1. INTRODUCTION

The dissipation of turbulent kinetic energy is of fundamental importance to the simulation of turbulent dynamics using Large Eddy Simulation (LES) (Meneveau and Katz 2000). Dissipation can be used in a diagnostic sense for model calibration (Lilly 1967), and to find model coefficients in a LES simulation through dissipation matching as in Porté-Agel et al. (2001). Thus, it is important to understanding the resulting dissipation from a particular subgrid-scale (SGS) model formulation.

Recent a priori studies exploiting the relative eigenvector alignment between the SGS stress, $\tau_{ij} = u_i u_j - \bar{u}_i \bar{u}_j$, and the filtered strain rate, $\bar{S}_{ij} = 0.5(\partial \bar{u}_i / \partial x_j + \partial \bar{u}_j / \partial x_i)$ (Tao et al. 2002, Higgins et al. 2002) have developed a geometric framework in which data can be interpreted. Within this framework, SGS models are decomposed into components akin to magnitude and direction and test only the fundamental assumptions within SGS model formulations (alignment between eigenvectors of the modeled and real SGS stress). In this paper we impose a similar geometric framework onto the dissipation equation and express the resulting formula in terms of alignments of eigenvectors and non-dimensional strain states. We then give an example of how the new formulation can be used to predict SGS dissipations when gross qualitative information about the alignment (given in Tao et al and Higgins et al) is known. This prediction is then compared to data from the atmospheric surface layer obtained from arrays of sonic anemometers.

2. EXPERIMENTAL DATA

Two previous studies analyzed the full three dimensional alignment between the filtered strain rate tensor and the SGS stress tensor. Tao et al. (2002) studied the turbulent flow a 5.7x5.7x4.5 cm$^3$ volume in the core of a turbulent square duct flow with holographic particle image velocimetry. They used a spatial filter size of $\Delta=3.3$ mm (the Kolmogorov scale was about 0.1 mm). The Taylor-scale Reynolds number was $R_{\lambda} \approx 260$. Higgins et al. 2002 studied the flow in the unstable atmospheric boundary layer (Obukhov length $L = -\frac{\langle u' \rangle}{\kappa g \langle T' \rangle}$ was in a range of $-30$ m to $-5$ m) with two arrays of sonic anemometers (Davis, California). A detailed account of the data set is provided in Porté-Agel et al 2001a. Yet, both studies produced strikingly similar qualitative results. Here we provide a brief summary of both experiments.

In this paper we present data from the same experimental setup as used in Higgins et al. 2002; however, the data used in this report were taken under neutral atmospheric stability. Data were classified as having neutral stability when the Obukhov length had an absolute value greater than $60$ m. The near neutral data represents about 30 minutes of data and ~40,000 time realizations taken in the summer in Davis, California 1999 over bare soil.

3. GEOMETRIC INTERPRETATION OF DISSIPATION

Dissipation can be written as $\Pi = -\tau_{ij} \bar{S}_{ij}$ which is equivalent to $\Pi = tr(-\bar{S} \bar{S}')$ for symmetric tensors. We can decompose each of the above matrices $(\bar{S}_{ij} = 0.5(\partial \bar{u}_i / \partial x_j + \partial \bar{u}_j / \partial x_i)$ and $\tau_{ij} = u_i u_j - \bar{u}_i \bar{u}_j$) into their respective eigenvectors and eigenvalues by the transform $\bar{S} = Q_\bar{S} \Lambda_{\bar{S}} Q_\bar{S}^T$ where $Q_\bar{S}$ is a matrix containing the eigenvectors of $\bar{S}$ and $\Lambda_{\bar{S}}$ is a diagonal matrix containing the corresponding eigenvalues. We are then left with:

$$\Pi = tr(Q_\bar{S} \Lambda_{\bar{S}} Q_\bar{S}^T \Lambda_{\bar{S}} Q_\bar{S}^T)$$

