EDDY COLLISION MODELS FOR TURBULENCE

Blair Perot and Chris Chartrand

Department of Mechanical and Industrial Engineering
University of Massachusetts, Amherst, MA 01003, USA

ABSTRACT

Simple fluids such as gases and liquids are the result of collisions between molecules. More complex fluids, such as granular flows and colloidal suspensions (non-Newtonian fluids), result from the more complex collision (or interaction) behaviors of their constituent particles. In this paper it is demonstrated that collision rules can be constructed for large chunks of fluid material (eddies) such that the resulting collective system behaves like the mean (RANS) flow of a turbulent fluid.

The collision model approach has a number of advantages over classic Reynolds stress transport (RST) models. For example, turbulent transport does not require a model and mathematical constraints like realizability are automatically satisfied. Using some ideas from lattice-Boltzmann methods and adaptive moving mesh algorithms for CFD it is shown that this modeling approach can be made computationally efficient and comparable in cost to classic Reynolds stress transport (RST) models. Finally, it is shown that the collisional approach to turbulence modeling can lead to some insights into turbulence and turbulence modeling that would probably not have been achieved via the traditional RST approach.

KEYWORDS

Turbulence, Modeling, RANS, Reynolds Stress Transport, Collision Model.

INTRODUCTION

The traditional approach to modeling turbulence or non-Newtonian fluids is to hypothesize equations for the unknown stress tensor (in turbulence this is the Reynolds stress tensor). Because, the eddies making up the flow are roughly the same size as the gradients in the mean flow these eddies respond on similar timescales as the mean flow. This means that algebraic models are rarely predictive, and evolution equations for the stress tensor must be hypothesized. In turbulence, these are the Reynolds stress transport (RST) equations. Simpler turbulence models, such as the k-ε model or algebraic Reynolds stress models, are simplifications of the RST equations.

There is a strong analogy between turbulent fluid flow and Non-Newtonian or granular flows. Very similar to turbulent flows, transport equations are very often developed for non-Newtonian stress tensors (the Oldroyd-B model and FENE-P models are examples). In fact, we note that many important turbulence modeling concepts (realizability, material frame indifference, tensor consistency) actually find their origins in the non-Newtonian literature at this transport equation level.

However, it has long been recognized in the non-Newtonian fluid community that transport equation models have serious limitations. An alternative approach is to model the fluid at the particle collision level rather than using a transport equation for the stress. This approach is more versatile, and in many ways, more fundamental. For example, modeling a gas as particles with binary elastic hard sphere collisions gives the Navier-Stokes equations and the perfect gas law when the density is high, as well as the correct gas behavior even when the density is low (when Navier-Stokes is not valid). In this work we investigate the possibility of modeling turbulence as a collection of interacting particles.

NUMERICAL SOLUTION OF COLLISION MODELS

Once a certain collision behavior has been hypothesized there are three very different ways to solve the particle system numerically and obtain a prediction of the fluid behavior. The most straightforward technique is the 'molecular dynamics' approach where one numerically tracks all the particles in the domain, and performs collisions when they occur. This approach has a computational cost equivalent to large eddy simulation (LES) and is not considered further. The other two approaches note that one does not really care what happens to individual particles but only what happens to particles on average. The quantity of interest then becomes the probability density function that describes the probability that a particle (at a certain place and time) has a certain velocity. The evolution of the probability distribution function, *f*, obeys the exact equation

$$\frac{\partial f}{\partial t} + v_i \frac{\partial f}{\partial x_i} + a_i \frac{\partial f}{\partial v_i} = \left. \frac{df}{dt} \right|_{collisions} \tag{1}$$

where a_i is the acceleration due to external forces (like gravity) and the right-hand side describes the average affect of the collisions on the PDF. It is this average collision behavior that we now wish the models to predict.

There are two different ways to solve this PDF equation. One way is to assume the collision model has a Fokker-Planck form (see equations 2 through 4). Then using the equivalence between the Fokker-Planck equation and the Langevin equation (Brownian motion), it is possible to construct a Lagrangian particle method. This is the approach extensively researched by Pope (1994, 2000) and coworkers. The Lagrangian particles move like Brownian dust particles. They move with the mean flow and are randomly perturbed using a prescription given by the model. In this way each particle is independent from all the others, and simply interacts with the average of all the other particles. This is less expensive than tracking and implementing individual collisions ('molecular dynamics' approach) but is still expensive because a large statistical sample of particles is required.

