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# Effects of molecular diffusion on the subgrid-scale modeling of passive scalars

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The spectral eddy-viscosity and eddy-diffusivity closures derived from the eddy-damped quasnormal Markovian (EDQNM) theory, and one of its physical space counterparts, i.e., the structure function model [Métais and Lesieur, *J. Fluid Mech.* **239**, 157 (1992)], are revisited to account for molecular viscosity and diffusivity effects. The subgrid-scale Schmidt number (usually set to  $Sc_t \approx 0.6$ ) is analytically derived from the EDQNM theory and shown to be Reynolds number dependent, a property of utmost importance for flows involving scalar transport at moderate Reynolds numbers or during the transition to turbulence. *A priori* tests in direct numerical simulation of homogeneous isotropic turbulence [da Silva and Pereira, *Phys. Fluids* **19**, 035106 (2007)] and in spatially evolving turbulent plane jets [da Silva and Métais, *J. Fluid Mech.* **473**, 103 (2002)], as well as *a posteriori* (large eddy simulation) tests in a round jet are carried out and show that the present viscous structure function model improves the results from the classical approaches and at a comparatively small computational cost. © 2008 American Institute of Physics.

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## I. INTRODUCTION

The large eddy simulation (LES) technique consists of describing the large-scale motions based on a spatial filtering operation while the effect of the subgrid-scales (SGS) needs to be modeled.<sup>1</sup> While many SGS models have been designed to close the resulting filtered Navier–Stokes equations for incompressible flows,<sup>2–4</sup> the corresponding problem applied to turbulent combustion, turbulent mixing, or compressible flow has not yet been fully addressed.<sup>5,6</sup> For these situations, the filtered transport equation of a scalar variable (e.g., mixture fraction, temperature) must be solved and a subgrid-scale scalar flux has to be modeled. The simplest way to address this issue consists in considering a constant SGS Schmidt number<sup>7</sup>  $Sc_t \approx 0.6$  and in determining an eddy-diffusivity term proportional to the eddy-viscosity model:  $\kappa_t = \nu_t / Sc_t$ . The main limitation of such a model is that  $Sc_t$  is set to a constant while it should be strongly affected by the slope of the kinetic energy spectrum.<sup>8</sup> Moin *et al.*<sup>9</sup> have shown indeed that a dynamically computed value of  $Sc_t$  could greatly improve the results of the simulations, since  $\kappa_t$  depends on the molecular Schmidt number  $Sc$  and on the local turbulence level of the flow. In the present work we revisit the eddy-viscosity and eddy-diffusivity models in spectral space<sup>8</sup> in order to integrate the molecular viscosity/diffusivity effects from the original eddy-damped quasnormal Markovian (EDQNM) equations. The new formulation/model is useful to address two related issues: (i) The effects of low Reynolds number and (ii) a variable SGS Schmidt number for transitional flows.

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## II. SGS MODELING IN SPECTRAL SPACE

In the Fourier space, the SGS transfers across the cutoff wave number  $k_c$  (which represents the smallest resolved scale for LES) are modeled based on eddy-viscosity and eddy-diffusivity concept defined as<sup>8</sup>

$$\nu_t^\infty = \frac{1}{15} \int_{k_c}^{\infty} \theta_{0pp} \left[ 5E(p) + p \frac{\partial E}{\partial p} \right] dp, \quad (1)$$

$$\kappa_t^\infty = \frac{2}{3} \int_{k_c}^{\infty} \theta_{0pp}^T E(p) dp, \quad (2)$$

where  $E(k)$  is the three-dimensional kinetic energy spectrum and  $\theta_{kpq}$  and  $\theta_{kpq}^T$  are the velocity and scalar-velocity triple correlation relaxation times, respectively,

$$\theta_{kpq} = \frac{1}{\mu(k) + \mu(p) + \mu(q) + \nu(k^2 + p^2 + q^2)}, \quad (3)$$

$$\theta_{kpq}^T = \frac{1}{\mu'(k) + \mu'(p) + \mu''(q) + \kappa(k^2 + p^2) + \nu q^2}. \quad (4)$$

