Stochastic Modeling of Fluid Particle Dispersion in Turbulent Flows

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Chapter 1

Introduction

A very common phenomenon in environmental science and engineering is particle-laden turbulent flow, where the particles can either be solid particles or liquid droplets. A few examples are smoke rising from a chimney, pollution in rivers and contaminated flows in a heat exchanger. In such flows, one is especially interested in the dispersion of the particles in the turbulent flow, i.e., how fast a point-source or cloud of particles will spread out in the carrying fluid. Hereof, knowledge of the turbulent fluid flow field is required.

In general Newtonian fluid flow in motion can manifest itself in three states. In the first state the flow is smooth and regular, which is known as "laminar". The flow moves in layers and there are no fluctuations of the physical properties such as the fluid velocity and pressure. In the second state there can locally be small fluctuations in the flow field and the flow is called "transitional". It means that the flow is between laminar and the third and final state which is called "turbulent". In this turbulent state, the subject of this thesis, physical properties fluctuate in both time and space.

In spite of the numerous examples of it and our everyday experience with it, turbulence is not easy to define precisely. One usually resorts to a phenomenological description of it to distinguish it from laminair flows. Whereas a laminair flow is characterized by a fluid flowing in parallel layers, with no disruption between the layers, turbulent flows seem very irregular, chaotic and unpredictable. Due to this complicated structure, turbulent flows are much more efficient in transferring momentum and heat and propagating chemical reactions. On the other hand, turbulence increases the drag considerable.

Besides the phenomenological description, there is no real mathematical or physical defintion for turbulence. A flow is usually categorized in either of the three states through its value of the Reynolds number, which indicates the ratio, or relative importance, of the flow’s inertial and viscous forces:

\[ Re = \frac{UD}{\nu} \]  

(1.1)
where $U$ and $D$ are characteristic velocity and length scale of the flow and $\nu$ is the kinematic viscosity of the fluid. In laminar flows, the viscous terms dominate the nonlinear inertial terms and gradients in the flow are damped out. Upon increasing the mass flux, either by increasing the fluid velocity or decreasing the flow area, the inertial forces become more dominant and the flow becomes more chaotic and irregular. When this mass flux reaches a critical value, inertial forces dominate the viscous forces and the flow becomes turbulent. A nice example of a laminar flow becoming turbulent is that of a uniform flow past a cylinder \cite{1}. At low fluid velocities the flow appears to possess left-right and up-down symmetries. When increasing the velocity, the flow first loses its left-right symmetry, then the flow starts to separate behind the cylinder resulting in the formation of recirculating standing eddies, then the well-known Von Kármán-street of alternating eddies occurs and finally the flow becomes chaotic.

The complete difference in appearance could lead to one suggesting laminar and turbulent flows are described by different equations. However, it is widely accepted that this is not true. The dynamics of both types of flows are governed by the well-known Navier-Stokes equation. For Newtonian incompressible fluids this equation has the following form:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{f},$$  \hspace{1cm} (1.2)$$

where $\mathbf{u}$ is the fluid velocity vector, $p$ is the pressure and $\mathbf{f}$ is an external force. This equation shows that for high Reynolds numbers the viscous force is negligible. Along with appropriate initial and boundary conditions, equation (1.2) in combination with the continuity equation, $\nabla \cdot \mathbf{u} = 0$ for incompressible fluids, can be solved to give a complete description of the flow for every type of flow, even for turbulence. So even for turbulent flows it suggests that the fluid flow is deterministic given initial and boundary conditions for the flow field. However, for turbulence, the evolving flow field is extremely sensitive to small fluctuations in the initial field; small differences in the initial or boundary conditions lead to completely different solutions within a finite time period and the solution becomes totally unpredictable. It is then said that the set of equations is ill-posed and the solution is called deterministic chaos \cite{2}.

The sensitivity of a turbulent flow on small variations in the initial and boundary conditions would be no problem if they are known with an infinite accuracy. Such initial and boundary conditions are also known as mathematically ideal initial and boundary conditions and give a unique solution of the Navier-Stokes equation. In practice, however, initial and boundary conditions can be determined with only a finite accuracy, called realistic initial and boundary conditions. This means that two solutions of a turbulent flow having the same realistic initial and boundary conditions will be completely different after some time, as the initial and boundary conditions
differ slightly. These two completely different solutions could therefore be seen as two possible realizations of the turbulent flow. It therefore stands to reason not to study every individual realization of the turbulent flow but to study its statistics.

It is this statistical description of turbulence that makes the use of a stochastic equation in a Lagrangian framework to model fluid particle dispersion in a turbulent flow as alternative to the Navier-Stokes equation so interesting. With such a stochastic equation a possible realization of a fluid particle path can be simulated. By choosing the correct expressions for the parameters present in the stochastic equation and taking an ensemble average over many individual realizations of fluid particle paths statistics of the turbulent flow can be recovered. The advantage of stochastic equations over the Navier-Stokes equation is its relative simplicity, making it far more easy to solve numerically. The goal of this thesis is to find consistent stochastic equations for the fluid velocity in fully-developed turbulent channel and pipe flows and verifying their consistency by comparing Eulerian and Lagrangian statistics from the stochastic equations with those obtained from Direct Numerical Simulations.

The lay-out of this report is as follows: an overview of the various methods that are used in literature to solve solid particle dispersion in turbulent flows is given in Chapter 2. One of these methods, a stochastic equation for the fluid velocity, is used in Chapter 3 to simulate fluid particle dispersion in a stationary fully-developed channel flow. In Chapter 4 the same method is applied to stationary fully-developed pipe flow. Finally, conclusions and recommendations are given in Chapter 5.
Chapter 2

Particle dispersion models

In this section an overview will be given of the various methods used in the literature to model particle dispersion. Basically, there are two main approaches taken to simulate particle dispersion, viz., the Eulerian and Lagrangian approach. In section 2.1 the Eulerian approach is pursued for both the carrying fluid and the dispersed particles. Section 2.2 still uses an Eulerian framework for the fluid, while now a Lagrangian model is used for the particles, whereas section 2.3 uses the latter approach for both phases.

2.1 Eulerian - Eulerian approach

A classical way to describe turbulence is by means of an Eulerian framework; a fixed volume in space is discretised and variables are calculated at fixed points of the discretised space, the so-called grid points. Both phases, the carrying fluid and the dispersed particles, are treated as interacting and interpenetrating continua. For the dispersed phase a mass balance is applied to the fixed volume [3, 4] and the result is an equation for the concentration distribution $C(x)$:

$$\frac{\partial C}{\partial t} + u \cdot \nabla C = D \nabla^2 C,$$  

(2.1)

where $t$ is the time, $u$ the fluid velocity and $D$ the molecular diffusion coefficient. This latter parameter is a property of both the fluid and the diffusing solute. Equation (2.1) is known as the advection-diffusion equation, closely analogous to the heat convection-conduction equation, and assumes incompressibility of the flow, i.e., $\nabla \cdot u = 0$. The name stems from the primary transport mechanisms: advective transport and molecular diffusion. The advection-diffusion equation can also be applied to turbulent flows. Hereto the concentration and fluid velocity are split into their mean and fluctuation parts, i.e., $C = \bar{C} + C'$ and $u = \bar{u} + u'$, substituted in equation
(2.1) and finally the result is time-averaged:
\[ \frac{\partial \bar{C}}{\partial t} + \overline{\mathbf{u}} \cdot \nabla \bar{C} = D \nabla^2 \bar{C} - \nabla \cdot (\overline{\mathbf{u}C'}). \] (2.2)

An extra term, \( \nabla \cdot (\overline{\mathbf{u}C'}) \), arises due to the transport of \( C \) by the turbulent fluctuations. This turbulent flux is usually much larger than molecular diffusion, so that the latter can be neglected. As this equation cannot be solved due to the extra unknowns \( (\overline{\mathbf{u}C'}) \), similar to the well-known closure problem in turbulence, a final step is to model these extra terms similar to the molecular diffusion:
\[ \overline{\mathbf{u}C'} = -\kappa \nabla \bar{C}, \] (2.3)

where \( \kappa \) is the eddy diffusivity coefficient. This equation assumes that the turbulent mass transport is proportional to the mean concentration gradient. Using this model for the turbulent flux along with the notion that \( \kappa \gg D \) equation (2.2) becomes
\[ \frac{\partial \bar{C}}{\partial t} + \mathbf{u} \cdot \nabla \bar{C} = \nabla \cdot (\kappa \nabla \bar{C}), \] (2.4)

where the bars indicating averages have been dropped. In some models, \( \mathbf{u} \) is replaced by the sum of the fluid velocity itself and the negative of the settling velocity \( V_T \) \([5]\). Using this as well for stationary fully developed horizontal channel flow, with \( \mathbf{u} = (U, 0, 0) \), this equation usually has the form \([6]\):
\[ -V_T \frac{dC}{dx_2} = d \left( \frac{\kappa_{x_2} dC}{dx_2} \right), \] (2.5)

where \( x_2 \) is the wall-normal coordinate and \( \kappa_{x_2} \) the eddy diffusivity coefficient in wall-normal direction. Here, the concentration \( C(x_2) \) is assumed to be fully developed too. Iliopoulos and Hanratty \([6]\) state that this approach suffers from three shortcomings. First of all, the particles might not be long enough in the fluid to reach the settling velocity. Secondly, an empirical relation for the boundary condition at the wall, i.e., at \( x_2 = 0 \) is required. And finally, there are no firm theoretical grounds for a specification of the turbulent diffusivity \( \kappa \). It is defined in a phenomenological sense, by analogy with the molecular diffusivity, and does not have any true physical meaning. It usually depends on the flow conditions instead of being a property of the fluid. Especially this latter flaw is a big disadvantage in using the Eulerian approach for particle dispersion. As \( \kappa \) is strongly flow dependent, it has to be derived for every type of flow and estimation of it often relies on empirical data.

People therefore have turned their attentions through the years more to the Lagrangian (or trajectory) approach. The following sections will summarize a few of the possible Lagrangian models used along with Eulerian models for the fluid flow, which are also needed in combination with equation (2.4) for a complete Eulerian-Eulerian description.
2.2 Lagrangian - Eulerian approach

In the Lagrangian approach a single particle is marked and followed during its motion through the carrying fluid. Dispersion is then calculated by ensemble averaging over many individual particles.

The first equations derived for particles moving in a fluid were equations for the motion of a sphere that settled out under gravity in a stationary fluid [7, 8, 9]. Several researchers [10, 11, 12] corrected or modified these equations to include among others the effects of unsteadiness and non-uniformity of the flow field. Maxey and Riley [13] finally developed an equation of motion for a small rigid sphere in a nonuniform flow that is widely used as a starting point for the dispersion of particles in a turbulent flow:

\[
\frac{1}{6} \rho_p d_p^3 \frac{dv_{p,i}}{dt} = \frac{1}{6} d_p^3 (\rho_p - \rho_f) g_i + \frac{1}{6} \rho_f d_p^3 \frac{Du_i}{Dt} - \frac{1}{12} \rho_f d_p^3 \frac{d}{dt} \left( v_{p,i} - u_i - \frac{1}{40} d_p^2 \nabla^2 u_i \right) \\
- \frac{3}{2} \rho_f d_p^2 \sqrt{\nu} \int_0^t \left( \frac{d}{d\tau} \left( v_{p,i} - u_i - \frac{1}{24} d_p^2 \nabla^2 u_i \right) \right) \sqrt{\pi(t - \tau)} d\tau,
\]

(2.6)

where \( d_p \) is the particle diameter, \( \rho_p \) the particle density, \( \rho_f \) the fluid density, \( g_i \) the gravitational acceleration, \( \nu \) the fluid kinematic viscosity, \( v_{p,i} \) the particle velocity and \( u_i \) the fluid velocity. Note that there are two different time derivatives present in the equation, \( \frac{d}{dt} \) and \( \frac{D}{Dt} \). They denote time derivatives following the particle and following the fluid, respectively. Equation (2.6) describes the balance of forces working on a particle that moves through the fluid, basically Newton’s well-known second law. The left-hand side is the mass of a particle multiplied by its acceleration. The forces on the right-hand side are respectively the gravity force, the force due to the fluid pressure gradient, inertia force of added mass, the viscous and pressure drag force and the viscous force due to unsteady relative acceleration (also known as the Basset history term). The equation assumes that the flow field remains undisturbed by the presence of the particles and it does not take particle-particle interaction into account. These assumptions are valid for very low particle volume fractions. Furthermore, the particle Reynolds number \( R_p \), based on the particle diameter and the magnitude of the relative velocity \( |u - v_p| \), has to be small such that a Stokes approximation is permitted for the viscous and pressure drag force. Due to this Stokes approximation, no lift force is present in the model [14]. If the Stokes approximation would not be allowed, no explicit equation of motion is known [15]. This paper also gives three requirements which equation (2.6) has to satisfy in order for it to be applied to turbulent flow. The particle Reynolds number being small (less than 0.5) is the most restrictive of them.