The eigenvalues are named according to their magnitudes as $\alpha \geq \beta \geq \gamma$. The eigenvalues also satisfy
the condition $\alpha + \beta + \gamma = 0$ (by mass conservation), this requires $\alpha \geq 0$, $\gamma \leq 0$, and $\beta$ be either positive or negative. Eigenvectors are named by their corresponding eigenvalues: $\hat{a}$ is the extensive eigenvector, $\hat{c}$ is the compressive eigenvector, and $\hat{b}$ is the intermediate eigenvector. After carrying out the multiplication in (1) we are left with:

$$
\Pi = \alpha \hat{a} \cdot \alpha \cdot (\alpha, \hat{a}) + \alpha \hat{b} \cdot \alpha \cdot (\alpha, \hat{b}) + \alpha \hat{c} \cdot \alpha \cdot (\alpha, \hat{c})
$$

$$
+ \beta \hat{b} \cdot \beta \cdot (\beta, \hat{b}) + \beta \hat{c} \cdot \beta \cdot (\beta, \hat{c}) + \beta \hat{c} \cdot \beta \cdot (\beta, \hat{b})
$$

$$
+ \gamma \hat{c} \cdot \alpha \cdot (\alpha, \hat{c}) + \gamma \hat{c} \cdot \beta \cdot (\beta, \hat{c}) + \gamma \hat{c} \cdot \gamma \cdot (\gamma, \hat{c})
$$

(2)

All nine inner products in equation 2 can be expressed in terms of angles: $(a, b) = \cos(\theta')$ when $\theta'$ is the angle between the vectors (here a and b are unit vectors). Equation 2 now contains nine distinct angles and six eigenvalues, but the alignment between the eigenvectors of two symmetric tensors is fixed with only three angles in Tao et al. 2002 and Higgins et al. 2002. There should exist an expression for all nine dot products in equation 3 as a function of three angles. First we non-dimensionalize the eigenvalues so that they can be expressed in terms of two non-dimensional state parameters:

$$
\Pi = \frac{1}{S} (\alpha', \beta', \gamma') + (\alpha', \beta', \gamma') + (\alpha', \beta', \gamma')
$$

$$
+ (\alpha', \beta', \gamma') + (\alpha', \beta', \gamma') + (\alpha', \beta', \gamma')
$$

$$
+ (\alpha', \beta', \gamma') + (\alpha', \beta', \gamma') + (\alpha', \beta', \gamma')
$$

(3)

where $S = \sqrt{\alpha^2 + \beta^2 + \gamma^2}$ and $|f| = \sqrt{\alpha^2 + \beta^2 + \gamma^2}$. The resulting nondimensional dissipation is now bounded between -1 and 1. From the Lund and Rogers 1994 paper there are relationships that express the nondimensional eigenvalues $(\alpha', \beta', \gamma')$ as functions of the strain state parameter $s'$ and the stress state parameter $s''$. Similar expressions exist for the nondimensional eigenvalues of the SGS stress to the stress state parameter $s'$. These parameters are bounded between -1 and 1 when the filtered strain rate tensor is trace free (incompressible flow), and the deviatoric part of the SGS stress tensor $\tau_0'' = 1/3 \delta_0 \tau_0$ is subtracted from each of the diagonal elements of the SGS stress tensor. This form of $s'$ is useful since it indicates the type of deformation occurring. For example, $s' = 1$ corresponds to axisymmetric extension (i.e. $\alpha = \beta > 0$, $\gamma < 0$), $s' = 0$ ($\beta = 0$) to plane shear, and $s' = -1$ to axisymmetric contraction (i.e. $\alpha > 0$, $\beta = \gamma < 0$). Probability density functions of $s'$ and $s''$ for the data sets of Tao et al. 2002 and Higgins et al. 2002 show qualitatively similar results (i.e. the most likely value of $s'$ was 1 in both data sets corresponding to axisymmetric extending motions and that the most likely value of $s''$ was also 1 corresponding to axisymmetric compressing motions in the positive SGS stress).

Next, we must express the nine individual dot products in equation 3 as a function of three angles. Here, we will choose angles similar to those used by Tao et al. 2002, and Higgins et al. 2002 in a priori studies. Briefly, the earlier analysis fixed the relative orientation between two tensors with a triplet of angles ($\theta$, $\phi$, and $\zeta$). The angle triplets were calculated for each point in the entire data set, and then a joint probability density function of the three angles was computed. By interpreting the peaks in the joint PDF Tao et al., and Higgins et al. were able to deduce the most likely orientation of the SGS stress and filtered strain rate eigendirections. The most likely angle configurations deduced from these studies are presented in figure 1.