They are introduced in the frame of the EDQNM theory, to close the evolution equation for the third-order moments of the velocity and temperature components<sup>1,10,11</sup> involving triadic interactions,

$$\left\{ \frac{\partial}{\partial t} + \nu(k^2 + p^2 + q^2) + [\mu(k) + \mu(p) + \mu(q)] \right\} \times \langle \hat{u}(\mathbf{k}) \hat{u}(\mathbf{p}) \hat{u}(\mathbf{q}) \rangle = \Sigma \langle \hat{u} \hat{u} \rangle \langle \hat{u} \hat{u} \rangle, \quad (5)$$

$$\left\{ \frac{\partial}{\partial t} + \kappa(k^2 + p^2) + \nu q^2 + [\mu'(k) + \mu'(p) + \mu''(q)] \right\} \times \langle \hat{T}(\mathbf{k}) \hat{T}(\mathbf{p}) \hat{u}(\mathbf{q}) \rangle = \Sigma \langle \hat{u} \hat{u} \rangle \langle \hat{T} \hat{T} \rangle, \quad (6)$$

where  $\mu(k)^2 = a_1^2 \int_0^k p^2 E(p) dp$ ,  $\mu'(k)^2 = a_2^2 \int_0^k p^2 E(p) dp$  and  $\mu''(k)^2 = a_3^2 \int_0^k p^2 E(p) dp$  are linear damping functions that approximate the fourth-order cumulants with  $a_1 = 0.218 C_k^{3/2}$ ,  $a_2 = 0$ , and  $a_3 = 0.7848 C_k^{3/2}$  so that  $(a_2 + a_3)/6a_1 = 0.6$ . In Eqs. (3) and (4), the role of the molecular viscosity/diffusivity terms  $\nu k^2$  and  $\kappa k^2$  is to partially inhibit the linear terms associated to  $\mu(k)$ ,  $\mu'(k)$ , and  $\mu''(k)$ . This contribution had been neglected in the original formulation of the spectral eddy-viscosity model<sup>8</sup> because the aim was to deal with high Reynolds number flows. It is presently reintroduced here to address the issue of modeling turbulent flows involving a transition to turbulence or a moderate Reynolds number. In order to evaluate the integrals defined in Eqs. (1) and (2), the shape of the energy spectrum  $E(k)$  for  $k > k_c$  must be known. In the present work we assume that the kinetic energy spectrum is modeled as  $E(k) = C_m k^{-m}$  for  $k > k_c$ , where  $5/3 \leq m < 3$ . The case  $m = 5/3$  is considered to be a good approximation for high Reynolds number flows. In particular, the accuracy of the approximation increases with the Reynolds number. For low Reynolds number flows, the spectrum exhibits only a dissipative range with a local slope that is always  $m > 5/3$ .<sup>8,12</sup> Despite the limitations of this approximation, particularly in low Reynolds number flows, it has yielded good results in numerous theoretical and numerical works.<sup>1</sup> It is interesting to note that the upper bound  $m = 3$  value in the present analytical developments corresponds to forced flow situations such as two-dimensional turbulence in geophysical flows.<sup>1</sup>

Thus, the relaxation times are<sup>8,12</sup>

$$\theta_{0pp} = \frac{1}{2} \frac{1}{\frac{a_1 \sqrt{C_m}}{\sqrt{3-m}} p^{(3-m)/2} + \nu p^2}, \quad (7)$$

$$\theta_{0pp}^r = \frac{1}{\frac{(a_2 + a_3) \sqrt{C_m}}{\sqrt{3-m}} p^{(3-m)/2} + (\kappa + \nu) p^2}. \quad (8)$$

