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Diagnostics for eddy viscosity models of turbulence including data-driven/neural network based parameterizations

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ABSTRACT

Classical eddy viscosity models add a viscosity term with turbulent viscosity coefficient whose specification varies from model to model. Turbulent viscosity coefficient approximations of unknown accuracy are typically constructed by solving associated systems of nonlinear evolution equations or by data driven approaches such as deep neural networks. Often eddy viscosity models over-diffuse, so additional fixes are added. This process increases model complexity and decreases model comprehensibility, leading to the following two questions: *Is an eddy viscosity model needed? Does the eddy viscosity model fail?* This report derives diagnostic quantities of interest that answer these two questions. A notable quality of the derived quantities of interest for the eddy viscosity model is that they are *a posteriori* computable and require no *a priori* knowledge of the parameterization. For neural network based parameterizations these diagnostic quantities provide an indication of when the eddy viscosity model fails due to over diffusion of the flow.

1. Introduction

In computational fluid dynamics, turbulence [1], incomplete data, quantification of uncertainty [2], a finite predictability horizon [3], flow sensitivity [4] and other issues lead to the problem of computing *averages* (denoted $u(x,t)$) of under resolved (higher Reynolds number) solutions of the Navier–Stokes equations. The most common approach [5], among many, is to solve numerically an eddy viscosity[3] model for the fluid velocity $u(x,t)$ and pressure $p(x,t)$

$$u_t + u\cdot\nabla u - \nabla\cdot\left([2\nu+\nu_{turb}(\cdot)]\nabla^s u\right) + \nabla p = f(x) \text{ and } \nabla\cdot u = 0, \tag{1.1}$$

subject to initial and boundary conditions. Here, ν is the kinematic viscosity, $f(x)$ is the body force, $\nabla^s u$ is the symmetric part of ∇u, and $\nu_{turb}(\cdot)$ is the eddy or turbulent viscosity. We let U and L denote a characteristic velocity and length scales respectively (defined precisely in Section 2). The usual Reynolds number is then $\mathcal{R}e = LU/\nu$. This holds in a 3d, bounded, regular flow domain Ω subject to no-slip boundary conditions ($u = 0$ on $\partial\Omega$) and initial condition $u(x,0) = u_0(x)$. We assume $f(x)$ is smooth, $\nabla\cdot f = 0$ in Ω, and $f(x) = 0$ on $\partial\Omega$.

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3 The model arises after averaging (e.g., ensemble averages, time averages, local space averaging) the NSE in which a non closed term arises. After adjusting the pressure, eddy viscosity models replace that term by $-\nabla\cdot(\nu_{turb}\nabla^s u)$.

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Herein, u' denotes the fluctuation about the mean velocity u. Thus, the induced turbulent kinetic energy (TKE) density is $k'(x,t) := \frac{1}{2}|u'|^2(x,t)$. The Kolmogorov–Prandtl relation for $\boldsymbol{\nu}_{turb}$ (see [6] p.369, Section 10.3, for a derivation) is

$$\boldsymbol{\nu}_{turb}(l,k') = \sqrt{2}\mu l\sqrt{k'}, \tag{1.2}$$

where $l(x,t)$ has units of length (a mixing length or turbulent length scale) and μ is a calibration parameter. Determining $\nu_{turb}(\cdot)$ then reduces to modeling the unknowns l, k' in terms of computable flow variables and then calibrating μ.

In all cases, two central questions, addressed herein via *a posteriori* computable conditions, arise: *Is an eddy viscosity necessary?* and *Does the model fail?*

Question 1. Is an eddy viscosity model necessary? Phenomenology and many numerical tests suggests that an under-resolved simulation will be under-diffused and energy will accumulate in the smallest resolved scale (non-physical $O(\triangle x)$ oscillations). The classical interpretation has been that eddy viscosity is necessary if the mesh does not resolve energetically significant eddies ($\triangle x \simeq \mathcal{R}e^{-3/4}L$, the Kolmogorov micro-scale). Answering question 1, Theorem 1, Section 3 shows, surprisingly, that *if the mesh resolves the Taylor microscale (if* $\triangle x \simeq \sqrt{15}Re^{-1/2}L$ *) then the flow in the aggregate is not under diffused*. Then added eddy viscosity to correct aggregate under diffusion is not necessary.

