TWO-PHASE MODELS ASSESSMENT VIA DNS

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ABSTRACT

In this paper, to assess the existing statistical models, we use our direct numerical simulation (DNS) data for the two-phase situations of homogeneous shear and plane strain incompressible turbulent flows laden with spherical particles. Two statistical models derived in the framework of kinetic or probability density function (pdf) approach by Reeks (1991, 1992, 1993) and Zaichik (1999) are considered for the purpose of assessment. The closed set of equations for statistical average quantities of interest for particles are presented for these models in case of homogeneous plane strain flow. Their predictions along with the models predictions in case of homogeneous shear flows are compared with the DNS data.

INTRODUCTION

The accurate analytical description of dispersion of solid particles and liquid droplets (the dispersed phase) in turbulent fluid flows (the carrier phase) imposes many challenges mainly due to the numerous degrees of freedom associated with turbulent flows, which inevitably demands a very large computational effort. Despite significant increase in the computational power in recent years, it seems unlikely that, at least for a foreseeable future, turbulent flows of practical interest can be simulated in an exact manner such as DNS. Therefore, modeling is needed to decrease the number of degrees of freedom such that they can be resolved numerically with a (preferably) much less computational effort. The models are generally derived following a long and complex mathematical procedure, subject to simplifying assumptions; thus they must be assessed against more accurate data. Laboratory measurements can be used to generate the data for model validation, however, they are mostly limited to somewhat global and average flow variables.

An alternative can be provided by DNS data of simple flows (such as isotropic, homogeneous shear and plane strain) whose simulation is feasible with the available computational resources. Although these simple flows do not exhibit all the complexities involved in practical situations, they can be considered as basic flows locally prevailing in more general inhomogeneous configurations. Consequently, model validation in these flows can be considered as a logical 'first step'. A relatively rich database is now available for most of these flows, and they have already been implemented by various investigators to validate turbulence models at different stages (Simonin et al., 1995, Taulbee et al., 1999, Hyland et al., 1999a). In recent attempts (Zaichik, 1999, Hyland et al., 1999a), models, derived from kinetic approach, for dispersed phase in two-phase turbulent flows have been assessed against LES results for the homogeneous shear flow. Their further assessment, against DNS data, in homogeneous shear and plane strain flows is considered in this paper.

In the next section we discuss briefly the DNS methods. Next we discuss the models proposed by Zaichik (1999) and Reeks (1991, 1992, 1993) and present the model equations for particle-related statistical properties in the case of homogeneous plane shear flows. We do not write the equations for homogeneous shear flows as they are given in detail by Zaichik (1999) and Hyland et al. (1999). Finally we compare the predictions of models equations

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against the DNS data.

DNS OF HOMOGENEOUS FLOWS

We consider DNS of homogeneous shear and plane strain two-phase turbulent flows. In homogeneous shear flow, the instantaneous carrier-phase velocity $\widehat{U}_i$ ($i = 1, 2, 3$ denoting the components of the velocity) is described as

$$\widehat{U}_i = S_{sh} x_2 \delta_{i1} + u_i, \tag{1}$$

where u_i is the fluctuating carrier-phase velocity, δ_{ij} is the Kroneker delta function and $S_{sh} = dU_1/dx_2 =$ constant, with x_1 and x_2 indicating the streamwise and cross-stream flow directions, respectively. The mean velocity U_i is calculated by Eulerian ensemble averaging over the number of grid points. In homogeneous plane strain flow:

$$\widehat{U}_i = S_{ps} x_1 \delta_{i1} - S_{ps} x_2 \delta_{i2} + u_i, \tag{2}$$

$$S_{ps} = \frac{dU_1}{dx_1} = -\frac{dU_2}{dx_2} = \text{constant}. \tag{3}$$

All the variables are normalized using reference scales for length (L_0), velocity (U_0), and density (ρ_0). L_0 is chosen such that the normalized volume of the simulation box is $(2\pi)^3$, and the fluid density is used as the scale for density. U_0 is found from the box Reynolds number, $Re_0 = \rho_0 U_0 L_0/\mu$ (μ is the fluid viscosity) which is specified based on the grid resolution adopted in the simulations.

