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DIRECT-NUMERICAL AND LARGE-EDDY SIMULATIONS OF A NON-EQUILIBRIUM TURBULENT KOLMOGOROV FLOW*

S.L. WOODRUFF†, J.V. SHEBALIN‡, AND M.Y. HUSSAINI§

Abstract. A non-equilibrium form of turbulent Kolmogorov flow is set up by making an instantaneous change in the amplitude of the spatially-periodic forcing. It is found that the response of the flow to this instantaneous change becomes more dramatic as the wavenumber of the forcing is increased, and, at the same time, that the faithfulness with which the large-eddy-simulation results agree with the direct-numerical results decreases.

Key words. turbulence, modeling, large-eddy simulation

Subject classification. Fluid Mechanics

1. Introduction. How, and by how much, one must modify present steady-state sub-grid models in order to perform large-eddy simulations of non-equilibrium turbulent flows is very much an open question. The ever-growing computational resources at our disposal provide the opportunity for applying large-eddy simulations to non-equilibrium as well as other increasingly-complex flows, but there is no guarantee that the sub-grid models currently in use will be up to the task of adequately representing the effect of the sub-grid scales on the resolved flow. In the case of the non-equilibrium flows of interest here, for which the statistical state of the turbulence varies with time, there is clearly a failure of a steady-state model — one which bases its prediction of the Reynolds stress on the current, instantaneous, resolved velocity field — to reflect the finite time lag inherent in the reaction of the actual sub-grid dynamics to temporal changes in the resolved field. The extent to which this effect actually affects the large-eddy simulation results is another question, and clearly one strongly influenced by the rapidity of the resolved-field variations. The present investigation seeks to answer this question for one simple flow.

The choice of a turbulent flow to use in the study of this question is not a trivial one, given our desire to work with a flow whose computation does not require too much computer time, whose numerical analysis does not require especially-sophisticated numerical techniques and whose physics bears the closeset possible relationship to turbulent flows of real technological interest. Homogeneous, isotropic, turbulence is the simplest choice, but the applicability of results for this flow to real flows is problematic, at best. Homogeneous shear flow is a possibility, but the additional complexity of the numerical techniques required to deal with the cumulative shearing (*i.e.*, regridding, [8, 2, 9, 11]) make it an unappealing one. Simulations of even the simplest of those turbulent flows realizable in the laboratory, such as channel flow, are both computationally intensive and require special attention near walls, both to the numerics and to the modelling.

Shebalin and Woodruff [14] have advocated the study of turbulent Kolmogorov flow as a way to learn about turbulent shear flows without the excessive numerical difficulties and computational expense of the flows referred to above. This flow, in which fluid in an infinite domain is driven by a periodic body force,

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was proposed by Kolmogorov as a model problem for the study of stability issues, and a significant body of literature addresses the stability aspects of this flow (see, for example, [16], and the references therein). Additionally, there has been some work in the numerical simulation of turbulent Kolmogorov flow in two dimensions [13, 12] and in three dimensions [14].

In addition to the computational and numerical advantages afforded by the Kolmogorov flow, it has a further advantage for the testing of turbulence models in that there is the potential for allowing many different turbulent flow features to be studied, due to the freedom to choose the body force as one pleases. In the present work, use is made of this freedom to investigate the response of the flow to instantaneous changes in the amplitude of the forcing at different shear magnitudes.

A number of approaches have been proposed for the development of time-dependent models for non-equilibrium flows. Yakhot and Smith [15] presented a time-dependent eddy viscosity for $k-\epsilon$ models; a more general expression of the idea behind this model provided the basis for the stress-relaxation model of Yakhot *et al.* [18]. The two-scale Direct Interaction Approximation approach to the development of turbulence models proposed by Yoshizawa [20] was employed by Yoshizawa and Nisizima [21] to derive a time-dependent model; Rubinstein [10] also used Kraichnan's DIA [4], to motivate time-evolution equations for the Reynolds stresses. The general approach to developing turbulence models examined in [17], based on the fundamental idea behind Yoshizawa's work, was used to derive a history-integral model for non-equilibrium turbulent flows, independently of any time-scale-separation assumptions. Two simplified versions of this model were tested numerically in large-eddy simulations of plane-channel flow by Nwafor and Woodruff [6]; they found that the large-eddy simulations with the Smagorinsky model did in fact fail to reproduce the DNS results, and the new models did improve the results in several respects.

Reported in this paper are results of a comparison test for Kolmogorov flow similar to that of Nwafor and Woodruff. Simulations for Kolmogorov flows with spatially-sinusoidal forcing at three different wave numbers are set up and run until a steady state is reached; then the forcing amplitude is doubled and the relaxation of the flow to a new steady state is examined. These three non-equilibrium turbulent Kolmogorov flows were solved by direct numerical simulation and large-eddy simulation with the plane-averaged history-integral model (a simplified model proposed in [6]), with the dynamic sug-grid scale model [7] and with the Smagorinsky model using two values of the Smagorinsky constant: one consistent with the predictions of the history-integral model (C_h) and the other consistent with the predictions of the dynamic model (C_d). (The latter is different for the three values of forcing wave number, the former is not.)

In contrast to the findings of [6], it was found that there was little difference between the results of the LES with the new model and those of the LES with the Smagorinsky model employing C_h. What differences there were increased as the wavenumber of the forcing increased. The LES reproduced the DNS results fairly well at the lowest wave-number forcing, but became progressively worse as the wave number of the forcing increased. The dynamic model was an improvement over the Smagorinsky model with C_h and the history-integral model at the higher-wave-number forcings, but it, too, exhibited discrepancies when compared with the DNS. The Smagorinsky model with C_d did nearly as well as the dynamic model, indicating that the primary advantage of the dynamic model in this application is its automatic initial determination of the Smagorinsky constant; once the constant has been determined near the beginning of the simulation, there seems to be little advantage gained from the dynamical model's ability to further modify the constant in time or space.