Question 2. Does the model fail? Eddy viscosity models most commonly[4] fail by over damping the solution, either producing a lower $\mathcal{R}e$ flow or even driving the solution to a nonphysical steady state. One can compute the aggregate model dissipation, $\int \nu_{turb}|\nabla^s u|^2 dx$, and signal failure if too large. (Like a diagnosis that a patient "looks sick", this offers little insight into the cause or its correction.) Theorem 2, Section 4 separates out the effect of the chosen turbulent viscosity parameterization from the symmetric gradient, proving

$$\text{time-average model energy dissipation} \le \left(\frac{1}{2} + \mathcal{R}e^{-1} + \frac{avg(\boldsymbol{\nu}_{turb})}{LU}\right)\frac{U^3}{L},$$

where $avg(\boldsymbol{\nu}_{turb})$ denotes the **average turbulent viscosity** defined as

$$avg(\boldsymbol{\nu}_T) = \lim\sup_{T\to\infty} \frac{1}{T}\int_0^T \frac{1}{|\Omega|}\int_\Omega |\boldsymbol{\nu}_{turb}(x,t)|dx.$$

The term $avg(\nu_{turb})/LU$ is *a computable quantity which, if* $O(1)$, *implies the eddy viscosity model does not over diffuse the flow*. Answering Question 2, the model then does not fail due to over diffusing the flow in the aggregate. From (1.2), $\boldsymbol{\nu}_{turb}$ has two contributors: the parameterization of l and k'. Further, Theorem 2, Section 4 shows $avg(\boldsymbol{\nu}_{turb})/LU = O(1)$ if $avg(l)/L = O(1)$, where $avg(l)$ denotes the **average length scale** defined as

$$avg(l) = \lim\sup_{T\to\infty} \frac{1}{T}\int_0^T \frac{1}{|\Omega|}\int_\Omega |l(x,t)|^2 dx$$

and the model's predicted turbulent intensity $I_{\text{model}} = O(1)$ as $Re \to \infty$ with I_{model} defined as

$$\left(\frac{\lim\sup_{T\to\infty}\frac{1}{T}\int_0^T\int_\Omega 2k'dx}{\lim\sup_{T\to\infty}\frac{1}{T}\int_0^T\int_\Omega |u'|^2dx}\right)^{1/2}.$$

This follows from estimate (4.1) in Theorem 3, Section 4:

$$\frac{avg(\boldsymbol{\nu}_{turb})}{LU} \le \mu\frac{avg(l)}{L}\sqrt{I_{\text{model}}},$$

indicating the evolution of *the model length scale and the model's predicted turbulent intensity are determining quantities of interest to monitor*. The importance of this result is that the three computable quantities

$$\frac{avg(\boldsymbol{\nu}_{turb})}{LU}, \frac{avg(l)}{L}, I_{\text{model}},$$

can all be monitored in a calculation. As long as they are $O(1)$, the aggregate eddy viscosity is not over dissipating the (aggregate) flow. If too large, their spatial distribution can be checked and the resulting information used to isolate the cause and improve its parameterization. **Neural network (NN) based parameterizations** have seen an explosion of interest in determining these quantities, e.g., [8,9]. While NN based approximations have been successful, they lack theoretical guarantees of stability and convergence. These quantities of interest can be used to indicate the need to retrain the neural network parameterization or incorporated as a constraint into the training procedure of the neural network.

[4] Other failure modes, not considered herein, do occur intermittently when reproducing observed flow phenomena requires brief intervals of negative eddy viscosity values, resulting in numerical instabilities, Starr [7]. Simulations can also fail by having a correct aggregate model dissipation but an incorrect distribution.

We therefore consider the eddy viscosity model (1.1). Let $\|\cdot\|$ denote the L^2 spatial norm. Taking the dot product with the solution and integrating in space and time shows that a classical solution satisfies the energy equality (e.g. [10])

$$\frac{1}{2}\|u(T)\|^2 + \int_0^T \int_\Omega [2\nu + \nu_{turb}(x,t)]|\nabla^s u(x,t)|^2 dxdt = \\ = \frac{1}{2}\|u_0\|^2 + \int_0^T (f, u(t))\, dt. \tag{1.3}$$

The model's space-averaged energy dissipation rate is thus $\varepsilon = \varepsilon_0 + \varepsilon_{turb}$ where

$$\varepsilon_0 = \frac{1}{|\Omega|}\int_\Omega 2\nu|\nabla^s u(x,t)|^2 dx \text{ and } \varepsilon_{turb} = \frac{1}{|\Omega|}\int_\Omega \nu_{turb}(x,t)|\nabla^s u(x,t)|^2 dx.$$

We assume that solutions exist for the model and satisfy a standard energy inequality. There has been slow but steady progress on an existence theory for eddy viscosity models, summarized in Chacón–Rebollo and Lewandowski [11], but many open questions remain since the number of models seems to be increasing faster than their analytic foundations develop.

