PROBABILITY DENSITY FUNCTION MODELING OF SCALAR MIXING FROM A CONCENTRATED SOURCE IN TURBULENT CHANNEL FLOW

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INTRODUCTION

In engineering industry and atmospheric transport and dispersion modelling there is an increasing use of computational methods to calculate complex turbulent flow fields. Many of these computations depend on the k-e turbulence model, while some are based on second-moment closures. For some flows these models provide an adequate description of the turbulent processes, but for many others a more complete and accurate representation is required. The development of probability density function (PDF) methods is an effort to meet this need.

The mean velocity and Reynolds stresses are the first and second moments of the PDF of velocity. In PDF methods, a transport equation is solved directly for the PDF of the turbulent velocity field, rather than for its moments as in Reynolds stress closures. Therefore, in principle, a more complete statistical description can be obtained. While for some flows (e.g. homogeneous turbulence) this higher level description may provide little benefit over second moment closures, in general the fuller description is beneficial in allowing more processes to be treated exactly and in providing more information, which can be used in the construction of closure models. Convection, for example, can be exactly represented mathematically in the PDF framework, eliminating the need for a closure assumption (*Pope, 2000)*. Similarly, defining the joint PDF of velocity and species concentrations in a chemically reactive turbulent flow allows for the treatment of chemical reactions without the burden of closure assumptions for the highly nonlinear chemical source terms (*Fox, 2003)*. This latter advantage has been one of the most important incentives for the development of PDF methods, since previous attempts to provide moment closures for the chemical source terms resulted in errors of several orders of magnitude (*Pope, 1990)*. Applying this technique in atmospheric transport and dispersion modelling allows the source term of moisture content to be represented without turbulence closure.

In the case of turbulent flows around complex geometries the presence of walls requires special treatment, since traditional turbulence models are developed for high Reynolds numbers and need to be modified in the vicinity of walls. Possible modifications involve damping functions (*van Driest, 1956; Rodi & Mansour, 1993)* or wall-functions (*Launder & Spalding, 1974; Rodi, 1980*). In those turbulent flows where a higher level of statistical description is necessary close to walls, adequate representation of the near-wall anisotropy and inhomogeneity is crucial. *Durbin (1993)* proposed a Reynolds stress closure to address these issues. In his model, the process of pressure redistribution is modelled through an elliptic equation, by analogy with the Poisson equation, which governs the pressure in incompressible flows. This represents the non-local effect of the wall on the Reynolds stresses. In an effort to extend PDF methods to wall-bounded turbulent flows, Durbin's elliptic relaxation method has been combined with the generalized Langevin model *(Haworth & Pope, 1986)* by *Dreeben & Pope (1997; 1998)*. This approach is closely followed throughout the present study to model the joint PDF of the turbulent velocity field.

As a first step towards the application of PDF modelling for atmospheric flows on complex geometries, a PDF hydrodynamic solver has been developed to model a fully developed, inhomogeneous, turbulent channel flow. A widely used model to incorporate the effects of small scale mixing on the scalar in the PDF framework is the interaction by exchange with the mean (IEM) model *(Villermaux & Devillon, 1972)*. While this model has the virtue of being simple and efficient, it fails to comply with several physical constraints and desirable properties of an ideal mixing model *(Fox, 2003)*. Although a variety of other mixing models have been proposed to satisfy these properties, (see *Dopazo, 1994,* for a review), the IEM model remains widely used in practice. Recently, increasing attention has been devoted to the interaction by exchange with the conditional mean (IECM) model. *Sawford (2004*) has done a comparative study of scalar mixing from line sources in homogeneous turbulence employing both the IEM and IECM models, wherein he demonstrated that the largest differences between the two models occur in the near-field. He also investigated the two models in a double scalar mixing layer *(Sawford, 2006)* with an emphasis on those conditional statistics that frequently require closure assumptions. Based on the IECM model, a PDF micromixing model has been developed by *Cassiani et al. (2005, 2005b)* for dispersion of passive pollutants in the atmosphere. They compute scalar statistics in homogeneous turbulence and in neutral and convective boundary layer by assuming a joint PDF for the turbulent velocity field. However, no previous studies have been conducted on modelling the joint PDF of velocity and a passive scalar from a concentrated source in inhomogeneous flows.

