Kinetic energy spectrum of low-Reynolds-number turbulence with polymer additives

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Abstract. The effects of polymer additives on the behavior of the kinetic energy spectrum in isotropic decaying turbulence were numerically investigated by hybrid Eulerian-Lagrangian simulations making full use of large-scale parallel computation. The kinetic energy spectrum was found to obey the power-law \(E(k) \sim k^{-\alpha}\) in the range below the Kolmogorov length \(l_K\) when the turbulence decayed. The exponent \(\alpha\) satisfied \(4 < \alpha < 5\) and decreased with the increase in the Weissenberg number \(W_i\). The value of \(\alpha\) obtained by the largest \(W_i\) run was close to the values obtained in previous experimental and numerical studies on elastic turbulence, which is characterized by a larger \(W_i\) and a Reynolds number of less than unity. The relationship between the results of the present study and the results obtained for elastic turbulence is also discussed.

Small amounts of polymers added to a fluid significantly affect large-scale flow structures. Turbulence drag reduction [1, 2] is one of the most important phenomena related to polymer solution flows because this phenomenon has a broad range of industrial applications involving turbulent transport. On the other hand, the polymer solution flow characterized by both a smaller Reynolds number and higher elasticity indicates chaotic fluctuations in space and time. This phenomenon is referred to as elastic turbulence [3]. It is vital to examine the meso-scale dynamics of polymers in order to clarify the peculiar nature of polymer solution flows because the origin of the turbulence modifications or the origin of the appearance of random motions for low-Reynolds-number flow are due to the strong elasticity of polymers in flows.

Dilute polymer solution flows have been extensively investigated using constitutive equations, such as the Oldroyd-B or FENE-P models [4]. These are the evolution equations for the tensor field representing the polymer conformation and are constructed based on a simple polymer model. The constitutive equations are widely used in numerical studies of the above-mentioned phenomena [2] because of the ease of handling the polymer effects on fluid motions for a reasonable computational cost.

Another method by which to numerically investigate the polymer solution flow is a hybrid approach, e.g. [5]: the fluid motion is computed using the Navier–Stokes (NS) equations, while the polymer dynamics are determined by molecular or Brownian dynamics simulations (BDSs) using an appropriate polymer model [6]. In a previous study [7], we developed a two-way coupled simulation method using this approach, in which a BDS for a dumbbell model coupled with a direct numerical simulation (DNS) of turbulent flow was performed using large-scale parallel computations. A number of dumbbells, on the order of ten billion \((O(10^{10}))\), were dispersed in a turbulent flow, and their advection and deformation were tracked during the time evolution of
the system. We then examined the modification of the decaying turbulence for various polymer concentration and Weissenberg number, $W_i = \tau_i/\tau_K$, which is the ratio of the polymer relaxation time $\tau_i$ to the Kolmogorov time $\tau_K \equiv (\nu_s/\varepsilon)^{1/2}$ for the smallest eddy in turbulence ($\nu_s$ and $\varepsilon$ are respectively the kinematic viscosity of the solvent fluid and the average rate of the energy dissipation of turbulence).

Fundamental quantity characterizing the fluctuations of the solvent fluid is the kinetic energy spectrum which is defined by

$$E(k, t) = \sum_{k} \frac{1}{2} |\mathbf{u}(k, t)|^2$$

in terms of the Fourier amplitude $\mathbf{u}(k, t)$ where $\sum'_{k'}$ is the summation taken over the spherical shell within $k - \Delta k/2 < |k| \leq k + \Delta k/2$ in the wavenumber space. One of the most remarkable results reported in [7] is the fact that when turbulence sufficiently decays and $W_i > 1$ the kinetic energy spectrum obeys the power-law decay of $E(k, t) \sim k^{-\alpha}$ with $\alpha = 4.7$ at wavenumbers higher than the Kolmogorov wavenumber $1/l_K \equiv (\varepsilon/\nu_s^2)^{1/4}$. On the other hand, previous studies on elastic turbulence revealed experimentally that $E(k) \sim k^{-3.5}$ [3] and by the DNS of the Oldroyd-B model under a two-dimensional Kolmogorov flow that $E(k) \sim k^{-3.8}$ [8]. Thus, the power-law exponent obtained in a previous study (approximately 4.7) is larger than the exponents obtained for elastic turbulence, although this result is consistent with the theoretical prediction using the simplified viscoelastic model, where the scaling exponent $\alpha$ must be greater than 3 [9].