Using Eqs. (1), (2), (7), and (8), the eddy-viscosity and eddy-diffusivity are now obtained as<sup>13</sup>

$$\nu_t^\infty = \nu_{t_i}^\infty \left[ 1 - \frac{\ln(1+X)}{X} \right], \quad (9)$$

$$\kappa_t^\infty = \kappa_{t_i}^\infty \left[ 1 - \frac{\ln(1+Y)}{Y} \right] \quad (10)$$

with

$$X = \frac{15a_1^2 m + 1}{5-m} \frac{\nu_{t_i}^\infty}{3-m} \frac{1}{\nu}, \quad (11)$$

$$Y = \frac{3(a_2 + a_3)^2 m + 1}{2} \frac{\kappa_{t_i}^\infty}{3-m} \frac{1}{\nu + \kappa}. \quad (12)$$

The present formulation leads to a damping effect with respect to the basic inviscid eddy-viscosity and eddy-diffusivity defined as<sup>8</sup>

$$\nu_{t_i}^\infty = \frac{5-m}{15a_1} \frac{\sqrt{3-m}}{m+1} \sqrt{\frac{E(k_c)}{k_c}}, \quad (13)$$

$$\kappa_{t_i}^\infty = \frac{4}{3(a_2 + a_3)} \frac{\sqrt{3-m}}{m+1} \sqrt{\frac{E(k_c)}{k_c}}. \quad (14)$$

The new model equations (9)–(14) are first assessed using kinetic energy spectra  $E(k)$  from DNS of homogeneous isotropic turbulence<sup>14</sup> for  $\text{Re}_\lambda = 39$ – $96$ ,  $\text{Sc} = 0.2$ – $0.7$ – $3$ . Explicit filtering is obtained with a sharp cutoff filter in Fourier space applied with filter sizes ranging from  $\bar{\Delta} = 2\Delta$  to  $\bar{\Delta} = 10\Delta$ , where  $\Delta$  is the size of the grid from the DNS in each direction. In practice, the  $m$  slope is obtained by interpolation using a least-squares method<sup>12</sup> applied on the three-dimensional energy spectra in the wave number range  $k_c/2 \leq k \leq k_c$ . In this sense,  $m$  is a function of the global slope of the kinetic energy spectrum in the neighborhood of the cutoff wave number. For low Reynolds number flows no inertial range exists and the cutoff filter is located in the dissipative region of the kinetic energy spectrum. Therefore,  $m$  becomes steeper as the filter size decreases. Figures 1(a) and 1(b) show indeed that the spectral eddy-viscosity  $\nu_t^\infty$  and diffusivity  $\kappa_t^\infty$  are strongly damped for low Reynolds numbers, e.g., for  $\text{Re}_\lambda = 39$ , in comparison with their inviscid counterparts  $\nu_{t_i}^\infty$  and  $\kappa_{t_i}^\infty$ , respectively. The inviscid SGS Schmidt number is defined<sup>8</sup> as

$$\text{Sc}_{ii}^{(m)} = \frac{\nu_{t_i}^\infty}{\kappa_{t_i}^\infty} = (5-m) \frac{a_2 + a_3}{20a_1}. \quad (15)$$

Introducing  $Q$  as the ratio between  $Y$  and  $X$ ,

$$Q = \frac{Y}{X} = 2 \frac{a_2 + a_3}{a_1} \frac{\nu}{\nu + \kappa} = 12 \text{Sc}_{ii}^{(m=5/3)} \frac{\text{Sc}}{1 + \text{Sc}}, \quad (16)$$

we obtain an expression for the SGS Schmidt number,

$$\text{Sc}_t^{(m)} = \frac{\nu_t^\infty}{\kappa_t^\infty} = \text{Sc}_{ii}^{(m)} \frac{QX - Q \ln(1+X)}{QX - \ln(1+QX)}. \quad (17)$$

In the limit of small  $X$ ; i.e., small Reynolds number, the SGS Schmidt number is

$$\text{Sc}_t^{(m)} = \frac{(5-m)}{40} \left( 1 + \frac{1}{\text{Sc}} \right)$$

instead of its inviscid value defined in Eq. (15). Thus, the new model provides a damping adjustment of the SGS