The specifics of the physical problem to be solved are given in the following section. Section 3 gives information about the models employed in the large-eddy simulations and Section 4 is concerned with

numerical details, in particular, details of the implementation of the new model. The results are described in Section 5 and the implications of these results for the modelling of non-equilibrium turbulent flows are discussed in Section 6.

2. Description of the Flow and Its Properties. The Kolmogorov flow to be considered in this work is contained within a periodic box whose sides are of length 2π. Energy is input by an external, artificial, deterministic, body force which is introduced into the equations on the right-hand side. We use a Cartesian coordinate system, with axes x, y and z.

The external forces to be used throughout this work involve a single non-zero component in the x direction which depends only on the z coordinate. As a result, the flows to be examined are parallel, as are Couette and Poiseuille flow, in the sense that the mean motion is in one direction and varies in a perpendicular direction. The flow corresponds to Kolmogorov flow if the non-zero component of the force is sinusoidal in z and we shall here consider only sinusoidal forcing at various wavenumbers. We are thus interested in solving the Navier-Stokes equations with a force of the form $\mathbf{f} = k_f v_0^2 \sin k_f z \; \hat{\imath}$ inserted on the right-hand side. The characteristic velocity v_0 and the forcing wavenumber k_f may be used to nondimensionalize the equations of motion:

$$\frac{D\mathbf{u}}{Dt} = -\nabla p + \frac{1}{Re}\nabla^2 \mathbf{u} + \sin z \; \hat{\imath}; \tag{2.1}$$

the Reynolds number Re is $v_0/k_f\nu$.

In addition to the parallel nature of the flow, we may conclude from the fact that nothing depends on the y coordinate that the flow properties must not vary under an inversion of the y coordinate ($y \to -y$; the origin is at the midplane of the box.) This implies, for example, that all Reynolds averages involving the y component of velocity must be zero. The only nonzero off-diagonal term of the Reynolds stress tensor is thus the $< uw >$ term, and consequently this term is the one which produces energy for the turbulent velocity field.

3. Description of the Models. In this section, we briefly review the reasoning behind the Smagorinsky model, examine the issue of whether a time-dependent model is necessary for large-eddy simulations of non-equilibrium turbulent flows, and review the derivations of the history-integral model [5] and the plane-averaged history-integral model [6], a simplification which allows us to incorporate the history integral into a calculation in a computationally-feasible manner. Finally, we describe the application of the dynamic sub-grid scale model to this flow.

The well-known Smagorinsky model may be motivated by an appeal to the isotropy of the modeled subgrid scales, which leads to the form

$$R_{ij} = \frac{2}{3}k\delta_{ij} + \nu_e S_{ij}; \tag{3.1}$$

k being the kinetic energy of the subgrid scales, ν_e the turbulent eddy viscosity and S_{ij} the rate-of-strain tensor of the resolved velocity field U_i:

$$S_{ij} = \frac{1}{2}\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right). \tag{3.2}$$

One then has to determine the form of the eddy viscosity, ν_e, and dimensional analysis tells us that once we have chosen to assume that the modeled subgrid scales depend only on the dissipation rate (following Kolmogorov's analysis [3]) the eddy viscosity must have the form $\nu_e = \text{const.}\ \epsilon^{2/3}$. The dissipation rate for the subgrid scales is determined by assuming that the energy balance for the subgrid scales is dominated by

the local production $R_{ij}S_{ij}$ and the local dissipation ϵ. If this assumption is valid, then the kinetic energy equation for the subgrid scales reduces to a statement of the equality of the local production and the local dissipation. This relation may be used along with the Smagorinsky model itself (3.1) to eliminate ϵ, giving an expression in terms of the rate-of-strain tensor only:

$$R_{ij} = \frac{2}{3}k\delta_{ij} + (C_s\Delta)^2(S_{mn}S_{mn})^{1/2}S_{ij} \tag{3.3}$$

Here Δ is a length scale characterizing the grid size employed in the calculation and the constant is determined empirically by fitting with experiments or direct-numerical simulation data; its value is typically taken to be 0.1.

The crucial point about the Smagorinsky model for the present discussion is that it is based on scale-separation assumptions, both in space and in time. Gradient-transport models in general result from scale-separation assumptions: for example, the Newtonian-fluid viscous-stress relation is derived in the Chapman-Enskog formulation by taking advantage of the large separation in scales between the continuous fluid motion and the discrete molecular motion. Formal derivations of the Smagorinsky model also employ such a scale assumption (see, for example, [20, 17]).

Since there is in turbulence no spectral gap — a range of scales between the largest and the smallest in which the energy is neglegible — the scale-separation assumption is fundamentally not valid and we have to ask whether it should be removed. Certainly the success of the Smagorinsky model in simulations of many different types of flows suggests that it at least provides a useful formula, independently of the invalidity of the scale-separation assumption. The question of concern is really whether or not there are flows which are simulated better by a model which does not embody this scale separation assumption then they are simulated by the Smagorinsky model.

A model which removes the temporal scale-separation assumption has been derived by Woodruff [17], and has been applied to the non-equilibrium turbulent flow problem of accelerated plane-channel flow by Nwafor and Woodruff [6]. There it was found that there are in fact significant features of that flow which compare better with direct numerical simulatioins when simulated with the new model than when simulated with the Smagorinsky mdoel. Thus, there is some evidence that, from a purely practical standpoint, there are situations for which a time-dependent model does improve the results of large-eddy simulations of non-equilibrium turbulent flows. In the present paper, we examine whether this is true for Kolmogorov flow.

