Subgrid Scale Variance and Dissipation of a Scalar Field in Large Eddy Simulations

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Abstract

Subgrid scale (SGS) variance of a scalar field in Large Eddy Simulations is only properly defined in relation to a probability density function. This solves a reported problem in the variance definition[1,2] and allows to write a simple evolution equation for the scalar variance. This equation shows that a recently proposed model for scalar dissipation in terms of the large scale gradients[3] implies dissipation and production cancelling out, preventing variance decay and complete mixing at SGS level. An alternative simple model for dissipation in terms of a SGS mixing characteristic time is proposed and tested here.

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Extension of combustion models established in Reynolds averaged (RANS) calculations to Large Eddy Simulations (LES) has been investigated in recent works.[1–8] As in RANS, the key point of a LES combustion model is the determination of at least joint statistics of the reacting scalars and temperature at the subgrid scale (SGS) level. A whole category of models for non–premixed combustion is based on the description of SGS joint statistics as related to the SGS statistics of a conserved scalar, namely the mixture fraction Z. Different assumptions (the infinitely fast chemistry, the flamelet[9] or the CMC[10] assumptions), can be used to establish such relation, while it is generally agreed that the SGS statistics of Z can be described by a beta function, parametrized by its mean and variance.[1,6] A third parameter, the scalar dissipation, is usually needed to establish the reactants/mixture fraction structure by relating mixing and chemical times.

Thus the description of nonpremixed combustion at the SGS level relies for the mentioned models on the proper determination of the mean, variance and dissipation rate of the mixture fraction at the SGS level. The mean value coincides with the local large scale value $\overline{Z}$ and is directly computable in a LES. Different approaches have been proposed for the variance and dissipation modeling, most of them based on independent scale similarity assumptions. We show in this paper that reported problems in the variance modeling and calculation stem from an inadequate definition in terms of the square of SGS fluctuations. Once the proper definition is established, its evolution equation can be written without ambiguity. It shows that variance and dissipation can not be independently modeled without risk, being intimately related through mixing. We propose here to add an equation for scalar variance to the LES system of equations, so that a single model is needed to represent dissipation and effects of mixing in the variance evolution. Using for that purpose a recently proposed model for scalar dissipation[3] implies that dissipation and production of variance cancel out. This would lead to unphysical simulations in which the SGS scalar variance would not decay and complete mixing of reacting species would not be attainable. As a consequence, reaction rates would be underestimated in the associated combustion calculation. An alternative simple model is proposed here, based on assuming the SGS characteristic mixing time as proportional to the SGS turbulent characteristic time, as an extension of a model widely used in RANS. A priori tests and results of actual Large Eddy Simulations are presented that confirm the adequate behavior of such a model.

1 Variance definition

In RANS calculations, the variance of a scalar field Z under an averaging operation $\langle \quad \rangle$ is defined as the average of the square fluctuations about the mean value:

$$V_{RANS} = \left\langle Z'^2 \right\rangle = \left\langle (Z - \langle Z \rangle)^2 \right\rangle,$$

which is equivalent to the difference between the mean square value and the square of the mean value:

$$V_{RANS} = \left\langle (Z - \langle Z \rangle)^2 \right\rangle = \left\langle Z^2 \right\rangle + \langle Z \rangle^2 - 2 \langle Z \rangle \langle Z \rangle = \left\langle Z^2 \right\rangle - \langle Z \rangle^2,$$

and both forms can be used.

In LES, the analogous definitions in terms of filtering are not equivalent, as due to the properties of general filter operators $\overline{\overline{Z}} \neq \overline{Z}$. By analogy with the most common definition in RANS, and given the somewhat easier interpretation of the variance as related to fluctuations, one would define the SGS scalar variance in terms of SGS fluctuations, as:

$$\overline{Z'^2} = \overline{\left(Z - \overline{Z}\right)^2}. \tag{1}$$

This expression for the scalar variance was detected to give problems in practical calculations. A restriction of the allowed filtering operators to projectors, for which $\overline{\overline{Z}} = \overline{Z}$, was then adopted,[1,2] so that the SGS variance could be identically defined as:

$$\overline{Z^2} - \overline{Z}^2. \tag{2}$$

In fact the filter restriction is not needed if care is taken to define the scalar variance, a statistical quantity, in terms of a probability density function (PDF). Only the definition in equation 2 corresponds to the variance of a PDF. It can be shown that it is the variance of the *filtered probability density function* introduced by Gao and O'Brien:[11,12]

$$\overline{P}(\Gamma, x, t) = \int G(\vec{x}, \vec{x}')\delta(\Gamma - Z(\vec{x'}, t))d\vec{x'}, \tag{3}$$

where $G(\vec{x}, \vec{x'})$ represents the filtering kernel and δ the Dirac delta function.