Equation (2.6) has no closed form solution for a turbulent flow, even if all
terms on the right-hand side are neglected except for the Stokes force. This is caused by the nonlinearity of the equation, which requires the fluid velocity, \( u_i \), to be evaluated at the new, and yet unknown, particle position. The only case which has a solution is the trivial case of an invariant and uniform fluid velocity field, which rules out the fluid being turbulent [15]. Therefore, for particle-laden turbulent flow, this equation has to be included in a numerical simulation. However, it can become quite complicated to evaluate all terms and large computational efforts are needed. Fortunately, for heavy particles, \( \rho_p \gg \rho_f \), the only forces that have a significant contribution are the drag and gravity forces; all others have negligible magnitudes [6, 13, 15]. This simplifies the equation to

\[
\frac{dv_p}{dt} = \frac{3}{4} \rho_f C_D |v_p - u| (v_p - u) - g \left( 1 - \frac{\rho_f}{\rho_p} \right),
\]

(2.7)

where \( C_D \) is the drag coefficient. This parameter is given by the following semi-empirical correction to Stokes law [16]:

\[
C_D = \frac{24}{Re} \left( 1 + 0.15 \times 10^{-0.687} \right).
\]

(2.8)

The position of a particle can be found by solving

\[
\frac{dy_p}{dt} = v_p.
\]

(2.9)

Combining equations (2.7) and (2.9) along with initial conditions at \( t = t^0 \) for the particle position, \( y_p^0 \), and velocity, \( v_p^0 \), gives a possible realization of a particle trajectory. Dispersion can then be found by averaging over a large number of particle trajectories. The main problem, however, in simulating particle dispersion numerically is the need for the fluid velocity at the particle position, \( u(y_p(t), t) \), as the velocity of the fluid that a particle encounters on its path is needed to solve equation (2.7). The following sections will introduce several methods to calculate this fluid velocity through an Eulerian approach.

### 2.2.1 Direct Numerical Simulation

The most straightforward method to calculate the fluid velocity is by applying conservation of mass and momentum on a fluid continuum. For an incompressible and Newtonian fluid the resulting set of equations is

\[
\nabla \cdot u = 0, \tag{2.10a}
\]

\[
\frac{\partial u}{\partial t} + u \cdot \nabla u = -\frac{1}{\rho_f} \nabla p + \nu \nabla^2 u + f, \tag{2.10b}
\]

where \( u \) is the fluid velocity vector, \( p \) the pressure and \( f \) an external force. The first two are in general a function of place and time. Derivation and
more details regarding these equations can be found in [17]. This set of equations can be solved numerically by discretising the geometry in space and time and by specifying appropriate initial and boundary conditions. This reduces (2.10) to a set of algebraic equations and upon solving it numerically a complete three dimensional field of the fluid velocity and pressure is available. This method of calculating the fluid velocity is called a Direct Numerical Simulation (DNS). A review paper on DNS is written by Moin and Mahesh [18]. Even though this seems like the most logical way to calculate the fluid velocity, the drawback is that it puts serious strain on the computer. As turbulence is described by motion on scales ranging from the macrostructure, which has a characteristic length scale $L$ equal to the size of the geometry, to the microstructure, having a characteristic length scale $\eta$ equal to the Kolmogorov length scale, the computational grid has to be very dense such that all features of the turbulence are resolved accurately. This means that the number of grid points has to be at least equal to $N_c \sim (L/\eta)^{3/4}$ in a three-dimensional grid.

The Kolmogorov length scale can be written as $\eta = (\nu^3/\epsilon)^{1/4}$, with $\nu$ being the fluid kinematic viscosity and $\epsilon$ the mean rate of dissipation of turbulence kinetic energy. Kolmogorov’s relation states that a turbulent eddy, a coherent patch of swirling fluid, with energy $\sim U^2$ breaks down into smaller eddies due to instability in a timescale $T \sim L/U$ (the eddy turnover time), where $U$ is the typical velocity scale of the macrostructure [2]. Therefore, the dissipation rate should scale like $\epsilon \sim U^3/L$. Defining a Reynolds number based on macrostructure scales, $Re = UL/\nu$, it means that $\eta/L \sim Re^{-3/4}$. Based on this derivation it can be seen that the total number of grid point needed for an accurate simulation is proportional to the Reynolds number:

$$N_c \sim \left(\frac{L}{\eta}\right)^3 \sim Re^{3/4}.$$  \hspace{1cm} (2.11)

This result shows that the required number of grid points increases very rapidly with increasing Reynolds numbers and as turbulent flows are characterized by high Reynolds numbers it means, even with the supercomputers of nowadays, numerical simulations based on DNS are limited to Reynolds numbers of the order of $10^4$, with computational times of the order of weeks/months.

### 2.2.2 Large Eddy Simulation

An alternative to Direct Numerical Simulation is so-called Large Eddy Simulation, which was first applied to turbulent flows by Deardorff [19]. The famous self similarity theory by Kolmogorov [20] states that the large eddies of the flow are dependent on the flow geometry while the smaller, energy consuming, eddies are self similar and have a universal character. Therefore, in LES the equations are solved for the large, energy containing, eddies while
the effects of the smaller eddies on the larger ones are modeled. An equation for the larger eddies can be obtained by filtering the microstructure from the turbulent field through a filter operation:

\[ \hat{u}(x) = \int_V G(x; y)u(y)d^3y, \]  

(2.12)

where \( \hat{u} \) denotes the spatially filtered fluid velocity, \( V \) the domain and \( G(x; y) \) the filter function; e.g., the top-filter or spectral cutoff filter. In this way only the spatially filtered fluid velocity, also called the resolved fluid velocity, is calculated and a model for the scales that are filtered out, the subgrid scales, is needed. Several subgrid scale models have been proposed with good results for various single-phase turbulent flows [21, 22, 23, 24, 25]. However, for the solution of (2.7) the instantaneous fluid velocity is needed. It is justified to use the filtered fluid velocity as long as the particle relaxation time \( \tau_p = \rho_p d_p^2/18\mu \) is large compared to the Kolmogorov time scale and the smallest time scale resolved in LES [26], but results improve if a defiltered fluid velocity is used instead in the particle equation of motion [27, 28, 29]. Especially turbophoresis, i.e. particle deposition at the walls, cannot be predicted accurately if the filtered fluid velocity is used.

Even though LES requires models for the subgrid scales and the defiltered velocity is needed for particle-laden turbulent flows its great advantage over DNS is that less computational effort is needed due to the filtering.

2.2.3 Reynolds Averaged Navier Stokes

A second alternate to using Direct Numerical Simulations is the Reynolds Averaged Navier Stokes (RANS) model. In this method the Navier Stokes equations are averaged and only average properties are resolved. This method is hardly used for particle-laden turbulent flows as only the average fluid velocity is obtained while the instantaneous fluid velocity is needed in (2.7), meaning that one relies on empirical information to provide models for the fluctuating part of the fluid velocity.

2.3 Lagrangian - Lagrangian approach

The methods for the fluid velocity described in section 2.2 are based on the Eulerian approach; the fluid velocity is calculated at fixed points (the grid points) in space and to get the fluid velocity at the position of a particle one has to interpolate between these grid points. The counterpart of this type of approach is the Lagrangian (or trajectory) approach, where one solves for the trajectory of a finite size fluid particle that moves with the fluid, similar to what has been done for a solid particle in section 2.2. In this approach, the current position of a fluid particle \( \mathbf{x}(t) \) is a function only of its initial position \( \mathbf{x}^0 \) and the time \( t \) passed since marking the fluid particle.
Its velocity is equal to the Eulerian velocity \( u(x, t) \) evaluated at the current position and this enables one to calculate the new particle position simply by integration of

\[
\frac{dx}{dt} = u(x, t). \tag{2.13}
\]

A review article regarding the Lagrangian description of turbulence has been written by Yeung [30]. What remains is to find a suitable model for the fluid velocity. As the flow in the turbulence regime has a chaotic and irregular character an interesting way to model the Lagrangian statistics is by means of a stochastic equation. A stochastic equation is an equation that contains a stochastic process that can be described by a probability distribution. This section introduces the stochastic equations that have been used in literature to describe turbulent flows.

### 2.3.1 Stochastic Lagrangian model for position of a fluid particle

The pioneering work for applying stochastic equations to turbulent flows was done by Taylor [31]. He derived an equation for the mean-squared displacement of a large number of particles originating from a point source for stationary homogeneous isotropic turbulence:

\[
\bar{X}^2 = 2\bar{u}^2 \int_0^T \int_0^t R_\xi d\xi dt, \tag{2.14}
\]

where \( X \) is the distance traversed by a particle in time \( T \), \( \bar{u}^2 \) is the mean-squared fluid velocity and \( R_\xi \) is defined by

\[
\int_0^t u(t) u(t + \xi) dt = \bar{u}^2 \int_0^t R_\xi d\xi, \tag{2.15}
\]

i.e., it is the correlation coefficient between the value of \( u \) for a particle at any instant and the value of \( u \) for the same particle after a time interval \( \xi \). This equation implies that for this case, a stationary homogeneous isotropic turbulent field, dispersion can be described by one unknown parameter: the Lagrangian velocity correlation coefficient. For short times, when \( R_\xi \) does not differ appreciably from 1, \( \int_0^T \int_0^t R_\xi d\xi dt = \frac{1}{2} T^2 \) and equation (2.14) reduces to:

\[
\bar{X}^2 = \bar{u}^2 T^2, \tag{2.16}
\]

Thus the standard deviation of \( X \) is proportional to \( T \) for small \( T \). For large times such that \( T > T_1 \), where \( T_1 \) is a time interval chosen such that at the end of this time interval the velocity of a particle is uncorrelated with its initial value, equation (2.14) reduces to:

\[
\frac{d\bar{X}^2}{dt} = 2\bar{u}^2 \tau_L, \tag{2.16}
\]

where \( \tau_L = \lim_{t \to \infty} \int_0^t R_\xi d\xi \), i.e., \( \tau_L \) is the Lagrangian time scale.
The results of Taylor’s analysis can also be derived from the following stochastic equation for the position of a fluid particle:

\[ dX = u dt + \gamma dW(t), \tag{2.17} \]

where \( \gamma \) is the diffusion coefficient and \( dW(t) \) is the incremental Wiener process \([32]\). The increments of \( dW(t) \) are Gaussian with mean zero and variance \( dt \) and its successive values are uncorrelated. The results of Taylor’s analysis given by equations (2.15) and (2.16) can be derived from equation (2.17) by first multiplying the latter equation by \( X \), then taking an ensemble average and finally noting that the increments of \( dW(t) \) are uncorrelated with \( X \). The result then is

\[ \frac{dX}{dt} X = uX, \tag{2.18} \]

where the equation has been written in the derivative form for convenience. As a next step, on the left hand side the averaging bar and \( X \) will be brought inside the time derivative, resulting in:

\[ \frac{1}{2} \frac{dX^2}{dt} = uX. \tag{2.19} \]

Finally, the right hand side of this equation can be rewritten by using

\[ \bar{u} = \frac{1}{t} \int_0^t R_{\tau \tau} \, d\xi \]

\[ = \frac{1}{t} \int_0^t u \, d\xi \]

\[ = u \frac{1}{2} \int_0^t \frac{1}{2} \int_0^t u \, d\xi \]

Equation (2.14) is then recovered by integrating equation (2.19) over time.

In equation (2.17) the particle position is approximated by a stochastic process that has the Markov property. A stochastic process has the Markov property if the conditional probability distribution of future states of the process, given the present state and all past states, depends only upon the present state and not on any past states, i.e. it is conditionally independent of the past states (the path of the process) given the present state. A process with the Markov property is usually called a Markov process, and may be described as Markovian.

Next to stochastic differential equations like equation (2.17) Markov processes can also be described by an equation for the particle distribution, better known as the Fokker-Planck equation. When the particle position is assumed to be Markovian, like is done in this section, the Fokker-Planck equation reduces to the advection-diffusion equation presented in section 2.1. Equation (2.17) is equivalent to equation (2.4) if \( \kappa = \gamma^2 / 2 \) \([33]\).
When modeling only the position of a fluid particle as a Markov process, all memory effects are neglected because the velocity is assumed to be $\delta$-correlated. This is also known as the diffusion approach. Brouwers [34] shows that this approximation is only valid for times $t \gg \tau_L$ in the case of stationary, homogeneous turbulence. Furthermore, he derived the Fokker-Planck equation for the probability density of fluid particle position in inhomogeneous unsteady turbulence from the general kinematic relationship between particle velocity and displacement and applying exact asymptotical analysis. He concluded that the diffusion approach is only valid when, next to $t \gg \tau$,  

$$\varepsilon = \frac{\tau \tilde{u}}{L} \gg 1,$$  

(2.21)

where $\tau$ is correlation time of fluid particle velocity, $\tilde{u}$ represents the order of magnitude of the fluctuating part of the fluid velocity (e.g., the standard deviation of the fluid velocity) and $L$ is the external length scale. Condition (2.21) implies that the random displacement of a fluid particle measured over a time period which corresponds to the correlation time of fluid particle velocity is required to be small compared to the external length scale. As for most practical cases of turbulence $\varepsilon = O(1)$, the limit process of $\varepsilon \to 0$ for $Re \to \infty$ by which the diffusion approximation would become exact does not exist.