The time-dependent model used in the present investigation was derived in [17], by employing a fairly general technique for the derivation of turbulence models using ideas from the analytical theory of turbulence. The fundamental idea behind the approach goes back to Yoshizawa [20] and even further to Crow [1] and is a sort of rheological approach to turbulence wherein one separates the motion into the modeled portion and the resolved portion and treats those portions as distinct entities. A solution is derived for the modeled portion which involves functions characterizing the resolved portion; this solution may be used to give expressions for the modeled contributions to the resolved portions of the flow. Specifically, for the modelling of turbulence we divide the flow into the resolved portion and the subgrid, modeled, portion and derive a perturbative solution for the subgrid velocities, substitute that perturbative solution into the definition of the Reynolds stress and so derive an expression for the Reynolds stress which may be inserted into the Reynolds-averaged equations (or, in the case of large-eddy simulations, the filtered equations). The particular approximate solution for the subgrid velocities used in [17] was based on the assumption that if the commonly held assumptions about the universality of turbulence at the small scales are valid, we can approximate the sub-grid scale velocities in terms of a dominant part which is the contribution to the velocity from the universal

component and depends (according to the assumption of universality) only on a small number of descriptors of the resolved flow, such as the dissipation rate. Corrections to this dominant term arise from more specific details of the resolved flow, such as the rate-of-strain tensor. Thus, we have what is essentially an expansion in the magnitude of the rate of strain. The terms in this expansion may in principle be computed by any means that is available and convenient, using the theory of turbulence, or even using numerical or laboratory experiments. The models developed in the examples of Woodruff [17] were derived on the basis of turbulence approximations derivable from the Direct Interaction Aproximation of Kraichnan [4]. The one employed in the present numerical calculations, as well as the calculations of Nwafor and Woodruff [6], is based on the ϵ-expansion renormalization-group results of Yakhot and Orszag [19]. In fact, any specific theory used to make a computation along these lines would lead to a history-integral model of the type discussed below, the only differences would be in the details of the kernal function and it is likely that these differences would not affect the results of a tubulence model calculation drastically. The reader is referred to [17] for details of this derivation.

It is helpful in understanding the assumptions underlying this new model to sketch a more intuitive derivation. In this derivation, we make several assumptions and then ask what is the most general form an expression for the Reynolds stress may take consistent with those assumptions. The assumptions are that the Reynolds stress is linear in the strain rate, that the model is isotropic and and that the model is, spatially, a gradient transport model. The consequences of these three assumptions are that the proposed model must be identical in form to the Smagorinsky model, as far as the spatial dependence goes. The difference lies in the temporal dependence, which may be represented without loss of generality as a linear integral operator:

$$R_{ij}(t) = \frac{2}{3}k\delta_{ij} + \int_0^t K(t,s)\ S_{ij}(s)\ ds; \tag{3.4}$$

for clarity, we have shown explicitly only the time dependence of R_{ij} and S_{ij}.

The kernal $K(t,s)$ is determined by the analysis of [17] in terms of the response function and correlation function of the modeled subgrid velocity field and the expressions derived there will be used in the calculations to follow. It is, however, possible to argue from dimensional considerations that the kernal has the form

$$K(t,s) = \tau_c^{-2} k_c^{-2} F\left(\frac{t-s}{\tau_c}\right) \tag{3.5}$$

where k_c is the wavenumber of the smallest resolved eddies in the numerical calculation and τ_c is the corresponding eddy turn-over time. It is natural to expect that more recent history is more important than less recent history, so the non-dimensional function F should be a monotonically decreasing function of its argument. The analysis of [17] gives

$$F(x) = x\int_x^\infty dz \cdot z^{-2}e^{-2z} = e^{-2x} + 2xEi(-2x), \tag{3.6}$$

and this expression will be used in the present calculations.

If the history-integral model were simplified on the basis of a scale-separation assumption in time, it would reduce to the Smagorinsky model as a sort of steady-state limit. (That is, the rate-of-strain tensor is assumed to be essentially constant as far as the evaluation of the history-integral is concerned.) This calculation was performed in [17], where the predicted value of the Smagorinsky constant was found to be quite close to the value traditionally used in channel flows.

The computations required to actually compute this history-integral expression for the Reynolds stress in the course of a numerical calculation would be quite extensive, and certainly prohibitive for a practical

calculation. For this reason, we choose to take advantage of the homogeneity of the Kolmogorov flow under consideration here in the x and y directions to consider the possibility that most of the history effects may be captured by considering only the time history of the rate-of-strain tensor averaged over $x - y$ planes. This approach was also employed in the plane-channel calculations of Nwafor and Woodruff [6]. Such a plane-averaged approach may not be implemented rigorously, because it is not possible to rewrite equation (3.4) in terms of only plane-averaged quantities without breaking up some averages of products of quantities into products of averages. Once this is agreed to, however, and once the basic Smagorinsky model is added and subtracted from the history-integral model, the plane-averaged form of the history-integral model may be written

$$R_{ij} - \frac{2}{3}k\delta_{ij} \sim \nu(t)S_{ij} + \left[\int_0^t dt'\, K_p(t-t') < S_{ij}(t') >_p - < \nu(t) >_p < S_{ij} >_p\right] \tag{3.7}$$

(The notation $< \cdot >_p$ indicates plane averaging and the subscript on the kernal indicates that the kernal is computed using the plane-averaged dissipation rate.) This expression has been specifically constructed so as to be the basic Smagorinsky model plus a history-integral correction term, to aid in the numerical implementation of the model. The implementation will be sketched in the following section.