The numerical approach used in this project was to solve the PDF equation using a standard Eulerian mesh in physical space, **x**, as well as in velocity space, **v**. Normally, this approach would be rejected outright since 10 mesh points in each direction then requires a million mesh points (10^6) to mesh all six variables (**x** and **v**) and is too expensive. The resolution to this problem is to use an extremely coarse mesh in the velocity space (3 points in each direction). This means we are solving 27 equations for each point in space. For comparison, a RST model solves 3 velocity,

1 pressure, and 6 stress equations (10 equations) per point in space. However, since the RST equations are highly coupled and nonlinear, and the PDF equations are not, the solution times are very comparable.

A very coarse mesh in velocity space is an idea borrowed from Lattice-Boltzmann methods for solving the Navier-Stokes equations. These methods solve a PDF equation with a very simple collision term that is intended to give Navier-Stokes (Newtonian) fluid behavior. The difference here is that we solve a PDF equation with a much more complex collision term, which results in RANS behavior for the fluid. The coarse mesh is acceptable in both cases because the interest is not in the PDF itself but in its lowest order moments - the mean flow and the stresses. These low order moments can be reasonably extracted from a very coarse approximation of the PDF. Note that the Langevin approach is equivalent to approximating the PDF with a random sample, and a large sample is needed even to approximate the low order moments reasonably well. The Langevin approach is slower because it provides more information (about the higher order moments). Unfortunately, we have little interest, in engineering turbulence models, in the extra information the Langevin solution method provides.

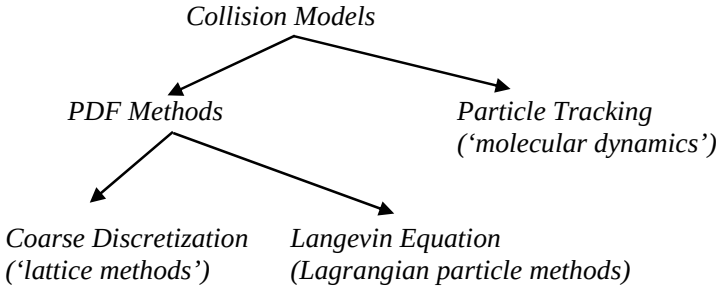


Figure 1. Taxonomy of collision model approaches.

While the approach taken in this work is inspired by the success of lattice-Boltzmann numerical methods, the approach is significantly different. This is because the PDF governing molecular interactions (Lattice-Boltmann) has a variance (width) that is much larger than the mean and which is essentially constant (related to the speed of sound). In contrast, the PDF for turbulence has a variance which is much smaller than the mean (turbulence intensities are measured in percent), and which can vary significantly (in time or space). This is illustrated in Figure 2.

To capture the turbulence PDF with only three points it is necessary to have a moving adaptive

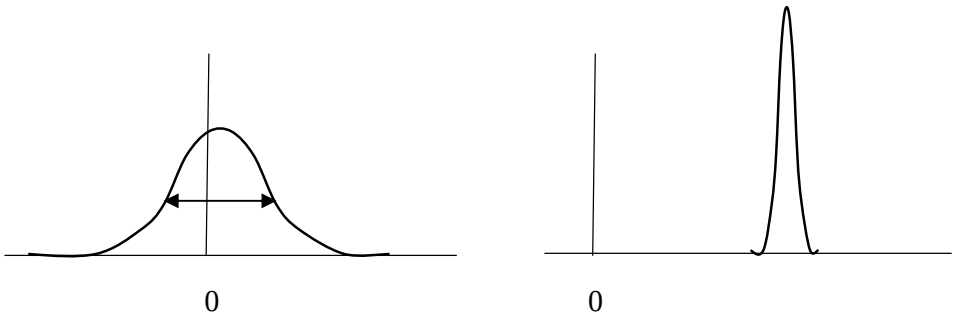


Figure 2: Left: typical PDF for molecules. Right: typical PDF for turbulence.

mesh in velocity space. In order to avoid losses due to interpolating one mesh to another as the mesh moves, we implemented a fully conservative scheme in which the mesh moves continuously in time (during the timestep). This uses technology previously developed by Perot & Nallapati (2003) for moving meshes in physical space. In actual practice the PDF is three-dimensional. An isosurface of an actual PDF (the 50% value) is shown in Figure 3. This PDF is modeling the behavior of the Le Penven et al (1985) return-to-isotropy Case III > 0 experiment. Note the fairly

large changes in the shape and size of the distribution even for this simple experiment. It can also be seen in this figure that a spherical PDF corresponds to isotropic turbulence.