The first moment or mean of $\overline{P}$ at $\vec{x}$ is the sum of possible values weighted by their probability, and coincides with the values of the filtered scalar at $\vec{x}$:

$$\int \Gamma\overline{P}(\Gamma;\vec{x})d\Gamma = \int\int \Gamma G(\vec{x},\vec{x}')\delta(\Gamma - Z(\vec{x'}))d\Gamma d\vec{x'} = \int Z(\vec{x}')G(\vec{x},\vec{x}')d\vec{x}' = \overline{Z}(\vec{x}).$$

The second centered moment, the variance, is defined as the sum of the square of fluctuations around the mean value weighted by their probability:

$$\int \left[\Gamma - \overline{Z}(\vec{x})\right]^2 \overline{P}(\Gamma;\vec{x}))d\Gamma = \int\int \left[\Gamma - \overline{Z}(\vec{x})\right]^2 G(\vec{x} - \vec{x}')\delta(\Gamma - Z(\vec{x}'))d\Gamma d\vec{x}'$$

$$= \int \left[Z^2(\vec{x}') + \overline{Z}^2(\vec{x}) - 2Z(\vec{x}')\overline{Z}(\vec{x})\right] G(\vec{x},\vec{x}')d\vec{x}'$$

$$= \overline{Z^2}(\vec{x}) + \overline{Z}^2(\vec{x}) - 2\overline{Z}(\vec{x})\overline{Z}(\vec{x}) = \overline{Z^2}(\vec{x}) - \overline{Z}^2(\vec{x}),$$

Thus the unique definition for the SGS scalar variance if SGS statistics are based on the filtered PDF above is:

$$\overline{V}_z = \overline{Z^2} - \overline{Z}^2, \tag{4}$$

while $\overline{Z'^2} = \overline{Z^2} - 2\overline{Z\overline{Z}} + \overline{Z}^2$ can not be related to the second moment of any one point PDF, as it includes correlations between $\overline{Z}$ and Z at different points.

2 Evolution equation for the SGS scalar variance

When an evolution equation for $\overline{Z'^2}$ is derived, several open correlation terms appear that make its closure a difficult task. This is probably the reason why SGS variance evolution simulations are not found in literature and most approaches use a similarity model for the variance and an independent model for the scalar dissipation.[2,3] The relation between the scalar variance and the scalar dissipation, that should model the mixing phenomenon, is not evident in such an approach.

Once the correct definition of the SGS scalar variance stated, a simple evolution equation for it can be obtained from the corresponding equations for $\overline{Z^2}$ and $\overline{Z}^2$ or from integration of the evolution equation for the PDF. In any case the resulting equation is:

$$\frac{\partial\left(\overline{Z^2}-\overline{Z}^2\right)}{\partial t}+\frac{\partial\overline{u_i}\left(\overline{Z^2}-\overline{Z}^2\right)}{\partial x_i}=\frac{\partial}{\partial x_i}\left(D\frac{\partial\left(\overline{Z^2}-\overline{Z}^2\right)}{\partial x_i}\right)-\underbrace{2D\overline{\frac{\partial Z}{\partial x_i}\frac{\partial Z}{\partial x_i}}}_{I}$$
$$+2D\frac{\partial\overline{Z}}{\partial x_i}\frac{\partial\overline{Z}}{\partial x_i}-\underbrace{\frac{\partial}{\partial x_i}\left(\overline{u_iZ^2}-\overline{u_i}\overline{Z^2}\right)}_{II}+\underbrace{2\overline{Z}\frac{\partial}{\partial x_i}\left(\overline{u_iZ}-\overline{u_i}\overline{Z}\right)}_{III} \tag{5}$$

Three open terms appear in it, representing dissipation of scalar variance by both resolved and SGS scale gradients (I), transport of the square of the scalar field by the SGS turbulence (II) and transport of the scalar field itself by the SGS turbulence (III). Modeling SGS transport of scalars by the classical gradient assumption through an eddy diffusivity gives for the last two terms:

$$-\frac{\partial}{\partial x_i}\left(\overline{u_iZ^2}-\overline{u_i}\overline{Z^2}\right)=\frac{\partial}{\partial x_i}\left(D_T\frac{\partial\overline{Z^2}}{\partial x_i}\right),$$

and

$$2\overline{Z}\frac{\partial}{\partial x_i}\left(\overline{u_iZ}-\overline{u_i}\overline{Z}\right)=-2\overline{Z}\frac{\partial}{\partial x_i}\left(D_T\frac{\partial\overline{Z}}{\partial x_i}\right)=-\frac{\partial}{\partial x_i}\left(D_T\frac{\partial\overline{Z}^2}{\partial x_i}\right)+2D_T\frac{\partial\overline{Z}}{\partial x_i}\frac{\partial\overline{Z}}{\partial x_i}.$$