An alternative to the Markovian approximation for the particle position is treating the position and velocity of a fluid particle as a continuous joint Markov process. This will be the basis of the stochastic models in the next section.

### 2.3.2 Stochastic Lagrangian model for velocity of a fluid particle

The main assumption made in section 2.3.1 is that the particle position is Markovian, implying that the particle velocity is $\delta$-correlated. Besides Brouwers’ proof that this assumption does not become exact with increasing Reynolds number, it does not seem reasonable to assume that the position of a particle is a Markov process as the velocity of a particle, with its timescale determined by the largest eddies, is not determined locally. It is more plausible to assume the position and velocity as jointly Markovian as the acceleration of a particle, having a very short correlation timescale, should have properties that are determined by the particle velocity and the local conditions. This is because for turbulence characterized by a high Reynolds number, the Lagrangian acceleration correlation is significant only for time lags in the order of the Kolmogorov timescale $\tau_\eta = (\nu/\eta)^{1/2}$ [35]. According to the definition of the turbulence Reynolds number, $Re_t = (\tau/\tau_\eta)^2$, $\tau_\eta \sim Re_t^{-1/2} \tau$, which means that for $Re_t \to \infty$, $\tau_\eta \to 0$. Thus the changes of the particle velocity are only weakly correlated over successive time in-
tervals $\Delta t$. However, they cannot be completely independent as this would mean that the variance of $u$ would grow indefinitely. By approximating the particle acceleration as a Markov process this dependence is assumed to be taken into account by allowing the velocity increments to depend on the particle’s velocity and (for inhomogeneous turbulent flow fields) on the particle’s position [36].

A model based on the Markovian assumption for the acceleration of a particle, however, cannot describe a particle motion accurately over timescales of order $\tau_\eta$. This will become more apparent later on in this report.

A stochastic differential equation for the velocity fluctuation of a fluid particle based on the joint Markovian assumption for the position and velocity has the following general form:

$$
\text{d}v'_i = a_i(v, x, t) \text{d}t + b_{ij}(v, x, t) \text{d}W_j(t),
$$  

(2.22)

where $\text{d}v'(t) \equiv v'(t + \text{d}t) - v'(t)$ is the infinitesimal increment of the fluctuating fluid particle velocity. The symbol $v$ is used to indicate that it is the Lagrangian fluid velocity, whereas $u$ was used for the Eulerian fluid velocity. The usual distinction between the mean $\langle v \rangle$ and the fluctuating part $v'$ of the total velocity $v \equiv \langle v \rangle + v'$ is made, where the brackets signify ensemble averaging. Furthermore, $a$ is called the drift tensor or damping tensor, $b$ is the diffusion tensor and $\text{d}W_j(t)$ are the infinitesimal increment of a vector-valued Wiener process, which was introduced in section 2.3.1. For inhomogeneous turbulence $a$ and $b$ are dependent on the particle position $x$.

In his treatment of Brownian motion Langevin derived an equation for the change of the velocity of a particle with time due to a damping force that is proportional to the velocity and a random force caused by the collisions of the individual molecules of the surrounding fluid [37], see also [38]. This equation is very similar to equation (2.22), with $a_i = \alpha_i v'_i$. That is why nowadays stochastic equations are often also called Langevin equations.

**Specification of $a$ and $b$**

The main problem in using equation (2.22) to model turbulence is the actual form of the functions $a_i$ and $b_{ij}$. If a complete description of the Lagrangian behavior of the turbulent field is known from either a Direct Numerical Simulation or measurements, expressions could be derived for these functions from the obtained Lagrangian statistics. However, as DNS calculations are limited to low Reynolds numbers and obtaining Lagrangian information of a turbulent flow by means of measurements requires complex measurement techniques, people have tried to derive expressions for $a_i$ and $b_{ij}$ based on theoretical grounds. The two main ideas that are usually applied to equation (2.22) to specify $a_i$ and $b_{ij}$ are developed by Van Dop et al. [39] and Thomson [36]. The former derived an expression for $b_{ij}$ that is consistent with
Kolmogorov’s similarity theory [20]. According to this theory, the second order Lagrangian structure function

\[ D_{ik}(t) = \langle (v'_i(t + \Delta t) - v'_i(t))(v'_k(t + \Delta t) - v'_k(t)) \rangle = \delta_{ik} C_0 \epsilon \Delta t \]  

(2.23)
in the inertial subrange \( \tau_\eta \ll \Delta t \ll \tau \) and for high Reynolds numbers. Furthermore, \( C_0 \) is the universal Kolmogorov constant. For time scales in this inertial subrange equation (2.22) implies

\[ D_{ik}(t) = b_{ij}b_{kj} \Delta t + O(\Delta t)^2. \]  

(2.24)

Matching equation (2.23) with equation (2.24) to leading order gives

\[ b_{ij} = \sqrt{C_0 \epsilon} \delta_{ij}. \]  

(2.25)

This was the expression found by Van Dop et al. [39] for a model in which \( a \) is a linear function of \( v \). Thomson [36] derived the same expression by using a general damping tensor. This result implies that the diffusion tensor is an isotropic diagonal matrix, i.e., a matrix containing only diagonal terms that are independent of the direction.

The second theoretical idea stems from work done by Thomson [36]. To ensure that the damping tensor is consistent with the prescribed, single-time Eulerian statistics, he showed that a model should satisfy the well-mixed condition. This condition requires that, for an initially well-mixed scalar field, the turbulence should not produce mean concentration gradients, nor should it produce concentration fluctuations [40]. A model that satisfies the well-mixed condition is called a model from the well-mixed class [36]. Applying the well-mixed conditions to equation (2.22), along with equation (2.25), for stationary, homogeneous, isotropic turbulence gives

\[ a_i = -\frac{1}{2} C_0 \epsilon \sigma^2 v'_i, \]  

(2.26)

where \( \sigma^2 \) is the variance of the velocity. The term on the right hand side is the inverse of a time scale times the velocity component. Therefore, equation (2.27) can also be written as

\[ a_i = -\frac{v'_i}{\tau_L}, \]  

(2.27)

where \( \tau_L \) is the Lagrangian correlation time or integral time scale:

\[ \tau_L = \frac{2\sigma^2}{C_0 \epsilon}, \]  

(2.28)

Using this expression in equation (2.25) results in the following alternative expression for the diffusion coefficient:

\[ b_{ij} = \left( \frac{2\sigma^2}{\tau_L} \right)^{1/2} \delta_{ij}. \]  

(2.29)
Substituting equations (2.26) and (2.29) in equation (2.22) gives the classical Langevin-equation
\[
dv'_{i} = -\frac{v'_{i}}{\tau_{L}} dt + \left(\frac{2\sigma^{2}}{\tau_{L}}\right) dW_{i}(t).
\] (2.30)

For this model the Lagrangian autocorrelation function is given by
\[
\rho(s) \equiv \frac{\langle v'_{i}(t)v'_{i}(t+s) \rangle}{\sigma^{2}} = e^{-|s|/\tau_{L}}.
\] (2.31)

From this expression for the autocorrelation it can be seen that there is only one time scale \(\tau_{L}\) present in the model, which is characteristic for the large, energy containing eddies. Furthermore, it does not depend on the Reynolds number and the slope is discontinuous at \(s = 0\).

A consideration of the average behavior of a large number of particle paths generated by equation (2.30) along with \(dx_{i}/dt = v'_{i}\) gives the same result as Taylor’s analysis presented in section 2.3.1. This can also be verified by substituting equation (2.31) in equation (2.14) and differentiating both sides, resulting in equation (2.16).

**Non-uniqueness problem**

Even though Kolmogorov’s similarity theory and the well-mixed conditions give analytical relations for the damping and diffusion coefficients for the stationary homogeneous isotropic case, the formulation of these coefficients for a more general inhomogeneous and anisotropic turbulent field is not straightforward. This is called the non-uniqueness problem. Borgas and Sawford [41] showed that there is a unique model provided that the flow is isotropic and homogeneous, even for the non-stationary case. However, it is not possible to define a unique model in three dimensions in terms of Eulerian statistics when the symmetry of the flow is relaxed even slightly. Borgas et al. [42], for example, showed that a rotational term of arbitrary magnitude can be added to a model applied to axisymmetric turbulence without reflection symmetry and that this term dramatically affects the dispersion predicted by the model. For the more general case of inhomogeneous turbulence, Sawford and Guest [43] showed that there are at least two models consistent with the prescribed Eulerian velocity statistics. This reduced many investigations to finding the ”best” or the ”correct” model out of the many that are consistent with these prescribed Eulerian velocity statistics. A possible discriminator between the various possible models is the mean rate of rotation of trajectories by the turbulence, where zero- or low-rotation models are possibly the ”best” models [44, 45, 46]. However, to date there is no theoretical proof for this.

Possibly the simplest flow for which the non-uniqueness problem is manifested is for homogeneous turbulence in uniform shear flow. Sawford and
Yeung [47] compared Eulerian acceleration statistics obtained by Direct Numerical Simulations for this type of turbulence with two different Lagrangian stochastic models; Thomson’s model [36] and one due to Borgas [43]. They found that Thomson’s model agrees very well with the DNS data, however, Borgas’ model showed some major discrepancies and therefore they concluded that these Eulerian acceleration statistics provide a means of discriminating between several models. In a later paper [48] Sawford and Yeung compared as well Lagrangian statistics from these two models with DNS results and found again that Thomson’s model was the better performing one. They attributed the deviations found in Borgas’ model to an excessively large mean rotation in the trajectories in the plane of shear, whereas Thomson’s model is rotation free. Pope [49] used a linear stochastic differential equation for the fluctuating fluid velocity for homogeneous turbulent shear flow and showed that there is a unique specification of the drift matrix and diffusion matrix such that the covariance matrix and time scale matrix match those obtained from DNS. Furthermore, he found that the diffusion matrix is significantly anisotropic, which is in contradiction with Kolmogorov’s hypotheses and conventional modeling. He notes though that this could be a low Reynolds-number effect.

Mito and Hanratty [50] implemented a jointly Gaussian forcing function, resulting in a non-diagonal anisotropic diffusion matrix, into a stochastic model for the fluid velocity and compared calculations of the dispersions and velocities of particles originating from a point source with DNS results of fully-developed inhomogeneous turbulent flow in a channel. Their damping coefficient is linear in the velocity and independent of the other two velocity components and depends on the wall-normal coordinate \(x_2\), i.e., \(a_i(v, x, t) = -v_i/\tau_i(x_2)\). Here \(\tau_i\) is not the Lagrangian integral timescale but a rather loosely defined ”local decorrelation timescale” [36]. They concluded that the use of jointly Gaussian, rather than uncorrelated Gaussian, forcing functions greatly improves the results. It is only recently though that people have started to develop models for inhomogeneous and anisotropic turbulence using the well-mixed approach.

**Kolmogorov constant**

Another problem that needs to be addressed when simulating particle paths using a stochastic model for the particle velocity is the exact value of the Kolmogorov constant \(C_0\). In principle, it can be determined from DNS computations, Lagrangian velocity measurements or tracer particle dispersion studies by using equation (2.23). An overview of some important results is given by Lien and D’Asaro [51]. Kolmogorov’s theory of local isotropy for high Reynolds-numbers states that \(C_0\) ought to be a universal constant, having the same value for all flows and in all three directions. However, this is not yet true for the relatively low Reynolds-numbered turbulence
that is being studied in practice. It therefore stands to reason to define a direction dependent $C_0^i$, something Pope [49] found as well for his study on homogeneous turbulent shear flow.