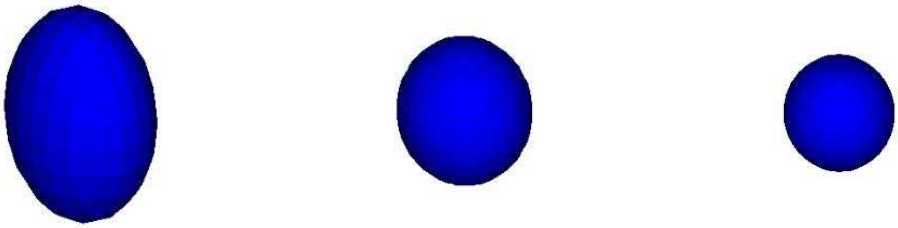


Figure 3: Evolution of the 50% isosurface of the PDF for the return-to-isotropy experiment of Le Penven *et al*. (case III > 0).

THEORETICAL ANALYSIS

Lundgren (1967) first derived the exact expression for the collision term in the PDF evolution equation for turbulence. As might be expected, this collision term can not be expressed solely in terms of the PDF, and solution of the PDF evolution equation requires a model for the collision term. In this work we have focused on generalizations of the Fokker-Plank collision term. In its simplest form this collision term has the form,

$$\left.\frac{df}{dt}\right|_{collision} = -\frac{\partial}{\partial v_i}\left[a\left(v_i - u_i\right) f\right] + b\frac{\partial^2 f}{\partial v_i^2} \tag{2}$$

where $u_i = \int v_i f d\mathbf{v}$ is the mean velocity and *a* and *b* are model constants. For turbulence this needs to be generalized. Pope and coworkers use the form,

$$\left.\frac{df}{dt}\right|_{collision} = -\frac{\partial}{\partial v_i}\left[G_{ij} v'_j f\right] + b\frac{\partial^2 f}{\partial v_i^2} + \nu\frac{\partial^2 f}{\partial x_i^2} \tag{3}$$

where $v'_j = v_j - u_j$ is the fluctuating velocity and the first term (the drift term) now has a matrix model parameter G_{ij}, and a viscous term has been added for near wall (low Re number) calculations. The conversion of these Fokker-Planck models to a Langevin equation for numerical solution dictates that the diffusion term (with *b*) be isotropic and not have a tensor coefficient.

In this paper we analyzed the following even more generalized Fokker Plank model.

$$\begin{aligned}\left.\frac{df}{dt}\right|_{collision} = &-\frac{\partial}{\partial v_i}\left[G_{ij} v'_j f\right] + \frac{\partial}{\partial v_i}\left[H_{ij}\frac{\partial f}{\partial v_j}\right] + \frac{\partial}{\partial v_i}\left[\left(J_{ij} + \nu u_{i,j}\right)\frac{\partial f}{\partial x_j}\right] \\ &+ \frac{\partial}{\partial x_i}\left[\nu\frac{\partial f}{\partial x_i}\right] + \frac{\partial}{\partial v_i}\left[\nu K_{,n}\frac{\partial\left(f v'_i / K\right)}{\partial x_n}\right] + \left.\frac{dv_i}{dt}\right|_{mesh}\frac{\partial f}{\partial v_i}\end{aligned} \tag{4}$$

The last term on the right hand side accounts (exactly) for the mesh motion. The first three terms involve model tensors. Sometimes, these tensors are isotropic and governed by a single parameter.

The viscous terms account for low Reynolds number effects and strong inhomogeneity. They do not involve any additional parameters and were derived via analysis and the condition that the model be exact as it approaches a wall (in the laminar sub layer).