Assumption. We assume that weak solutions of (1.1) exist[5] for any divergence free $u_0, f \in L^2$ and satisfy the energy inequality

$$\frac{1}{2}\frac{1}{|\Omega|}\|u(T)\|^2 + \\ + \int_0^T \frac{1}{|\Omega|}\int_\Omega 2\nu|\nabla^s u(x,t)|^2 + \nu_{turb}(x,t)|\nabla^s u(x,t)|^2 dxdt \\ \le \frac{1}{2}\frac{1}{|\Omega|}\|u_0\|^2 + \int_0^T \frac{1}{|\Omega|}(f, u(t))\, dt. \tag{1.4}$$

1.1. Related work

The energy dissipation rate is a fundamental quantity of interest of turbulence, e.g., [6,12]. In 1992, Constantin and Doering [13] established a direct link between phenomenology and NSE predicted energy dissipation. This work builds on [14,15] (and others) and has developed in many important directions subsequently e.g., [12,15–17]. For some simple turbulence models, *a priori* analysis has shown that $avg(\boldsymbol{\varepsilon}) = O(U^3/L)$, e.g., [18–29]. Often these models are significantly simpler than ones used in practice. For example, most of the models presented in Wilcox [5] evolve to high complexity. Many require different parameterizations of l and k' in different subregions (that must be identified *a priori* through previous flow data). Since the number of models seems to be growing faster than their *a priori* analytical foundation, there is a need for *a posteriori* model analysis identifying (as herein) computable quantities of interest for model assessment.

2. Notation and preliminaries

Let Ω be an open, regular domain in $\mathbb{R}^d (d = 2$ or $3)$. The $L^2(\Omega)$ norm and the inner product are $\|\cdot\|$ and $(\cdot,\cdot)$. Likewise, the $L^p(\Omega)$ norms is $\|\cdot\|_{L^p}$. C represents a generic positive constant independent of ν, $\mathcal{R}e$, other model parameters, and the flow scales U, L defined below.

Definition 1. The finite and long time averages of a function $\phi(t)$ are defined by

$$\langle\phi\rangle_T = \frac{1}{T}\int_0^T \phi(t)dt \text{ and } \langle\phi\rangle_\infty = \lim\sup_{T\to\infty} \langle\phi\rangle_T.$$

These satisfy

$$\langle\phi\psi\rangle_T \le \left\langle|\phi|^2\right\rangle_T^{1/2}\left\langle|\psi|^2\right\rangle_T^{1/2}, \langle\phi\psi\rangle_\infty \le \left\langle|\phi|^2\right\rangle_\infty^{1/2}\left\langle|\psi|^2\right\rangle_\infty^{1/2} \\ \text{and } \left\langle\langle\phi\rangle_\infty\right\rangle_\infty = \langle\phi\rangle_\infty. \tag{2.1}$$

5 Even in the absence of a complete existence theory, the analysis of energy dissipation rates can be performed for variational discretizations in space (such as finite element methods or spectral methods). The same sequence of steps shows that the discrete solutions satisfy the same energy dissipation rate bounds uniformly in any space discretization parameter (such as mesh width or frequency cutoff). Since the primary utility of turbulence models is to account for breaking the communication between the inertial range and dissipation range in numerical simulations after space discretizations, this analysis is highly relevant for the uses of the models. It however adds significant notational complexity without requiring any new mathematical ideas or even steps, we shall assume the above about the continuum model for purposes of greater clarity.

Definition 2. The viscous and turbulent viscosity energy dissipation rate (per unit volume) are

$$\varepsilon_0(u) = \frac{1}{|\Omega|}\int_\Omega 2\nu|\nabla^s u(x,t)|^2 dx \text{ and } \varepsilon_{turb}(u) = \frac{1}{|\Omega|}\int_\Omega \nu_{turb}(x,t)|\nabla^s u(x,t)|^2 dx.$$

The force, large scale velocity, and length scales, F, U, L, are

$$F = \frac{1}{|\Omega|^{\frac{1}{2}}}\|f\|,\ U = \left\langle \frac{1}{|\Omega|}\|u\|^2 \right\rangle_\infty^{\frac{1}{2}},\ \ U' = \left\langle \frac{1}{|\Omega|}\|u'\|^2 \right\rangle_\infty^{\frac{1}{2}} \tag{2.2}$$

$$L = \min\left\{ |\Omega|^{\frac{1}{3}}, \frac{F}{\|\nabla f(\cdot)\|_\infty}, \frac{F}{\frac{1}{|\Omega|^{\frac{1}{2}}}\|\nabla f\|} \right\}.$$

L has units of length and satisfies

$$\|\nabla f\|_\infty \le \frac{F}{L} \text{ and } \frac{1}{|\Omega|}\|\nabla f\|^2 \le \frac{F^2}{L^2}. \tag{2.3}$$

Dimensional consistency (the Kolmogorov–Prandtl relation) requires $\boldsymbol{\nu}_{turb}(l,k') = \sqrt{2}\mu l\sqrt{k'}$. Thus, picking $\boldsymbol{\nu}_{turb}$ means a choice for $l(x,t)$ and a model k'_{model} for k' are induced. Since $k' = \frac{1}{2}|u'|^2$ this determines a model for $|u'| \simeq |u'|_{\text{model}} = \sqrt{2k'}_{\text{model}}$.