The evolution equation for the variance once this modelization introduced reads:

$$\frac{\partial \overline{V}_z}{\partial t} + \frac{\partial \overline{u_i} \overline{V}_z}{\partial x_i} = \frac{\partial}{\partial x_i} \left((D + D_T) \frac{\partial \overline{V}_z}{\partial x_i} \right) - 2D \overline{\frac{\partial Z}{\partial x_i} \frac{\partial Z}{\partial x_i}} + 2 (D + D_T) \frac{\partial \overline{Z}}{\partial x_i} \frac{\partial \overline{Z}}{\partial x_i}. \tag{6}$$

SGS turbulent transport effects appear in the diffusion and production terms, while the remaining open term $\overline{\chi} = 2D\overline{\frac{\partial Z}{\partial x_i}\frac{\partial Z}{\partial x_i}}$, the filtered scalar dissipation, represents mixing at the SGS level. This equation shows the relation between the scalar variance decay and the scalar dissipation mentioned above. Using a scale similarity model for the variance and an independent model for the dissipation can result in situations in which the variance evolves in a way incompatible with the local scalar dissipation. On the other hand, the SGS scalar variance can be computed along the simulation by addition of this equation to the LES system of equations, once the dissipation term is modeled. This approach would lead to a LES in which mixing is well represented by the correct relation between variance and dissipation with just a small increase in cost.

3 Modeling the scalar dissipation

A recent model for the filtered scalar dissipation reads:[3,13]

$$\overline{\chi} = 2D\overline{\frac{\partial Z}{\partial x_i}\frac{\partial Z}{\partial x_i}} = 2\left(D + D_T\right)\frac{\partial \overline{Z}}{\partial x_i}\frac{\partial \overline{Z}}{\partial x_i}. \tag{7}$$

This model can not be used to close the variance equation, as it was derived from a local equilibrium assumption in it that implies that the unsteady, convective and diffusive terms are negligible and estimates the dissipation as equal to the production. If used in equation 6, the production and dissipation terms would cancel out and it would become a convection–diffusion equation, by which the total SGS variance would be conserved in a closed system. This does not correspond to the real behavior of the SGS scalar variance, that should decay by the effect of turbulence, leading asymptotically to a completely mixed state in which variance is zero. This model was developed to be used as a model for the scalar dissipation rate in a context in which no variance equation is solved and $\overline{\chi}$ is only needed to determine the underlying flamelet regime.[3] The full model therein contains an independent scale similarity model for the variance, which is thus not affected by the local equilibrium assumption.

The dissipation model above is the first term in a model derived in,[13] whose complete expression is quite complex to be incorporated into the simulation of equation 6. A simple and general alternative model can be taken from RANS modeling of dissipation in terms of a characteristic mixing time assumed proportional to the turbulent characteristic time. In LES, the SGS scalar mixing time can be defined as:

$$\frac{1}{\tau_Z} = \frac{\overline{\chi}}{\overline{Z^2} - \overline{Z}^2}. \tag{8}$$

An equivalent SGS turbulent characteristic time $\overline{\tau}$ can be introduced as the ratio between the SGS kinetic energy $\kappa = 1/2\,(\overline{u_i u_i} - \overline{u_i}\,\overline{u_i})$ and the filtered kinetic energy dissipation rate $\overline{\epsilon} = \overline{\nu \frac{\partial u_i}{\partial x_j}\frac{\partial u_i}{\partial x_j}}$. Assuming a proportionality between both times, a model for $\overline{\chi}$ can be derived as:

$$\frac{\overline{\chi}}{\overline{Z^2} - \overline{Z}^2} = \frac{1}{\tau_Z} \sim \frac{C}{\overline{\tau}} = C\frac{\overline{\epsilon}}{\kappa} \tag{9}$$

where C is a parameter to be determined.

A test of this modeling assumption has been performed by comparing exact and predicted $\overline{\chi}$ values extracted from direct numerical simulation (DNS) data. DNS was conducted using a high–order compact finite differences parallel code[14] and corresponds to an inert scalar mixing in homogeneous isotropic turbulence at $Re_T \sim 64$ with $Sc = .75$ on a 150^3 grid. A box filter of characteristic size 10 times the grid size ($\overline{\Delta} = 10\Delta x$) was used to extract the relevant data and results for local and averaged values are presented in Fig. 1. A value for the parameter $C = 1/.75 = 1/Sc$ was found to be adequate. Further tests based in different Schmidt number scalars are needed to support this, but for the rest of this note and in all results presented a value $C = 1/Sc$ was assumed.

But unlike in RANS k-ϵ calculations, when it comes to a practical LES, quantities such as the SGS kinetic energy or its dissipation are not available. The implementation of the proposed model has to use approximations of $\overline{\kappa}$ and $\overline{\epsilon}$ derived from SGS turbulence models. If a Smagorinsky–type eddy viscosity model is used for the SGS stresses, and the Yoshizawa model is used for the SGS kinetic energy:

$$\overline{\epsilon} = 2\left(\nu + C_S\overline{\Delta}^2\left|\overline{S}\right|\right)\overline{S}_{ij}\overline{S}_{ij}, \qquad \overline{\kappa} = 2C_I\overline{\Delta}^2\overline{S}_{ij}\overline{S}_{ij}, \tag{10}$$

the actual implementation of the model for $\overline{\chi}$ would read:

$$\overline{\chi} = \frac{\left(\nu + C_S\overline{\Delta}^2\left|\overline{S}\right|\right)}{Sc\, C_I\overline{\Delta}^2}\left(\overline{Z^2} - \overline{Z}^2\right), \tag{11}$$

resulting in a well-conditioned expression, provided that C_S and C_I are not zero.