The zeroth moment of the PDF equation (Eqn 4) is the mass conservation equation. The first velocity moment of the PDF equation gives the momentum equation,

$$\frac{\partial u_n}{\partial t}+\frac{\partial(u_i u_n+R_{in})}{\partial x_i}-a_n=\frac{\partial}{\partial x_i}\left[\nu u_{n,i}\right] \tag{5}$$

This implies that the acceleration is given by $a_n=-p_{,n}+(\mu u_{i,n})_{,i}$. The viscous contribution to this acceleration is necessary only if the viscosity is not constant. Taking the moment of the modeled PDF equation with respect to $v'_n v'_m$ gives the Reynolds stress transport equation,

$$\begin{aligned}\frac{\partial R_{nm}}{\partial t}+\frac{\partial(u_i R_{nm})}{\partial x_i}+\frac{\partial T_{nmi}}{\partial x_i}+(u_{m,j}R_{jn}+u_{n,j}R_{jm})=(G_{mj}R_{jn}+G_{nj}R_{jm})+(H_{nm}+H_{mn})\\ -(J_{mj}u_{n,j}+J_{nj}u_{m,j})+\frac{\partial}{\partial x_i}\left[\nu\frac{\partial R_{jm}}{\partial x_i}\right]-2\nu K_{,j}\frac{\partial\left(R_{mn}/K\right)}{\partial x_j}\end{aligned} \tag{6}$$

where $T_{nmi}=\int v'_n v'_m v'_i\, f d\mathbf{v}$ and $K=\frac{1}{2}R_{ii}$ is the turbulent kinetic energy. The tensors G_{ij}, H_{ij}, and J_{ij} determine the model. Complex dissipation and pressure-strain models can be implemented via these tensors.

The equation for the total resolved (or mean) kinetic energy, $E_r=\int\frac{1}{2}v_i v_i\, f d\mathbf{v}-\frac{1}{2}R_{ii}$, is

$$\frac{\partial E_r}{\partial t}+\frac{\partial}{\partial x_i}\left[u_i E_r+u_k(R_{ik}-\nu u_{i,k})\right]=-(pu_i)_{,i}+u_{n,j}R_{jn}-\nu u_{i,j}(u_{i,j}+u_{j,i})+\frac{\partial}{\partial x_i}\left[\nu\frac{\partial E_r}{\partial x_i}\right] \tag{7}$$

The resolved kinetic energy correctly loses energy as a result of large scale dissipation, and via turbulence production. It is completely specified and does not depend on the model coefficients. The details of these derivations can be found in Chartrand (2004).

When implementing the Fokker-Planck collision model (Eqn. 4) on a coarse mesh, it is attractive to make the change of variables $\hat{f}=\ln(f)$. If f is close to Gaussian (which is expected) then $\hat{f}$ will be close to parabolic. This parabola can be accurately resolved and interpolated by the three points available in our scheme. The evolution equation for $\hat{f}$ is,

$$\begin{aligned}\frac{\partial\hat{f}}{\partial t}+v_i\frac{\partial\hat{f}}{\partial x_i}+\left(a_i-a_{mesh}\right)\frac{\partial\hat{f}}{\partial v_i}=-G_{ii}-G_{ij}v'_j\frac{\partial\hat{f}}{\partial v_i}+\frac{\partial}{\partial v_i}\left[H_{ij}\frac{\partial\hat{f}}{\partial v_j}\right]+H_{ij}\frac{\partial\hat{f}}{\partial v_i}\frac{\partial\hat{f}}{\partial v_j}\\ +\frac{\partial}{\partial v_i}\left[(J_{ij}+\nu u_{i,j})\frac{\partial\hat{f}}{\partial x_j}\right]+(J_{ij}+\nu u_{i,j})\frac{\partial\hat{f}}{\partial x_j}\frac{\partial\hat{f}}{\partial v_i}+\frac{\partial}{\partial x_i}\left[\nu\frac{\partial\hat{f}}{\partial x_i}\right]+\nu\frac{\partial\hat{f}}{\partial x_i}\frac{\partial\hat{f}}{\partial x_i}\\ +\nu K_{,n}\left[\frac{\partial}{\partial x_n}+\frac{\partial\hat{f}}{\partial x_n}\right]\left\{\frac{3}{K}+\frac{v'_i}{K}\frac{\partial\hat{f}}{\partial v_i}\right\}\end{aligned} \tag{8}$$

While there are more terms to compute in this version, the equation for $\hat{f}$ is much more accurate to solve numerically. In addition, low order methods and simple (3 point) difference stencils suffice because $\hat{f}$ is expected to be very close to quadratic.