To determine the Kolmogorov constant accurately from the second order Lagrangian velocity structure function, the Taylor microscale Reynolds number $R_\lambda = \sqrt{20k^2/(3\epsilon\nu)}$, where $k = \langle u_i u_i \rangle / 2$ is the turbulent kinetic energy, has to be bigger than $10^5$ so that the inertial subrange of the structure function is sufficiently wide. It is therefore better to determine $C_0 = \pi \beta$ by first determining the inertial subrange constant for the Lagrangian acceleration spectrum $\beta$, as values of $R_\lambda$ greater than $10^2$ are sufficient to determine $\beta$ [51]. According to Kolmogorov’s similarity theory, a plateau of $C_0$ should be observed for high Reynolds numbers in the inertial subrange. For the more practical Reynolds numbers, such plateaus are not present and a local maximum value, $C_0^*$, appears when the structure function is scaled with $\epsilon t$. This local maximum is found to increase with $R_\lambda$ [51, 52] and reaches an asymptotic value of approximately 6 to 7. These findings are in agreement with the relation proposed by Fox and Yeung [53]:

$$C_0 = 6.5 \left[ 1 + \frac{8.1817}{R_\lambda} \left( 1 + \frac{110}{R_\lambda} \right) \right]^{-1}. \quad (2.32)$$

Fluid velocity along particle trajectory

Finally, when applying stochastic models for the fluid velocity to solid particle dispersion, it has to be noted that these solid particles do not follow the fluid particles. In other words, when using equation (2.7) the fluid velocity is needed along the solid particle trajectory, while with a stochastic model like equation (2.22) a trajectory of a fluid particle can be simulated. These two trajectories are fundamentally different, as the solid particle moves through the carrying fluid, not with it. Therefore, this discrepancy has to be taken into account when using equation (2.22) for solid particle dispersion. One possible solution explored by a number of investigators is to use two step stochastic models [54, 55, 56]. These models calculate the new velocity of a fluid particle using a stochastic model, while using a spatial correlation to relate the new fluid velocity to the fluid velocity at the new position of a solid particle that was initially in contact with this fluid particle. This method however lacks theoretical justification, while Pozorski and Minier [57] showed that the models wrongly predicts the turbulent kinetic energy of the fluid "seen" by the particles as well as the inertia and crossing trajectory effects. Furthermore, Ushijima [58] suggests that the use of Eulerian space correlation in a two-step analysis is fundamentally wrong. Another method was explored by Iliopoulos and Hanratty [6]. They adjusted their spatially varying local decorrelation time $\tau_i$ to take account of the discrepancy between the velocity history of fluid particles and the velocity history of the fluid "seen" by solid particles along a trajectory.
2.3.3 Stochastic Lagrangian model for acceleration of a fluid particle

A deficiency of a stochastic model for the velocity of a fluid particle is its short-time behavior. This is due to the application of Kolmogorov’s similarity theory in specifying the diffusion tensor and causes the model to wrongly predict particle motion in timescales on the order of the Kolmogorov timescale $\tau_\eta$. This became apparent in the Lagrangian autocorrelation function, given by equation (2.31) for isotropic and homogeneous turbulence. The logical step therefore is assuming the position, velocity and acceleration of a fluid particle as jointly Markovian, opposed to a Markovian particle position used in section 2.3.1 and a jointly Markovian particle position and velocity in section 2.3.2. That assumption gives rise to a stochastic model for the Lagrangian acceleration of the fluid. Such a model was proposed by Sawford [59, 60] and is also designated as a second-order model [59].

By formulating a stochastic equation for the Lagrangian acceleration of a fluid particle, an extra timescale is introduced, namely the Kolmogorov timescale $\tau_\eta$, which is representative of the dissipative scales of motion. In that way a Reynolds dependence is also built into the model, as the turbulence Reynolds number, defined as

$$R_{e_t} = \left(\frac{\tau_L}{\tau_\eta}\right)^2$$

appears as a parameter at second order. Sawford [59] found, among others, the correct quadratic behavior of the velocity autocorrelation function for small time lags using a stochastic equation for the particle acceleration. However, the objection to using such a model is that there is no physical basis for approximating the acceleration by a Markov process; there is no physical process acting on a time scale smaller than $\tau_\eta$ which can "smooth out" the singular behavior inherent in the Markov approximation.

2.4 Turbulent relative dispersion

The last method to model particle dispersion in turbulence that has been studied to some extent in literature and that will briefly be discussed here is relative dispersion. Instead of dealing with individual particle, relative dispersion aims at modeling the mean-square separation of a pair of particles. A review article about relative dispersion has been written by Sawford [40].

One of the most important results regarding relative dispersion has been derived by Batchelor [61]. He found that the mean-square separation of a pair of particles, $\Delta$, in the inertial subrange, $\eta \ll \Delta_0 \ll L$, and for times, $\tau_\eta \ll t \ll \tau_L$, where $\eta$ and $\tau_\eta$ are Kolmogorov’s length- and time scale respectively, $L$ and $\tau_L$ are the length- and time scale of the large energetic
eddies and $\Delta_0$ is the initial separation of the particle pair, is given by

$$\Delta^2(t) - \Delta_0^2 \approx \begin{cases} 
\frac{11}{3} C (\bar{\epsilon} \Delta_0)^2 t^2 & \text{if } \tau_\eta \ll t \ll t_0 \\
g \bar{\epsilon} t^3 & \text{if } t_0 \ll t \ll \tau_L,
\end{cases} \quad (2.34)$$

where $C$ is the universal constant in the inertial subrange similarity form of the longitudinal Eulerian velocity structure function, $t_0 = (\Delta_0^2 / \bar{\epsilon})^{1/3}$ is the time for which the initial separation is important and $g$ is the Richardson constant. The $t^3$ law in the inertial subrange is important because of its universality. Furthermore, the value of the Richardson constant is of great interest and varies throughout the different approaches taken.

One of these approaches is very similar to the one discussed in section 2.3.2, i.e., assuming that the position and velocity are jointly Markovian resulting in the following stochastic differential equations

$$\begin{align*}
\frac{dv_i'}{dt} &= a_i(v, x, t)dt + b_{ij}(v, x, t)dW_j(t), \\
\frac{dx_i}{dt} &= v_i dt.
\end{align*} \quad (2.35)$$

The vectors $v$, $x$ and $W$ are now six-dimensional with the first three components representing particle one and the second three representing particle two. Thomson [33] extended his theory initially developed for one particle models to particle pair models. Because many of the ideas are similar to the ones elaborated in section 2.3.2 they will not be repeated here.

Other approaches used in the literature are the so-called two-point or spectral closures, which yields the diffusion equation for the separation probability function but where the diffusivity varies depending on assumptions made [62, 63], and the kinematic solution, where the Eulerian velocity field is approximated by a Fourier series with a finite number of modes and Lagrangian statistics are obtained by tracing particle trajectories through this synthetic Eulerian velocity field [64, 65]. However, the stochastic approach is the one mostly used in literature.
Chapter 3

Linear stochastic model for channel flow

In this thesis, the Lagrangian-Lagrangian approach is pursued for the simulation of particle dispersion as that approach requires the least computational effort. The biggest problem is to specify a consistent stochastic model to obtain the fluid velocity. Section 2.3 showed that there are mainly four methods used in literature to solve this problem; stochastic models for either the position, velocity or acceleration of a fluid particle or stochastic models for fluid particle pairs. That section also argued that stochastic models for the position or acceleration lack physical foundation, while relative dispersion models require additional models for the correlation of the velocities of the two particles. Therefore, stochastic Lagrangian models for the velocity of a fluid particle will be used, the one that is also mostly studied in literature.

In this chapter stochastic models for fluid particles will be presented for turbulent channel flow. The flow considered is fully-developed, so that the only non-zero mean velocity component is in streamwise direction, i.e., \( \langle v \rangle = (U_1, 0, 0) \), and statistical properties of the turbulence are only a function of \( x_2 \). Variables are expressed in wall units, meaning they are made dimensionless using the fluid kinematic viscosity \( \nu \) and the friction velocity \( u_\tau \). The Reynolds number of the flow based on these two parameters and half the channel height \( h \) is 150, i.e., \( Re_\tau = \frac{u_\tau h}{\nu} = 150 \).

This chapter starts with the mathematical description of a stochastic model for the fluid velocity for turbulent channel flow, in Section 3.1. Details of the numerical methods used to solve the model are given in Section 3.2. Finally, results are given in Section 3.3.
3.1 Model features

In this subsection the derivation and some properties of the linear stochastic model are discussed. The derivation starts with the Navier-Stokes equations for incompressible Newtonian fluids in a Cartesian frame of reference:

\[
\frac{\partial u_i}{\partial t} + u_j \frac{\partial}{\partial x_j} u_i + \frac{1}{\rho} \frac{\partial p}{\partial x_i} = \nu \frac{\partial^2 u_i}{\partial x_j^2}, \quad (3.1)
\]

The subscript \(i = 1, 2, 3\) refers to the streamwise, wall-normal and spanwise component, respectively. As usual, the velocity and pressure are decomposed into its mean and fluctuating part

\[
u_i(t) = u_i^0(x) + u_i'(x, t) \quad \text{and} \quad p = p^0(x) + p'(x, t).
\]

Substituting this into equation (3.1) leads to:

\[
\frac{\partial u_i'}{\partial t} + u_j^0 \frac{\partial}{\partial x_j} u_i' + u_j' \frac{\partial}{\partial x_j} u_i^0 + \frac{1}{\rho} \frac{\partial p^0}{\partial x_i} + \frac{1}{\rho} \frac{\partial p'}{\partial x_i} = \nu \frac{\partial^2 u_i^0}{\partial x_j^2} + \nu \frac{\partial^2 u_i'}{\partial x_j^2}. \quad (3.2)
\]

Here we already used the properties \(u_j^0(\partial u_i^0)/(\partial x_j) = 0\) and \((\partial u_i^0)/(\partial t) = 0\) which hold for stationary unidirectional flows, such as pipe and channel flow. Equation (3.2) can be ensemble averaged which results in the Reynolds averaged Navier-Stokes equations for the mean flow:

\[
\frac{\partial}{\partial x_j} \langle u_j' u_i' \rangle + \frac{1}{\rho} \frac{\partial p^0}{\partial x_i} = \nu \frac{\partial^2 u_i^0}{\partial x_j^2}. \quad (3.3)
\]

In the Lagrangian frame of reference, the Lagrangian velocity of a fluid particle is given by

\[
u_i(t) = u_i(x(t), t), \quad (3.4)
\]

and the fluctuating Lagrangian velocity component by

\[
v_i'(t) = u_i(x(t), t) - u_i^0(x(t)). \quad (3.5)
\]

The Lagrangian acceleration of a fluid particle is then equal to

\[
\frac{dv_i'(t)}{dt} = \frac{\partial u_i}{\partial t} + \frac{\partial u_i}{\partial x_j} \frac{dx_j}{dt} - \frac{\partial u_i^0}{\partial x_j} \frac{dx_j}{dt} = \frac{\partial u_i}{\partial t} + u_j \frac{\partial}{\partial x_j} u_i - u_j \frac{\partial}{\partial x_j} u_i^0. \quad (3.6)
\]

Substitution of equation (3.1) leads to

\[
\frac{dv_i'(t)}{dt} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i^0}{\partial x_j^2} - u_j \frac{\partial}{\partial x_j} u_i^0
\]

\[
\quad = -\frac{1}{\rho} \frac{\partial p^0}{\partial x_i} + \nu \frac{\partial^2 u_i^0}{\partial x_j^2} - \frac{1}{\rho} \frac{\partial p'}{\partial x_i} + \nu \frac{\partial^2 u_i'}{\partial x_j^2} - u_j \frac{\partial}{\partial x_j} u_i^0
\]

\[
\quad \quad = \frac{\partial}{\partial x_j} \langle u_j' u_i' \rangle - \frac{1}{\rho} \frac{\partial p^0}{\partial x_i} + \nu \frac{\partial^2 u_i'}{\partial x_j^2} - u_j' \frac{\partial}{\partial x_j} u_i^0. \quad (3.7)
\]
The average acceleration of the Lagrangian velocity is obtained by ensemble averaging this equation. This results in the simple relation

\[
\langle \frac{dv'_i}{dt} \rangle = \frac{\partial}{\partial x_j} \langle u'_j u'_i \rangle .
\] (3.8)

For the fluctuating velocity of a fluid particle a simple Markov model, or -equivalently- Langevin equation, reads

\[
\begin{aligned}
dv'_i &= g_i(v', x, t)dt + (C'_i e)^{1/2} dW_i(t) \\
dx_i &= v_i dt = v'_i dt + v'_i dt
\end{aligned}
\] (3.9)

This equation is already introduced in Section 2.3.2, viz. equation (2.22) along with equation (2.25), except that now a direction dependent \(C'_i\) is used, which seems to be a characteristic for relatively low Reynolds-numbered turbulence, see also Section 2.3.2. There it was also discussed that the form of the damping functions \(g_i(v', x, t)\) is not known for inhomogeneous flow. Initially, this function is assumed to be linear in \(v'_i\), \(g_i(v', x, t) = g^0_i(x) + a_i(x)v'_i\) with \(a_i\) damping coefficients. Using equation (3.8) and the property \(\langle dW_i(t) \rangle = 0\), the ensemble average of equation (3.9) yields

\[
g^0_i(x) = \langle dv'_i \rangle = \frac{\partial}{\partial x_j} \langle u'_j u'_i \rangle ,
\] (3.10)

This leads to the following expression for the damping function:

\[
g_i(v', x, t) = \frac{\partial}{\partial x_j} \langle u'_j u'_i \rangle + a_i v'_i 
\] (3.11)

For channel flow the first term on the right hand side of equation (3.11) appears as \(d \langle u'_2 u'_\mu \rangle / dx_2\) since averaged quantities do not depend on the streamwise or spanwise direction in a stationary fully-developed flow. This term represents the average acceleration for a large number of trajectories due to the nonhomogeneity of the field and have to be added to ensure that the well-mixed condition is not violated. In other words, it prevents particles from drifting from one wall-normal position to another on average. Therefore they are also referred to as drift terms. They balance the convective term that arise when treating the left hand side of the velocity equation in equation (3.9) as a material derivative following the fluid, i.e., \(dv'_i = \partial u'_i + u \cdot (\nabla u'_i) dt\). The first term on the right hand side of this equation is zero due to the stationarity of the flow while the fluid velocity vector \(u\) in the second term on the right hand side can be taken inside the gradient operator for incompressible flows. Equation (3.10) is then recovered after taking an ensemble average.
If one assumes a model with linear damping function in Cartesian coordinates then the complete first order Langevin model is given by

\[
\begin{align*}
    dv_1' &= a_1v_1' dt + \frac{d}{dx_2} \langle u_1' u_2' \rangle dt + \left(C_0^1 \epsilon \right)^{1/2} dW_1(t) \\
    dv_2' &= a_2v_2' dt + \frac{d}{dx_2} \langle u_2'^2 \rangle dt + \left(C_0^2 \epsilon \right)^{1/2} dW_2(t) \\
    dv_3' &= a_3v_3' dt + \left(C_0^3 \epsilon \right)^{1/2} dW_3(t).
\end{align*}
\] (3.12)

Since the spanwise direction is decoupled from the streamwise and wall-normal directions, the cross-correlations \( \langle u_1' u_3' \rangle \) and \( \langle u_2' u_3' \rangle \) are equal to zero.