Definition 3. Define the velocity scales U, U', U'_{model} by

$$U = \left\langle \frac{1}{|\Omega|}\|u\|^2 \right\rangle_\infty^{1/2}, U'_{\text{model}} = \left\langle \frac{1}{|\Omega|}\int_\Omega 2k' dx \right\rangle_\infty^{1/2} \text{ and } U' = \left\langle \frac{1}{|\Omega|}\int_\Omega |u'|^2 dx \right\rangle_\infty^{1/2}.$$

It has not been necessary herein to specify the initial average leading to the eddy viscosity term and used to define U'. Our intuition is that for a properly defined (and commonly used) averaging operations $U' \le U$ and thus $0 \le I(u) \le 1$.

Definition 4. The models' predicted **turbulent intensity** is

$$I_{\text{model}}(u) = \left(\frac{U'_{\text{model}}}{U}\right)^2.$$

The average **model length-scale** and **average turbulent viscosity** are

$$avg(l) = \left\langle \frac{1}{|\Omega|}\|l(x,t)\|^2 \right\rangle_\infty^{1/2},$$

$$avg(\boldsymbol{\nu}_T) = \left\langle \frac{1}{|\Omega|}\int_\Omega |\boldsymbol{\nu}_{turb}(x,t)| dx \right\rangle_\infty.$$

3. Is an eddy viscosity model necessary?

This is a question that can only be sensibly asked after discretization in space in a standard way on a spatial mesh or grid with mesh size denoted h and with $\boldsymbol{\nu}_T = 0$. (Thus in this section U represents the NSE velocity scale.) For the chosen numerical (spatial) discretization, we assume that (i) *no model or numerical dissipation is present* (A1 below), (ii) *the largest discrete gradient representable is proportional to* $1/meshwidth$ (A2 below, see [30,31], and [32] for proofs in specific settings) and, as kinetic energy is concentrated in the largest scales, (iii) *the discrete kinetic energy is comparable to the true kinetic energy* (A3 below).

A1. [No model or numerical dissipation] *The total energy dissipation rate of* u^h *is* $\varepsilon_0(u^h)$.

A2. [Inverse Assumption] *There is a parameter* $h = \triangle x$*, representing a typical meshwidth, and an* $O(1)$ *constant* C_I *such that for all discrete velocities* u^h

$$\|\nabla^s u^h\| \le C_I h^{-1}\|u^h\|.$$

A3. [Assumption on energy of approximate velocity]. *There are constants* c_E, C_E *such that the kinetic energy of the true and approximate velocities satisfy*

$$0 < c_E \le \frac{U_h}{U} = \sqrt{\frac{\langle \|u^h\|^2\rangle_\infty}{\langle \|u\|^2\rangle_\infty}} \le C_E < \infty,$$

where U_h *is defined analogously to* U *in Definition 3.*

Definition 5. The Taylor microscale λ_T (e.g., [6,33–35]) of the fluid velocity $u(x,t)$ is

$$\lambda_T(u) := \left(\frac{\frac{1}{15}\left\langle \|\nabla u\|^2 \right\rangle_\infty}{\left\langle \|u\|^2 \right\rangle_\infty} \right)^{-1/2}. \tag{3.1}$$

For fully developed, 3d turbulent flows (away from walls), it is known, e.g., [6,33,34], that λ_T is significantly larger than the Kolmogorov microscale and scales with the Reynolds number as

$$\lambda_T \simeq \mathcal{R}e^{-1/2}L. \tag{3.2}$$

The Taylor microscale $\lambda_T(u)$ represents an average length of the velocity u. For example, one can have $\mathcal{R}e \gg 1$, but $\lambda_T = O(1)$ for artificially constructed/manufactured laminar velocities, such as the Taylor–Green vortex [36,37].

We then have the following.

Theorem 1. *Let A1, A2 and A3 hold. If the meshwidth* $h \gg 2(C_I C_E)\sqrt{15}\mathcal{R}e^{-1/2}L$, *then*

$$\left\langle \varepsilon(u^h) \right\rangle_\infty \ll \frac{U^3}{L} \text{ and } \left\langle \varepsilon(u^h) \right\rangle_\infty \to 0 \text{ as } \mathcal{R}e \to \infty.$$

Contrarily, $\left\langle \varepsilon(u^h) \right\rangle_\infty \simeq \frac{U^3}{L}$ *if the Taylor microscale of the computed solution* u^h *satisfies*

$$\lambda_T(u^h) \le \frac{\sqrt{30}}{2}\mathcal{R}e^{-1/2}L.$$

Proof. *By A1, A2*

$$\begin{aligned}
\left\langle \varepsilon(u^h) \right\rangle_\infty &= 2\nu \left\langle \|\nabla^s u^h\|^2 \right\rangle_\infty \le 2\nu C_I^2 h^{-2} \left\langle \|u^h\|^2 \right\rangle_\infty \\
&\le 2\nu C_I^2 h^{-2} U_h^2 = \frac{\nu}{LU} C_I^2 \left(\frac{h}{L}\right)^{-2} \left(\frac{U_h}{U}\right)^2 \frac{U^3}{L} \\
&\le 2\left[\mathcal{R}e^{-1} C_I^2 C_E^2 \left(\frac{h}{L}\right)^{-2} \right] \frac{U^3}{L}, \text{ by A3.}
\end{aligned}$$