We have developed a complete PDF-IECM model for a fully developed, turbulent, long-aspect-ratio channel flow, where a passive scalar is continuously released from concentrated sources. The joint PDF of velocity, characteristic turbulent frequency and concentration of a passive scalar is computed using stochastic equations. The flow is explicitly modelled down to the viscous sublayer by imposing only the no-slip and impermeability condition on particles without the use of damping, or wall-functions. The high level inhomogeneity and anisotropy of the Reynolds stress tensor at the wall are captured by the elliptic relaxation method. A passive scalar is released from a concentrated source at the channel centreline and in the viscous wall-region. The effect of small-scale mixing on the scalar is modelled by the IECM model. Velocity and scalar statistics are computed in physical and composition spaces. The results are compared to DNS and experimental data.

GOVERNING EQUATIONS

The governing equation for a viscous, incompressible flow is the Navier-Stokes equation

$$\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} + \frac{1}{r}\frac{\partial p}{\partial x_i} = n\nabla^2 U_i, \quad (1)$$

where U_i, p, r and n are the Eulerian velocity, pressure, constant density and kinematic viscosity, respectively. Based on Equation (1), an exact transport equation can be derived for the Eulerian joint PDF of velocity *(Pope, 1985; 2000)*. The PDF transport equation is seldom solved with traditional numerical methods due to its high dimensionality. More economical are Monte-Carlo methods, in which the flow is represented by a large number of Lagrangian particles governed by stochastic differential equations. Incorporating the generalized Langevin model of *Haworth & Pope (1986)* as the turbulence closure, the position and velocity of each particle are governed by

$$\mathrm{d}X_i = U_i \mathrm{d}t + (2n)^{1/2}\mathrm{d}W_i, \quad (2)$$

$$\mathrm{d}U_i = -\frac{1}{r}\frac{\partial\langle p\rangle}{\partial x_i}\mathrm{d}t + 2n\nabla^2\langle U_i\rangle\mathrm{d}t + (2n)^{1/2}\frac{\partial\langle U_i\rangle}{\partial x_j}\mathrm{d}W_j + G_{ij}\left(U_j - \langle U_j\rangle\right)\mathrm{d}t + (C_0 e)^{1/2}\mathrm{d}W_i', \quad (3)$$

where $\mathrm{d}W_i$ is an isotropic Wiener-process, G_{ij} is a second order tensor function of velocity statistics, C_0 is a positive constant and e is the turbulent kinetic energy dissipation rate. G_{ij} and C_0 are determined by solving an elliptic equation to incorporate the effects of the wall on the particles. Details can be found in (*Dreeben & Pope, 1998)*. A remarkable feature of this formulation is that the effects of convection and viscous diffusion have exact mathematical representations, therefore need no closure assumptions. Only pressure redistribution and dissipation, which are jointly modelled by the last two terms of Equation (3), require closure hypotheses. The dissipation rate is modelled by a stochastic equation for the characteristic turbulent particle frequency w. To model the concentration of a transported scalar the interaction by exchange with the conditional mean (IECM) model is employed:

$$\mathrm{d}y = -\frac{y - \langle j \mid U\rangle}{t_m}, \quad (4)$$

where t_m is the micromixing timescale, y is the sample space variable of the scalar concentration j, while $\langle j \mid U\rangle$ denotes the scalar mean conditioned on the velocity field.