The dynamic sub-grid scale model is implemented following [7]. A test filter is defined which filters the resolved velocity field such that the smallest resolved length and time scales are eliminated. One then seeks a value for the Smagorinsky constant which yields the same values for the modeled Reynolds stress from both the resolved velocity field and the test-filtered velocity field. Given that there are six independent components of the stress tensor and but one Smagorinsky constant, this requirement leads to an overdetermined system of equations; of the several approaches to finding the "best" value for the Smagorinsky constant under these constraints [7], that proposed by Lilly [5], where the square of the residual error is minimized, is employed here. Additionally, as is common in this sort of parallel-flow shear-layer problem, the computation of the Smagorinsky model is performed with quantities averaged over $x - y$ planes in order to ensure numerical stability.

4. Numerical Considerations. The DNS code used in the present work is that of Shebalin and Woodruff [14]. The code is spectral with Fourier modes in all three spatial directions and incorporates the viscous term implicitly in time-stepping based on a predictor-corrector algorithm. The nonlinear terms are handled by fast-Fourier transforming back into physical space, multiplying and then transforming into Fourier space. It was found that a resolution of 64^3 was sufficient for an accurately-resolved solution for the parameters employed in this study.

In order to perform large-eddy simulations of the Kolmogorov flow, subroutines were added to the DNS code which compute the Reynolds stress based on the Smagorinsky model, the dynamic model and the plane-averaged history integral model. For the runs described here, the original time-stepping of the DNS code was retained, where only the (molecular) viscous terms are treated implicitly; the entire Reynolds stress term is treated explicitly. Some experimentation was done with a time-stepping algorithm incorporating the eddy viscosity averaged over $x - y$ planes into the implicit part of the computation, but the second-order differences employed in the z direction in this altered algorithm were found to degrade the accuracy of the calculation over long times at higher values of shear and this algorithm was abandoned.

The Reynolds stress for the Smagorinsky model is computed by calculating the rate-of-strain tensor for the resolved velocity field and then computing the Smagorinsky approximation for the stress according to (3.3). The dynamic model is computed similarly, with the addition of the computation of the Smagorinsky constant itself.

Implementation of the plane-averaged history integral model is of course more complex, since it is necessary to store the history of the rate-of-strain tensor and compute its integral. As described in Section 3, we implement the plane-averaged history integral model by inserting it as a correction factor to the Smagorinsky model so the routines described above for the Smagorinsky model remain intact. In addition, we add routines to calculate the plane-averaged rate of strain tensor, the kernal of the history integral and the history integral itself. The dissipation for use in the computation of the history integral kernal is computed according to the local production — local dissipation equivalence discussed in Section 3.

5. Results. We present results for the response of the Kolmogorov flow to an instantaneous change in the amplitude of the forcing at three different wave numbers. In each case, four runs were made: a direct numerical simulation, a large-eddy simulation with the Smagorinsky model with a value for the Smagorinsky constant consistent with that predicted by the history-integral model (C_h), a large-eddy simulation with the plane-averaged history-integral model, a large-eddy simulation with the dynamic model and, finally, a large-eddy simulation with the Smagorinsky model employing a value for the constant (C_d) consistent with that predicted by the dynamic model for each case. The direct-numerical simulations were performed with a resolution of 64^3 and the large-eddy simulations were performed with a resolution of 32^3.

The reason for two separate Smagorinsky-model simulations at each of the forcing wave numbers is our desire to make the truest possible comparison between the Smagorinsky model and the two more sophisticated models considered. Thus, the history-integral-model simulation is most appropriately compared with a Smagorinsky-model simulation performed with a Smagorinsky constant equal to that attained by the history-integral model in the steady-state limit. Similarly, in view of the circumstance that the Smagorinsky constant predicted by the dynamic model varies little in time, it is most appropriate to compare the dynamic-model predictions with those of the Smagorinsky model using a value for the Smagorinsky constant fitted as best one can to the time-history of the Smagorinsky constant generated by the dynamic model. This ambivalence in the Smagorinsky model, with its arbitrary constant, is, of course, one of its more significant weaknesses, and the fact cannot be ignored that it was by using the results of the dynamic-model calculation that an appropriate value of the Smagorinsky model was determined without the expensive trial-and-error searching of parameter space that would otherwise be necessary.

In attempting to compare turbulence simulations of different types with different resolutions, it is necessary to choose a method of making all simulations start at the same state. This initial state should not be too far in advance of the step change in forcing amplitude whose response we want to look at, given the inevitable deviations of the large-eddy simulations from the direct-numerical simulations even for steady-state turbulence, and yet, if we take a 32^3 velocity field from the large-eddy simulations and use it to start the 64^3 direct numerical simulations (or *vice versa*), there is bound to be some period of adjustment while the velocity field orients itself to the new resolution. Both starting the DNS with LES data and starting the LES with DNS data was tried in the course of this work and it was found that the DNS started with LES data continued the steady state with almost no discernible adjustment period, but the LES started with the DNS data experienced an almost 20% drop in turbulent kinetic energy as soon as the simulation began. As a result of these tests, all comparisons reported in this paper were made by attaining a steady state with the LES code and using the velocity field from this run as the initial state for both LES and DNS runs.