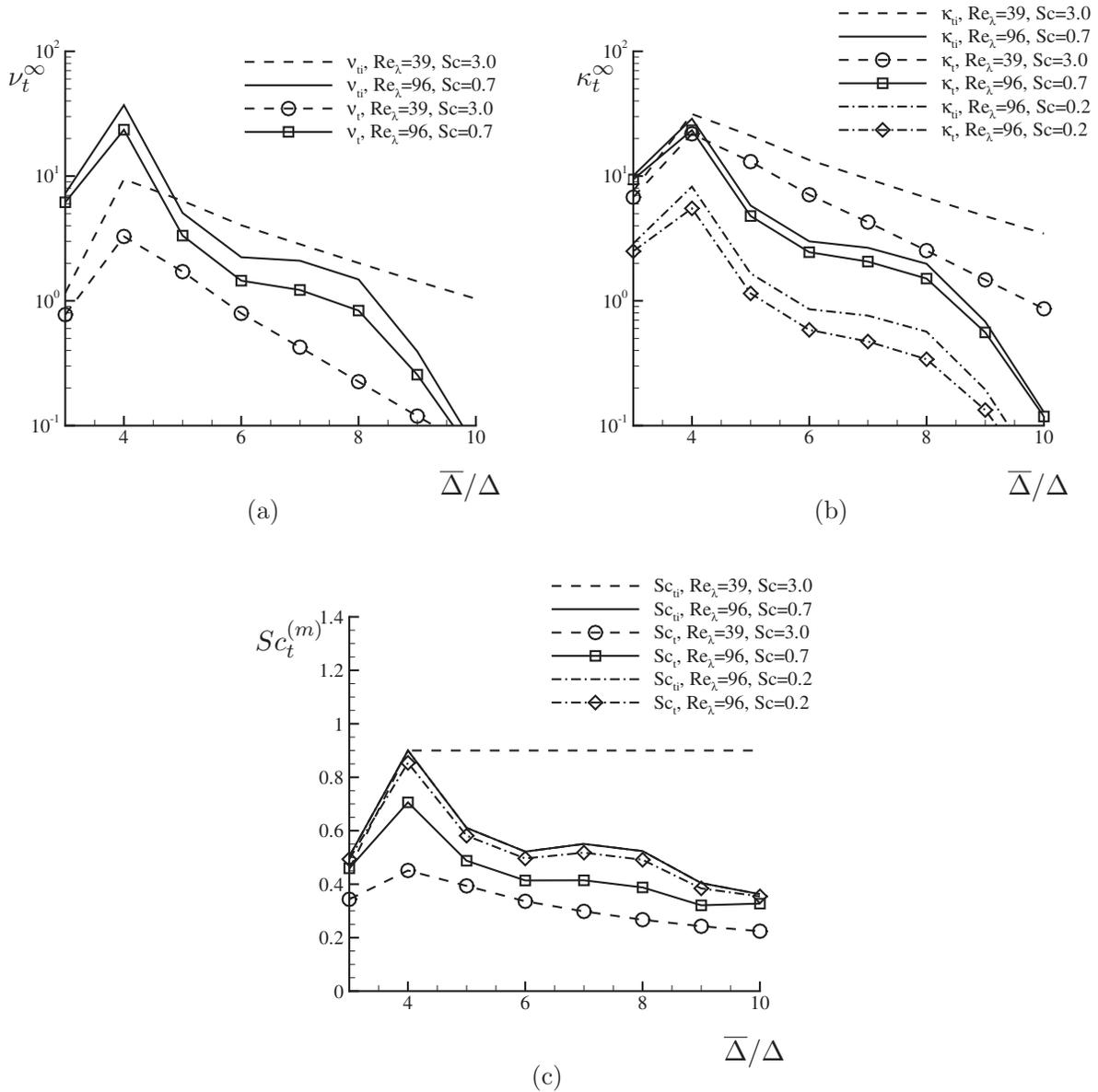


FIG. 1. *A priori* tests on isotropic turbulence with passive scalar for  $Re_\lambda=39-96$  and  $Sc=0.2-0.7-3$ . A sharp cutoff filter with filter widths equal to  $\bar{\Delta}/\Delta \in [2; 10]$  was used. The results were obtained with Eqs. (9), (10), and (17). (a) Spectral eddy-viscosity  $\nu_t^\infty$  and  $\nu_t^\infty$ . (b) Spectral eddy-diffusivity  $\kappa_t^\infty$  and  $\kappa_t^\infty$ . (c) SGS Schmidt number  $Sc_t^{(m)}$  and  $Sc_t^{(m)}$ .

Schmidt number, which includes the effects of the global slope of the kinetic energy spectrum  $m$  around the cutoff wave number and of the molecular diffusion (accounted for by the Schmidt number). These two effects are expected to be of critical importance in the simulation of flows involving scalar transport in low to moderate Reynolds numbers or during the transition to turbulence. As an example of application using Eqs. (15) and (17), consider the case  $m=5/3$  and  $Sc=0.7$ . We get  $Sc_{t_i}=0.6$  and  $Sc_t=0.2$ , with these equations, respectively, while for  $m=3$  and  $Sc=0.7$ , we obtain  $Sc_{t_i}=0.36$  and  $Sc_t=0.12$ ; i.e., the damping functions lead to a reduction in the SGS Schmidt number to about one third. These effects are well illustrated in Fig. 1(c), where again the shape of the energy spectra from isotropic turbulence<sup>14</sup> were used.

### III. SGS MODELING IN PHYSICAL SPACE

#### A. Viscous structure function model

In LES carried out in the physical space, the filtered Navier–Stokes equations and a corresponding filtered scalar transport equation have to be evaluated,

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j} (\bar{u}_i \bar{u}_j) = - \frac{1}{\rho} \frac{\partial \bar{P}}{\partial x_i} + 2\nu \frac{\partial \bar{S}_{ij}}{\partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j}, \quad (18)$$