The intrinsic difference between the previous study [7] and studies on elastic turbulence [3, 8] is that the former was performed with a smaller $W_i$ and a larger Reynolds number, on the order of $R_\lambda \approx 3.5$, than in [3, 8], where $R_\lambda$ is the Taylor microscale Reynolds number defined by (9). This raises the question of how the scaling behavior of the kinetic energy spectrum varies with the variation of parameters $W_i$ and $R_\lambda$ in the hybrid simulation.

The purpose of the present study is to examine the scaling behavior of the kinetic energy spectrum $E(k, t)$ in isotropic decaying turbulence with polymer additives for a wider parameter space. We investigate the power-law behavior of $E(k, t)$ for cases of larger $W_i$ values than those in our previous study [7]. This means that the system more closely resembles elastic turbulence.

The dumbbell model used in the present study is given by

$$\frac{dR^{(n)}(t)}{dt} = u^{(n)}_1 - u^{(n)}_2 - \frac{1}{2\tau} f \left( \frac{|R^{(n)}|}{L_{\text{max}}} \right) R^{(n)} + \frac{r_{eq}}{\sqrt{2\tau}} \left( W^{(n)}_1 - W^{(n)}_2 \right),$$

$$\frac{dt^{(n)}_h}{dt} = -2 \left( u^{(n)}_1 + u^{(n)}_2 \right) - \frac{r_{eq}}{\sqrt{8\tau}} \left( W^{(n)}_1 + W^{(n)}_2 \right), \quad u^{(n)}_h = u(x^{(n)}_h(t), t),$$

where $R^{(n)}(t)$ and $t^{(n)}_h(t)$ are, respectively, the end-to-end vector and the center-of-mass vector of the $n$-th dumbbell. We adopt the finitely extensible nonlinear elastic (FENE) model $f(z) = 1/(1 - z^2)$ for the elastic force of a dumbbell. In equation (2), $L_{\text{max}}$ is the maximum extension length of the dumbbell because $f(z \to 1) = \infty$. The term $W^{(n)}_{1,2}(t)$ indicates a random force representing the Brownian motion of particles in the solvent fluid, which obeys Gaussian statistics with a white-in-time correlation of $\langle W^{(n)}_{\alpha,i}(t) \rangle = 0$ and $\langle W^{(m)}_{\alpha,i}(t) W^{(n)}_{\beta,j}(s) \rangle = \delta_{\alpha,\beta} \delta_{ij} \delta_{mn} \delta(t - s)$, where $\langle \cdots \rangle$ denotes the ensemble average. The subscripts $\alpha, \beta, i, j, m$, and $n$ take the values $(\alpha, \beta) = 1$ or 2, $(i, j) = 1, 2$, and 3, and $(n, m) = 1, 2, \cdots, N_t$, respectively. Moreover, $\delta_{ij}$ denotes the Kronecker delta, and $\delta(t)$ is the Dirac delta function. The constants $\tau \equiv \zeta/4k$ and $r_{eq} \equiv \sqrt{KT}/k$ are, respectively, the relaxation time and the equilibrium length.
of the dumbbell under \( \mathbf{u}(\mathbf{x}, t) = 0 \). Here, \( k \) is the spring constant, and \( \zeta \equiv 6\pi \nu_s \rho_s a \) (\( \rho_s \) is the density of the solvent fluid). Also, \( k_B \) and \( T \) are the Boltzmann constant and temperature, respectively.

The turbulent velocity field obeys the continuity equation for an incompressible fluid and the NS equations
\[
\nabla \cdot \mathbf{u} = 0, \quad \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \nu_s \nabla^2 \mathbf{u} + \nabla : \mathbf{T}^p,
\]
where \( p(\mathbf{x}, t) \) is the pressure field. Here, \( \rho_s \) is set to unity and is equal to the density of bead \( \rho_p \), representing the polymer, and \( \mathbf{T}^p(\mathbf{x}, t) \) is the polymer stress tensor due to the force acting on the fluid from the dispersed dumbbells and is defined by
\[
\mathbf{T}_{ij}^p(\mathbf{x}, t) = \frac{\nu_s \eta_s}{\tau_s} \left( \frac{L_{box}^3}{N_t} \right) \sum_{n=1}^{N_t} \left( \frac{R_i^{(n)} R_j^{(n)}}{r_{eq}^2} f \left( \frac{R_{ij}^{(n)}}{L_{max}} \right) - \delta_{ij} \right) \delta(\mathbf{x} - \mathbf{r}_{ij}^{(n)}),
\]
where \( N_t \) is the total number of polymers required to realize the experimental situation, \( \eta \equiv (3r_{eq}^2/4a)^2 \Phi_v \) is the zero-shear viscosity ratio of the polymer \( \nu_p \) to the solution viscosity (\( \eta = \nu_p/\nu_s \)), and \( \Phi_v \equiv (8\pi N_t/3)(a/L_{box})^3 \) represents the volume fraction of the ensemble of dumbbells.