The models for the tensors G_{ij}, H_{ij}, and J_{ij} require a time scale to be dimensionally correct. For this reason an additional transport equation for the timescale must be included in the model. We have used the standard epsilon transport equation for this purpose since it is very commonly used in RST models as well.

SUMMARY OF THE MODEL

The collision model used in this paper is given by,

$$G_{ij} = C^s_{p2} S_{ij} + C^w_{p2} \overline{W}_{ij} + \tfrac{1}{2} C^s_{p2} \frac{P}{K} \delta_{ij} - \frac{\hat{\varepsilon}}{R_{nm} R_{mn}} R_{ij} - \frac{\hat{\varepsilon}}{K} C_d \delta_{ij} \tag{9a}$$

$$H_{ij} = \tfrac{\hat{\varepsilon}}{K} C_d R_{ij} \tag{9b}$$

$$J_{ij} = -\tfrac{2}{3} K C^*_{p2} \delta_{ij} \tag{9c}$$

where $\hat{\varepsilon} = \varepsilon \left(1 + 10\nu \left| \left(\sqrt{K} \right)_{,i} \right| / K \right)^{-1}$ is the modified dissipation that goes to zero in regions of strong inhomogeneity such as near walls, and $P = -R_{nm} u_{n,m}$ is the standard turbulent production rate. The frame invariant strain-rate and rotation-rate tensors are respectively $S_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$ and $\overline{W}_{ij} = \frac{1}{2}(u_{i,j} - u_{j,i}) + \varepsilon_{ijk} \Omega_k$, where Ω_k is the rotation rate of a non-inertial frame of reference.

For comparison with classic RST models, the equivalent Reynolds stress transport equation would be,

$$\begin{aligned} &\frac{\partial R_{mn}}{\partial t} + \frac{\partial}{\partial x_i} u_i R_{mn} + \frac{\partial}{\partial x_i} T_{imn} + \left(u_{m,j} R_{jn} + u_{n,j} R_{jm} \right) = \\ &\quad \left(C^s_{p2} S_{mj} + C^w_{p2} W_{mj} \right) R_{jn} + \left(C^s_{p2} S_{nj} + C^w_{p2} W_{nj} \right) R_{jm} + C^s_{p2} \frac{P}{K} R_{mn} - 2 \frac{\hat{\varepsilon}}{R_{ij} R_{ji}} R_{ms} R_{sn} \\ &\quad + \tfrac{4}{3} K C^*_{p2} S_{mn} + \frac{\partial}{\partial x_i} \nu \frac{\partial R_{mn}}{\partial x_i} - 2\nu \frac{\partial K}{\partial x_l} \left(\frac{R_{mn}}{K} \right)_{,l} \end{aligned} \tag{10}$$

Note that the model constant C_d does not effect the Reynolds stress transport equation. However, it does have an effect on the higher order moments (such as T_{imn}) and the turbulent transport term. This constant can be related to the Kolmorgorov constant (Pope, 2000). The other model constants are actually parameters and are given by,

$$C^s_{p2} = \frac{\nu_t}{\nu + \nu_t} - .2F\,, \qquad C^w_{p2} = \frac{\nu_t}{\nu + \nu_t} - .4F\,, \qquad C^*_{p2} = -0.2F^2 + .006 \frac{P}{\hat{\varepsilon}} \tag{11}$$

where the eddy viscosity is given by $\nu_t = .12F\frac{K^2}{\hat{\varepsilon}}$ and $F = \frac{27}{8}\det(R_{ij}/k)$ is the standard two-component parameter that is 1 in isotropic turbulence and 0 for two-component turbulence.