A priori tests of this model are presented in Fig. 2, in which exact $\overline{\chi}$ values are compared to those given by eq. 11, with constant C_I and C_S

parameters, estimated from DNS data by averaging (both in space and time) the relations in equation 10. In Fig. 3 the space averaged values of these parameters (and of Sc_T) are presented for reference. While Sc_T and C_S appear as approximately constant in time, C_I varies from a .09 to a .06 value along the simulation. An intermediate value $C_I = .07$ was used to produce results in Fig. 2. It appears that dissipation is accurately predicted both locally and on average even when this rough parameter estimation is used.

4 Simulation Results

A Large Eddy Simulation of a scalar mixing in homogeneous isotropic turbulence was performed to further test the dissipation modeling in a real SGS variance calculation. The large scale equations of the velocity and scalar fields plus the equation of the SGS variance:

$$\begin{aligned}
\frac{\partial \overline{u}_i}{\partial t} + \frac{\partial \overline{u}_i \overline{u_j}}{\partial x_j} &= -\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_k}\left((\nu + \nu_T) \frac{\partial u_i}{\partial x_k} \right) \\
\frac{\partial \overline{Z}}{\partial t} + \frac{\partial \overline{Z}\overline{u_j}}{\partial x_j} &= \frac{\partial}{\partial x_k}\left((D + D_T) \frac{\partial \overline{Z}}{\partial x_k} \right) \\
\frac{\partial \overline{V}_z}{\partial t} + \frac{\partial \overline{V}_z \overline{u_j}}{\partial x_j} &= \frac{\partial}{\partial x_k}\left((D + D_T) \frac{\partial \overline{V}_z}{\partial x_k} \right) - 2\,(D + D_T) \frac{\partial \overline{Z}}{\partial x_k}\frac{\partial \overline{Z}}{\partial x_k} + \overline{\chi}
\end{aligned} \tag{12}$$

were solved on a 30^3 grid by the same DNS high–order finite-difference code,[14] to which eddy viscosity and diffusivity terms were added, and production and dissipation of variance incorporated as source terms. Filtered fields obtained from DNS by applying a box filter operator of size $\overline{\Delta} = 10\Delta x$ and then projecting into the 30^3 grid were imposed as the initial conditions for the LES.

Several models enter such a calculation: an eddy viscosity (ν_T) model and an eddy diffusivity (D_T) model were used to close the momentum and scalar equations, while the variance equation was closed by the same eddy-diffusivity model plus the dissipation model in equation 11. The SGS variance calculation is thus affected by the eddy viscosity model (through the large scale convection velocity), the eddy diffusivity model (both directly and through its effect on $\overline{Z}$), and the dissipation model. In order to assess the performance of the dissipation model, independent tests for the three models were needed. This could be achieved by comparison of LES and DNS results for some particular magnitudes:

- A Smagorinsky model with constant C_s (obtained from a priori tests) was used to close the momentum equation, and tested by comparing LES and DNS results for the decay of the global resolved kinetic energy

$\int \frac{1}{2}\overline{u_i}^2$. This comparison is presented in Fig. 4, and agreement is quite good, as expected from the well–documented good behavior of this model in homogeneous isotropic turbulence.

- An eddy diffusivity model derived from the above Smagorinsky model as $D_T = \nu_T / Sc_T$ with $Sc_T = .3$ (as obtained from a priori tests), was used to close the $\overline{Z}$ equation. The study of the decay of the "scalar energy" $\overline{Z}^2$, a large scale quantity equivalent to the kinetic energy, constitutes an independent test of this model, as:

$$\frac{d}{dt}\int \overline{Z}^2 = \int 2\,(D + D_T)\,\frac{\partial \overline{Z}}{\partial x_i}\frac{\partial \overline{Z}}{\partial x_i}.$$

Comparison of LES and DNS results for the decay of the global scalar energy is presented in Fig. 4, while instantaneous isosurfaces of the $\overline{Z}$ field obtained from filtering the DNS data and from the LES calculation at time ~ 3 are shown in Fig. 5. Again a good agreement is found. Slight deviations in the $\int \overline{Z}^2$ decay rate indicate, however, that Sc_T should not be taken as constant. The space averaged value of Sc_T obtained in a priori tests is constant in time (see Fig. 3), but local spatial variations should be allowed, as the initial condition for the scalar field has a cylindrical shape, and is thus not homogeneous or isotropic. Probably a local determination of Sc_T through a dynamic procedure would give better results.