The dissipation rate, \( \epsilon \), is calculated from DNS data according to:

\[
\epsilon = 2\nu \langle S_{ij}^2 \rangle,
\]

where \( S_{ij} \) is the strain tensor, defined as:

\[
S_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right).
\] (3.13)

As a first attempt, the damping coefficients are set equal to the negative of the reciprocal of the local decorrelation time, i.e., \( a_i = -1/\tau_i \), with \( \tau_i = \tau_i(x_2) \). Furthermore, equation (2.28) is used to write \( C_0^i \epsilon = 2\sigma_i^2 / \tau_i \), where \( \sigma_i \) is the standard deviation of the fluid velocity component \( v'_i \).

In Section 3.3 the Langevin model given by equation (3.12) will be modified by using another random process in the forcing term (Section 3.3.1) and by making another choice for the damping functions \( g_i(v', x, t) \) (Section 3.3.2). This latter modification automatically leads to different damping coefficients.

### 3.2 Numerical method

In this section the numerical method is introduced that is used to solve the Langevin model given by equation (3.12). This same numerical method is used to solve the models that result from modifications made to this initial model. Results of these models will be compared to results from a DNS. The description of this DNS is also given in this section.

#### 3.2.1 Time advancement scheme for Langevin models

The particles move through a channel with a height coordinate of \( 0 \leq x_2 \leq 300 \), with walls located at each extremum. As the problem is symmetric with respect to \( x_2 = 150 \), only the bottom part of the channel is modeled and the symmetric property is applied for particles that cross the channel center line. Particle collisions at the wall, i.e., at \( x_2 = 0 \), are assumed to be elastic. The Eulerian mean velocity and (co)variances are obtained by a
DNS. Covariances of the spanwise velocity component with the other two are zero, so the only non-zero covariance is \( \langle u_1' u_2' \rangle \).

A simulation is started by choosing the initial conditions \( x_0^i \) and \( v_0^i \) such that the initial velocity field has the correct (co)variances. The particles are homogeneously distributed over the height and the initial position in streamwise and spanwise direction are set to zero. The new particle position is calculated using the first-order Euler explicit method:

\[
x_i^{n+1} = x_i^n + v_i^n \, dt,
\]

where \( n \) indicates the number of the time step, which starts at zero and stops when it reaches the value of \( N_t \), the final time step. Higher order methods were tested but no significant differences were found. Next, Eulerian properties such as \( U_1, \sigma_i, \langle u_1' u_2' \rangle \) at the new particle wall-normal position \( x_{i+1}^2 \) are found by using a first-order interpolation method of the DNS results. This means that the mean streamwise velocity has changed by an amount

\[
dU_1^{n+1} = U_1^{n+1} - U_1^n
\]

To find \( \tau_i^{n+1} \) a polynomial is fit through the data points found by [66]. For the drift terms, which are derivatives with respect to the wall-normal coordinate, central differences are applied to the two DNS data points, along with its corresponding values of \( \langle u_1' u_2' \rangle^{n+1} \), surrounding the particle position.

The total change in the velocity at \( t^{n+1} \) can then be found with

\[
dv_i^{n+1} = a_i^{n+1} v_i^n \, dt + \left( \frac{d}{dx_2} \langle u_1' u_2' \rangle^{n+1} \right) dt + \left( C_0^{n+1} \epsilon^{n+1} \right)^{1/2} dW_i(t),
\]

while the new velocity is given by:

\[
v_i^{n+1} = v_i^n + dv_i^{n+1} + dU_i^{n+1}.
\]

### 3.2.2 Description of the DNS of channel flow

The geometry of the channel is \( 0 < x_1/H < L, -1 < x_2/H < 1 \) and \( 0 < x_3/H < W \), where \( x_1 \) is the streamwise direction, \( x_2 \) the direction normal to the walls of the channel and \( x_3 \) the spanwise direction. Hence, walls are at position \( x_2 = \pm H \). In the computer program \( L = 4\pi \) and \( W = 2\pi \).

The incompressible Navier-Stokes equation that is solved numerically is

\[
\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \times \mathbf{u} + \nabla P = \nu \Delta \mathbf{u} - \mathbf{f},
\]

where \( \mathbf{u} \) denotes the fluid velocity vector, \( P = p/\rho_f + \frac{1}{2} \mathbf{u}^2 \) is the total pressure, \( p \) the static pressure, \( \rho_f \) the fluid mass density, \( \mathbf{u} \) is the vorticity of the fluid and \( \nu \) is the fluid kinematic viscosity. Incompressibility of the flow is described by \( \nabla \cdot \mathbf{u} = 0 \). The boundary conditions read
\( u(x_1, \pm H, x_3) = 0, u(x_1, x_2, x_3 + WH) = u(x_1 + LH, x_2, x_3) = u(x_1, x_2, x_3) \) for all \( x_1, x_2 \) and \( x_3 \). The first condition implies no slip at the walls while the second results in periodicity. Finally, \( f \) is the external force, necessary to maintain the flow. \( f \) has only a component in the \( x_1 \)-direction and is taken constant in space and time. The expression for this component can be found by integration of equation (3.18) over the total domain and averaging over time. This yields:

\[
fx_1 = \frac{\nu}{2H} \left( \frac{\partial u_{x_1}}{\partial x_2}(1) - \frac{\partial u_{x_1}}{\partial x_2}(-1) \right),
\]

(3.19)

where the bar denotes averaging over time and the periodic directions.

The equations are non-dimensionalized by taking a certain velocity \( U_0 \) as velocity scale and half the channel height \( H \) as length scale. Hence the Reynolds number \( Re = \frac{U_0 H}{\nu} \) is introduced, which has a value of 3500 in the current simulation. Due to the non-dimensionalization, the walls are positioned at \( x_2 = \pm 1 \).

In order to solve the equations numerically a Fourier-Chebyshev spectral method is adopted. In the periodic directions \( x_1 \) and \( x_3 \) a Fourier expansion is used and in \( x_2 \)-direction a Chebyshev expansion is introduced. The collocation points are chosen as

\[
x_{2,j} = \cos\left(\frac{j\pi}{N_{x_2}}\right),
\]

(3.20)

where \( j = 0, 1, \ldots, N_{x_2} \). This method increases the spatial resolution of the computational domain close to the wall where steep gradients prevail. The number of grid points is \( N_{x_1} \times N_{x_2} \times N_{x_3} = 128 \times 129 \times 128 \).

The time integration is a combination of an explicit three-stage Runge-Kutta method and the implicit Crank-Nicolson method. Only the nonlinear term is treated explicitly, for all others the implicit method is used. The total method is second-order accurate in the time step. This computational time step is \( \Delta t u^2 / \nu = 0.032 \).

Eulerian Statistics of the fluid velocity are obtained by time averaging over 908 statistically independent fluid velocity fields.

To obtain Lagrangian statistics from a DNS a different approach has to be taken as fluid particles have to be tracked. As these statistics of the flow vary in wall-normal direction, particles have to be injected at several wall-normal positions. Hereto, in one simulation particles are initially distributed between \(-1\) and \(1\) as:

\[
x^0_{2,j} = \pm \frac{1}{32}, \pm \frac{3}{32}, \ldots, \pm \frac{31}{32}.
\]

(3.21)

As the lower half of the channel is statistically symmetric with the upper half, we have two realizations for every \( x_2 \)-position. This number can be further increased by using the spanwise and streamwise directions as well. Utilizing
the total length, \( L = 4\pi \) and width, \( W = 2\pi \) of the channel, particles are injected at the following initial streamwise and spanwise positions for every initial wall-normal position:

\[
x_0^0 = 0, \frac{1}{4}\pi, \ldots, \frac{15}{4}\pi
\]  

(3.22)

and

\[
x_3^0 = 0, \frac{1}{4}\pi, \ldots, \frac{7}{4}\pi.
\]  

(3.23)

Hence particles are separated by a distance of \( \pi/4 \) in both directions, which is large enough to ensure that particle trajectories are independent.

Since the particle position will in general not coincide with a grid point, a fourth-order interpolation scheme is used to calculate the Eulerian fluid velocity at the particle position. This interpolation scheme is a combination of Hermite polynomials, used for the periodic direction, and Lagrange polynomials, which is used for the normal direction [67]. The new particle position can then be found by integration of:

\[
\frac{dx}{dt} = u(x,t).
\]  

(3.24)

Numerically, this equation will be solved using Heun’s method, which is a two-stage Runge-Kutta method.

Finally, one simulation results in \( 2 \times 8 \times 16 = 256 \) statistically independent records for every \( x_3 \) in a single simulation. Lagrangian statistics are obtained by averaging over 20 such simulations.

### 3.3 Results

In this section the results will be presented which were obtained by using the numerical model outlined in Section 3.2. A time step of \( 0.25\nu/u_x^2 \) is used with a total number of time steps \( N_t = 16000 \). Eulerian statistics of the model are obtained by injecting 25000 particles and taking an ensemble average over all particles after every 800 time steps. This gives 20 statistically independent ensemble averages as the velocities of the fluid particles are uncorrelated with their corresponding values of 800 time steps earlier, see later on in this report for correlation function plots. Final statistics result then from averaging over these 20 statistically independent ensemble averages. The comparison of the Eulerian statistics with DNS data will be made by dividing the height of the channel in 300 equally spaced bins and taking an ensemble average of all particles present in each bin.

Results show that the particle distribution along with most of the first- and second-order statistics turn out to be calculated correctly, except for the mean velocity in streamwise direction (see Figure (3.1)) and the covariance \( \langle u'_1 u'_2 \rangle \), the latter turning out to be equal to zero. These deviations
are caused by the absence of a correlation between the streamwise and wall-normal velocity component in the model. Two different options to implement this covariance will now be proposed and the resulting models will be tested numerically.

Figure 3.1: Eulerian mean velocity in streamwise direction as function of the height

3.3.1 Correlated forcing term

The problems that arose by using the model elaborated in Section 3.2 are caused by the absence of the covariance $\langle u'_1 u'_2 \rangle$ in the model. As the variances of the different velocity components are included in the model by means of the forcing term, it would be straightforward to try to implement the covariance in this way as well. As mentioned before, the random process used in the forcing term is the incremental Wiener process, which is very similar to a normal process, i.e., $dW_i(t) \sim \sqrt{\Delta t} N(0, 1)$. In the model of Section 3.2, the random processes in the Langevin equation for each velocity are uncorrelated, but by using a multivariate random process instead the desired covariance can be included. For this random process a vector with mean values (in this case one containing three zeros) and a covariance matrix of size $3 \times 3$ has to be specified. The diagonal of this matrix contains the variances of the three velocity components and the off-diagonal terms are the covariances between the different components. The only non-zero off-diagonal terms are the term on the first row in the second column and the one on the second row in the first column, both being equal to $\langle u'_1 u'_2 \rangle$. All others are zero as the spanwise velocity component is uncorrelated with
the other two. Note that this same multivariate random process is used to initialize the velocity field.

To test this new model 50,000 particles are injected and a time step of $0.25\nu/u_1^2$ is used. The total number of time steps is 64,000 and an ensemble average is taken after every 800 time steps, resulting in 80 independent ensemble averages. Eulerian statistics are then obtained by averaging over these independent ensemble averages. In order to obtain them as function of the wall-normal coordinate, the height is divided into 300 equally spaced bins.

![Figure 3.2](image)

Figure 3.2: Eulerian mean velocity in streamwise direction as function of the height using a multivariate random process in the Langevin equation.