The data to be examined in comparing the runs are global quantities of the flow: the kinetic energy, the dissipation (resolved and subgrid, in the case of the large-eddy simulations) and the work done by the force on the fluid. The three elements of the overall energy balance are the kinetic energy, $k = 1/2 \int_{\text{box}} (u^2 + v^2 +$

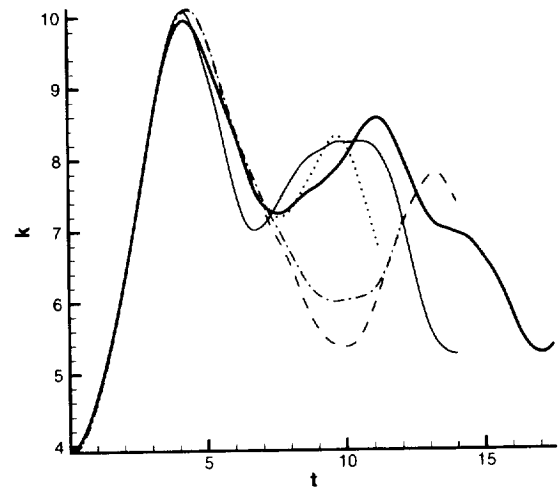

FIG. 5.1. *Case 1: Energy k versus time. DNS, thin solid line; Smagorinsky LES with history-integral-model constant, dashed line; history-integral LES, dash-dot line; Smagorinsky LES with constant generated by dynamic model, thick solid line; dynamic-model LES, dotted line.*

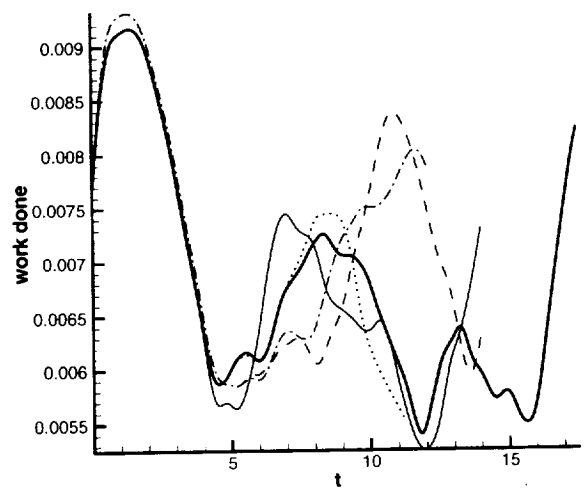

FIG. 5.2. *Case 1: Work done by external force versus time. Line types as in Figure 5.1.*

$w^2)d\mathbf{x}$, the dissipation, ϵ, and the work done by the force, $w_f = Re^{-1}k_f^3 \int_0^{2\pi} < u >_p \sin(k_f z)\, dz$:

$$\frac{dk}{dt} = w_f - \epsilon. \tag{5.1}$$

In the case of the large-eddy simulations, both the dissipation of the resolved-scale motion and the dissipation of the sub-grid scales (computed in the course of computing the modeled Reynolds stresses) will be examined.

In Case 1, the forcing wave number is $k_f = 1$ and the initial turbulent state corresponds to $Re = 28.2$. Doubling the amplitude corresponded to changing the Reynolds number to $R = 39.9$, and it may be seen from Figures 5.1–5.4 that the time histories of the observed global quantities are affected fairly gradually by

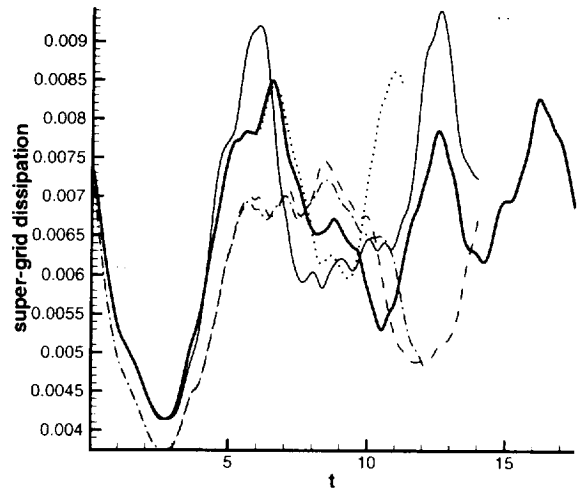

FIG. 5.3. *Case 1: Super-grid dissipation versus time. Line types as in Figure 5.1.*

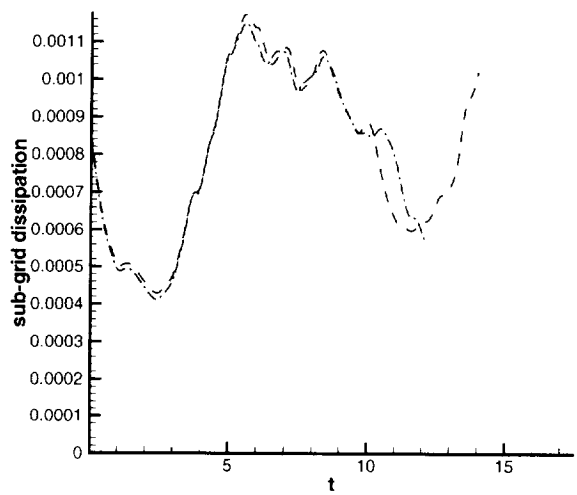

FIG. 5.4. *Case 1: Sub-grid dissipation versus time. Line types as in Figure 5.1.*

the abrupt change in forcing. (The exception is the work done, which jumps simply because it is computed directly from the force.) All the LES runs follow the DNS results fairly closely until $t \sim 6$ or 7, after which the runs with the dynamic model and with the Smagorinsky model with the constant suggested by the dynamic-model run continue to represent the DNS results tolerably well, but the history-integral model and the Smagorinsky run with C_h deviate significantly from the DNS results.