- The dissipation model in equation 11 with $C_I = .06$ was used to close the dissipation term in the variance equation, while the eddy-diffusivity model above was used for the SGS transport terms. Results of global SGS scalar variance decay and instantaneous scalar variance fields from LES and DNS are presented in Figs. 4 and 5. Again some deviations in the decay rate can be observed, especially in the first steps of the simulation. The use of a constant value for C_I, much closer to the final values than to the initial values in Fig. 3 is in part responsible for that deviations, together with effects of constant Sc_T. In the first steps of the simulation $\overline{Z}^2$ decays too rapidly and $\overline{Z^2} - \overline{Z}^2$ too slowly. This is an effect of a too large production term $(2\,(D + D_T)\,\frac{\partial \overline{Z}}{\partial x_i}\frac{\partial \overline{Z}}{\partial x_i})$ at this period, as can be seen in Fig. 6, and which is possibly caused by the use of a spatially constant Sc_T. Dissipation appears to be slightly overestimated at the same initial time (Fig. 6 left), due to the use of a $C_I = .06$ value, smaller than that estimated a priori as adequate for that time. Later, both values appear to be closer to the DNS values and both the scalar energy and the variance decay at the correct rate.

These results appear to confirm the adequacy of the proposed model, as even with approximate C_I and Sc_T parameters the adequate global variance decay rate is reproduced and the instantaneous field presents the appropriate shape. Estimations of these parameters by a dynamic procedure[15,16] in combination with the present model for dissipation would lead to a complete model for the system in eq. 12 in which no external input would be needed.

As suggested by one of the reviewers of this work, a comparison with existing models for the variance is needed to assess the performance of the present modelisation. A comparison of the global SGS variance evolution obtained by the present model and by the scale similarity model in:[3]

$$\overline{V}_z = C_s \left(\widehat{\overline{Y}^2} - \widehat{\overline{Y}}^2 \right) \tag{13}$$

with C_s a dynamically determined coefficient, is presented in Fig. 7. Circles represent there the actual value of the variance obtained by filtering DNS data (void circles) and the value obtained in the LES described above (full circles). Square symbols represent the values given by the scale similarity dynamic model in an a priori estimation based in filtering DNS data at two levels (void squares) and by an actual LES of the velocity and scalar field that computes variance by the same model (full squares). The scale similarity dynamic model appears to overestimate the variance when DNS data are used and to underestimate it in the case of the LES calculation. This different behavior indicates again some need for a better model to close the scalar evolution equation in LES (note that only the variance is estimated dynamically in the LES calculation, while a constant turbulent Schmidt number is used to close the $\overline{Z}$ evolution equation). But even when the DNS data are used, the scale similarity model appears to be a worse estimation of the variance than the simulation of the closed variance equation presented here. Of course, there is also the cost issue, which could in some cases make the estimation of the variance through a scale similarity model more appropriate than the resolution of an additional equation. This depends on the numerical scheme adopted, as for some of them the cost of a filtering operation can be very close or even greater than the cost of solving a scalar equation. In the present case both the scale similarity dynamic model estimation and the addition of an equation for the variance represent an increase in CPU time of about 20 % (19 % and 18 % resp.).

5 Conclusion

The formal derivation of the SGS scalar variance definition presented here allows to write an evolution equation for it in which the only open term is the filtered scalar dissipation, which represents SGS mixing effects. This equation can be added to the LES equations of a reacting flow so that SGS reactant statistics are determined by a single model for dissipation, while variance and dissipation appear as correctly related through mixing. Modeling the dissipation as in equation 7 would imply identical dissipation and production of variance and thus can not be used for the purpose of closing this equation. An alternative simple model has been proposed and tested here for a scalar mixing in homogeneous isotropic turbulence. Model parameters have been obtained from space and time averaged values of fitted parameters extracted from DNS data and the obtained model has been shown to behave appropriately. Existing dynamic procedures to determine C_S, Sc_T and C_I along the simulation could give better results, but even when roughly estimated constant parameters are used the proposed model gives the correct magnitude for the variance decay.