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0, \quad (19)$$

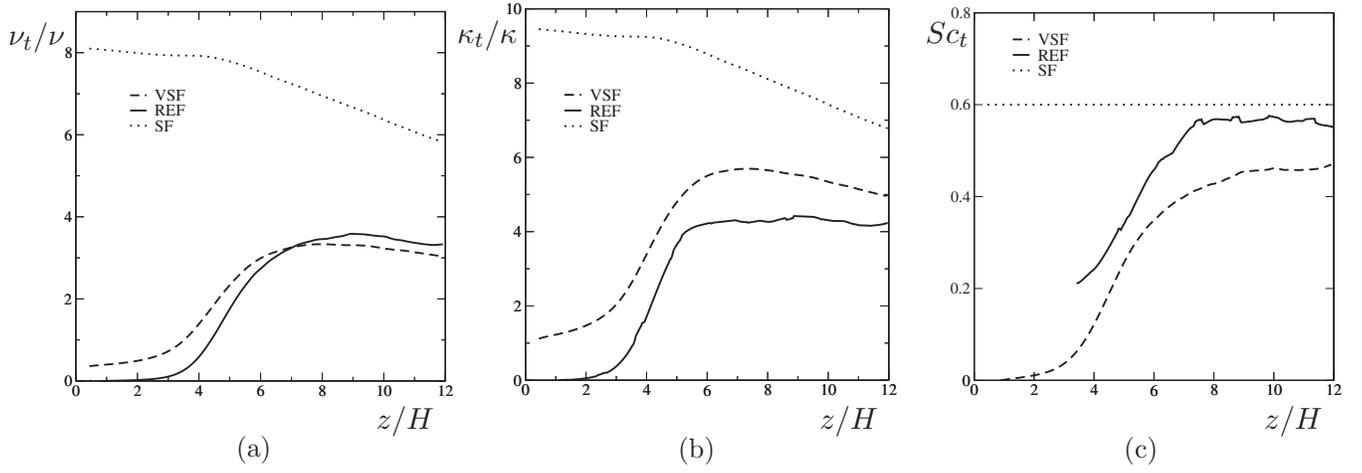


FIG. 2. Downstream evolution at  $y/H=0.5$  of the (a) eddy-viscosity  $\nu_t$ , (b) eddy-diffusivity  $\kappa_t$ , and (c) SGS Schmidt number  $Sc_t$  in *a priori* tests on a plane jet for  $Re_H=3000$  and  $Sc=0.7$ . The reference values (REF) were obtained by box filtering the DNS, and using Eqs. (27), while results for the classical structure function model (SF), and viscous structure function model (VSF) were obtained with Eqs. (23)–(26), respectively.

$$\frac{\partial \bar{T}}{\partial t} + \frac{\partial}{\partial x_i} (\bar{T} \bar{u}_i) = \kappa \frac{\partial \bar{G}_i}{\partial x_i} - \frac{\partial q_i}{\partial x_i}, \quad (20)$$

where  $\bar{S}_{ij} = \frac{1}{2}(\partial \bar{u}_i / \partial x_j + \partial \bar{u}_j / \partial x_i)$  is the strain rate tensor and  $\bar{G}_i = \partial \bar{T} / \partial x_i$  is the scalar gradient. The subgrid-scale stresses tensor  $\tau_{ij} = u_i u_j - \bar{u}_i \bar{u}_j$  and the subgrid-scale scalar flux  $q_i = T u_i - \bar{T} \bar{u}_i$  are unknown quantities requiring modeling. The use of the eddy-viscosity and eddy-diffusivity concepts permits one to relate these unknowns to a turbulent eddy-viscosity  $\nu_t(\mathbf{z}, t)$  and a turbulent eddy-diffusivity  $\kappa_t(\mathbf{z}, t)$ ,

$$\tau_{ij} - \frac{1}{3} \delta_{ij} \tau_{kk} = -2 \nu_t \bar{S}_{ij}, \quad (21)$$

$$q_i = -\kappa_t \bar{G}_i. \quad (22)$$