Thus, the first case of under-dissipation occurs when the bracketed term

$$\mathcal{R}e^{-1} C_I^2 C_E^2 \left(\frac{h}{L}\right)^{-2} \ll \frac{1}{2} \Leftrightarrow h \gg \sqrt{2}\,(C_I C_E)\,\mathcal{R}e^{-1/2}L = \mathcal{O}\left(\lambda_T(u)\right).$$

For the second claim, by A1, A3,

$$\begin{aligned}
\left\langle \varepsilon(u^h) \right\rangle_\infty &= 2\nu \left\langle \|\nabla^s u^h\|^2 \right\rangle_\infty = 2\nu \frac{\left\langle \|\nabla^s u^h\|^2 \right\rangle_\infty}{\left\langle \|u^h\|^2 \right\rangle_\infty} \left\langle \|u^h\|^2 \right\rangle_\infty \\
&= 30\frac{\nu}{LU}\lambda_T(u^h)^{-2} LUU_h^2 \\
&= 30\mathcal{R}e^{-1}\left(\frac{\lambda_T(u^h)}{L}\right)^{-2}\left(\frac{U_h}{U}\right)^2 \frac{U^3}{L} \le 30C_E^2 \left[\mathcal{R}e^{-1}\left(\frac{\lambda_T(u^h)}{L}\right)^{-2} \right] \frac{U^3}{L}.
\end{aligned}$$

The bracketed term is $\mathcal{O}(1)$ *provided* $\lambda_T(u^h) \simeq \sqrt{30}Re^{-1/2}L$, *as claimed.* ■

4. Does the eddy viscosity model fail?

The most common failure mode of eddy viscosity models is model over dissipation. Model dissipation can be studied at the level of the continuum model (1.1), that is, without a spatial discretization. Since this simplifies notation, we do so in this section. Consider therefore the model (1.1) and recall that the data $u_0(x), f(x)$ is smooth, divergence free, and both vanish on $\partial\Omega$. The next theorem establishes that model dissipation is independent of solution gradients and controlled by the average of the chosen eddy viscosity parameterization $avg(\boldsymbol{\nu}_{turb})$

$$avg(\boldsymbol{\nu}_{turb}) = \left\langle \frac{1}{|\Omega|}\int_\Omega |\boldsymbol{\nu}_{turb}(x,t)|dx \right\rangle_\infty.$$

Theorem 2. *The time averaged rate of total energy dissipation for the eddy viscosity model satisfies the following. For any* $0 < \beta < 1$,

$$\langle \varepsilon_0 + \varepsilon_{turb} \rangle \le \left(\frac{2}{2-\beta} + \frac{2}{\beta(2-\beta)}\mathcal{R}e^{-1} + \frac{1}{\beta(2-\beta)}\frac{avg(\boldsymbol{\nu}_{turb})}{LU} \right)\frac{U^3}{L}.$$

The key term is $\frac{avg(\boldsymbol{\nu}_{turb})}{LU}$. For this term we can further separate the effects of the choice of l and k' in the model as follows.

Theorem 3. *We have*

$$\frac{avg(\boldsymbol{\nu}_{turb})}{LU} \le \mu \frac{avg(l)}{L}\sqrt{I_{model}(u)} = \mu \frac{avg(l)}{L}\frac{U'_{model}}{U'}\sqrt{I(u)}. \tag{4.1}$$

As a consequence there follows.

Corollary 1. *The time averaged energy rate of total energy dissipation for the general eddy viscosity model satisfies the following. For any* $0 < \beta < 1$,

$$\langle \varepsilon_0 + \varepsilon_{turb}\rangle_\infty \le \left(\frac{2}{2-\beta} + \frac{2}{\beta(2-\beta)}\mathcal{R}e^{-1} + \frac{1}{\beta(2-\beta)}\mu\frac{avg(l_m)}{L}\frac{U'_m}{U}\right)\frac{U^3}{L}$$

and

$$\langle \varepsilon_0 + \varepsilon_{turb}\rangle_\infty \le \left(\frac{2}{2-\beta} + \frac{2}{\beta(2-\beta)}\mathcal{R}e^{-1} + \frac{1}{\beta(2-\beta)}\mu\frac{avg(l)}{L}\frac{U'_m}{U'}\sqrt{I(u)}\right)\frac{U^3}{L}.$$

Proof. The claim follows by rearranging the last term in the estimate using the definition of the turbulent intensity $I(u) = (U'/U)^2$. ∎

As noted above, the importance of this result is that the three quantities

$$\frac{avg(\boldsymbol{\nu}_{turb})}{LU}, \frac{avg(l)}{L}, \frac{U'_m}{U},$$

are computable. If too large, their spatial distribution can be checked and the resulting information used to improve the model.