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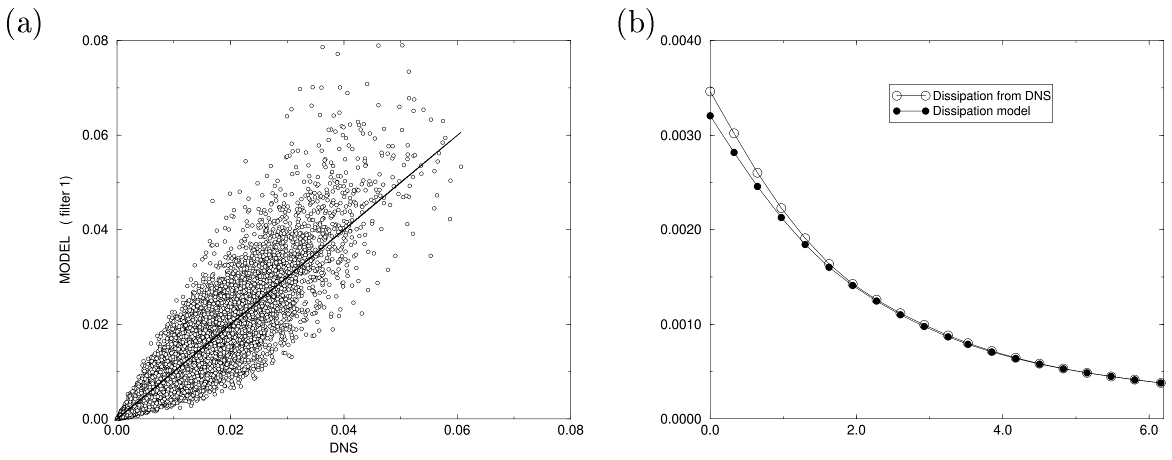

Figure 1: C. Jiménez, Physics of Fluids

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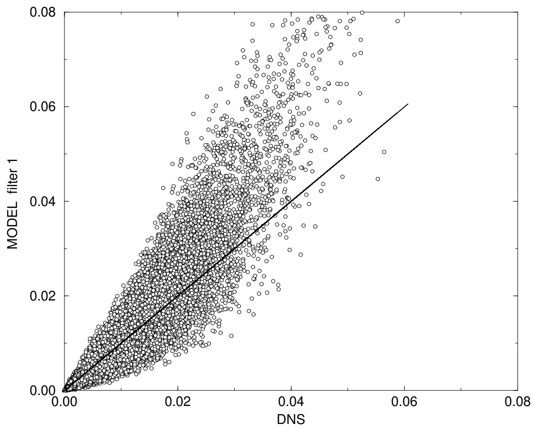

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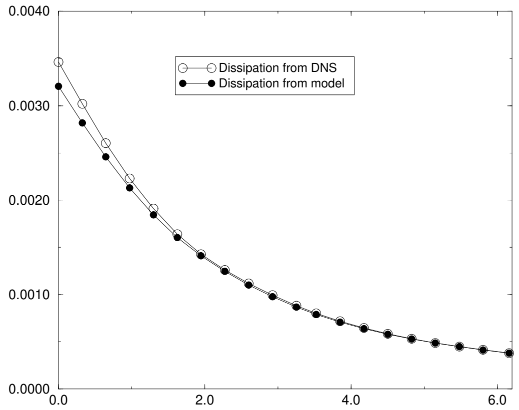

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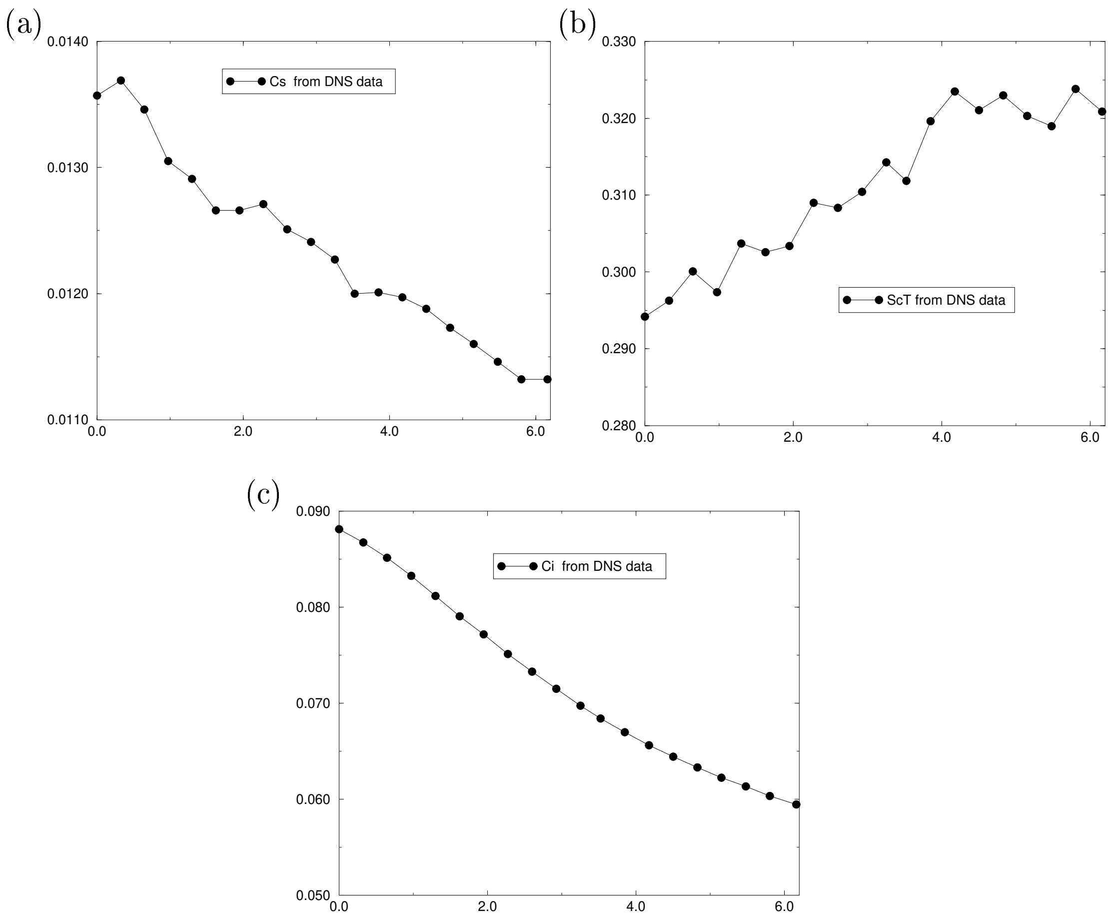