The structure function (SF) model<sup>8</sup> was developed as a physical space representation of the spectral eddy-viscosity model derived from the EDQNM closure. It seems, therefore, natural to assess the present model in the physical space using the SF model as a starting point. The eddy-viscosity for the SF model is given by

$$\nu_t^{sf} = 0.105 C_K^{-3/2} \bar{\Delta} \sqrt{F_2(\mathbf{z}, \bar{\Delta}, t)}, \quad (23)$$

where  $F_2(\mathbf{z}, \bar{\Delta}, t)$  is the local second-order velocity structure function computed on a shell of diameter equal to  $\bar{\Delta}$ . This model showed good results in a number of turbulent shear flows.<sup>8</sup> The extension to the physical space of the present low Reynolds number model consists in the *viscous structure function* model (VSF) developed by Brun *et al.*<sup>13</sup> In this model the (physical space) eddy-viscosity<sup>13</sup> and eddy-diffusivity are given by

$$\nu_t^{VSF} = \nu_t^{SF} \left[ 1 - \frac{1}{x} \ln(1+x) \right], \quad (24)$$

$$\kappa_t^{VSF} = \frac{\nu_t^{SF} \left[ 1 - \frac{1}{Qx} \ln(1+Qx) \right]}{Sc_t^{(m)}}, \quad (25)$$

respectively, where  $Q$  is given by Eq. (16), and  $x$  is a function of the angle  $\alpha$  between the local vorticity  $\boldsymbol{\omega}$  and the mean vorticity  $\boldsymbol{\omega}_m$  averaged over a shell of radius equal to  $\bar{\Delta}$  (see Sagaut<sup>4</sup>),

$$x = \tan\left(\frac{\alpha}{2}\right) \frac{\nu_t^{SF}}{\nu} \quad \alpha = \arccos\left(\frac{\boldsymbol{\omega}_m \cdot \boldsymbol{\omega}}{\|\boldsymbol{\omega}_m\| \|\boldsymbol{\omega}\|}\right). \quad (26)$$