The numerical simulations of equations (2) through (5) are performed in a periodic box with periodicity \( L_{box} = 2\pi \) using the pseudo-spectral method in space and the second-order Runge–Kutta method in time. A total of 128\(^3\) grid points are set to solve the NS equations. The total number of dumbbells in computation is \( N_{comp} = N_t/b = 5.04 \times 10^8 \), where \( b \) is the artificial parameter representing the number of replica dumbbells. This reduces the computational cost of the computation of \( N_t = O(10^{12}) \) dumbbells [7]. The initial velocity field is given by the random solenoidal field obeying Gaussian statistics, with an energy spectrum
\[
E(k, 0) = 16 \left( \frac{2}{\pi} \right)^{1/4} \left( \frac{u_0}{k_0} \right)^4 \left( \frac{k}{k_0} \right)^4 \exp \left( -2 \left( \frac{k}{k_0} \right)^2 \right) \quad (u_0 = 1, k_0 = 2).
\]
In this setting, the initial value of \( R_\lambda \) is \( R_\lambda(0) = 52 \). The dumbbells are uniformly and randomly distributed over the computational domain. The initial configuration of each dumbbell is set according to \( \mathbf{R}^{(m)}(0) = \sqrt{3} r_{eq} \mathbf{n}^{(m)} \), where \( \mathbf{n}^{(m)} \) is a random unit vector, which is isotropically distributed.

Parallel computations are performed in order to evaluate the convection and deformation of the dispersed dumbbells. The program is parallelized using Message Passing Interface (MPI). The maximum number of MPI processors is 64, and the total number of dumbbells in computation, \( N_{comp} \), is divided into 63 groups, with each group assigned one processor that computes the temporal evolution of the group. One processor is also assigned to perform the DNS of the solvent fluid. Figure 1 shows the schematic diagram of the parallel computation in the hybrid simulations. The field data of the fluid velocity \( \mathbf{u}(\mathbf{x}, t) \) and \( \mathbf{u}(\mathbf{x} + \Delta \mathbf{x}/2, t) \) from the process dedicated to the time integration of the turbulence is transferred to all of the other 63 processes for the computation of the dumbbells. The fluid velocity at the bead positions is then interpolated using the TS13 scheme [10], whereas the polymer stress term is evaluated as follows:

(i) The polymer stress field \( \mathbf{T}_{ij}^p(\mathbf{x}) \quad (m = 1, \ldots, 63) \) is computed according to (5) for each processor.

(ii) The results are gathered by the processor \( (m = 0) \) for the turbulence DNS and are summed as \( \mathbf{T}^p(\mathbf{x}) = \sum_{m=1}^{63} \mathbf{T}_{ij}^p(\mathbf{x}) \).

(iii) The obtained \( \mathbf{T}^p(\mathbf{x}) \) is incorporated into the DNS of the NS equations.
In step (i), since the center-of-mass vector $r_g^{(n)}$ for each of the dumbbells is not on the grid points for the DNS computation, we need an approximate expression instead of (5). The delta function in (5) is approximated by the weight function $\delta_\Delta(x - r_g^{(n)})$ used for the tri-linear interpolation scheme [11]. The other parameter settings are described in detail in [7]. We examine three cases of decaying turbulence for three values of $W_i$ while fixing the other parameters. The values of the numerical parameters are listed in Table 1.

### Table 1. Parameters for the hybrid simulations of decaying turbulence and Brownian dynamics for dispersed dumbbells. The values of $\tau$ listed below are determined using the values of $W_i$ given in the table and the minimum value of $\tau_K(t)$ during the simulation without the polymer additives (one-way coupling simulation).

| Run  | $N_{comp}$ ($\times 10^9$) | $b$ ($\times 10^5$) | $\Phi_V (\times 10^{-4})$ | $\eta$ | $W_i$ | $\tau$ |
|------|--------------------------|---------------------|---------------------------|-------|-------|-------|
| D1   | 0.504                    | 0.9                 | 1.01                      | 0.1045| 25    | 4.903 |
| D2   | 0.504                    | 0.9                 | 1.01                      | 0.1045| 50    | 9.806 |
| D3   | 0.504                    | 0.9                 | 1.01                      | 0.1045| 100   | 19.612|