The carrier and dispersed phases are simulated in the Eulerian and Lagrangian frames, respectively. Let $\widehat{P}$, X_i, and $\widehat{V}_i$ denote the instantaneous fluid pressure, particle position, and particle velocity, respectively. The governing equations are described by the instantaneous continuity and momentum equations for the incompressible fluid:

$$\frac{\partial \widehat{U}_j}{\partial x_j} = 0, \tag{4}$$

$$\frac{\partial \widehat{U}_i}{\partial t} + \frac{\partial(\widehat{U}_i \widehat{U}_j)}{\partial x_j} = -\frac{\partial \widehat{P}}{\partial x_i} + \frac{1}{Re_0} \frac{\partial^2 \widehat{U}_i}{\partial x_j \partial x_j} - \frac{f}{\Delta V} \sum^{n_p} \frac{m_p(\widehat{U}_i^* - \widehat{V}_i)}{\tau_p}, \tag{5}$$

along with the Lagrangian equations of motion for a single particle:

$$\frac{dX_i}{dt} = \widehat{V}_i, \ \frac{d\widehat{V}_i}{dt} = \frac{f}{\tau_p}(\widehat{U}_i^* - \widehat{V}_i), \ \beta = \frac{1}{\tau_p}, \tag{6}$$

where m_p is the particle mass and superscript $*$ denotes the fluid property value at particle's location. The nondimensional particle time constant $\tau_p = Re_0 \rho_p d_p^2/18$ where ρ_p and d_p are the particle density and diameter, respectively. The function $f = 1 + 0.15 Re_p^{0.687}$ in (5) and (6), represents a correction to the Stokes drag relation at high particle Reynolds number ($Re_p = Re_0 d_p |U_i^* - V_i| \leq 1000$). The last term in (5) describes the effects of the particles on the fluid (i.e. the two-way coupling). This Eulerian source/sink term is calculated from the Lagrangian particles by summing over the number of the particles, n_p, present in the Eulerian cell of volume ΔV. f is taken equal to 1 in the case of the plane strain flow. The details of DNS in these homogeneous flows are given elsewhere (Taulbee et al.,1999, Barré et al. 2000).

Two different cases (denoted by SM1, SM2) for homogeneous shear flow are considered and the values for τ_p, number of particles N_p in SM1 and SM2 are $(0.5, 1 \times 10^5)$ and $(0.5, 6.67 \times 10^5)$ respectively. One-way coupling is considered in SM1 and mass loading ratio Φ_m (defined as the ratio of the mass of the particles and the mass of the fluid) is 0.5 for two-way coupling in SM2. The simulations are performed using a Fourier spectral method with 96^3 collocation points, and $\rho_p = 721.8$, $Re_0 = 200$ and $S_{sh} = 2$.

For homogeneous plane strain flow, two different cases (denoted by PS1, PS2) are considered with the values for τ_p, N_p and initial conditions for $\frac{\partial V_1}{\partial x_1}, \frac{\partial V_2}{\partial x_2}, \frac{\partial V_3}{\partial x_3}$ as (PS1: $0.112, 1.2 \times 10^5, 0.686, -0.739, 0$) and (PS2: $0.434, 1.2 \times 10^5, 0.588, -0.739, 0$) respectively. The simulations are performed using 160^3 collocation points with $\rho_p = 721.8$, $Re_0 = 536.1$, $S_{ps} = 0.739$. One-way coupling is considered in PS1 and PS2.

The statistical quantities of interest, namely, particle velocities correlations and particle-fluid velocities correlations are calculated, during the simulation, along with the values of kinetic energy ($k = \ll u_i u_i \gg /2$) and dissipation (ϵ) (see Fig. 1) which are needed to assess different models. Here $\ll \gg$ denotes ensemble average in DNS. Figure 1a shows the temporal variations of $\ll u_1 u_1 \gg$, $\ll u_2 u_2 \gg$, $\ll u_3 u_3 \gg$, ϵ for SM1 (one-way coupling) and SM2 (two-way coupling). It can be inferred that the k and ϵ values are less in SM2 as compared to SM1 because of the turbulence intensity dampening when the particles are considered in the fluid motion. Since we have considered only one-way coupling in the plane strain flow, curves in Fig. 1b are applicable for both PS1 and PS2.

MODELS FOR DISPERSED PHASE

We consider two statistical models derived in the kinetic or probability density function (pdf) framework which are proposed by Zaichik (1999) and Reeks and coworkers (Reeks, 1991, 1992, 1993, Hyland et al., 1999a).

