IMPLEMENTING SCHMIDT NUMBER DEPENDENCE IN A STOCHASTIC LAGRANGIAN MODEL FOR THE SCALAR GRADIENT

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ABSTRACT

A stochastic Lagrangian model for the scalar gradient (Gonzalez, 2009) is extended to Schmidt numbers larger than unity as a necessary step to make the approach valid for a wider range of mixing problems. The basic idea is to derive the damping time scale of the modelled molecular diffusion from the phenomenology of stretched scalar layers. In this context, the diffusive damping rate is itself given by a non-linear stochastic equation. Although the model has to be checked further and improved in some respects – for instance, as regards the scaling of the scalar gradient intermittency with the Reynolds number –, first results in isotropic turbulent flow agree with the standard physics of scalar turbulence.

INTRODUCTION

The gradient of a scalar rules molecular diffusion and also gives a detailed insight into the small-scale structure of scalar fields and mixing patterns. It is actually the finest level at which micromixing in fluid flows can be investigated. In fact, the efficiency of micromixing is revealed by the mean dissipation rate of the energy of scalar fluctuations – or scalar dissipation – which directly involves the variance of the scalar gradient. The study of the mechanisms of scalar gradient production is therefore closely connected to the concerns of modelling and predicting small-scale mixing in process and chemical engineering or in combustion flows.

In this context, a number of studies have addressed the small-scale structure of scalar fields (Pumir, 1994; Buch & Dahm, 1996; Vedula *et al.*, 2001; Brethouwer *et al.*, 2003; Su & Clemens, 2003; Schumacher & Sreenivasan, 2005; Kushnir *et al.*, 2006); see also Warhaft (2000) for a review on scalar turbulence. Because scalar gradient production is a matter of both strain level and scalar gradient 'geometry' through orientation in the strain eigenframe, the mechanisms promoting scalar dissipation are not that simple. In particular, they indirectly involve the tight interaction of strain and vorticity (Vedula *et al.*, 2001; Brethouwer *et al.*, 2003; Gonzalez, 2012) and may also be deeply affected by the dynamics of the scalar gradient orientation (Smyth, 1999; Lapeyre *et al.*, 2001; Brethouwer *et al.*, 2003; Gonzalez & Paranthoën, 2010).

Accounting for such detailed mechanisms in the prediction of small-scale mixing thus needs models which are directly based either on a presumed local flow structure (Pullin & Lundgren, 2001) or on the behaviour of the scalar gradient derived from the computation of the small-scale velocity field. The latter approach was used in the stochastic modelling (Gonzalez, 2009; Li, 2011) which was shown to retrieve a number of detailed properties of the scalar gradient.

In the present study the stochastic Lagrangian model devised in Gonzalez (2009) is extended to Schmidt number larger than unity to make the approach suitable for addressing a wider range of mixing problems. Exploring high-Schmidt number flows may also shed new light on basic phenomena such as small-scale anisotropy (Yeung *et al.*, 2002; Brethouwer *et al.*, 2003; Gonzalez & Paranthoën, 2004). The paper details the modelling of the molecular diffusion of the scalar gradient as well as the way in which it is implemented into the stochastic model. First results of this approach are then presented and discussed.

MODELLING MOLECULAR DIFFUSION OF THE SCALAR GRADIENT

The exact equation for the gradient, $\boldsymbol{G} = \nabla\theta$, of a scalar θ is:

$$\frac{d\boldsymbol{G}}{dt} = -\boldsymbol{A}^T\boldsymbol{G} + D\nabla^2\boldsymbol{G} \qquad (1)$$

where $\boldsymbol{A} = \boldsymbol{\nabla} u$ is the velocity gradient tensor and D is the molecular diffusivity of the scalar in the fluid. Provided that the velocity gradient is known for instance, through an additional equation – see below –, the stretching term – first one on right-hand side – does not need to be modelled. A model, however, has to be devised for the molecular diffusion term.