4.1. Proof of Theorem 1

From (1.3)

$$\frac{1}{2T}\frac{1}{|\Omega|}\|u(T)\|^2 + \langle \varepsilon_0 + \varepsilon_{turb}\rangle_T \le \frac{1}{2T}\frac{1}{|\Omega|}\|u_0\|^2 + \left\langle \frac{1}{|\Omega|}(f, u(t))\right\rangle_T, \tag{4.2}$$

and standard arguments, it follows that, uniformly in T,

$$\sup_{T\in(0,\infty)} \|u(T)\|^2 \le C(data) < \infty \text{ and } \langle \varepsilon_0 + \varepsilon_{turb}\rangle_T \le C(data) < \infty. \tag{4.3}$$

For the RHS of the energy inequality, from (2.1) there follows

$$\left\langle \frac{1}{|\Omega|}(f, u(t))\right\rangle_T \le F\sqrt{\left\langle \frac{1}{|\Omega|}\|u(t)\|^2\right\rangle_T},$$

which, from (4.2), implies

$$\langle \varepsilon_0 + \varepsilon_{turb}\rangle_T \le \mathcal{O}(\frac{1}{T}) + F\left\langle \frac{1}{|\Omega|}\|u\|^2\right\rangle_T^{\frac{1}{2}}. \tag{4.4}$$

To bound F in terms of flow quantities, take the inner product of the model (1.1) with $f(x)$, integrate by parts (using $\nabla\cdot f = 0$ and $f(x) = 0$ on $\partial\Omega$), and average over $[0, T]$. This gives

$$F^2 = \frac{(u(T) - u_0, f)}{T|\Omega|} - \left\langle \frac{1}{|\Omega|}(uu, \nabla f)\right\rangle_T + \left\langle \frac{1}{|\Omega|}\int_\Omega 2\nu\nabla^s u : \nabla^s f + \boldsymbol{\nu}_{turb}(x,t)\nabla^s u : \nabla^s f dx\right\rangle_T. \tag{4.5}$$

Analysis of the first three terms on the RHS parallels the NSE case in, e.g., [12,13,15–17]. The fourth is the key, model-specific term. The first term on the RHS is $\mathcal{O}(1/T)$ by (4.3). The second is bounded by Holders inequality, (2.1), and (2.3) as follows

$$\left\langle \frac{1}{|\Omega|}(uu, \nabla f)\right\rangle_T \le \left\langle \|\nabla f(\cdot)\|_\infty \frac{1}{|\Omega|}\|u(\cdot,t)\|^2\right\rangle_T \le \|\nabla f(\cdot)\|_\infty \left\langle \frac{1}{|\Omega|}\|u(\cdot,t)\|^2\right\rangle_T \le \frac{F}{L}\left\langle \frac{1}{|\Omega|}\|u(\cdot,t)\|^2\right\rangle_T.$$

The third term is bounded by analogous steps to the second. For any $0 < \beta < 1$, we have

$$\left\langle \frac{1}{|\Omega|} \int_\Omega 2\nu \nabla^s u(x,t) : \nabla^s f(x) dx \right\rangle_T$$
$$\leq \left\langle \frac{4\nu^2}{|\Omega|} \|\nabla^s u\|^2 \right\rangle_T^{\frac{1}{2}} \left\langle \frac{1}{|\Omega|} \|\nabla^s f\|^2 \right\rangle_T^{\frac{1}{2}} \leq \langle \varepsilon_0 \rangle_T^{\frac{1}{2}} \sqrt{2\nu} \frac{F}{L} \leq \frac{\beta F}{2U} \langle \varepsilon_0 \rangle_T + \frac{UF}{\beta} \frac{\nu}{L^2}.$$