We use $(\mathbf{v}, \mathbf{x})$ to represent phase space variables corresponding to $(\widehat{\mathbf{V}}, \mathbf{X})$. The equation for phase space density $p(\mathbf{v}, \mathbf{x}, t)$ can be written, by using Liouville's theorem and equation (6), as (Hyland et al., 1999a)

$$\frac{\partial p}{\partial t} + \frac{\partial}{\partial x_i}[v_i p] + \frac{\partial}{\partial v_i}\Big[\frac{1}{\tau_p}(\widehat{U}_i - v_i)p\Big] = 0. \quad (7)$$

The ensemble average (denoted by $\langle\ \rangle$) of (7) over all realizations gives

$$\frac{\partial P}{\partial t} + \frac{\partial}{\partial x_i}[v_i P] + \frac{\partial}{\partial v_i}\Big[\frac{1}{\tau_p}(U_i - v_i)P\Big] = - \frac{\partial}{\partial v_i}\Big[\frac{1}{\tau_p}\langle u_i p\rangle\Big], \quad (8)$$

which contains unknown correlation term $\langle u_i p\rangle$. Here U_i is ensemble average of $\widehat{U}_i$ and u_i is fluctuation over U_i in the vicinity of particles along their trajectories. The unknown term poses the problem of closure.

Whereas Zaichik (1999) solved the closure problem and obtained the pdf equation using the functional formalism, Reeks (1991, 1992, 1993) obtained pdf equation by using Kraichnan's Lagrangian History Direct Interaction Approximation (LHDIA) (Kraichnan, 1965) and the same equation has recently been derived in functional formalism approach (Hyland et al., 1999b). The "fluid" equations for dispersed phase for homogeneous flows, which are obtained by various moments of pdf equation, are given by Zaichik as:

$$\frac{d\langle v_i' v_j'\rangle}{dt} = 2\beta(f_u\langle u_i u_j\rangle - \langle v_i' v_j'\rangle) - \langle v_i' v_k'\rangle\frac{\partial V_j}{\partial x_k} - \langle v_j' v_k'\rangle\frac{\partial V_i}{\partial x_k} + \langle u_i u_k\rangle\left(l_u\frac{\partial U_j}{\partial x_k} - g_u\frac{\partial V_j}{\partial x_k}\right) + \langle u_j u_k\rangle\left(l_u\frac{\partial U_i}{\partial x_k} - g_u\frac{\partial V_i}{\partial x_k}\right), \quad (9)$$

$$\langle u_i v_j'\rangle = f_u\langle u_i u_j\rangle + \tau_p\langle u_i u_k\rangle\left(l_u\frac{\partial U_j}{\partial x_k} - g_u\frac{\partial V_j}{\partial x_k}\right). \quad (10)$$

Reeks' equations (Hyland et al. 1999b) in case of homogeneous flows are written as

$$\frac{d\langle v_i' v_j'\rangle}{dt} = -2\beta\langle v_i' v_j'\rangle - \frac{\partial V_i}{\partial x_k}(\langle v_j' v_k'\rangle + \lambda_{kj}) - \frac{\partial V_j}{\partial x_k}(\langle v_i' v_k'\rangle + \lambda_{ki}) + \mu_{ij} + \mu_{ji}, \quad (11)$$

$$\langle u_i v_j'\rangle = \tau_p\left(\mu_{ji} - \lambda_{ki}\frac{\partial V_j}{\partial x_k}\right). \quad (12)$$

Here

$$V_i \int P d\mathbf{v} = \int v_i P d\mathbf{v}, \quad (13)$$

$$\langle v_i' v_j'\rangle \int P d\mathbf{v} = \int (v_i - V_i)(v_j - V_j) P d\mathbf{v}, \quad (14)$$

$$\langle u_i v_j'\rangle \int P d\mathbf{v} = \int \langle u_i (v_j - V_j) p\rangle d\mathbf{v} \quad (15)$$

and

$$l_u = \frac{\beta^3 T^3}{(\beta T + 1)^2}, \; g_u = \frac{\beta^2 T^2}{\beta T + 1}, \; f_u = \frac{\beta T}{\beta T + 1} \quad (16)$$

