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A structure-based model for the transport of passive scalars in homogeneous turbulent flows

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ABSTRACT

A structure-based model has been constructed, for the first time, for the study of passive scalar transport in turbulent flows. The scalar variance and the large-scale scalar gradient variance are proposed as the two turbulence scales needed for closure of the scalar equations in the framework of the Interacting Particle Representation Model (IPRM). The scalar dissipation rate is modeled in terms of the scalar variance and the large-scale enstrophy of the velocity field. Model parameters are defined by matching the decay rates in freely isotropic turbulence. The model is validated for a large number of cases of deformation in both fixed and rotating frames, showing encouraging results. The model shows good agreement with DNS results for the case of pure shear flow in the presence of either transverse or streamwise mean scalar gradient, while it correctly predicts the presence of direct cascade for the passive scalar variance in two dimensional isotropic turbulence.

1. Introduction

The transport of passive scalars is of great scientific interest since it plays a role in physical phenomena such as atmospheric dispersion and in engineering applications involving turbulent mixing. The term passive scalar refers to the simplified case where a scalar is present in such a low concentration that it does not influence the evolution of the fluid flow. Hence, the transport of passive scalars is also a convenient simplified starting point for the study of processes where one expects a more complex interaction between the scalar and the fluid flow, such as reacting flows with concentration gradients and heat release.

At sufficiently high Reynolds numbers, the predominant theory for the description of the velocity field statistics is based on Kolmogorov's 1941 idea of local isotropy, which assumes that the small scales remain mostly isotropic, independently of the presence of any large-scale anisotropies. By analogy, similar arguments were extended by Obukhov (1949) and Corrsin (1951) to describe the statistics of a passive scalar in homogeneous and isotropic turbulent flow at high Reynolds and Peclet numbers. The assumption of local isotropy enables the drastic simplification of the governing transport equations and leads to similarity solutions for the passive scalar and velocity fields, even in the presence of mean scalar gradients (Chasnov, 1993). The simplicity and elegance of such solutions has motivated a large amount of work in the literature (Danaila et al., 2012; Ma and Warhaft, 1986).

Yet, deviation from small-scale isotropy has been observed experimentally by a number of workers. For example, (Tong and Warhaft, 1994) considered the case of isotropic turbulence in the presence of a transverse mean scalar gradient, finding that $\overline{(\phi'_{,y})^2} \sim 1.4\overline{(\phi'_{,x})^2}$ where ϕ' denotes the fluctuating passive scalar and y is the direction of the mean gradient. A similar observation was published some years earlier by Sreenivasan et al. (1977) for shear turbulence, again in the presence of transverse mean scalar gradient. The departure from isotropy for small-scale second-order statistics that was reported in these studies was relatively small. However, in the case of third order small-scale statistics, the assumption of small-scale isotropy breaks down entirely, as first reported by Stewart (1969) for high Reynolds and Peclet number measurements in the atmospheric boundary layer. Stewart observed that the scalar-derivative skewness, defined as

$$S_{\phi'_{,x}} = \overline{(\phi'_{,x})^3}/[\overline{(\phi'_{,x})^2}]^{3/2}, \tag{1}$$

was of order one and not zero, as small-scale isotropy requires. Based on experimental observations, (Sreenivasan and Tavoularis, 1980) argued that the skewness should vanish only when the mean shear and the mean scalar gradient are both zero. In all other cases, it was found that:

(a) $sgn(S_{\phi'_{,x}}) = -sgn(S)sgn(S_\phi)$ [1],

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[1] Also mentioned in Mestayer (1982)

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(b) $|S_{\phi'_x}|$ varies linearly with the magnitude of $\ell_0 S_\phi/(\overline{\phi'^2})^{1/2}$,
(c) $|S_{\phi'_x}|$ depends on the history of S,

where ℓ_0 is the characteristic lengthscale of the large eddies, S_ϕ is the magnitude of the mean scalar gradient and S is the magnitude of the mean velocity gradient, both imposed transverse to the mean flow direction. Clearly the three above observations show that scalar derivative skewness *is directly linked to both the mean field and the large-scale structure.*

The aforementioned efforts addressed passive scalar transport in non-rotating flows. Recently, however, significant effort has been directed to the study of passive scalar transport in shear flows in rotating frames as well. Brethouwer (2005) performed a number of DNS computations at different frame rotation rates for the case of homogeneous shear flow in the presence of mean scalar gradient. Particularly, for the case of a transverse mean scalar gradient, he observed that scalar flux in the mean flow direction tends to become much larger compared to the flux in transverse direction. The DNS study of Kassinos et al. (2007) provided additional supporting evidence for the strong dependency of the passive scalar transport on the relative strength of the frame rotation rate and the mean shear rate and emphasized the role played by the large-scale turbulence structure in determining passive scalar transport.

1.1. General approach and objectives

The significant effect that the large-scale structures have on the evolution of the small-scale scalar statistics (Shraiman and Sigga, 2000) has motivated us to construct a structure-based model (SBM) for passive scalar transport with the ability to account for these effects. Such an SBM for passive scalar transport could be based either on the Interacting Particle Representation Model (IPRM) (Kassinos and Akylas, 2012) or a simplified engineering SBM such as the Algebraic Structure-Based Model (ASBM) (Panagiotou and Kassinos, 2015). In either case, the intent is to take advantage of the turbulence structure information carried in these models in order to provide improved predictions of scalar transport. In order to accomplish this in a self-consistent framework, we found it necessary to develop a set of transport equations for the scales of the passive scalar field that are sensitized to the structure of the large scales.