In Gonzalez (2009) the modelling of $D\nabla^2\boldsymbol{G}$ was achieved consistently with the approach used by Jeong & Girimaji (2003) and Chevillard & Meneveau (2006) for the viscous term of the velocity gradient equation. It comes to model the molecular diffusion term expressed in Lagrangian coordinates by a friction term based on a constant time scale. In Eulerian coordinates, however, the effective friction time scale is not constant as it includes information on fluid elements deformation through the Cauchy-Green tensor – see Eq. (10) for the velocity gradient.

The present approach is different in that the molecular diffusion term is directly modelled in connection to the structure of the scalar gradient field. It is indeed taken for granted that this small-scale structure is sheet like and can be pictured by stretched scalar layers which eventually fade out as their thickness reaches the diffusive lengthscale (Buch & Dahm, 1996; Su & Clemens, 2003; Kushnir *et al.*, 2006).

As in Gonzalez (2009), a friction model is assumed for the molecular diffusion term, $D\nabla^2\boldsymbol{G} \equiv -f_d\boldsymbol{G}$, but the derivation of f_d, this time, proceeds as follows:

1. we consider the one-dimensional problem of a scalar layer initially defined by a gaussian profile, $C(y,0) = C_0\exp(-y^2/s_0^2)$, and undergoing a normal strain rate γ ($\gamma < 0$ for compressional strain). The solution of the advection-diffusion equation for $C(y,t)$ is:

$$C(y,t) = C_0(1+4\tau)^{-1/2}\exp[-(y^2/s^2)/(1+4\tau)] \quad (2)$$

with:

$$d\tau = \frac{D}{s^2}dt \quad \text{and} \quad \frac{ds}{dt} = \gamma s \qquad (3)$$

From Eq. (2), the gradient of C is easily derived as:

$$G(y,t) = -2C_0 s^{-2}(1+4\tau)^{-3/2} y\exp[-(y^2/s^2)/(1+4\tau)] \qquad (4)$$

2. the molecular diffusion time scale, T_d, of the scalar gradient is estimated as:

$$T_d^{-1} = f_d = D\left|\frac{\partial^2 G/\partial y^2}{G}\right|(y_m,t) \qquad (5)$$

where y_m is time dependent and define the position of the extrema of $G(y,t)$; from Eq. (4):

$$y_m^2(t) = \frac{s^2(1+4\tau)}{2} \qquad (6)$$

From Eq. (5), with the equation for $\partial^2G/\partial y^2$ – which is easily derived from Eq. (4) and is not given – and Eqs. (4) and (6):

$$f_d = \frac{2D}{y_m^2} \qquad (7)$$

3. the diffusive rate, f_d, has to be included in a stochastic model to account for variable strain experienced by the scalar gradient; an equation for f_d is thus needed and derived by differentiating Eq. (7) accounting for Eqs. (3) and (6) and again for the definition of f_d; the equation for f_d is finally written as:

$$df_d = -f_d(f_d + 2\gamma)dt \qquad (8)$$

In the stochastic model γ is the effective strain rate experienced by the scalar gradient, $\gamma = G_\alpha S_{\alpha\beta} G_\beta/\boldsymbol{G}^2$ – with $S_{\alpha\beta}$ the components of the strain tensor, $\boldsymbol{S} = (\boldsymbol{A}+\boldsymbol{A}^T)/2$ – and is negative or positive for compressional or extensional events, respectively.

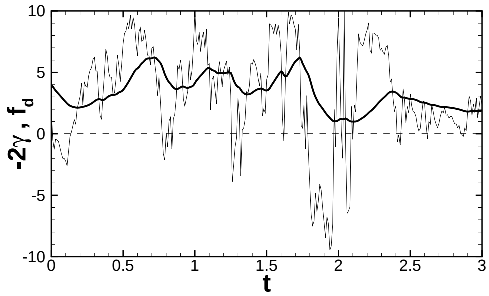

Figure 1. Sample signals of f_d (thick line) and -2γ; in the figure positive values of -2γ correspond to compressional strain and negative ones to extensional strain.