are obtained by using exponential (with fluid integral time scale T) form for two-time correlation function (Zaichik, 1999). The expressions for λ_{ji} and μ_{ji} are given later in this section for homogeneous plane strain flow. Though equation (9) is a simplified version of equation derived for shear flow (Zaichik, 1999), we assume the same equation to remain valid in case of the plane strain flow. The equations (9)-(11) can be further simplified in case of homogeneous shear flows and the final equations are given by Zaichik (1999), Hyland et al. (1999a) and are not repeated here. We now present the closed set of equations in case of homogeneous plane strain flow. In this case the exact expressions for $\frac{\partial V_1}{\partial x_1}$ and $\frac{\partial V_2}{\partial x_2}$ as given by Barré et al. (2000) will be used in computation of models. Zaichik's equations simplify to the following:

$$\frac{d\langle v_1' v_1'\rangle}{dt} = -2\langle v_1' v_1'\rangle\frac{\partial V_1}{\partial x_1} + 2\langle u_1 u_1\rangle\Big(l_u\frac{\partial U_1}{\partial x_1} - g_u\frac{\partial V_1}{\partial x_1}\Big) + 2\beta(f_u\langle u_1 u_1\rangle - \langle v_1' v_1'\rangle), \quad (17)$$

$$\frac{d\langle v_3' v_3'\rangle}{dt} = 2\beta(f_u\langle u_3 u_3\rangle - \langle v_3' v_3'\rangle), \quad (18)$$

$$\frac{\langle u_1 v_1'\rangle}{\langle u_1 u_1\rangle} = f_u + \tau_p\Big(l_u\frac{\partial U_1}{\partial x_1} - g_u\frac{\partial V_1}{\partial x_1}\Big), \quad (19)$$

$$\langle u_3 v_3' \rangle = f_u \langle u_3 u_3 \rangle, \quad (20)$$

and equations for $\langle v_2' v_2' \rangle$ and $\langle u_2 v_2' \rangle$ can be obtained by changing subscripts from 1 to 2 in equations for $\langle v_1' v_1' \rangle$ and $\langle u_1 v_1' \rangle$.

We obtained the closed set of equations, in Hyland et al. (1999a, 1999b) framework, for the plane strain case, written as

$$\frac{d\langle v_1' v_1' \rangle}{dt} = -2\langle v_1' v_1' \rangle \frac{\partial V_1}{\partial x_1} - 2\beta \langle v_1' v_1' \rangle$$

$$-2\lambda_{11} \frac{\partial V_1}{\partial x_1} + 2\mu_{11}, \quad (21)$$

$$\frac{d\langle v_3' v_3' \rangle}{dt} = -2\beta \langle v_3' v_3' \rangle + 2\mu_{33}, \quad (22)$$

$$\langle u_1 v_1' \rangle = \frac{1}{\beta}(\mu_{11} - \lambda_{11} \frac{\partial V_1}{\partial x_1}), \ \langle u_3 v_3' \rangle = \frac{1}{\beta} \mu_{33}, \quad (23)$$

and equations for $\langle v_2' v_2' \rangle$ and $\langle u_2 v_2' \rangle$ can be obtained by changing subscripts from 1 to 2 in equations for $\langle v_1' v_1' \rangle$ and $\langle u_1 v_1' \rangle$.

For the usual exponential form for two-time correlation function with $T = 0.482k/\epsilon$ (Hyland et al., 1999a) and initial fluctuating velocity of the particle $v_i' = a u_i$, the required expressions for λ_{ji} and μ_{ji} are as follows:

$$\lambda_{11} = \beta^2 \frac{\langle u_1 u_1 \rangle}{A_1 - A_2} \Big[\frac{T}{A_1 T - 1} \left(e^{(A_1 T - 1)t/T} - 1 \right)$$

$$+ \frac{T}{A_2 T - 1} \left(1 - e^{(A_2 T - 1)t/T} \right) \Big]$$

$$+ a\beta \langle u_1 u_1 \rangle e^{-t/T} \frac{(e^{A_1 t} - e^{A_2 t})}{A_1 - A_2}, \quad (24)$$

$$\mu_{11} = \beta^2 \frac{\langle u_1 u_1 \rangle}{A_1 - A_2} \Big[\frac{A_1 T}{A_1 T - 1} \left(e^{(A_1 T - 1)t/T} - 1 \right)$$