The fourth, *model dependent* term, is estimated successively as follows

$$\left\langle \frac{1}{|\Omega|} \int_\Omega \boldsymbol{\nu}_{turb} \nabla^s u(x,t) : \nabla^s f(x) dx \right\rangle_T \leq \left\langle \frac{1}{|\Omega|} \int_\Omega \sqrt{\boldsymbol{\nu}_{turb}} \left(\sqrt{\boldsymbol{\nu}_{turb}} |\nabla^s u| \right) |\nabla^s f| dx \right\rangle_T$$
$$\leq \|\nabla^s f\|_{L\infty} \left\langle \left(\frac{1}{|\Omega|} \int_\Omega \boldsymbol{\nu}_{turb} dx \right)^{1/2} \left(\frac{1}{|\Omega|} \int_\Omega \boldsymbol{\nu}_{turb} |\nabla^s u|^2 dx \right)^{1/2} dx \right\rangle_T$$
$$\leq \|\nabla^s f\|_{L\infty} \left\langle \left(\frac{1}{|\Omega|} \int_\Omega \boldsymbol{\nu}_{turb} dx \right)^{1/2} \varepsilon_{turb}^{1/2} \right\rangle_T$$
$$\leq \frac{F}{L} \left(\frac{U}{F} \left\langle \frac{1}{|\Omega|} \int_\Omega \boldsymbol{\nu}_{turb} dx \right\rangle_T \right)^{1/2} \left(\frac{F}{U} \langle \varepsilon_{turb} \rangle_T \right)^{1/2}$$
$$\leq \frac{\beta}{2} \frac{F}{U} \langle \varepsilon_{turb} \rangle_T + \frac{1}{2\beta} \frac{UF}{L^2} \left\langle \frac{1}{|\Omega|} \int_\Omega \boldsymbol{\nu}_{turb} dx \right\rangle_T.$$

Using these estimates in the bound for F^2 yields

$$F^2 \leq \mathcal{O}\left(\frac{1}{T}\right) + \frac{F}{L} \left\langle \frac{1}{|\Omega|} \|u\|^2 \right\rangle_T + \frac{\beta}{2} U^{-1} F \langle \varepsilon_0 \rangle_T + \frac{1}{\beta} UF \frac{\nu}{L^2}$$
$$+ \frac{\beta}{2} \frac{F}{U} \langle \varepsilon_{turb} \rangle_T + \frac{1}{2\beta} \frac{UF}{L^2} \left\langle \frac{1}{|\Omega|} \int_\Omega \boldsymbol{\nu}_{turb} dx \right\rangle_T.$$

Thus, we have an estimate for $F \left\langle \frac{1}{|\Omega|} \|u\|^2 \right\rangle_T^{\frac{1}{2}}$

$$F \left\langle \frac{1}{|\Omega|} \|u\|^2 \right\rangle_T^{\frac{1}{2}} \leq \mathcal{O}\left(\frac{1}{T}\right) + \frac{1}{L} \left\langle \frac{1}{|\Omega|} \|u\|^2 \right\rangle_T^{\frac{3}{2}} + \frac{\beta}{2} \frac{\left\langle \frac{1}{|\Omega|} \|u\|^2 \right\rangle_T^{\frac{1}{2}}}{U} \langle \varepsilon_0 \rangle_T$$
$$+ \frac{1}{\beta} \left\langle \frac{1}{|\Omega|} \|u\|^2 \right\rangle_T^{\frac{1}{2}} U \frac{\nu}{L^2} + \frac{\beta}{2} \frac{\left\langle \frac{1}{|\Omega|} \|u\|^2 \right\rangle_T^{\frac{1}{2}}}{U} \langle \varepsilon_{turb} \rangle_T$$
$$+ \frac{1}{2\beta} \left\langle \frac{1}{|\Omega|} \|u\|^2 \right\rangle_T^{\frac{1}{2}} \frac{U}{L^2} \left\langle \frac{1}{|\Omega|} \int_\Omega \boldsymbol{\nu}_{turb} dx \right\rangle_T.$$

These four estimates then imply that

$$\left[1 - \frac{\beta}{2} \frac{\left\langle \frac{1}{|\Omega|} \|u\|^2 \right\rangle_T^{\frac{1}{2}}}{U} \right] \langle \varepsilon_0 + \varepsilon_{turb} \rangle_T$$
$$\leq \mathcal{O}\left(\frac{1}{T}\right) + \frac{1}{L} \left\langle \frac{1}{|\Omega|} \|u\|^2 \right\rangle_T^{\frac{3}{2}} + \frac{1}{\beta} \left\langle \frac{1}{|\Omega|} \|u\|^2 \right\rangle_T^{\frac{1}{2}} U \frac{\nu}{L^2} +$$
$$+ \frac{1}{2\beta} \left\langle \frac{1}{|\Omega|} \|u\|^2 \right\rangle_T^{\frac{1}{2}} \frac{U}{L^2} \left\langle \frac{1}{|\Omega|} \int_\Omega \boldsymbol{\nu}_{turb} dx \right\rangle_T.$$

The limit superior as $T \to \infty$, which exists by (4.3), yields the following

$$\left[1 - \frac{\beta}{2} \right] \langle \varepsilon_0 + \varepsilon_{turb} \rangle_\infty \leq \frac{U^3}{L} + \frac{1}{\beta} U^2 \frac{\nu}{L^2} + \frac{avg(\boldsymbol{\nu}_{turb})}{2\beta} \frac{U^2}{L^2}$$
$$\leq \frac{U^3}{L} \left(1 + \frac{1}{\beta} \frac{\nu}{LU} + \frac{1}{2\beta} \frac{avg(\boldsymbol{\nu}_{turb})}{LU} \right).$$