An inherent bimodal structure in the tensor alignment was observed. Notice though, that in both cases, the angle between the two compressive directions (the angle between $\hat{c}_3$ and $\hat{c}_-3$) is approximately the same ($\sim 30^\circ$ for Tao et al. $\sim 30^2$ for Higgins et al. 2002), and in configurations the compressive direction $\hat{c}_3$ is perpendicular to the intermediate direction of the filtered strain rate, $\hat{b}_3$. 
The angles of interest in previous studies and the angles used here can be defined as: \( \theta = \cos^{-1}(\langle \alpha_s, \alpha_g \rangle) \),
\( \phi = (\vec{y}_5 \times \vec{\beta}_g) \cdot (\hat{\alpha}_{s', \alpha}_{g}) \cos^{-1}(\langle \alpha_{s'}, \vec{\beta}_g \rangle) \),
\( \zeta = -(\vec{y}_5 \times \vec{\beta}_g) \cdot (\hat{\gamma}_{s', \gamma}_{g}) \cos^{-1}(\langle \gamma_{s'}, \vec{\gamma}_g \rangle) \). Where \( \alpha_{s'} \) is the projection of \( \alpha_s \) onto the \( \gamma_{s'} - \beta_{g'} \) plane and \( \gamma_{s'} \) is the projection of \( \gamma_s \) on the \( \gamma_{s'} - \beta_{g'} \) plane.

We circumscribe the set of eigendirections given by the filtered strain rate, and the SGS stress with the unit sphere. The intersection of this sphere and a plane defined by any two eigendirections forms a great circle that connects the two respective points on the sphere. The radius of this great circle must be 1; therefore, the arc-length on a great circle between two points on the unit sphere is identical to the angle between the corresponding vectors. Once this transformation is made, we can use the standard tools of spherical trigonometry to find distances on the sphere.

The law of cosines for spherical triangles can be used to simplify equation 3 so it contains only four inner products:

\[
\frac{6\Pi}{\|S\|} = (\hat{\alpha}_{s', \alpha}_{s}) \cdot (\gamma_{s'} - \beta_{g'}) (\gamma_{s'} - \beta_{g'}) + (\vec{y}_5, \vec{\gamma}_{s'}) \cdot (\gamma_{s'} - \beta_{g'}) (\gamma_{s'} - \beta_{g'}) + (\vec{y}_5, \vec{\beta}_{s'}) \cdot (\gamma_{s'} - \beta_{g'}) (\gamma_{s'} - \beta_{g'}) + (\vec{y}_5, \vec{\beta}_{s'}) \cdot (\gamma_{s'} - \beta_{g'}) (\gamma_{s'} - \beta_{g'}) - 3\beta_{s'}^2 \beta_{g'}^2.
\]

And from our particular angle definitions we have:

\[
(\hat{\alpha}_{s', \alpha}_{s}) \cdot (\gamma_{s'} - \beta_{g'}) = \cos^2 \theta
\]
\[
(\vec{y}_5, \vec{\gamma}_{s'}) \cdot (\gamma_{s'} - \beta_{g'}) = \sin^2 \theta \sin \phi
\]
\[
(\vec{y}_5, \vec{\beta}_{s'}) \cdot (\gamma_{s'} - \beta_{g'}) = \cos^2 \zeta (\cos^2 \theta \sin^2 \phi + \cos \phi \sin \phi \zeta)^2 \sin^2 \theta
\]
\[
(\vec{y}_5, \vec{\beta}_{s'}) \cdot (\gamma_{s'} - \beta_{g'}) = \cos \theta \sin \phi \cos \zeta + \cos \phi \sin \phi \zeta \sin^2 \theta
\]
\[
1 - \sin^2 \theta \sin^2 \phi
\]

We omit the final form of the equation for brevity, as it is often more convenient to start from the compact form given in equation 4.