$$+ \frac{A_2 T}{A_2 T - 1} \left(1 - e^{(A_2 T - 1)t/T} \right) \Big]$$

$$+ a\beta \langle u_1 u_1 \rangle e^{-t/T} \frac{(A_1 e^{A_1 t} - A_2 e^{A_2 t})}{A_1 - A_2}, \quad (25)$$

where

$$A_1 = \frac{-1 + \sqrt{1 + 4 S_{ps} \tau_p}}{2\tau_p}, \quad (26)$$

$$A_2 = \frac{-1 - \sqrt{1 + 4 S_{ps} \tau_p}}{2\tau_p} \quad (27)$$

and

$$\mu_{33} = \beta^2 \langle u_3 u_3 \rangle \frac{T}{\beta T + 1} \left[1 - e^{-(\beta T + 1)t/T} \right]$$

$$+ a\beta \langle u_3 u_3 \rangle e^{-\frac{t}{T}(1 + \beta T)}. \quad (28)$$

For $\tau_p < \frac{1}{4 S_{ps}}$

$$\lambda_{22} = \beta^2 \frac{\langle u_2 u_2 \rangle}{C_1 - C_2} \Big[\frac{T}{C_1 T - 1} \left(e^{(C_1 T - 1)t/T} - 1 \right)$$

$$+ \frac{T}{C_2 T - 1} \left(1 - e^{(C_2 T - 1)t/T} \right) \Big]$$

$$+ a\beta \langle u_2 u_2 \rangle e^{-t/T} \frac{(e^{C_1 t} - e^{C_2 t})}{C_1 - C_2}, \quad (29)$$

$$\mu_{22} = \beta^2 \frac{\langle u_2 u_2 \rangle}{C_1 - C_2} \Big[\frac{C_1 T}{C_1 T - 1} \left(e^{(C_1 T - 1)t/T} - 1 \right)$$

$$+ \frac{C_2 T}{C_2 T - 1} \left(1 - e^{(C_2 T - 1)t/T} \right) \Big]$$

$$+ a\beta \langle u_2 u_2 \rangle e^{-t/T} \frac{(C_1 e^{C_1 t} - C_2 e^{C_2 t})}{C_1 - C_2}, \quad (30)$$

where

$$C_1 = \frac{-1 + \sqrt{1 - 4 S_{ps} \tau_p}}{2\tau_p}, \quad (31)$$

$$C_2 = \frac{-1 - \sqrt{1 - 4 S_{ps} \tau_p}}{2\tau_p}. \quad (32)$$

For $\tau_p = \frac{1}{4 S_{ps}}$

$$\lambda_{22} = \beta^2 \langle u_2 u_2 \rangle \left[\frac{1 - e^{-tP}}{P^2} - \frac{t e^{-tP}}{P} \right]$$

$$+ a\beta \langle u_2 u_2 \rangle e^{-t/T} t e^{-\beta t/2}, \quad (33)$$

$$\mu_{22} = \beta^2 \langle u_2 u_2 \rangle \Big[\frac{1 - e^{-tP}}{P} +$$

$$+ \frac{\beta}{2P^2} \left(tP e^{-tP} + e^{-tP} - 1 \right) \Big]$$

$$+ a\beta \langle u_2 u_2 \rangle e^{-t/T} \Big[e^{-\beta t/2} - \frac{\beta t}{2} e^{-\beta t/2} \Big], \quad (34)$$

where

$$P = \frac{\beta T + 2}{2T}. \quad (35)$$

For $\tau_p > \frac{1}{4 S_{ps}}$

$$\lambda_{22} = \frac{\beta^2 \langle u_2 u_2 \rangle}{\omega} \Big[\frac{\omega}{P^2 + \omega^2} \left(1 - \cos(\omega t) e^{-Pt} \right)$$

$$- \frac{P}{P^2 + \omega^2} \sin(\omega t) e^{-Pt} \Big]$$

$$+ a\beta \langle u_2 u_2 \rangle e^{-t/T} e^{-\beta t/2} \frac{\sin(\omega t)}{\omega}, \quad (36)$$

$$\mu_{22} = \frac{\beta^2 \langle u_2 u_2 \rangle}{P} \left(1 - \cos(\omega t) e^{-tP} \right)$$