The resulting VSF model constitutes therefore a continuous formulation of the selective structure function model.<sup>2,15</sup>

## B. *A priori* tests

*A priori* tests were performed on a DNS of a turbulent plane jet<sup>16</sup> for  $Re_H=3000$  and  $Sc=0.7$ . Explicit filtering was made with a top-hat filter for the evaluation of the SGS model in the physical space for  $\bar{\Delta}/\Delta=3, 5$ , and  $7$ . The results demonstrated that  $\nu_t$  and  $\kappa_t$  are roughly proportional to  $(\bar{\Delta}/\Delta)^{4/3}$  as expected from the literature<sup>1</sup> (not shown). For comparison we computed reference values for the eddy-viscosity and eddy-diffusivity from the DNS data through

$$\nu_t^{REF} = -\frac{\langle \tau_{ij} \bar{S}_{ij} \rangle}{2 \langle \bar{S}_{kl} \bar{S}_{kl} \rangle}, \quad \kappa_t^{REF} = -\frac{\langle q_i \bar{G}_i \rangle}{\langle q_j q_j \rangle}, \quad (27)$$

where  $\langle \cdot \rangle$  means a temporal averaging. Figure 2(a) compares the new viscous SF eddy-viscosity  $\nu_t^{VSF}$ , the classical SF eddy-viscosity<sup>8</sup>  $\nu_t^{SF}$ , and the reference eddy-viscosity  $\nu_t^{REF}$  obtained with Eq. (27). As can be seen the VSF model has the expected behavior along the jet streamwise direction; i.e., it damps the influence arising from the presence of a strong mean velocity gradient during the transition stage. Similar results are obtained for the eddy-diffusivity [see Fig. 2(b)]. Figure 2(c) displays the evolution of the SGS Schmidt num-

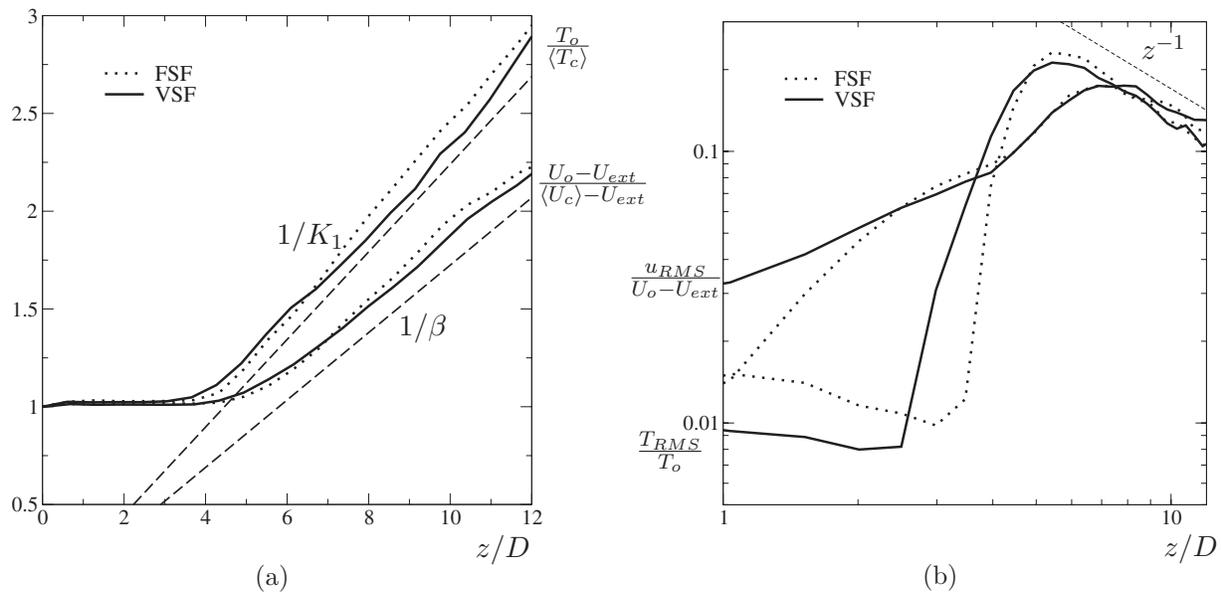


FIG. 3. Centerline evolution of the (a) mean velocity and passive scalar field and (b) RMS velocity and RMS passive scalar field for LES of spatially evolving round jets at  $Re_D=25\,000$  and  $Sc=0.2$ .