The transport model for the epsilon equation is standard and is given by,

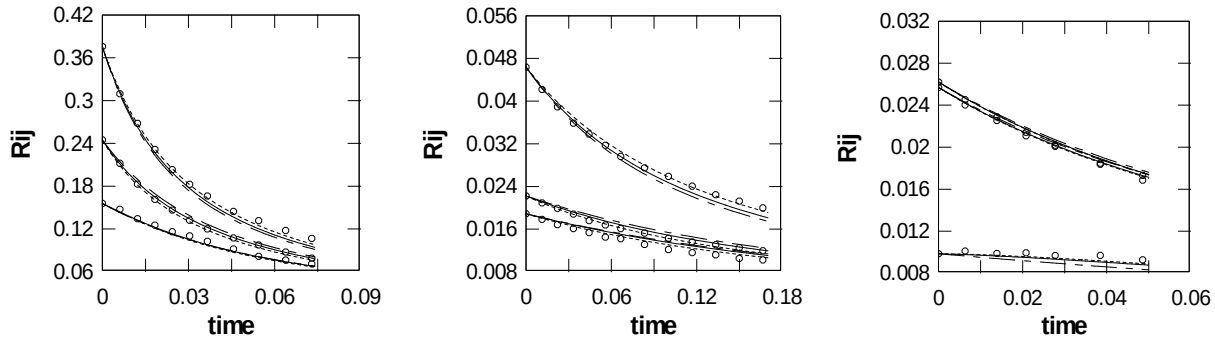
$$\frac{\partial \varepsilon}{\partial t} + u_i \frac{\partial \varepsilon}{\partial x_i} = \frac{\hat{\varepsilon}}{K}(C_{\varepsilon 1}P - C_{\varepsilon 2}\varepsilon) + \frac{\partial}{\partial x_i}(\nu + C_{\varepsilon 3}\nu_T)\frac{\partial \varepsilon}{\partial x_i} \tag{12}$$

where $C_{\varepsilon 1} = 1.43$, $C_{\varepsilon 2} = 11/6$, $C_{\varepsilon 3} = 0.83$, and fairly standard values.

SUMMARY OF RESULTS

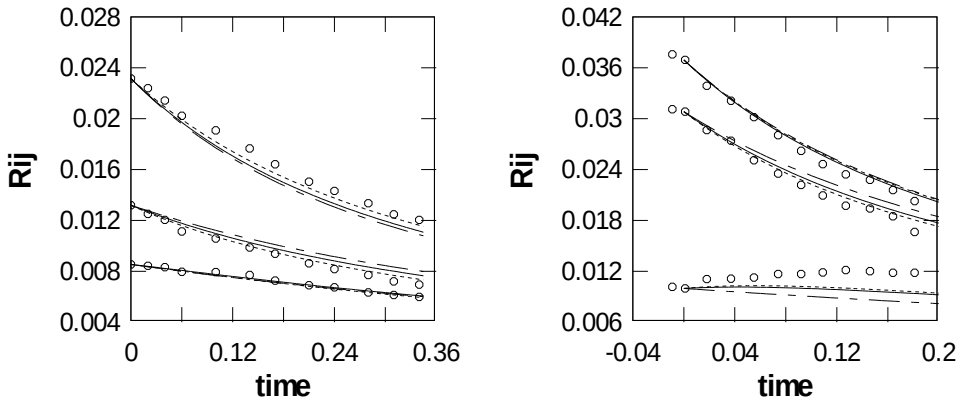
The model was tested on anisotropic decaying turbulence. This is essentially a test of the models ability to correctly predict slow pressure-strain or return-to-isotropy. The eddy collision model has no model constants associated with return to isotropy. In classic RST models, return to isotropy is parameterized by at least the Rotta constant (Rotta, 1951), and quite frequently by an additional return constant to parameterize nonlinear return effects. The Sarkar & Speziale (1990) model is an example of a two parameter nonlinear return model. The derivation of the parameter-free eddy collision return model is found in Perot & Chartrand (2004). This parameter-free model is nonlinear, and strongly realizable, and was discovered as a direct result of the collisional model framework.

Two different experiments (Choi & Lumley (2001) and Le Penven et al (1985)) and five different data sets were used to evaluate the performance of the model in figures 4 and 5. Except for Le Penven case III<0 (where all models show difficulty) the parameter-free model agrees well with experimental data.