4. DEPENDENCE OF MODE DISSIPATION ON STRAIN STATE

In equation 4 there is a single filtered scale quantity: the strain state parameter \( s' = 1 \) (nondimensional eigenvalues are a function of this quantity). Angles combine information from filtered and SGS quantities, and the SGS stress state, \( s_{s', \gamma} \), is a purely SGS scale quantity. Therefore, we must choose a tensor alignment and a value for the SGS stress state parameter if we wish to explore the dependence of dissipation on filtered scale quantities.

If we assume that the value of the stress state parameter \( s' = 1 \), then we are guaranteed to capture both alignment modes as \( s_{s', \gamma} = 1 \) corresponds to \( \alpha_s = \beta_{s'} > 0 \), and \( \beta_{s'} < 0 \). The value of \( s_{s', \gamma} = 1 \) is the most likely value of this parameter in the atmospheric data set of Higgins et al. and in the square duct turbulence investigated by Tao et al. By inspection of figure 1 we see that \( \gamma_{s'} \perp \vec{\beta}_{s'} \). Substituting these two conditions into equation 4 \( s_{s', \gamma} = 1 \) and \( \gamma_{s'} \perp \vec{\beta}_{s'} \) the normalized dissipation becomes:

\[
\Pi = \frac{(\vec{y}_5, \vec{\gamma}_{s'})^2 (\gamma_{s'} - \beta_{g'}) - \alpha_{s'}^2}{\|S\|^2}
\]

which is a function of a single angle (the angle \( \vec{y}_5, \vec{\gamma}_{s'} \) that persists in both alignment configurations and the strain state parameter. We can then use the most likely value of this angle as observed from data \( (\vec{y}_5, \vec{\gamma}_{s'})^2 = 0.75 \) (the value reported by Higgins et al. 2002). Equation 5 reduces to:

\[
\Pi = \frac{\beta_{s'}^2 - 2\gamma_{s'}^2}{8}
\]

Equation 6 varies in a range between 1/8 when \( s' = -1 \) to 5/8 when \( s' = 1 \), and is now a prediction of the normalized dissipation based on only filtered scale quantities. The choice of \( (\vec{y}_5, \vec{\gamma}_{s'})^2 \) also determines if this prediction of dissipation allows for any negative values. The first negative dissipation values are allowed when \( (\vec{y}_5, \vec{\gamma}_{s'})^2 \leq 2/3 \), and the prediction gives only negative values when \( (\vec{y}_5, \vec{\gamma}_{s'})^2 \leq 1/3 \). This prediction of the mode of dissipation conditioned on the value of \( s' \) can be compared to the sonic anemometer data obtained from the near neutral atmospheric surface layer in the Davis 1999 experiment.

A joint probability density function of normalized dissipation with the strain state parameter is presented in figure 2 (a similar joint PDF is presented in Tao et al 2002 figure 9a). The dashed black line denotes the prediction based on equation 6.

This theoretical line tracks very well, but slightly over-predicts, the most likely normalized dissipation for any given strain state. Picking larger values for \( (\vec{y}_5, \vec{\gamma}_{s'})^2 \) moves the alignment closer to “eddy viscosity,” which is the maximum dissipation prediction. Picking smaller values for \( (\vec{y}_5, \vec{\gamma}_{s'})^2 \) eventually shifts the prediction curve downward the minimum.
5. DISCUSSION AND CONCLUSIONS

The geometry developed by Tao et al. 2002 and later used by Higgins et al. 2002 provided an initial framework in which to examine the effect of the eigenvector alignments of SGS stress and filtered strain rate on dissipation. Through a Spherical Trigonometry formulation a nondimensional form of the dissipation equation is attained which has only 5 degrees of freedom (three angles and two nondimensional parameters). Using observations obtained from experimental data of previous studies the behavior of the normalized dissipation with respect to the strain state is well reproduced. The formula also predicts a unique value of  for which this prediction first allows negative dissipation,  and a unique value when the prediction of dissipation is negative for all strain states . The results show the potential of interpreting turbulent parameters within a geometric framework, and make a clear and immediate connection between observable flow properties and the resulting dissipation.

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