In Case 2, the forcing wave number is $k_f = 4$ and the initial and final Reynolds numbers are $Re = 28.0$ and $Re = 39.6$. In this case, the response of the measured global quantities (Figures 5.5–5.8) is more abrupt: there is a rapid rise in most of the plotted quantities when the forcing is changed. We begin to see more serious discrepancies between the LES and DNS runs, and the discrepancies appear earlier. For example,

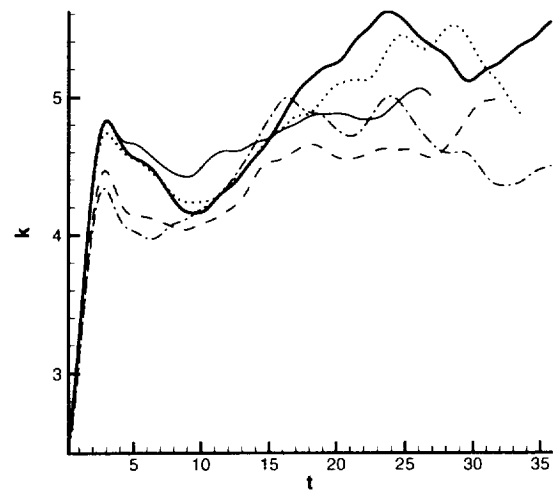

FIG. 5.5. *Case 2: Energy k versus time. Line types as in Figure 5.1.*

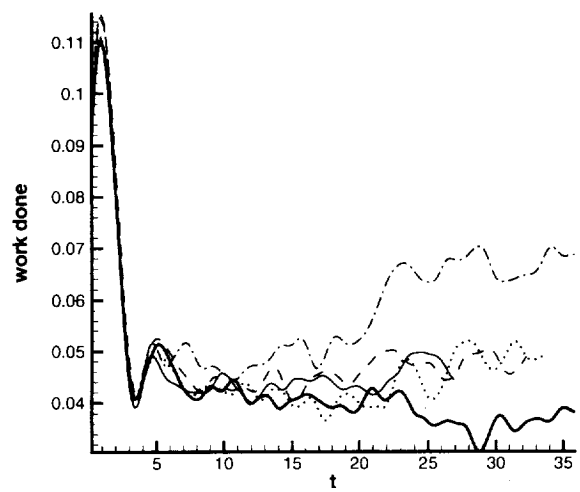

FIG. 5.6. *Case 2: Work done by external force versus time. Line types as in Figure 5.1.*

the history-integral-model run and the associated Smagorinsky-model run fail to attain the proper level of kinetic energy very early in the run. The dynamic-model run and its associated Smagorinsky run do correctly predict the initial peak in the kinetic energy, but begin to deviate from the DNS results fairly soon afterward. The other plotted quantities show similar deviations.

Case 3 is for a wave number $k_f = 6$. The initial and final Reynolds numbers are $Re = 28.1$ and $Re = 39.7$. Figures 5.9–5.12 show that the deviations noted in Case 2 become even more pronounced in this case: the history-integral-model run and its associated Smagorinsky run underestimate the kinetic energy throughout the run; the dynamic-model run and its associated Smagorinsky-model run overestimate the kinetic energy for most of the run, overshooting the initial peak significantly, as well.

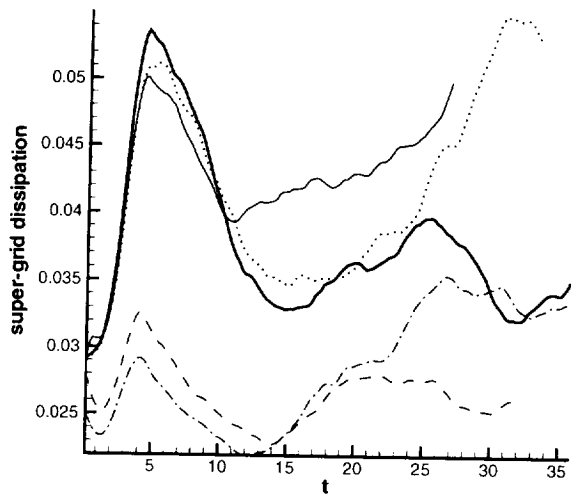

FIG. 5.7. *Case 2: Super-grid dissipation versus time. Line types as in Figure 5.1.*

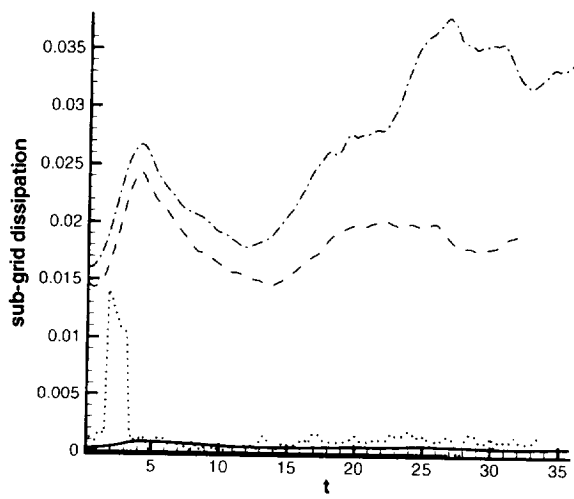

FIG. 5.8. *Case 2: Sub-grid dissipation versus time. Line types as in Figure 5.1.*

These results indicate strongly that the plane-averaged history-integral model provides no significant improvement over the Smagorinsky model for this problem. The dynamic model does predict the time histories of global quantities studied here significantly better than the history-integral model and its associated Smagorinsky model, but significant deviations from the direct-numerical simulations are still present, particularly for the higher-wavenumber forcing. However, the Smagorinsky-model run whose constant was fixed at the dynamic-model level did nearly as well; this would seem to indicate that the strength of the dynamic model for this problem is its ability to automatically choose a good value for the Smagorinsky constant, rather than its ability to accomodate spatial and temporal variations in that "constant."