(a) (b) (c)

Figure 4: Reynolds stresses for Choi and Lumley. (a) Case A, (b) Case B, (c) Case C-2. Symbols are the experimental data, lines are the Rotta model predictions (CR = 0.8), the dashed lines are the SS model predictions (CR=0.8, CN=0.8), and large dashed lines are the current model



(a) (b)

Figure 5: Reynolds stresses from Le Penven, Gence and Comte-Bellot.
(a) case III>0, (b) case III<0. See Figure 4 for Legend.

Next the model was tested in a variety of homogeneous shear flows. They key to predicting these flows correctly is in the modeling of the fast pressure-strain. In the current model three parameters are devoted to the modeling of the fast pressure-strain. The performance of the model is shown in figure 6. In the absence of rotation, the current model performs well. The final figure shows the turbulent kinetic energy in a shear flow as a function of time at three different rotation rates. Only the zero rotation case (upper curve) is well predicted.

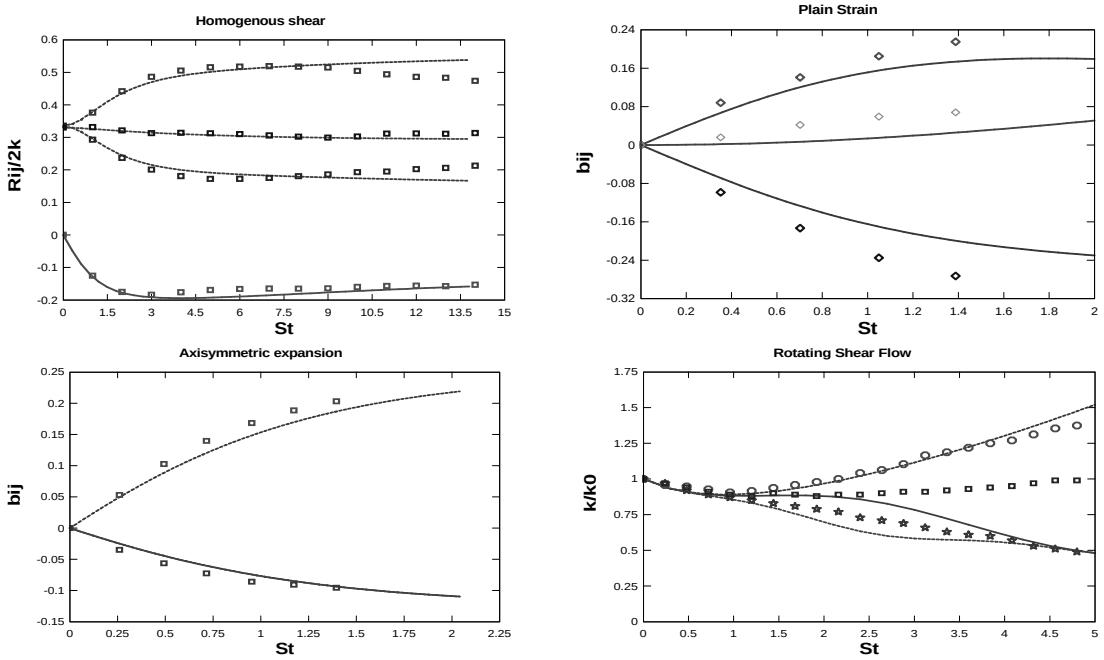


Figure 6: Eddy collision model applied to homogeneous shear flows. Symbols are experimental or DNS data. Lines are the model predictions.

Finally, the model was implemented and tested in fully developed channel flow at Re=590. The results are shown in figure 7. The issue in channel flow is to correctly account for inhomogeneity and low Reynolds number effects. In this situation, the modeling of the dissipation tensor requires close attention. This term dominates near the wall and balances viscous diffusion. Details of the dissipation model are found in Perot & Natu (2003). The model for the dissipation

tensor is exact in regions of strong inhomogeneity and involves no model parameters. The second to last term in Eqn. 4 is due to this dissipation model. The fact that the model is exact in this limit is important. It means that the diffusion is exactly balanced at the wall, and therefore that the Reynolds stresses always have the correct asymptotic limits near a wall. This means that elliptic relaxation approaches are not required. In addition, computational stability is significantly enhanced since this is the region where Reynolds stresses are close to becoming unrealizable.