Figure 3.2 shows the new Eulerian mean velocity in the streamwise direction, whereas the Eulerian covariance $\langle u'_1 u'_2 \rangle$ is plotted in Figure 3.3. Both agree very well with the values obtained by a DNS, which are also plotted in the figures. To check if the well-mixed criterion is satisfied, $\langle u'_2 \rangle$ is calculated. For the criterion to hold, this variable has to be (approximately) zero such that particles do not drift from one position to another on average. As can be seen from Figure 3.4, $\langle u'_2 \rangle$ fluctuates around zero for most wall-normal positions, except near the wall, where it is slightly positive. Even though this deviation is quite small, it will cause particles to drift away from the wall, something which will become apparent in very long simulations. The fluctuations in $\langle u'_2 \rangle$ decrease upon increasing the number of particles or increasing the simulation time. As expected, it is found that the amplitude decreases approximately proportional to $1/\sqrt{n}$, where $n$ is the total number of particles over which is averaged.
Figure 3.3: Covariance of $u'_1$ with $u'_2$ as function of the height using a multivariate random process in the Langevin equation.

Figure 3.4: Eulerian mean velocity in wall-normal direction as function of the height using a multivariate random process in the Langevin equation.

Eulerian mean-squared values of all velocity components are depicted in Figure 3.5. All agree very well with DNS data.

So far, only Eulerian statistics of the model have been compared with data from our DNS database. It is also possible to compare Lagrangian statistics like auto- and cross-correlation functions. Hereto, 50,000 particles
are injected at one position and are followed during 1000 time steps, using the same time steps as before, i.e., $\Delta t = 0.25\nu/u_\tau^2$. Figure 3.6 shows the auto- and cross-correlation functions for particles that initially had a wall-normal position $x_2 = 61$. All plots have the same initial value of $\rho_{ij}$ as the DNS results, which indicates that the initial (co)variances of the model are equal to those of the DNS data. Furthermore, the model predicts the behavior of the functions correctly for most of them, except for $\rho_{21}$, which deviates quite a lot from the DNS results, and $\rho_{11}$ to a lesser extent. These deviations are mainly caused by the short time behavior of the model, something that was already mentioned in Section 2.3.2. Due to the absence of a second time scale that is representative of motion on the smaller scales, the correlation functions will ignore small scale effects and drop off immediately, thus not predicting the quadratic short time behavior correctly. The slope, however, of the correlation functions agrees quite well with the DNS data, indicating that the large scale effects are correctly retrieved. Similar results are found for other initial wall-normal positions.

![Figure 3.5: Velocity MSV for channel flow as a function of the height for all velocity components using a multivariate random process in the Langevin equation.](image)

3.3.2 Cross term in $v'_i$-equation

So far, a damping term that is proportional to the velocity component itself has been used; no terms are included that contain the other velocity components. It can be expected that if there is a covariance between $v'_1$ and $v'_2$ the
equation for $dv'_1$ should depend on $v'_2$ as well. To make this dependency explicit the following model for the streamwise velocity fluctuation component is proposed:

$$
\begin{align*}
    dv'_1 &= a_{11}v'_1 dt + a_{12}v'_2 dt + \frac{d}{dx_2} \langle u'_1 u'_2 \rangle dt + \sqrt{\frac{2\sigma^2_1}{\tau_1}} dw_1(t) \\
    \text{(3.25)}
\end{align*}
$$

The equations for the other two velocity components stay the same (see Section 3.3.3), i.e.,

$$
\begin{align*}
    dv'_2 &= a_{22}v'_2 dt + \frac{d}{dx_2} \langle u'_2 u'_2 \rangle dt + \sqrt{\frac{2\sigma^2_2}{\tau_2}} dw_2(t), \\
    \text{(3.26a)} \\
    dv'_3 &= a_{33}v'_3 dt + \sqrt{\frac{2\sigma^2_3}{\tau_3}} dw_3(t). \\
    \text{(3.26b)}
\end{align*}
$$

The incremental Wiener processes present in the equations for the velocity components are again uncorrelated, in contrary to Section 3.3.1 where
a multivariate random distribution was used. Expressions for the four unknown parameters, i.e., $a_{11}, a_{12}, a_{22}$ and $a_{33}$, are derived using only Eulerian based statistics. For that, the following properties of the random process are used:

\[
\langle dw_i(t)dw_j(t) \rangle = \delta_{ij}(t - \tau), \quad (3.27a)
\]

\[
\langle v_i'(t)dw_j(t) \rangle = \frac{1}{2} \left( \frac{2\sigma_i^2}{\tau_i} \right)^{1/2} \delta_{ij}. \quad (3.27b)
\]

First the spanwise velocity component of equation (3.26) is multiplied with $v_3'$ and an ensemble average is taken

\[
\left\langle \frac{1}{2} v_3'^2 \right\rangle = a_{33} \langle v_3'v_3' \rangle dt + \sqrt{2\sigma_3^2/\tau_3} \langle dw_3(t)v_3' \rangle, \quad (3.28)
\]

where $dv_3'v_3' = d \left( \frac{1}{2} v_3'^2 \right)$ is used. Next, the definition of the material derivative is applied

\[
\left\langle \frac{1}{2} v_3'^2 \right\rangle = \left\langle \partial_t \frac{1}{2} u_3'^2 \right\rangle + \left\langle u \cdot \nabla \frac{1}{2} u_3'^2 \right\rangle dt. \quad (3.29)
\]

The first term on the right-hand-side of this equation is zero for stationary flow. Furthermore, for incompressible flow $\nabla \cdot u = 0$, so that $u$ can be brought inside the gradient operator. Using all this, along with the second property of (3.27) gives:

\[
\nabla \cdot \left\langle \frac{1}{2} u u_3'^2 \right\rangle = a_{33} \langle u_3'^2 \rangle + \frac{\sigma_3^2}{\tau_3}. \quad (3.30)
\]

As the streamwise and spanwise directions are homogeneous for channel flow the previous equation can be simplified to

\[
\frac{d}{dx_2} \left\langle \frac{1}{2} u_2'^2 u_3'^2 \right\rangle = a_{33} \langle u_3'^2 \rangle + \frac{\sigma_3^2}{\tau_3}. \quad (3.31)
\]

Moments of the spanwise velocity component with other velocity components are zero so that the left-hand-side of this equation vanishes. Also $\langle u_3'^2 \rangle = \sigma_3^2$, which finally results in:

\[
a_{33} = -\frac{1}{\tau_3}. \quad (3.32)
\]

So it results in the same expression as found in Section 3.1. This result should have been expected as the equation of the spanwise velocity component stayed unchanged and that velocity component is uncorrelated with the other two components.

Next, the equation of the wall-normal velocity component, the first equation in (3.26), is multiplied by $v_2'$ and a similar derivation is used, i.e., taking
an ensemble average, using the second property of equation (3.27), applying the definition of the material derivative and noting that channel flow is only non-homogeneous in wall-normal direction. The final result is:

$$a_{22} = -\frac{1}{\tau_2} + \frac{d}{dx_2} \langle \frac{1}{2} u_2'^2 \rangle. \quad (3.33)$$

This expression deviates from the one used before, i.e., from $a_{22} = -1/\tau_2$, as there is an additional term present. However, as the Langevin equation used in this paper does not contain any moments of third order or higher, the additional term can be neglected. This then gives again the same expression for the damping coefficient as used before.

To obtain an expression for $a_{11}$ equation (3.25) is multiplied with $v_1'$ and the same steps as before are taken. This yields:

$$a_{11} \langle u_1'^2 \rangle + a_{12} \langle u_1' u_2' \rangle = -\frac{\sigma_1^2}{\tau_1} + \frac{d}{dx_2} \left( \frac{1}{2} u_1'^2 u_2' \right). \quad (3.34)$$

It is apparent that this equation for $a_{11}$ cannot be solved because it contains the additional unknown $a_{12}$. Therefore, another equation that combines these two unknown damping coefficients is needed. For that equation (3.25) is multiplied with $v_2'$ and the first equation of (3.26) is multiplied with $v_1'$ and of both an ensemble average is taken. Adding the two results and applying a similar derivation as for the previous damping coefficients results in:

$$a_{11} \langle u_1' u_2' \rangle + a_{12} \langle u_2'^2 \rangle = -a_{22} \langle u_1' u_2' \rangle + \frac{d}{dx_2} \left( \frac{1}{2} u_1'^2 u_2'^2 \right). \quad (3.35)$$

This gives two equations for two unknowns, which is solvable. Neglecting again third order moments and rearranging terms in (3.35) gives:

$$a_{12} = -\frac{\langle u_1' u_2' \rangle}{\sigma_2^2} (a_{11} + a_{22}). \quad (3.36)$$

Replacing this expression for $a_{12}$ finally in (3.34) gives:

$$a_{11} = \left( -\frac{\sigma_1^2}{\tau_1} - a_{22} \frac{\langle u_1' u_2'^2 \rangle}{\sigma_2^2} \right) / \left( \sigma_1^2 - \frac{\langle u_1' u_2' \rangle^2}{\sigma_2^2} \right) \quad (3.37)$$

So the expression for the damping coefficients are:
\[ a_{11} = \left( -\frac{\sigma_1^2}{\tau_1} - a_{22} \frac{\langle u'_1 u'_2 \rangle^2}{\sigma_2^2} \right) / \left( \sigma_1^2 - \frac{\langle u'_1 u'_2 \rangle^2}{\sigma_2^2} \right), \]  

(3.38a)

\[ a_{12} = -\frac{\langle u'_1 u'_2 \rangle}{\sigma_2^2} (a_{11} + a_{22}), \]  

(3.38b)

\[ a_{22} = -\frac{1}{\tau_2}, \]  

(3.38c)

\[ a_{33} = -\frac{1}{\tau_3}. \]  

(3.38d)

To find the correct values for these coefficients the data obtained from a DNS is used again, as well as the polynomial function for $\tau_i$. Equations (3.38) show that $a_{22}$ is needed before being able to proceed with $a_{11}$ and finally $a_{12}$.

The expressions (3.38) along with the equations (3.25) and (3.26) are implemented in a numerical model. The time step is again $0.25\nu/u_2^2$, but the total number of time steps now is 80,000 while an ensemble average is taken after every 800 time steps. The number of particles is set equal to 60,000 and the height is divided again in 300 equally spaced bins. To estimate the error made in the averaging process, 10 of these simulations have been carried out. Eulerian statistics are then found by averaging over the ten individual simulations while the standard deviation of the estimated means gives an indication of the error. Where useful, these standard deviations will be presented in the figures by means of error bars.

The reason for some different values of the numerical parameters in this simulation compared with the one from Section 3.3.1 is the fact that using a multivariate random distribution greatly slows down the simulation, causing the simulation to run a lot longer if the same values are used.

Plots of the Eulerian mean streamwise velocity and the Eulerian covariance of the streamwise velocity component with the wall-normal velocity component can be found in Figures 3.7 and 3.8, respectively. The results from the numerical model agree very well with the DNS results. Error bars have been omitted from Figure 3.7 as the value of the error is very small compared with the value of the streamwise velocity: a maximum of 0.009 is found at $x_2 \approx 15$ dropping off to 0.002 at the wall and the center of the channel.

The Eulerian mean wall-normal velocity is plotted in Figure 3.9, which shows the same behavior as found for the model presented in Section 3.3.1, i.e., a generally around zero fluctuating $\langle u'_3 \rangle$, except near the wall where it has a relatively small positive value. The error bars indicate $\langle u'_3 \rangle$ is probably really positive near the wall, i.e., the observed behavior is not caused due to poor sampling. Eulerian mean-square values of all velocity components can be found in Figure 3.10; all agree pretty well with DNS data. The standard
Figure 3.7: Eulerian mean velocity in streamwise direction as function of the height using an extra term in the $v'_1$-equation.

Figure 3.8: Covariance of $u'_1$ with $u'_2$ as function of the height using an extra term in the $v'_1$-equation.

The deviation of the estimated means of the variance has a value between 0.0001 and 0.002 for the wall-normal and spanwise velocity components, while it has a maximum of 0.03 near the peak for the streamwise velocity component and falls down to values around 0.002 at the wall and channel center.
Finally, velocity auto- and cross-correlation functions are shown in Figure 3.11. Similar results are found as in Section 3.3.1; biggest deviations in $\rho_{11}$ and $\rho_{21}$ due to wrong short time behavior of the model, whereas the
large scale motion is predicted much better.

![Graphs showing velocity auto- and cross-correlation functions for channel flow for all velocity components at $y^+ = 61$ using an extra term in the $v'_1$ equation.](image)

**Figure 3.11:** Velocity auto- and cross-correlation functions for channel flow for all velocity components at $y^+ = 61$ using an extra term in the $v'_1$ equation.