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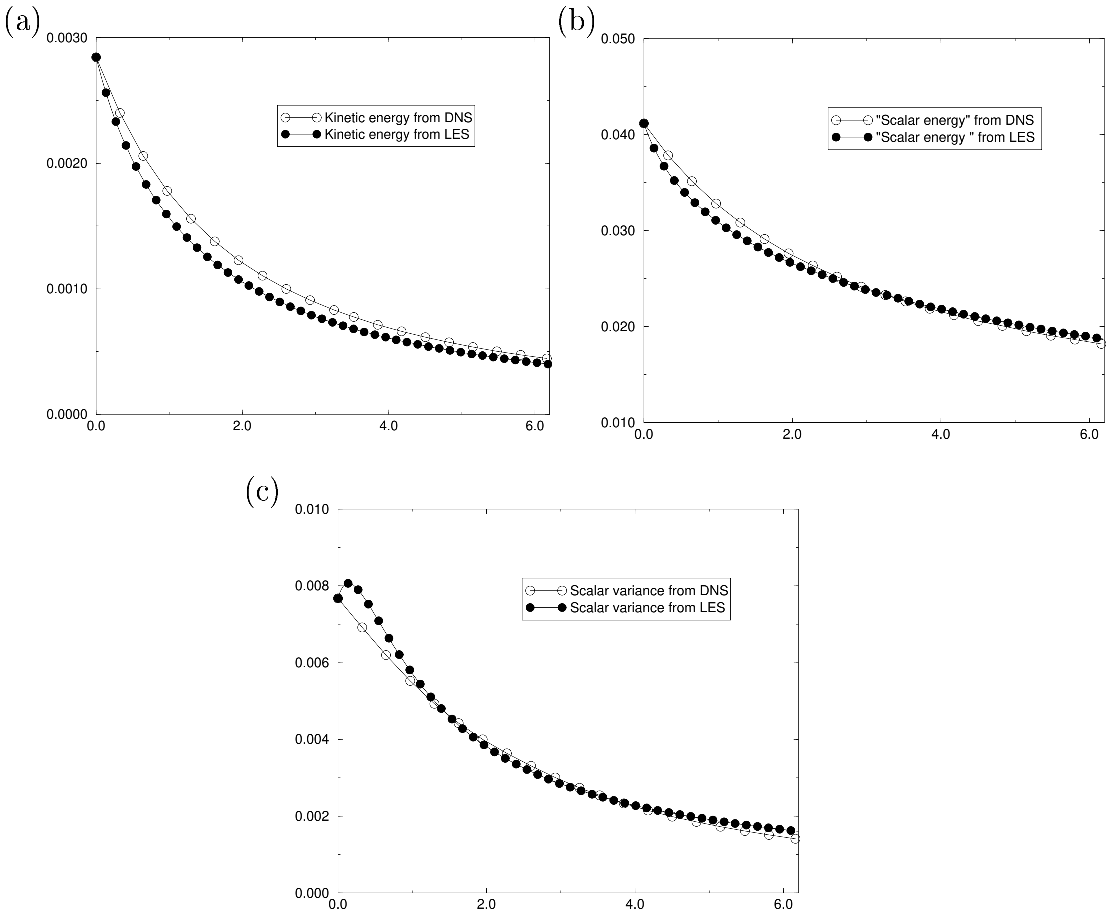