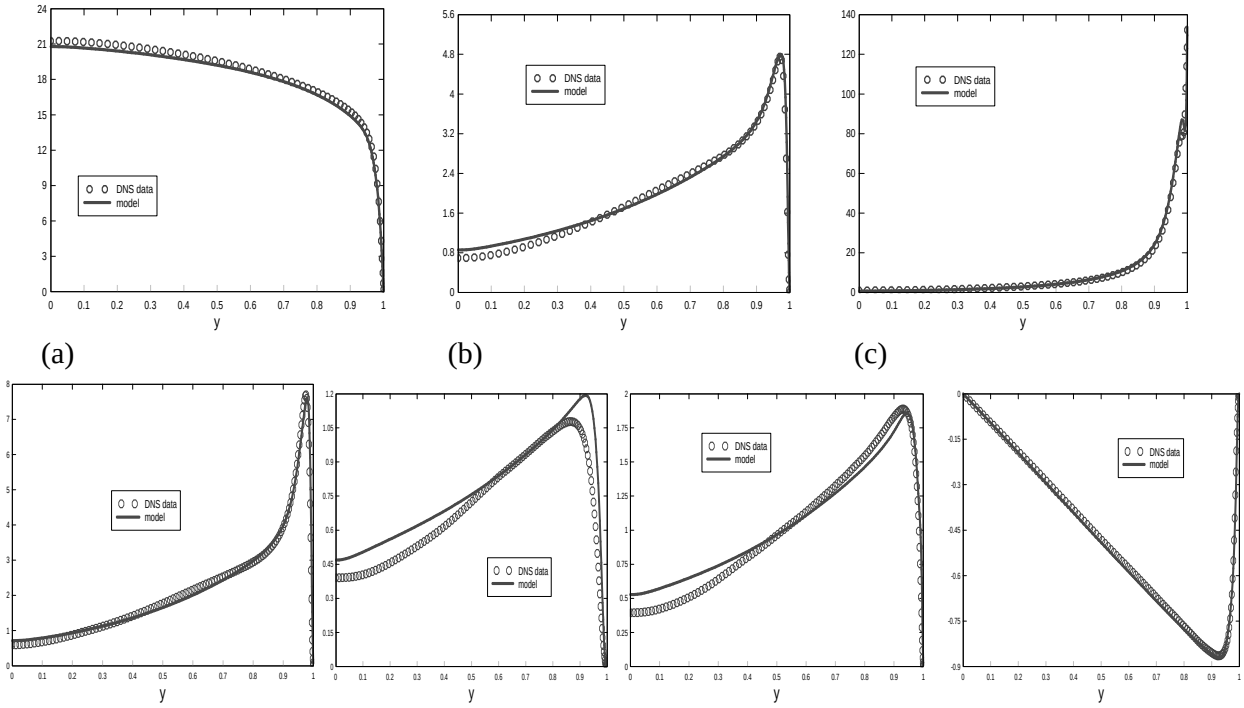


Figure 7: Turbulent channel flow at Re=590. Symbols are the DNS data of Moser et al., lines are the model predictions. (a) Mean velocity, (b) Turbulent kinetic energy, (c) Dissipation rate, (d) R_{11}, (e) R_{22}, (f) R_{33}, (g) R_{12}.

CONCLUSIONS

This paper demonstrates that collisional models are a viable alternative to RST models. In one instance, we have even been able to remove a model parameter due to insights gained from this viewpoint. However, it is also clear that this approach, as it stands, has most of the same difficulties and limitations of RST models. In particular, the fast pressure-strain model largely dictates the model's performance in flows with mean flow gradients (most flows). Fast pressure-strain models have many constants and a great deal of predictive uncertainty associated with them. In addition, the scale (or epsilon) transport equation remains (as with RST models) a source of significant error and parameterization (many constants). Finally, although we have used Lattice-Boltzmann discretization ideas, the implementation of these collision models is not as computationally efficient as classic Lattice-Boltzmann methods. A moving adaptive mesh is required making the method computationally comparable to RST models.

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