Figure 2 shows the temporal evolutions of the kinetic energy of fluid motion $E(t)$ and of the potential energy for the ensemble of dumbbells $U(t)$, which are defined, respectively, as follows:

$$E(t) = \frac{1}{2} \langle u(x,t)^2 \rangle_V$$

and

$$U(t) = -\frac{\nu_s \eta}{2\tau} \left( \frac{L_{max}}{r_{eq}} \right)^2 \frac{1}{N_{comp}} \sum_{n=1}^{N_{comp}} \ln \left[ 1 - \left( \frac{R^{(n)}(t)}{L_{max}} \right)^2 \right]$$

for all of the runs, where $\langle \cdots \rangle_V$ represents the volume average over the computational domain $V = L_{box}^3$. Hereinafter, figures are plotted using non-dimensional time $t^* \equiv k_0 u_0 t$. In figure 2 (a), $E(t)$ decays monotonically with time, and the curves collapse onto a single curve irrespective of $W_i$. The values of $E(t)$ at the end of the simulations are much smaller than their initial values, meaning that the turbulence adequately decayed at $t^* = 20$. On the other hand, $U(t)$ increases with time for $t^* < 7$, which indicates that the turbulence kinetic energy is transferred...
Figure 2. Comparison of the temporal evolutions of (a) the kinetic energy of fluid motion $E(t)$ and the potential energy for the ensemble of dumbbells $U(t)$ and of (b) the total energy $E(t) + U(t)$ for Runs D1, D2, and D3.

Figure 3. Comparison of the temporal evolutions of the Taylor microscale Reynolds number $R_\lambda(t)$ for Runs D1, D2, and D3.

Figure 4. Comparison of the temporal evolutions of the local Weissenberg number $W_i(t)$ for Runs D1, D2, and D3.

to the potential energy of the ensemble of dumbbells in addition to the heat. Moreover, $U(t)$ starts to decay at around $t^* = 7$, indicating that the portion of restored potential energy is also back-transferred to turbulence and is dissipated due to the viscosity. Note that $U(t)$ is larger than $E(t)$ in the range of $t^* > 10$ for all of the runs. Figure 2(b) shows the temporal variation of the total energy $E(t) + U(t)$ based on the data of figure 2(a). We confirmed that the total energy also decays monotonically with time.

The temporal evolutions of the Taylor microscale Reynolds number $R_\lambda(t)$, which is defined by using $E(t)$ (7) and $\varepsilon(t) = \nu_s \langle (\nabla u)^2 \rangle V$ as follows:

$$R_\lambda(t) = \sqrt{\frac{20}{3\nu_s \varepsilon(t)}} E(t),$$

are shown in figure 3. The curves almost collapse onto a single curve for $t^* < 10$, and the curve for Run D1 slightly deviates upward from the other curves for $t^* > 10$. Thus, $R_\lambda$ is almost insensitive to the variation of $W_i$, and the values at $t^* = 20$ are $R_\lambda = 3.5, 3.2$, and 3.1 for Runs D1, D2, and D3, respectively.

Figure 4 compares the temporal evolutions of the local Weissenberg number $W_i(t) = \tau/\tau_K(t)$
for all runs. Based on figure 4, we confirm that the curves reach their maximum values at approximately $t^* = 2$, and $W_i(t)$ decays with time for $t^* > 2$. The value obtained for Run D3 is the greatest among the three values in the entire time region. At the end of simulation ($t^* = 20$), we have $W_i = 1.7, 3.8, \text{and } 7.5$ for Runs D1, D2, and D3, respectively, which indicates that numerous dumbbells remain in the stretched configuration for Runs D2 and D3 because the values of $W_i$ are just above the critical value $W_i^c = 3 - 4$ at which the coil-stretch transition occurs [12].