### 3.3.3 Multiple cross terms

In Section 3.3.2 a cross term was added to the equation of the streamwise velocity component such that $v'_1$ would depend on $v'_2$, but it has not been explained why no cross term was added as well to the equation of the wall-normal velocity component. In fact, two cross terms could be added in each velocity component equation. That would have given the following equation for the velocity fluctuation component $v'_i$:

\[
dv_i = a_{ij}v'_j dt + \frac{d}{dx_2} \langle u'_i u'_j \rangle dt + \sqrt{\frac{2\sigma^2_{i}}{\tau_i}} dw_i(t), \tag{3.39}
\]

where the Einstein convention has been used for summation over the index $j$, however not for the index $i$. This gives in total nine damping terms; one in each equation containing the same velocity component and two cross terms in each equation. This gives also nine damping coefficients. As the
spanwise direction is uncorrelated with the two other directions, all damping coefficients containing a 3 in the index, i.e., $a_{13}, a_{23}, a_{31}$ and $a_{32}$, are equal to zero. It turns out that from measurements and numerical simulations on turbulent pipe flow the damping coefficient from the cross term in the wall-normal velocity component equation is very close to zero, i.e., $a_{21} \approx 0$, so that finally only four damping coefficients are non-zero. Expressions for these non-zero damping coefficients were found using Eulerian statistics through the method elaborated in Section 3.3.2. This wouldn’t have worked had $a_{21}$ not been approximately equal to zero, or if no other relation holds between the damping coefficients (e.g. $a_{12} = a_{21}$), as the four second order Eulerian moment ($\sigma^2_1, \sigma^2_2, \sigma^2_3$ and $\langle u'_1 u'_2 \rangle$) were used to derive expressions for the four unknown damping coefficient. Had there been five non-zero damping coefficients no independent expressions could have been found for each one of them, as there would be five unknowns and only four equations. This is the non-uniqueness problem mentioned in Section 2.3.2. So the reasoning behind including only one cross term is the fact the four of the six possible cross term are zero due to the independency of the spanwise velocity component on the other two and measurements and simulations showed that one of the remaining two is very close to zero.

3.3.4 Preferred model

Having found two properly working models one could wonder if there is a preference for either one of them. According to Kolmogorov’s theory the forcing term should become isotropic for high Reynolds numbers, see also Section 2.3.2. This means that the variance is equal for each direction and that the diffusion matrix does not contain any off-diagonal terms, which makes the use of a multivariate normal process impossible. So based on this theory there is a preference for the second one, i.e., the one containing the cross term.

Furthermore, DNS results show that the cross-correlation function $\rho_{12}$ decays immediately to zero, while $\rho_{21}$ first increases before dropping off to zero, see Walpot et al. [68] for an explanation of this phenomenon. When either one of them is mirrored and connected to the other one, the resulting correlation function should be differentiable at the connection point $t = 0$. This is not the case for the cross-correlations found from either Langevin model, which was expected as they do not predict the short time behavior correctly. However, the model containing a cross term in the $v_i'$ equation does recover the behavior of the cross-correlation function $\rho_{21}$ much better than the model using a multivariate random process in the forcing term; where it falls off immediately for the latter, it rises first before decaying for the former. This is another reason why the model with a cross term in the equation for the streamwise velocity component is preferred.
Chapter 4

Linear Stochastic Model for Pipe Flow

In this chapter the Lagrangian approach will be used to model fluid particle dispersion in turbulent pipe flow. The Langevin equation has mostly been used to simulate particle dispersion in either turbulent channel flow [66, 52] or turbulent shear flow [49, 48]. We are not aware of anyone attempting to apply it to turbulent pipe flow. In Section 4.1 the Langevin model will be derived for turbulent pipe flow in a similar way as was done for turbulent channel flow in Section 3.1. The circular geometry characteristic for pipe flow gives rise to additional (centrifugal) terms, which are proportional to $1/r$. How these terms are treated numerically will be discussed in Section 4.2, along with further details on how to solve the resulting stochastic equations numerically. Finally, in Section 4.3 results obtained from the Langevin model will be compared with calculations from a DNS.

4.1 Model Features

The derivation of the Langevin model outlined in Section 3.1 remains unchanged for turbulent pipe flow up to equation (3.10). In a cylindrical coordinate system the term after the second equal sign of that equation appears as $r^{-1} d \langle r u_r' u_r' \rangle / dr$ since averaged quantities do not depend on the tangential or axial direction in a stationary fully-developed flow. Furthermore, the damping functions will now be assumed to be linear in $v_j'$, i.e., $g_i(v', x, t) = g_i^0(v', x, t) + a_{ij}(x)v_j'$, similar to what is used in Section 3.3.3 for turbulent channel flow. The reason for this is that results on turbulent channel flow showed that models containing damping functions $g_i(v', x, t)$ linear in $v_i'$ only, $i = r, \phi, z$, do not predict the mean streamwise direction correctly, see Section 3.3.1. This can be overcome by using a multivariate random process. However, that process asks for much more computational effort and it is not consistent with Kolmogorov’s similarity theory, see Sec-
tion 3.3.4. Thus, the following expression for the damping functions results:

\[
g_i(v', x, t) = \frac{1}{r} \frac{d}{dr} \langle ru_r' u_i' \rangle + a_{ij} v_j',
\]

(4.1)

where the Einstein convention has been used for summation over repeated indices. If one assumes a model with linear damping function in Cartesian coordinates then in cylindrical coordinates the complete first order Langevin model is given by

\[
\begin{align*}
    dv_r' &= a_{rr} v_r' dt + a_{r\phi} v_\phi' dt + a_{rz} v_z' dt + \frac{1}{r} \frac{d}{dr} \langle ru_r'^2 \rangle dt - \frac{1}{r} \langle u_r'^2 \rangle dt \\
    &\quad + \frac{1}{r} v_\phi'^2 dt + (C_0^r \epsilon)^{1/2} dW_r(t) \\
    dv_\phi' &= a_{\phi r} v_r' dt + a_{\phi\phi} v_\phi' dt + a_{\phi z} v_z' dt - \frac{1}{r} v_r' v_\phi' dt + \left( C_0^\phi \epsilon \right)^{1/2} dW_\phi(t) \\
    dv_z' &= a_{z r} v_r' dt + a_{z \phi} v_\phi' dt + a_{zz} v_z' dt + \frac{1}{r} \frac{d}{dr} \langle ru_r' u_z' \rangle dt + (C_0^z \epsilon)^{1/2} dW_z(t).
\end{align*}
\]

(4.2)

The transformation procedure from Cartesian to cylindrical coordinates is similar to that of, for example, the Navier Stokes equations and gives rise to centrifugal terms, namely \( r^{-1} v_r'^2 \) and \( -r^{-1} v_r' v_\phi' \). Hence, a linear model in Cartesian coordinates automatically results in a nonlinear model in cylindrical coordinates. These terms would not be present if had been opted for a linear model in cylindrical coordinates, however, such a model gave far less accurate results than one linear in Cartesian coordinates. For example, the mean axial velocity was not calculated correctly.

The tangential direction is decoupled from the other two directions, meaning that correlations such as \( \langle u_\phi' u_z' \rangle \) and \( \langle u_\phi' u_r' \rangle \) are equal to zero. DNS calculations and 3D PTV measurement results indeed show them to be 2 orders of magnitude smaller than the correlations not containing \( u_\phi' \) [68]. Therefore, the damping coefficients in equation (4.2) containing a \( \phi \) are equal to zero, just as the additional term \( r^{-1} \langle u_\phi' u_\phi' \rangle \). Veenman [69] found by means of a DNS that the coefficient \( a_{rz} \) is close to zero. This was later on verified by Walpot [70] by using 3D particle tracking velocimetry (3D PTV). This enables us to use the well-mixed criterion again to find expressions for the four remaining damping coefficients based on Eulerian statistics. The derivation is similar to the one used in Section 3.3.2 and therefore only the result will be given here:

\[
a_{zr} \langle u_r' u_z' \rangle + a_{zz} \langle u_z'^2 \rangle = -\frac{1}{2} C_0^z \epsilon + \frac{1}{r} \frac{d}{dr} \left( \frac{1}{2} ru_r'^2 \right)
\]

(4.3)

\[
a_{zr} \langle u_z'^2 \rangle + a_{zz} \langle u_r' u_z' \rangle = -a_{rr} \langle u_r' u_z' \rangle + \frac{1}{r} \frac{d}{dr} \langle ru_r'^2 u_z' \rangle
\]

(4.4)

\[
a_{rr} = -\frac{1}{2} C_0^r \epsilon \langle u_r'^2 \rangle + \frac{1}{r} \frac{d}{dr} \left( \frac{1}{2} ru_r'^3 \right)
\]

(4.5)
\[ a_{\phi \phi} = -\frac{1}{2} \frac{C_{0}^{i} \epsilon}{\langle u_{\phi}^{2} \rangle} \] (4.6)

Terms of third- and higher-order will be neglected again when calculating the damping coefficients from the above given equations. Including them did not give significant differences in the results.

4.2 Numerical Method

This section describes the numerical technique used to solve the stochastic model of equation (4.2). The flow is stationary and fully-developed, so that \( \langle v \rangle = (0, 0, U_{z}) \) and statistical properties of the turbulence are only a function of the radius \( r \). All variables are non-dimensionalized using the radius \( R \) of the pipe and the friction velocity \( u_{\tau} \). Therefore, the radial position of a fluid particle is bounded by \( r = 0 \), the pipe axis, and \( r = 1 \), the wall. Symmetry is used for particles crossing the pipe axis, whereas particles experience elastic collisions when hitting the wall. All results are calculated at a Reynolds number based on bulk velocity \( U_{b} \) and pipe diameter \( D \) of \( Re_{b} = \frac{U_{b}D}{\nu} \approx 5300 \). Veenman \[69\] determined the Eulerian mean axial velocity, Eulerian velocity (co)variances, the mean dissipation rate \( \epsilon \) and \( C_{0}^{i} \) from a DNS at this Reynolds number and his results will be used where necessary.

Initially, the particles are homogeneously distributed over the radius and have axial and tangential positions equal to zero. It is less straightforward to obtain a homogeneous distribution in radial direction than it is to obtain such a distribution in wall-normal direction, as was needed for turbulent channel flow, due to flow area that increases with increasing radius \( r \). The radially homogeneous distribution is generated by taking the square root of a uniform distribution for the radius, resulting in the number of particles to increase linearly in radial direction. The initial velocity field is specified using the multivariate random process discussed in Section 3.3.1. A first order Euler explicit method is again used for time integration of the position, while the new velocity is found from equation (4.2) on a way analogous to Section 3.2. The only difference is that now the local decorrelation time \( \tau_{i} \) is not known, but instead \( C_{0}^{i} \) is known. The most straightforward solution would be to simply fit a polynomial through the DNS data available for this latter parameter and use that fit to obtain the corresponding value of \( C_{0}^{i} \) at the particle position needed in the Langevin model and in the equations for the damping coefficients, all given in Section 4.1. The problem in doing so is that \( C_{0}^{i} \) is found to be approximately constant over the pipe radius, except near the wall where it drops rapidly to zero. The behavior of \( C_{0}^{i} \) near the wall is not known, as it is assumed to be a universal constant for high Reynolds-numbered turbulence. \( \tau_{i} \) is related to \( C_{0}^{i} \) through the following
expression:
\[ \tau_i = \frac{2\sigma_i^2}{C_0^i \epsilon} \]  
and behaves much smoother throughout the whole domain. Equation (4.7) can be used to fit a polynomial through the data points available from a DNS and subsequently to find the value of \( C_0^i \epsilon \). However, \( C_0^i \) is only known at ten radial positions, which causes problems when fitting a polynomial, or alternatively, interpolating between the available data points. By using the polynomial of the local decorrelation time \( \tau_i \) that is used as well for channel flow in Chapter 3 instead, this problem is avoided. This is possible because the turbulent pipe flow has a Reynolds number based on wall units and the radius of \( Re_r = \frac{U_{\tau} R}{\nu} \approx 180 \), close to the one of 150 for turbulent channel flow.

Finally, as already mentioned in the introduction of this chapter, the terms containing \( 1/r \) in equation (4.2) can cause problems for particles near the pipe axis, where \( r = 0 \). The drift terms \( r^{-1}d \left< ru'_r u'_i \right>/dr \), included to prevent particles drifting from one radial position to another on average, remain finite. Therefore, those do not cause any problems. However, the others will go to infinity if \( r \) would be allowed to go to zero. To prevent this, the value of \( r \) in those terms has a lower bound of 0.01, i.e., if a particle is located within a circular duct of radius \( r = 0.01 \), \( r \) is set equal to 0.01 in those terms. Smaller values of \( r \) would be possible if \( \Delta t \) would be decreased, but as there are only a few particles having a radial position smaller than 0.01, it is more advantageous to let \( r \) not get too small in the terms \( \frac{1}{r} \left< u'_r u'_i \right> dt \), \( \frac{1}{r} \left< v'_r v'_i \right> dt \) and \( \frac{1}{r} \left< v'_r u'_i \right> dt \). After all, decreasing \( \Delta t \) implies that the calculation time has to increase to obtain the same number of statistically independent ensemble averages.

### 4.3 Results

In this section, results of the Langevin model given in Section 4.1 are compared with results from a DNS.