In summary, the flow is represented by a large number of Lagrangian particles representing a finite sample of all fluid particles in the domain. Each particle has a position ***X***, and with its velocity ***U*** carries its turbulent frequency w and concentration y. These particles can be thought of as different realizations of the turbulent flow, therefore all one-point statistics as well as the full joint PDF of velocity, frequency and scalar concentration are readily available from suitable lo-cal averages.

RESULTS

The model has been run for the case of fully developed channel flow at $\mathrm{Re} = \langle U\rangle h/n = 22800$ based on the streamwise centerline mean velocity and the channel half-width *h*, with a passive scalar released from a concentrated source at the centreline and in the viscous wall region. The equations to model the velocity and turbulent frequency have been solved on a 100-cell one-dimensional grid with 500 particles per cell, while to compute scalar concentration statistics a two-dimensional unstructured grid has been used. In Figure 1 the cross-stream profiles of mean streamwise velocity, the non-zero components of the Reynolds stress tensor and the dissipation rate of turbulent kinetic energy are compared with the DNS data of *Abe et al. (2004)*. The turbulence model combined with the elliptic relaxation technique reproduces well the high inhomogeneity and anisotropy in the low-Reynolds-number wall-region.

In fully developed turbulent channel flow the centre region of the channel can be considered approximately homogeneous *(Brethouwer & Nieuwstadt, 2001)*. Thus for a scalar released at the centreline, *Taylor's (1921)* theory of absolute dispersion is expected to describe the mean field of the passive scalar well up to a certain downstream distance from the source. This is demonstrated in Figure 2, where cross-stream mean concentration profiles at different downstream locations are depicted. Also shown in Figure 2 is a PDF of scalar concentration fluctuations at a location downstream of the source. The model for the joint PDF of velocity, turbulent frequency and scalar concentration accurately represents the full PDF and its statistics.