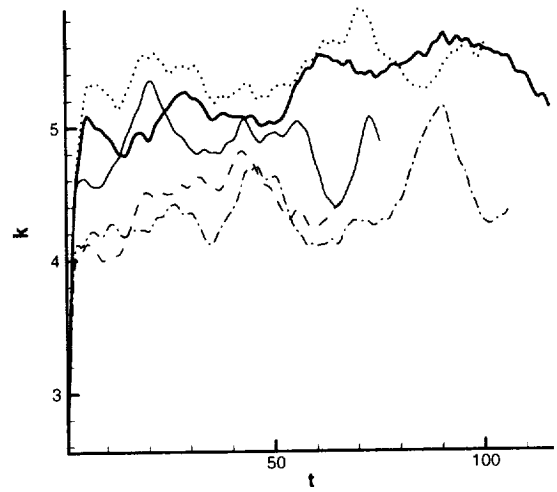

FIG. 5.9. *Case 3: Energy k versus time. Line types as in Figure 5.1.*

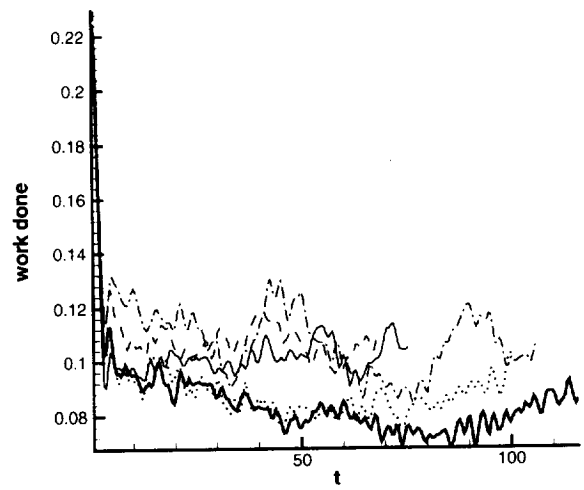

FIG. 5.10. *Case 3: Work done by external force versus time. Line types as in Figure 5.1.*

6. Conclusion. The purpose of this final section is to make some progress towards understanding the results of the previous section and their consequences for the large-eddy simulation of non-equilibrium turbulent flows. Contrasts with the analogous investigation of Nwafor and Woodruff [6] for accelerated plane channel flow will also be discussed.

We are concerned with two basic questions. The more fundamental question is the extent to which, and under what conditions, a steady-state model like the Smagorinsky model breaks down for non-equilibrium turbulent flows. The secondary question is whether or not the time-dependent history-integral model proposed in [6] represents any improvement over the Smagorinsky model.

Considering these questions in turn, it is clear from the results of the previous section that the agreement

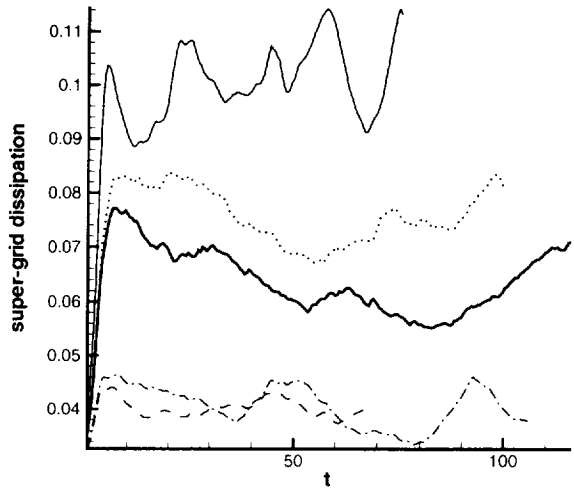

FIG. 5.11. *Case 3: Super-grid dissipation versus time. Line types as in Figure 5.1.*

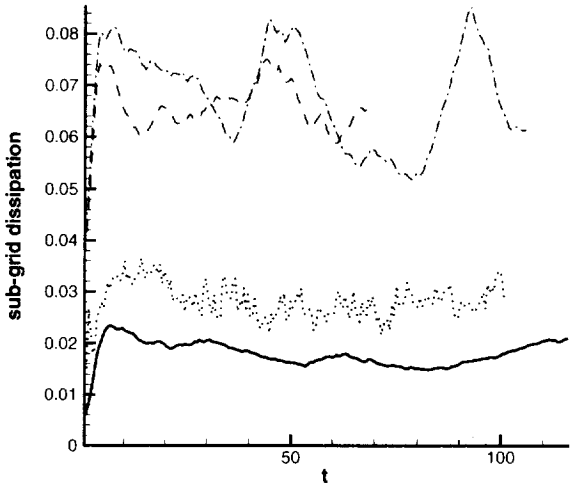

FIG. 5.12. *Case 3: Sub-grid dissipation versus time. Line types as in Figure 5.1.*

between LES and DNS deteriorates as the wavenumber of the forcing increases. It also seems fair to assert that even in the case of the best agreement between LES and DNS, that of Case 1, with $k_f = 1$, quantities based on the mean velocities, such as the bulk velocities, the work and the overall kinetic energy, are simulated more accurately by the LES than are quantities determined by the fluctuating velocity field, such as the dissipation. The present results thus suggest that the steady-state Smagorinsky model becomes less satisfactory for simulating non-equilibrium turbulent flows as the gradients in the flow become larger (a criterion we shall attempt to make more precise below) and as one's interests are concentrated on higher-order moments of the flow.