To obtain Eulerian statistics from the model, a method similar to the one used in Section 3.3.2 is carried out, i.e., averaging over ten individual simulations. This enables us again to calculate the standard deviation of the estimated means to assess the error made in the averages. For one individual simulation, 30,000 particles are homogeneously distributed over the radial direction. They are tracked for 100,000 time steps, given by \( \Delta t u_r R^{-1} = 0.001 \). Particles are ensemble averaged after every 400 time steps, resulting in 250 statistically independent ensemble averages. Averaging these ensemble averages then gives the Eulerian statistics of one individual simulation. The Eulerian statistics presented in the various figures are then obtained by taking the average of all ten simulations.
To check whether the model satisfies the well-mixed criterion, the mean radial velocity profile is plotted in Figure 4.1. As the mean radial velocity fluctuates rather strongly in this figure, two different smoothing operations have been applied to the data to capture the trend of the mean radial velocity better. The first smoothing operation is simply halving the number of bins, i.e., from 200 to 100. The value of $\langle u'_r \rangle = 0$ in one of these 100 bins can be found by taking the average of two neighboring bins. Its value is allocated to the average position of the two neighboring bins. The result is shown in Figure 4.2. The fluctuations clearly become smaller in amplitude, what was to be expected as basically the number of particles over which the average has been calculated has been doubled. An alternative smoothing operation is setting the value of the mean radial velocity in a certain bin equal to half its original value plus a quarter of its two neighboring bins, i.e.,:

$$
\langle u'_r \rangle_{\text{new}}^i = \frac{1}{4} \langle u'_r \rangle_{\text{old}}^{i-1} + \frac{1}{2} \langle u'_r \rangle_{\text{old}}^i + \frac{1}{4} \langle u'_r \rangle_{\text{old}}^{i+1},
$$

where $i$ is the number of the bin, i.e., $i = 1, 2, \ldots, 200$. This results in a further decrease of the amplitude of the fluctuations as well as a smoother profile, see Figure 4.3. This latter result is of course caused by the fact that the value of the mean radial velocity in a certain bin now depends directly on its neighbors.

If $\langle u'_r \rangle = 0$ for all $r$, the initially well-mixed particle distribution will stay well-mixed and the criterion holds. Especially Figure 4.3 shows that $\langle u'_r \rangle$ is slightly positive for nearly all radial positions, except close to the pipe wall, where it is negative. This would suggest that particles would
accumulate around $r \approx 0.8$. However, this has not been observed in particle distribution plots. Strangely enough, particle distribution plots show that particles accumulate at the wall, which implies that the mean radial velocity is actually positive near the wall. A possibility is that it is positive close to the wall, but that this trend is not recovered due to poor sampling. To check
this, error bars showing the standard deviation of the estimated means of the ten simulations have been included in the plots. The error bars suggest that $\langle u'_r \rangle$ is indeed negative close to the wall.

As the radial velocity is found by solving equation (4.1) ensemble averages for each term in the radial velocity component equation are calculated to see which term causes the deviations found in $\langle u'_r \rangle$. An ensemble average of the last term in that equation is per definition zero, while the terms $-\frac{1}{r}\langle u' \phi^2 \rangle$ and $\frac{1}{r} v'_r \phi$ should cancel when taking an ensemble average. And as $a_{r\phi} = a_{r\phi} = 0$ only three terms remain: $dv'_r/dt$, $a_{rr} v'_r$ and $\frac{1}{r} \frac{d}{dr} \langle ru'^2_r \rangle$. The first of these terms can be written as a local time derivative plus a convective derivative following the fluid, i.e., $dv'_r/dt = \partial u'_r/\partial t + u \cdot \nabla u'_r$. The local derivative is zero for stationary flow, while the second term on the right hand side appears as $\frac{1}{r} \frac{d}{dr} \langle ru'^2_r \rangle$ for fully-developed flow. This implies that the terms $dv'_r/dt$ and $\frac{1}{r} \frac{d}{dr} \langle ru'^2_r \rangle$ in equation (4.1) have to balance each other in order for $\langle u'_r \rangle$ to be zero, after all, that is why the latter of these two terms is included in the equation; to prevent particles drifting from one radial position to another on average. To verify if both terms are indeed equal, ensemble averages of $dv'_r$ and $a_{rr} v'_r$ have been calculated as well in the ten simulations. They are shown in Figure 4.4, along with $\frac{1}{r} \frac{d}{dr} \langle ru'^2_r \rangle$ obtained from a DNS. The profiles are only shown for $r > 0.1$ for clarity reasons, while $\langle a_{rr} v'_r \rangle$ has been magnified by 100 to make it visible in the figure. The figure shows that the convective term of $\langle dv'_r \rangle$ balances the drift term very well for every radial position, except maybe near the wall, where it is slightly smaller for $0.8 < r < 0.9$ and slightly bigger for $0.9 < r < 1.0$. Furthermore, $\langle a_{rr} v'_r \rangle$ is negligibly small compared to the other two curves. However, $\langle a_{rr} v'_r \rangle$ is positive near the pipe wall, meaning that $\langle v'_r \rangle$ is negative in that area as $a_{rr} = -1/\tau_r$ for every radial position. This is in line with the plots for $\langle v'_r \rangle$, as was expected. The figure does not explain though why particles drift towards the wall.

To further test the accuracy of the model, well-known Eulerian statistical properties of turbulent pipe flow have been calculated from the simulation described above. The mean axial velocity is shown in Figure 4.5. Results from the model agree very well with DNS results. Error bars showing the standard deviation of the estimated means of the ten simulations have been omitted from this figure as the standard deviation of the estimated means is very small; decreasing from a value of 0.018 at the pipe axis to 0.0006 at the wall. The mean square value (MSV) of all three velocity components is depicted in Figure 4.6, which shows that the MSV profiles are in agreement with DNS. The only deviations occur near $r/R = 0$ for all velocity components. These deviations could be caused by the relatively low number of particles near the wall. However, the standard deviation of the estimated means of the MSV is approximately 0.02 at the pipe axis for all three velocity components, not nearly enough to explain the deviation. A more valid
Figure 4.4: Ensemble averaged terms $d v'_r / dt$ and $a r r'_r$ from the stochastic model along with $\frac{1}{r} \frac{d}{dr} \langle u_r' r^2 \rangle$ from a DNS as a function of the dimensionless radius.

Figure 4.5: The mean axial velocity as a function of the dimensionless radius.

Explanation is the behavior of the terms in equation (4.2) containing a the radial coordinate in the denominator. To prevent them from going to infinite, $r$ has been given a lower-bound of 0.01 in those terms, see Section 4.2. This leads to incorrect values that possibly can cause (partly) the deviations
The MSV profiles for all three velocity components drop to zero near the pipe wall, meaning there is no big spread in particle velocities close to the wall. The mean square value of the radial velocity obtained from the Langevin equation is slightly bigger than the one obtained from a Direct Numerical Simulation, increasing the chance that a particle in the Langevin model has a high positive radial velocity compared with a DNS. This can cause particles to suddenly move to the wall due to its high radial velocity, but being unable to move away from it as it has moved to a position where the mean square value of the radial velocity is much lower. This could be an explanation for particles drifting towards the wall. In fact, results from a model with damping coefficients that have been adjusted such that both MSV profiles of the radial velocity nearly agree, show that the particles stay much better radially homogeneously distributed for that situation. However, changing the damping coefficients affects the time scales present in the model, leading to incorrect auto- and cross correlation functions. Furthermore, it does not explain why $\langle u'_r \rangle = 0$ is negative near the wall.

For the axial component the peak of the mean square value is shifted towards the wall for the model results. However, the magnitude of this peak is predicted well. The same observation holds for the covariance of the radial velocity component with the axial component, which can be seen in Figure 4.7 where it is compared with DNS results.

The stochastic model only contains a single time-scale, namely the integral time scale, thus assuming a high Reynolds number flow. This property is illustrated by Figures 4.8 and 4.9, where velocity correlation functions as calculated with the model are compared with DNS results for $Re_b = 5300$ at $r/R = 0.3$ and $r/R = 0.9$, respectively. For the model calculations, 50,000 particles are released at the radial position of interest and have initial tangential and axial positions equal to zero. These particles are tracked for 1000 time steps. The results of the model calculations do not change when further increasing the number of particles. The figures show the expected influence of the absence of the Kolmogorov time-scale in the model on the correlation functions: the correlation functions calculated by the Langevin model start with a non-zero slope at $\tau = 0$. For larger time separations, the agreement between the slopes of the corresponding correlation functions is better. The model results are generally reliable for times $t \gg \tau_\eta$, with the exception of the axial autocorrelation at $r/R = 0.9$ and the $rz$-cross correlations for $r/R < 0.6$. 

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Figure 4.6: Velocity MSV for pipe flow as a function of the dimensionless radius for all velocity components at $Re_b = 5300$. 
Figure 4.7: Covariance of $u'_r$ with $u'_z$ as a function of the dimensionless radius.

Figure 4.8: Velocity auto- and cross-correlation functions for pipe flow for all velocity components for $Re_b = 5300$ at $r/R = 0.3$. 

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Figure 4.9: Velocity auto- and cross-correlation functions for pipe flow for all velocity components for $Re_b = 5300$ at $r/R = 0.9$. 
Chapter 5

Conclusion

The goal of this thesis was to find consistent stochastic equations for the fluid velocity in fully-developed turbulent channel and pipe flows and verifying their consistency by comparing Eulerian and Lagrangian statistics from the stochastic equations with those obtained from Direct Numerical Simulations. Expressions for the diffusion coefficients present in the stochastic equations have been derived by using Kolmogorov’s similarity theory for high Reynolds-numbered turbulence. To be able to apply this theory to non-homogeneous turbulence characterized by a relatively low Reynolds number, the parameter $C_0$ has been assumed to be inhomogeneous and anisotropic, i.e., $C_0 = C_0(x_2)$, where $x_2$ is the wall-normal coordinate.

Initially, for turbulent channel flow, the damping function in the Langevin equation was assumed to be linear in $v'_i$, $g_i(v', x, t) = g_i^0(x) + a_i(x)v'_i$ with $a_i$ damping coefficients equal to the negative of the reciprocal of the local decorrelation time $\tau_i$, $a_i = -1/\tau_i$. Simulations from the model with these damping coefficients and a direction and wall-normal coordinate dependent $C_0$ resulted in deviations in the mean streamwise velocity component and in the covariance of $v'_1$ with $v'_2$. The deviations are caused by the absence of a correlation between the streamwise and wall-normal velocity components in the model. Two solutions were proposed.

In the first solution, the covariance was implemented by means of a multivariate random distribution in the forcing term. In the second solution, an additional damping term that is linear in $v'_2$ was added to the equation for the streamwise velocity component. Expressions for the four damping coefficients were then derived based on the well-mixed condition, i.e., ensuring Eulerian second-order moments of the model agree with those obtained from a DNS. Eulerian statistics of the two models agree very well with those from a DNS. The same applies to Lagrangian results for times $t \gg \tau_\eta$. However, the second solution is preferred as the first solution results in a diffusion matrix containing off-diagonal terms, something that does not comply with Kolmogorov’s similarity theory for high Reynolds numbers.
The second solution would suggest a damping function linear in $v'_j$, $g_j(v', x, t) = g^0_j(x) + a_{ij}(x)v'_j$, is a better choice than what was assumed initially. This would give rise to nine damping coefficients $a_{ij}$. Four of them are zero as the spanwise direction is decoupled from the other two. Calculations from a DNS and results from 3D PTV measurements on fully-developed pipe flow showed that one of the five remaining non-zero damping coefficients, $a_{rz}$, is close to zero for every radial position. Thus only four damping coefficients remain enabling us to find expressions for them using the well-mixed condition.

A model equivalent to the second one used for channel flow was applied to fully-developed turbulent pipe flow, i.e., damping functions linear in $v'_j$. The model was assumed to be linear in Cartesian coordinates as such a model gives far more accurate results than one linear in cylindrical coordinates. This assumption however does lead to additional centrifugal terms in the model. Special care has to be taken when solving them numerically as they contain the radial coordinate in the denominator. Results from the model agree fairly well with DNS results, although particle accumulation at the wall is found for long simulation times. Possible explanations are the assumption of $a_{rz} = 0$ not being totally correct or particles having a too high radial velocity in the model as a result of the mean square value of the radial velocity in the model being somewhat bigger than the one found in a DNS. This could cause fluid particles to suddenly jump towards the wall while being unable to move away from it. Results for the mean radial velocity component contradict this, however. Therefore, more investigation is needed on this.

In the models used for turbulent channel and pipe flow, one of the five non-zero damping coefficients was set to zero based on observations on fully-developed turbulent pipe flow. However, 3D PTV measurements show this damping coefficient is less close to zero for higher Reynolds numbers [70]. It is therefore recommended to study the behavior of the damping coefficients as function of the Reynolds number to see if $a_{rz}$ is really close to zero. Perhaps $a_{rz} = a_{zr}$ is a better assumption for high Reynolds numbers [71]. It is also recommended to solve the stochastic model for turbulent pipe flow in Cartesian coordinate as the terms linear in $r^{-1}$ cause numerical problems near the pipe axis. This should improve the results near the pipe axis.
Bibliography


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