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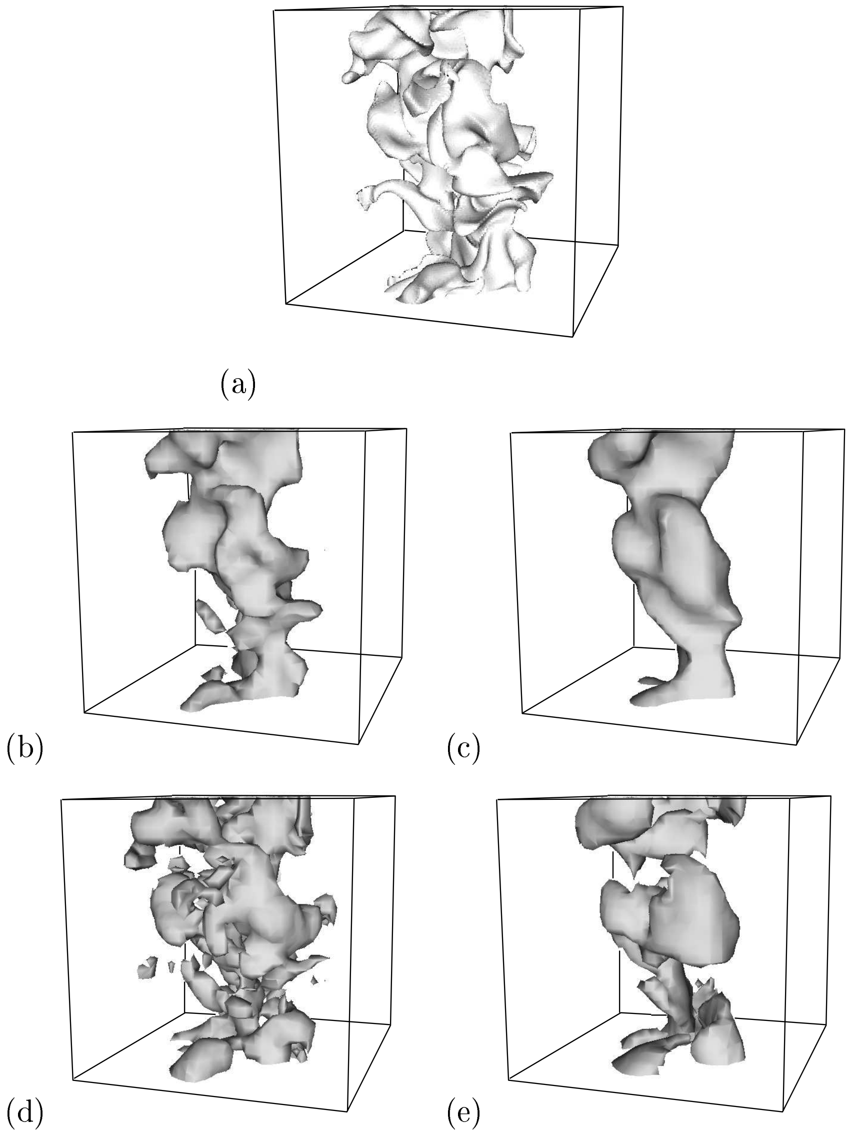

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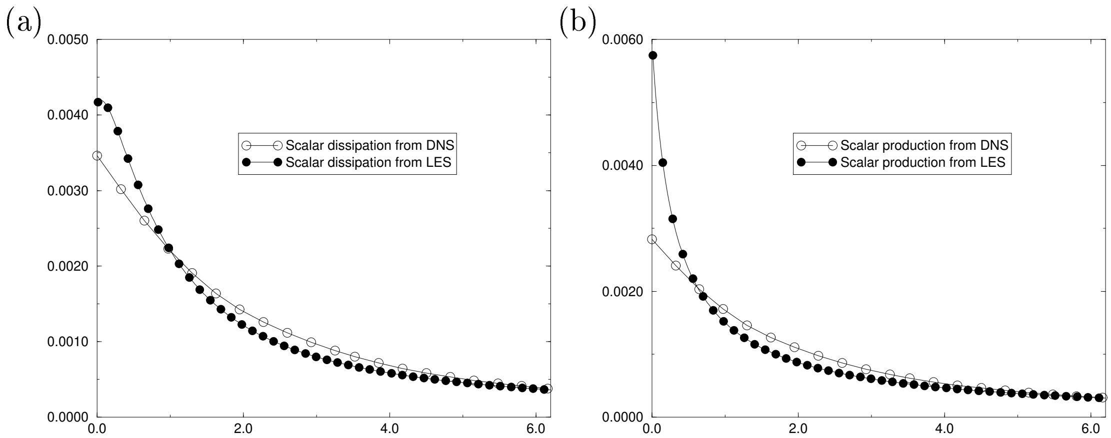

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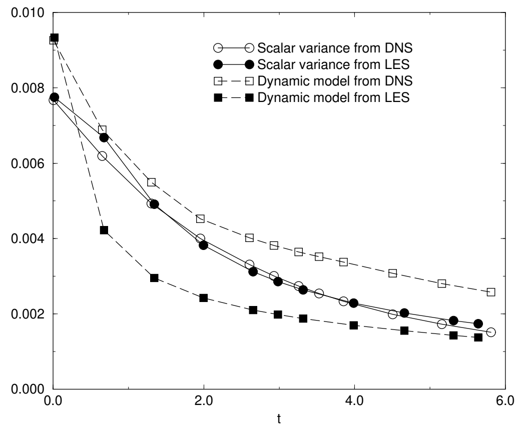

Figure 7: C. Jiménez, Physics of Fluids