$$- \omega \lambda_{22} \left(\frac{2\omega^2 + \beta P}{2\omega P} \right) + a\beta \langle u_2 u_2 \rangle e^{-t/T}$$

$$\times\left[\cos(\omega t)e^{-\beta t/2} - \frac{\beta}{2\omega}e^{-\beta t/2}\sin(\omega t)\right], \quad (37)$$

where

$$\omega = 0.5\beta\sqrt{4S_{ps}\tau_p - 1}. \quad (38)$$

COMPARISONS WITH DNS

First order differential equations for $\langle v_i' v_j' \rangle$, as given by the models, are solved using the Runge-Kutta numerical method for the known DNS statistics ($\langle u_i u_j \rangle = << u_i u_j >>$) for the carrier phase with $a = 1$. Data presented in Fig. 1 are used to compute $T = 0.482k/\epsilon$ for different cases, namely, SM1, SM2, PS1 and PS2. Calculation of $\langle u_i v_j \rangle$ is straightforward due to the algebraic structure of the models equations. In Figs. 2 and 3, DNS data for $<< v_i' v_j' >>$ and $<< u_i v_j' >>$ are compared with the models predictions for $\langle v_i' v_j' \rangle$ and $\langle u_i v_j' \rangle$.

For homogeneous shear case, f is replaced by its ensemble average value $\langle f \rangle \cong 1 + 0.15\left[Re_0 d_p \sqrt{\langle u_i u_i \rangle + \langle v_i' v_i' \rangle - 2\langle u_i v_i' \rangle}\right]^{0.687}$ which is calculated by using DNS data at discrete times. Figure 2 shows the temporal variations for $\langle v_i' v_j' \rangle$ (Fig. 2a,b) and $\langle u_i v_j' \rangle$ (Fig. 2c,d) vs. $S_{sh}t$ and shows the effects of two-way coupling. Zaichik model and Reeks model predictions are in good agreement with DNS data for $S_{sh}t >\sim 3$ and for $S_{sh}t <\sim 3$ differences in models predictions are observed. These differences are mainly because Zaichik model equations do not depend on a i.e. initial conditions for the particles velocity.

Figure 3 shows the temporal variations for $\langle v_i' v_j' \rangle$ (Fig. 3a,b) and $\langle u_i v_j' \rangle$ (Fig. 3c,d) vs. $S_{ps}t$ and shows the effects due to different values for τ_p . The predictions, except for $\langle v_2' v_2' \rangle$, $\langle u_2 v_2' \rangle$, are in good agreement for small value of $\tau_p = 0.112$ (Fig. 3a,c). For large value of $\tau_p = 0.434$ (Fig. 3b,d), Reeks model behavior is closer to DNS and properly captures the trend of $\frac{d<<v_2' v_2'>>}{dt}$ as compared to Zaichik model which does not include the effects of a.

CONCLUSIONS

Two different models, proposed by Zaichik and Reeks, for the dispersed phase are assessed against our DNS data in case of homogeneous shear and plane strain flows after deriving the equations for the case of plane strain flow. The models predictions have been found in good agreement with DNS data in homogeneous shear flows having particles with $\tau_p = 0.5$ for both the cases of one-way and two-way coupling. In the plane strain flow cases, though the models predictions are in error for large value of $\tau_p = 0.434$, Reeks and coworkers model has been found to capture the trend of $\frac{d<<v_2' v_2'>>}{dt}$.

ACKNOWLEDGEMENT

This work was in part supported by the National Science Foundation and the Office of Naval Research through Grants CTS-0096349 and N00014-01-1-0122, respectively.

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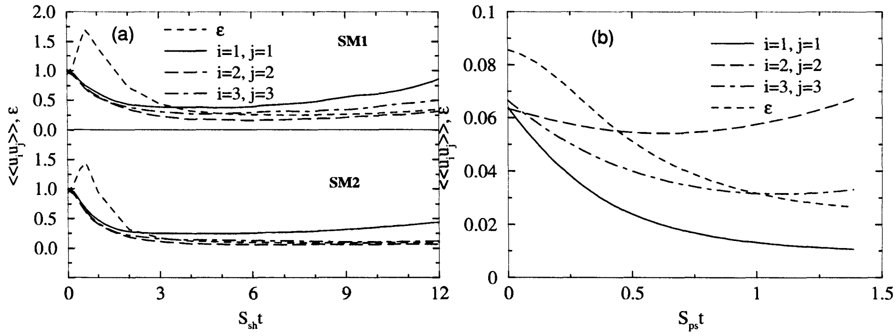

Figure 1: DNS data for temporal variations of $<< u_i u_j >>$ and ϵ.