Since the turbulence adequately decays for $t^* = 20$, where $W_i$ is larger than unity for all of the runs, we investigate the scaling behavior of $E(k, t)$ obtained at $t^* = 20$. Figure 5 compares the kinetic energy spectra obtained for all of the runs, where we plot the dimensionless form of spectra $\hat{E}(k, t)$ defined using the Kolmogorov scaling as

$$\hat{E}(k, t) = \frac{E(k, t)}{\varepsilon(t) 2^{-3/5} K(t)^{3/5}}.$$ (10)

As shown in figure 5, the normalized spectra generally collapse in the range of $kl_K(t) < 1$, and exhibit a power-law decay similar to $k^{-4.7}$ over one decade for $kl_K(t) > 1$. However, the spectrum becomes less steep with the increase of $W_i$. To see this point in more details, we make the compensated plot $k^\alpha E(k, t)$ in figure 6, where the exponent $\alpha$ is evaluated by using a least squares fit in the range $2 \leq kl_K(t) \leq 5$. This figure clearly indicates that the value of $\alpha$ decreases from 4.58 to 4.20 when $W_i$ is increased. For the greatest values of $W_i$, $\alpha = 4.20$, which is close to the values obtained for elastic turbulence [3, 8].

Next, we will comment on the difference between the hybrid DNS using FENE dumbbells and the DNS of the elastic turbulence using the Oldroyd-B model [8]. The FENE model has the upper limit of the dumbbell extension length, $L_{\text{max}}$. This means that many dumbbells tend to remain at around $L_{\text{max}}$ when $W_i$ is larger. Figure 7 shows the probability density function (PDF) for the end-to-end distance of dumbbell $r = |\mathbf{R}^{(n)}|/L_{\text{max}}$ at $t^* = 20$ for all of the runs. This figure indicates that there are more stretched dumbbells for larger $W_i$, even when $R_\lambda$ is sufficiently small. This also implies that the contribution of each dumbbell to the polymer stress tensor $\mathbf{T}^p$ becomes larger as $W_i$ increases because $f(z) \rightarrow \infty$ as $z \rightarrow 1$. In contrast, the Oldroyd-B model is a linear equation for the conformation tensor of the polymer, which corresponds to

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure5.png}
\caption{Comparison of the kinetic energy spectra normalized using the Kolmogorov scaling of (10) obtained at $t^* = 20$ for Runs D1, D2, and D3. The reference line shows the power law scaling of $k^{-4.7}$.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure6.png}
\caption{Compensated kinetic energy spectra $k^\alpha E(k, t)$ obtained at $t^* = 20$ for Runs D1, D2, and D3. The value of $\alpha$ is evaluated by using a least squares fit in the range of $2 \leq kl_K(t) \leq 5$. Plateaus are clearly confirmed in the range $kl_K(t) > 1$.}
\end{figure}
the case in which the linear spring model is adapted to (2) by setting $f(z) = 1$. In this case, the stretched dumbbells can exceed $L_{\text{max}}$, leading to a greater contribution to the increase in $T^p$ due to an increase in $|R^{(0)}|$. Thus, the mechanism for increasing the amplitude of $E(k, t)$ through the NS equations, differs significantly between the FENE model and the Oldroyd-B model.

Another important point is the nature of the isotropy of the flow field. In the present case, the flow field is regarded as nearly isotropic, so that the effect of anisotropy on the scaling behavior of $E(k, t)$ is negligible. In contrast, the flow field is strongly anisotropic for the DNS study under the Kolmogorov flow [8] and for the experimental viscoelastic flow within the rotating disks [3]. The persistent anisotropy leads to the modification of the spectral dynamics at small scales, so that we must carefully compare the present results to the previous results for elastic turbulence.

The above considerations raise the question of how the power-law form of the kinetic energy spectrum is universal for the changes in the mechanical properties of the chain polymer model or the degree of anisotropy. Moreover, since the flow field is nearly isotropic in the present study, it is appropriate to explore whether the power-law exponent is universal for $W_i \gg 1$ and $R_\lambda \ll 1$. We may need more computational resources to examine this problem because the case in which $W_i \gg 1$ requires much finer spatial resolution for computing the NS equation and much finer time steps for computing the dumbbell deformations in the Lagrangian frame with reasonable computational accuracy. This is perhaps the greatest computational challenge in examining the ultimate state of elastic turbulence by large-scale simulations.

We investigated the scaling behavior of the kinetic energy spectrum in decaying isotropic turbulence with polymer additives for various values of $W_i$. We obtained the power-law form of $E(k) \sim k^{-\alpha}$ in the range $kl_K > 1$, and $\alpha$ was approximately 4.2–4.6 and decreased with the increase in $W_i$. The value of 4.20 obtained for Run D3, which has the greatest value of $W_i$ in the present study, was similar to the values obtained in the study on elastic turbulence ($\alpha = 3.5$ experimentally [3] and $\alpha = 3.8$ by DNS of the constitutive equation [8]).

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