Thus, after rearranging,

$$\langle \varepsilon_0 + \varepsilon_{turb} \rangle_\infty \leq \frac{U^3}{L}\left(\frac{2}{2-\beta} + \frac{2}{\beta(2-\beta)}\mathcal{R}e^{-1} + \frac{1}{\beta(2-\beta)}\frac{avg(\boldsymbol{\nu}_{turb})}{LU}\right).$$

4.2. Proof of Theorem 2: estimating $\frac{avg(\boldsymbol{\nu}_{turb})}{LU}$

We now prove the estimate in Theorem 2 for $avg(\boldsymbol{\nu}_{turb})$. Since $\boldsymbol{\nu}_{turb} = \sqrt{2}\mu l \sqrt{\frac{1}{2}|u'|^2_{\text{model}}}$ we have

$$\begin{aligned}\frac{1}{LU}\left\langle \frac{1}{|\Omega|}\int_\Omega \boldsymbol{\nu}_{turb}(x,t)dx \right\rangle_T &= \frac{1}{LU}\left\langle \frac{1}{|\Omega|}\int_\Omega \sqrt{2}\mu l \sqrt{\frac{1}{2}|u'|^2_{\text{model}}}dx \right\rangle_T \\ &= \frac{\mu}{LU}\left\langle \frac{1}{|\Omega|}\int_\Omega l|u'|_{\text{model}}dx \right\rangle_T .\end{aligned}$$

By the Cauchy–Schwarz inequality in space and (2.1) we have

$$\frac{1}{LU}\left\langle \frac{1}{|\Omega|}\int_\Omega \boldsymbol{\nu}_{turb}dx \right\rangle_T \leq \frac{\mu}{LU}\left\langle \frac{1}{|\Omega|}\|l\|^2 \right\rangle_T^{1/2} \left\langle \frac{1}{|\Omega|}\||u'|_{\text{model}}\|^2 \right\rangle_T^{1/2}. \tag{4.6}$$

Taking the limit superior of (4.6) gives, as claimed,

$$\begin{aligned}\frac{avg(\boldsymbol{\nu}_{turb})}{LU} &\leq \frac{\mu}{LU} avg(l) U'_{\text{model}} = \mu \frac{avg(l)}{L}\frac{U'_{\text{model}}}{U} \\ &= \mu \frac{avg(l)}{L}\sqrt{I_{\text{model}}(u)} = \mu \frac{avg(l)}{L}\frac{U'_{\text{model}}}{U'}\sqrt{I(u)}.\end{aligned}$$

5. Conclusions and open problems

One basic challenge is that the analysis of models has advanced more slowly than new models have been developed to respond to the needs of predictive flow simulations. This means that models can evolve by more complex parameterizations rather than more careful representation of the effects of fluctuations on mean velocities. The gap between model complexity and model understanding is widening even further due to the current model development using machine learning and neural networks based eddy viscosity models [8,9,38]. Since turbulence models are used in many safety critical settings, there is an obvious need to assess models during a simulation. To this end, this report presents a new approach to assess model dissipation. The first result (Theorem 1) is that, surprisingly, the need for eddy viscosity depends on the mesh resolving the Taylor microscale rather than the Kolmogorov micro-scale. The second result (Theorem 2) is when an eddy viscosity model is used, its total dissipation can be estimated in terms of several computable flow quantities of interest. When the model over dissipates, these can be used to isolate the part of the model needing improvement; the estimates separate the effects of the different model choices so that, when over-dissipation occurs, the source in the various modeling decisions can be isolated. This is of particular interest for neural network based eddy viscosity parameterizations. Due to the data driven nature of these approximations nothing can be said *a priori* about the quality of the neural network based models. The computable quantities of interest derived in this work serve as a diagnostic tool for when these models fail due to over dissipation of the flow. In particular they inform which specific part of the eddy viscosity parameterization is causing over dissipation of the flow.

Open problems abound. Our analysis assumes that $f(x) = 0$ on the boundary. This means the effect of boundary layers is less than small scales generated by the system nonlinearity. To seek the right computable quantity of interest for turbulent boundary layers, an analysis of energy dissipation for shear flows is needed. There is a small number of eddy viscosity models where quantities like the turbulent quantities of interest identified herein can be performed. Expanding this list to models closer to those used in practice is an important collection of open problems. Numerical dissipation often is much greater than model dissipation. Thus, analysis including numerical dissipation is of great importance. Estimation of the effect of eddy viscosity terms on helicity dissipation rates is little studied but possibly critical for correct predictions of rotational flows. Neural network based eddy viscosity models are at a beginning point in their development. Thus, practically any question (analytical, theoretical of experimental) known for classic models is open for these.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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