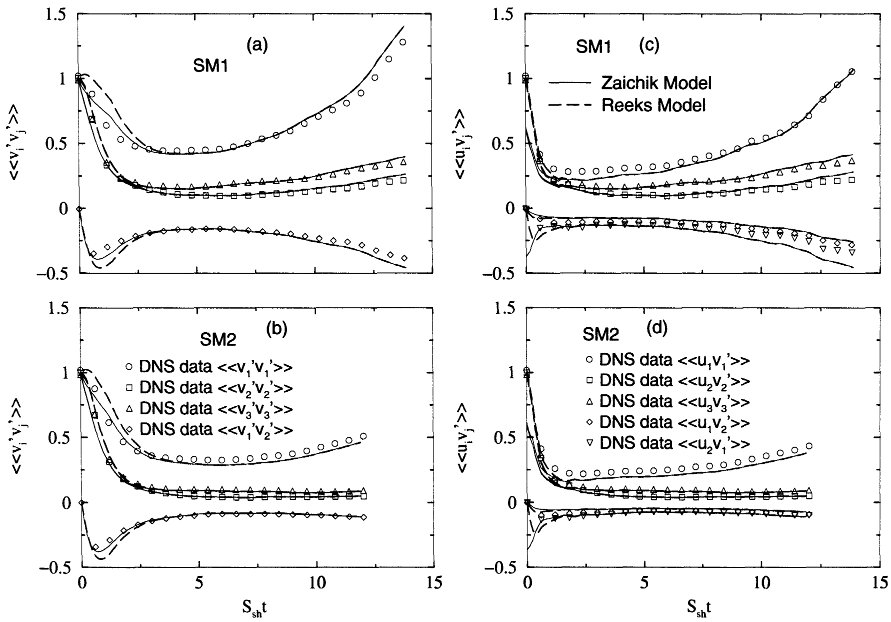

Figure 2: Comparison of models predictions with DNS data for homogeneous shear flow.

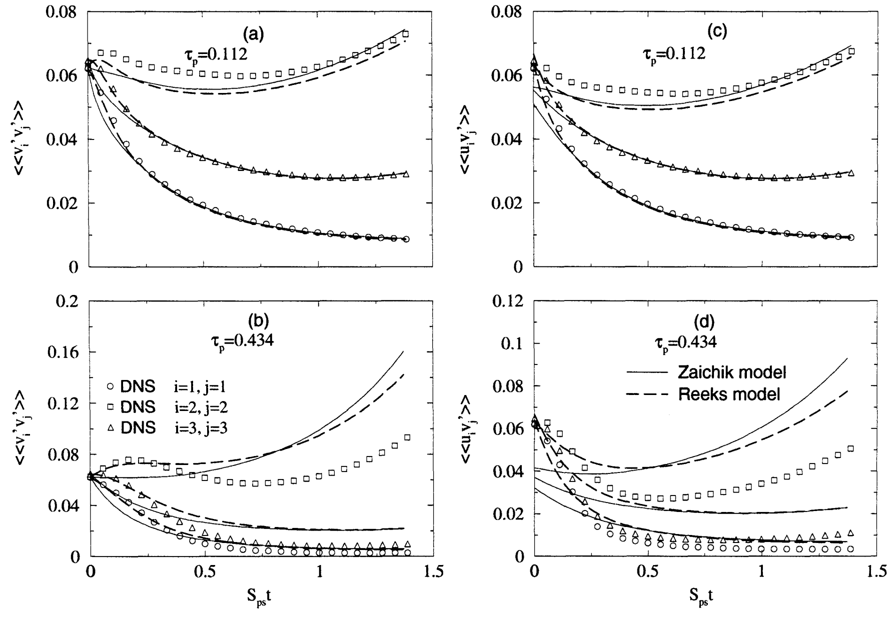

Figure 3: Comparison of models predictions and DNS data for homogeneous plane strain flow.