It is also clear that the plane-averaged history-integral model exhibits no improvement over the Smagorin-

TABLE 6.1
Summary of Cases.

Case	k_f	Initial Re	Final Re	$\|\|u\|\|$	Re_ϵ
1	1	28.2	39.9	1.00	2.2
2	4	28.0	39.6	0.85	15
3	6	28.1	39.7	0.85	34
Ref. [12]	*	*	*	*	43

sky model in the present investigation. In those cases where the results of the LES with the two models do deviate, the deviation is on the order of the noise in the signal and is often in the wrong direction, anyway. We consequently conclude that the discrepancies between the DNS and the Smagorinsky LES observed in the present calculations are not the result of history effects, at least insofar as history effects are represented by the plane-averaged history-integral model.

This second conclusion is in marked contrast to that indicated by the results of the accelerated plane channel flow simulations of Nwafor and Woodruff [6]. There, too, LES with the Smagorinsky and the plane-averaged history-integral models were compared with DNS for an impulsively-disturbed flow. Time-histories of global quantities contributing to the energy balance of the flow were examined (production and dissipation), as well as the time history of the wall shear stress. The simulations showed that the history-integral model significantly improved the LES predictions for the production and the dissipation in the initial stage of the response to the disturbance and qualitatively improved some aspects of the wall shear stress predictions.

In light of all this, it would be desirable to characterize as precisely as possible the differences between the three cases of the present investigation which lead to the increasing discrepancy between the LES and the DNS, as well as the differences between the present flow and the plane channel flow of [6] which cause the simulations of one to be improved by the history-integral model but not those of the other.

Other than the increasing discrepancy between the LES and DNS as the wave number of the forcing increases, the most obvious difference between the results of the three cases is the relative magnitude of the resolved and subgrid portions of the dissipation. These two quantities may be regarded as characteristic of the magnitudes of the viscous and Reynolds-stress terms in the filtered-averaged equations and so their ratio is likely to be an important non-dimensional parameter describing the interplay between the resolved and sub-grid dynamics. The ratio of local values of the sub-grid to the resolved dissipation is

$$\frac{\epsilon_{sg}}{\epsilon_R} = \frac{(c_s\Delta)^2 \left(S_{mn}S_{mn}\right)^{1/2} S_{ij}S_{ij}}{\nu S_{ij}S_{ij}} = \frac{c_s^2\Delta \left(\Delta S_{mn}\Delta S_{mn}\right)^{1/2}}{\nu} \tag{6.1}$$

A characteristic value of this ratio may be formed with a characteristic strain rate S_0,

$$c_s^2 \frac{\Delta \cdot \Delta S_0}{\nu}. \tag{6.2}$$

It may clearly be viewed as a Reynolds number based on the grid size Δ and the velocity ΔS_0. This last velocity scale may be regarded as a characteristic velocity difference induced by the shear for neighboring points on the grid. We will consequently define $Re_\epsilon = \Delta^2 S_0/\nu$ and examine the success of this parameter in predicting the behavior of the simulations. (The Smagorinsky constant c_s has been dropped; it is irrelevant to our purpose of comparing the relative magnitudes between cases.)

Let us assume that the magnitude of the shear in the flows studied here may be characterized by the magnitude of the shear of the (plane-averaged) mean-velocity profile. Then we may take $S_0 = k_f\|\bar{u}\|$,

where $\|\bar{u}\|$ is the mean peak value of the x-component of velocity in the initial turbulent state, and so find that in the three cases of the present investigation Re_ϵ has, just before the instantaneous change in forcing amplitude, the values 2.2, 15 and 34, respectively. (See Table 6.1) Correlating these values with the results described in the previous section, we see that smaller ($O(1)$) values of Re_ϵ seem to correspond to fairly good agreement between the LES and DNS, no measurable difference between the LES's with the history-integral model and with the Smagorinsky model with C_h and much more dissipation in the resolved scales than in the sub-grid scales. Intermediate values of Re_ϵ on the order of a dozen or so seem to correspond to larger discrepancies between LES and DNS and the resolved dissipation exceeds the sub-grid dissipation by an order of magnitude. Finally, values of Re_ϵ on the order of 30 or 40 seem to correspond to large deviations between LES and DNS and to a sub-grid dissipation that is commensurate with the dissipation of the resolved scales.

An additional data point comes from the channel-flow computations of Nwafor and Woodruff [6]; using the shear at the wall as the characteristic value of the shear, one finds that Re_ϵ at the initial state has the value 43. The discrepancy between the DNS and the Smagorinsky LES, as well as the differences between the Smagorinsky and plane-averaged history-integral model LES's, are consistent with the conclusions drawn in the previous paragraph for simulations with moderate values of Re_ϵ. The difference between these channel-flow results and the results of the present study, of course, is that the new model improved the LES results in the channel-flow simulations. No such improvement occured in the present investigation.

The Reynolds number Re_ϵ thus seems to provide some indication of whether a large-eddy simulation using a steady-state model like the Smagorinsky model will faithfully reproduce at least the global quantities in a non-equilibrium turbulent flow. It does not, however, help to explain when the history-integral model employed here will offer an improvement for an LES calculation.

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A non-equilibrium form of turbulent Kolmogorov flow is set up by making an instantaneous change in the amplitude of the spatially-periodic forcing. It is found that the response of the flow to this instantaneous change becomes more dramatic as the wavenumber of the forcing is increased, and, at the same time, that the faithfulness with which the large-eddy-simulation results agree with the direct-numerical results decreases.

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