In Section 2, we give a brief summary of the one-point turbulence structure tensors and the IPRM framework. In Section 3, we develop an extension of the IPRM model to account for the passive-scalar statistics. In order to bring the extended IPRM model into a closed form, a set of structure-based scales for the passive scalar field is derived and discussed in Section 4 through Section 6. The validation of the complete structure-based model equations for a large number of test cases is carried out in Section 7, leading to encouraging results. In Section 8, we outline our future plans to adapt the current approach for use with the ASBM and show preliminary results that appear to be promising. A summary and conclusions are given in Section 9.

2. Mathematical background

2.1. The governing equations

The transport of a passive scalar ϕ in an incompressible fluid with no buoyancy effects is governed by the continuity, momentum and passive scalar transport equations,

$$u_{i,i} = 0, \tag{2a}$$

$$\partial_t u_i + u_j u_{i,j} = -\frac{1}{\rho} p_{,i} + \nu u_{i,jj}, \tag{2b}$$

$$\partial_t \phi + u_j \phi_{,j} = \gamma \phi_{,jj}, \tag{2c}$$

where ρ is the density of the fluid and u_i, p, ϕ are the instantaneous velocity, pressure and passive scalar fields respectively. The fluid viscosity and scalar diffusivity are denoted by ν and γ respectively. Hereafter, we are using index notation whereby repeated indexes imply summation and an index following a comma denotes differentiation with respect to the corresponding spatial coordinate. Applying Reynolds' decomposition of the flow variables,

$$u_i = \overline{u}_i + u'_i, \quad p = \overline{p} + p', \quad \phi = \overline{\phi} + \phi', \tag{3}$$

to Eq. (2) leads to the set of equations governing the transport of the turbulence fluctuations. For the case of homogeneous turbulence these take the form,

$$u'_{i,i} = 0, \tag{4a}$$

$$\partial_t u'_i + \overline{u}_j u'_{i,j} = -G_{ik} u'_k - u'_j u'_{i,j} - \frac{1}{\rho} p'_{,i} + \nu u'_{i,jj}, \tag{4b}$$

$$\partial_t \phi' + \overline{u}_j \phi'_{,j} = -\Lambda_j u'_j - u'_j \phi'_{,j} + \gamma \phi'_{,jj}, \tag{4c}$$

where $G_{ij} = \overline{u}_{i,j}$ and $\Lambda_i = \overline{\phi}_{,i}$ are the mean velocity gradient tensor and mean scalar gradient vector respectively.

2.2. The one-point turbulence structure tensors

In the context of Reynolds Averaged Navier–Stokes (RANS), it is important to have good one-point measures of turbulence anisotropy. As shown by Kassinos and Reynolds (1994); Kassinos et al. (2001), such anisotropy measures must take into account the morphology of the large energy-containing eddies. These coherent structures tend to organize the fluctuating motion in their vicinity and in the process create anisotropy in both the componentality and the dimensionality of the turbulence. Here, componentality refers to information about the directions in which turbulent fluctuations are most energetic, while dimensionality refers to information about the alignment and extent of the coherent structures. One has to distinguish between the turbulence componentality and dimensionality because they are two distinct aspects of turbulence anisotropy that affect the dynamics of the turbulence in different ways (Kassinos et al., 2001). The structure of the turbulence field, i.e. the morphology of the large energy-containing eddies, can be characterized through a set of one-point turbulence structure tensors. Here, we summarize the key features of these tensors, but more details can be found in several works, such as (Kassinos et al., 2000; Reynolds and Kassinos, 1995; Stylianou et al., 2015).

The one-point structure tensors are defined through the fluctuating stream function vector ψ'_i, which is related to the fluctuating velocity u'_i and vorticity ω'_i through the expressions,

$$u'_i = \epsilon_{ijk} \psi'_{k,j}, \quad \psi'_{i,i} = 0, \quad \psi'_{i,nn} = -\omega'_i. \tag{5}$$

The Reynolds stress tensor R_{ij}, also called componentality tensor in the terminology of Kassinos et al. (2001), describes the spatial orientation of the velocity fluctuations, i.e. it allows one to know in which direction the velocity fluctuations are most energetic. The componentality tensor is related to the stream function vector through the identity

$$R_{ij} = \overline{u'_i u'_j} = \epsilon_{ist}\epsilon_{jpq}\overline{\psi'_{t,s}\psi'_{q,p}}, \quad r_{ij} = R_{ij}/R_{qq} = R_{ij}/(2\kappa), \tag{6}$$

where κ is the turbulent kinetic energy. Applying isotropic tensor identities (Mahoney, 1985) to Eq. (6) leads to a constitutive equation, which in the case of homogeneous turbulence reduces to

$$R_{ij} + D_{ij} + F_{ij} = R_{kk}\delta_{ij}. \tag{7}$$

Eq. (7) leads to the definitions of the one-point structure tensors,

$$\text{Componentality} \quad R_{ij} = \overline{u'_i u'_j}, \quad r_{ij} = R_{ij}/R_{kk}, \quad \tilde{r}_{ij} = r_{ij} - \delta_{ij}/3, \tag{8a}$$

$$\text{Dimensionality} \quad D_{ij} = \overline{\psi'_{k,i}\psi'_{k,j}}, \quad d_{ij} = D_{ij}/D_{kk}, \quad \tilde{d}_{ij} = d_{ij} - \delta_{ij}/3, \tag{8b}$$