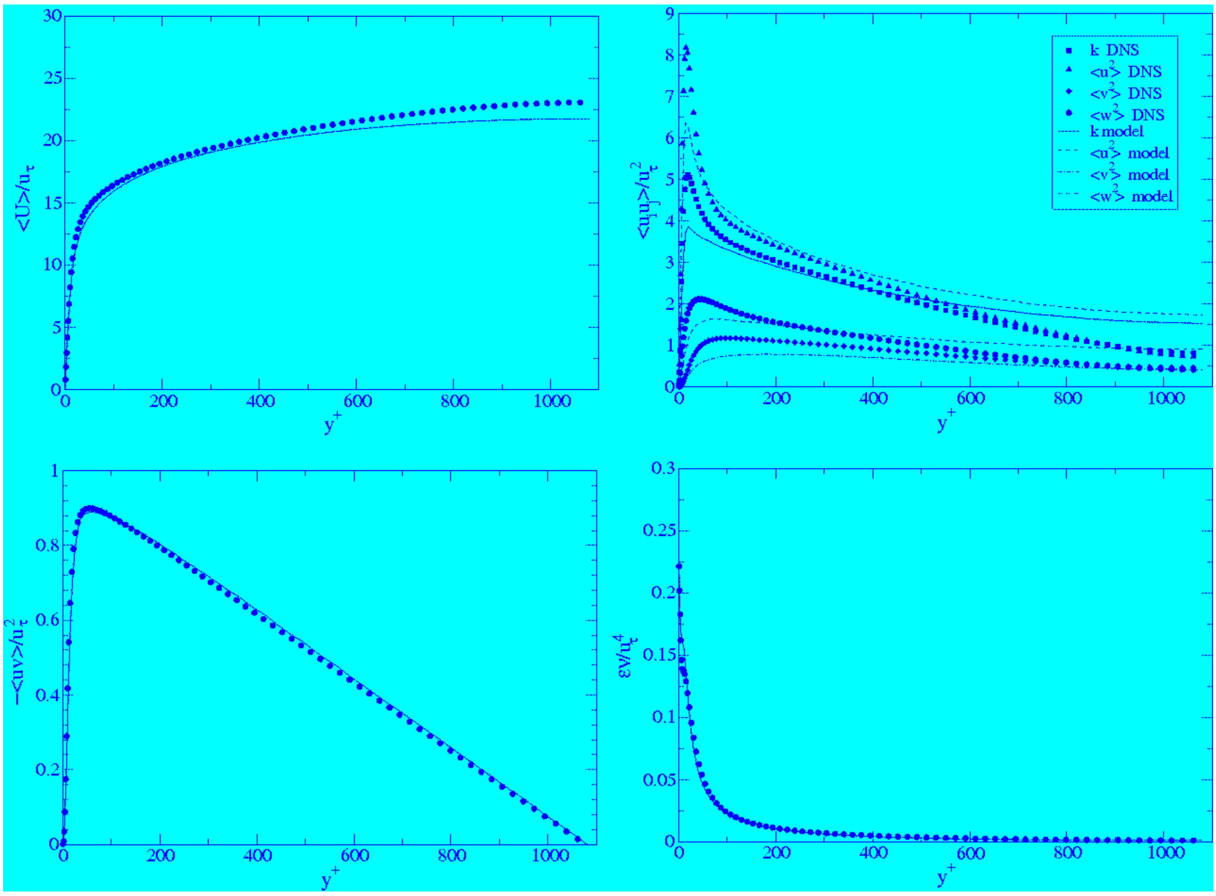

Fig. 1; Cross-stream profiles of (a) the mean streamwise velocity, (b) the diagonal components of the Reynolds stress tensor, (c) the shear Reynolds stress and (d) the rate of dissipation of turbulent kinetic energy. Lines - PDF calculation, symbols - DNS data of Abe et al. (2004). All quantities are normalized by the friction velocity and the channel half-width.

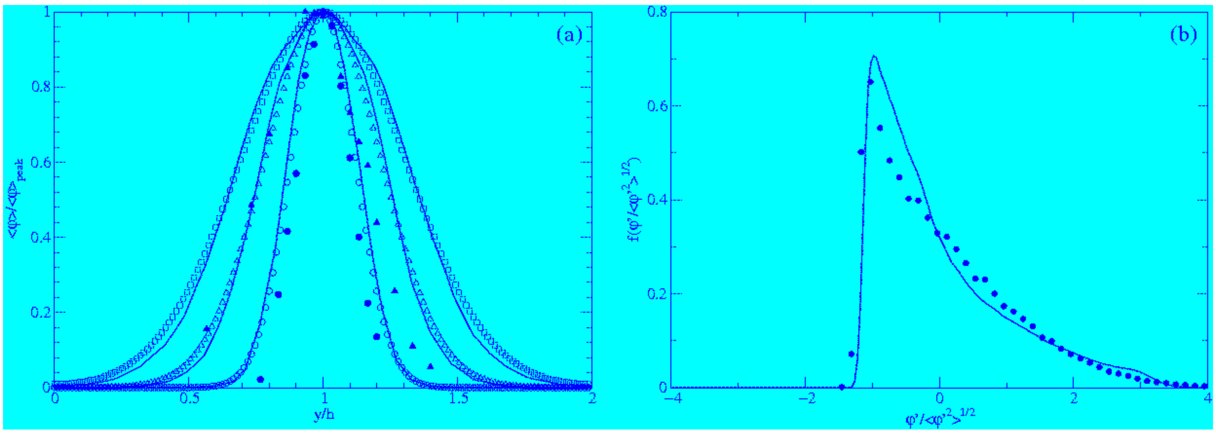

Fig. 2; (a) Cross-stream profiles of mean concentration at different downstream locations for the centreline release. Lines – PDF calculation, hollow symbols – analytical Gaussians according to Taylor's (1921) theory, filled symbols – experimental data of Lavertu & Midlarsky (2005). (b) PDF of concentration fluctuations at a downstream location at the centreline. Lines – computation, symbols – experimental data.

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