ber corresponding to Figs. 2(a) and 2(b). The constant value of  $Sc_t=0.6$  usually set in LES of passive scalar is also shown for comparison. The potential of the new model is clearly illustrated by the damping effect present in the initial stage of the plane jet development.

### C. A posteriori tests: LES of round jet at $Re_D=25\,000$

Finally, LES of spatially evolving turbulent round jet were carried out with the new model (VSF) using an accurate Navier–Stokes solver with pseudospectral methods and sixth-order compact schemes.<sup>16,17</sup> The Reynolds number is  $Re_D=25\,000$  based on the inflow velocity  $U_o$  of the jet and on the diameter  $D$ , and the molecular Schmidt number is  $Sc=0.2$ . The flow configuration consists of a co-flowing jet with about  $U_{ext}/U_o=7\%$  co-flow. Hyperbolic tangent profiles were applied as inflow conditions for both the velocity and the scalar,<sup>16</sup> with a momentum thickness  $\theta_o=D/40$ . Results are compared with the filtered structure function model<sup>2</sup> (FSF) with constant SGS Schmidt number  $Sc_t=0.6$ . Figure 3(a) shows the mean velocity  $\langle U_c \rangle$  and mean scalar  $\langle T_c \rangle$  decay rates along the centerline  $z$ , which are in good agreement with the experimental results<sup>18,19</sup> with  $\beta=5.8$  and  $K_1=4.48$  for the velocity and passive scalar fields, respectively. A good agreement is obtained also for the root-mean square (RMS) of the velocity and passive scalar fields [Fig. 3(b)] with respect to experimental results<sup>19,20</sup> including a linear decay behavior in the fully turbulent region. Notice that the transition to turbulence starts about  $1D$  earlier for both the velocity and the scalar fields [see Fig. 3(b)] due to the inhibition of the SGS model caused by the damping functions. The scalar RMS reaches a lower (about 10%) saturation value with the VSF model than with the FSF model, an effect which is related to the variation in SGS Schmidt number in the transition zone. In the experiments,<sup>19</sup> the transition to turbulence is strongly enhanced when the flow is issued from a smooth contraction and yields  $T_{RMS}/T_o \approx 3\%$  at about  $z$

$=2D$ . The present LES results show a clear improvement with a similar trend when the VSF model is used.

## IV. CONCLUSION

In the present study, we revisited the spectral eddy-viscosity and eddy-diffusivity closures derived from the EDQNM theory and accounted for molecular diffusion effects which were neglected in the original formulation dedicated to high Reynolds number flows.<sup>8</sup> Two related issues were addressed: (i) The effects of low Reynolds number and (ii) a variable SGS Schmidt number for transitional flows. The analytical present spectral formulation involves a damping of the inviscid eddy-viscosity and inviscid eddy-diffusivity which vanishes for increasing Reynolds number flows. The spectral model has been transposed to the physical space SGS modeling and yields a so-called *viscous structure function* (VSF) model, which consists of an improvement of the original *structure function* (SF) model<sup>8</sup> for flows involving transition to turbulence. The present VSF model is of particular interest for transitional flows with scalar transport since the resulting SGS Schmidt number is no longer constant and set to  $Sc_t=0.6$  but is reduced in low Reynolds number flow regions, as expected from analytical and numerical analysis. The new model was validated based on both *a priori tests* in DNS of homogeneous isotropic turbulence and DNS of turbulent plane jet and *a posteriori tests* in LES of round turbulent jet with scalar transport.

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