Equation (8) includes only time scales and is thus suitable for a pointwise, Lagrangian approach. It is also interesting to notice that it is a non-linear damping equation. The posivity of $f_d(t)$ is ensured provided that $f_d(0) > 0$; for an extensional strain rate ($\gamma > 0$) f_d does not tend to -2γ, but asymptotically to zero as a result of the non-linearity of Eq. (8). For a steady compressional strain rate ($\gamma < 0$) f_d tends to -2γ; this is consistent with the fact that in a stretched scalar layer the maximum of the scalar gradient norm eventually decays at the net rate $\gamma = -\gamma - f_d$ as a result of both enhancement by compression at the rate $-\gamma$ and damping by diffusion at the rate f_d.

Because γ is defined in terms of $\boldsymbol{G}$ itself, the friction term, $-f_d\boldsymbol{G}$, in the equation for $\boldsymbol{G}$ is implicit through f_d. It also responds to the effective, instantaneous strain experienced by the scalar gradient. Figure 1 shows sample signals of both -2γ and f_d.

Finally, Eq. (8) does not explicitly include the scalar diffusivity and thus Schmidt number effects. In fact, the latter are felt through the initial condition, in the transient regime and Eq. (8) has thus to be combined with a renewal of f_d; this is done at the start of each compressional cycle as $f_{d_0} = CD\boldsymbol{G}^2$ where C is a constant which has the dimension of θ^{-2}; $C = 2$ in the present calculations.

STOCHASTIC LAGRANGIAN MODEL
Stochastic Equations

The modelled stochastic Lagrangian equation for the scalar gradient is now written as:

$$d\boldsymbol{G} = -(\boldsymbol{A}^T\boldsymbol{G} + f_d\boldsymbol{G})dt + (2\mathrm{Sc}f_d)^{1/2}d\boldsymbol{W}_G \qquad (9)$$

with $d\boldsymbol{W_G} = dt^{1/2}\boldsymbol{\xi}$ the increment of a Wiener process where $\boldsymbol{\xi}$ is a vectorial, Gaussian noise such that $\langle\xi_i\rangle = 0$ and $\langle\xi_i\xi_j\rangle = \delta_{ij}$. Because f_d is not a constant, but is itself the solution of a stochastic equation, Eq. (9) is not in the standard form used in Gonzalez (2009). The presence of the Schmidt number, Sc, as a multiplying factor of f_d ensures that the amplitude of the forcing noise term is conserved when the Schmidt number is changed.

Equation (9) is solved together with Eq. (8) – allowing for the renewal of f_d – and the stochastic equation of Chevillard and Meneveau for the velocity gradient tensor (Chevillard & Meneveau, 2006; Chevillard *et al.*, 2008;

Meneveau, 2011):

$$dA = -\left(A^2 - \frac{Tr(A^2)}{Tr(C_{\tau_\eta}^{-1})}C_{\tau_\eta}^{-1} + \frac{Tr(C_{\tau_\eta}^{-1})}{3T}A\right)dt + \left(\frac{2}{T}\right)^{1/2} dW \quad (10)$$

Second and third terms including the modelled Cauchy-Green tensor, $C_{\tau_\eta} = \exp(\tau_\eta A)\exp(\tau_\eta A^T)$ – where τ_η is the Kolmogorov time scale – respectively model the pressure Hessian and the viscous term of the velocity gradient equation; T is the integral time scale. Forcing is ensured by the increment of a tensorial Wiener process, $dW = dt^{1/2}\zeta$, where ζ is a tensorial, Gaussian delta-correlated noise with $\langle\zeta_{ij}\rangle = 0$ and $\langle\zeta_{ij}\zeta_{kl}\rangle = 2\delta_{ik}\delta_{jl} - 1/2\delta_{ij}\delta_{kl} - 1/2\delta_{il}\delta_{jk}$.

Numerical Solution

Normalizing time scales by the integral time scale, T, two parameters are needed to run the model, namely the Kolmogorov timescale, τ_η, and the Schmidt number, Sc, or in other words, the Reynolds and the Péclet numbers. With $\tau_\eta = 0.1$, for instance, the microscale Reynolds number, Re_λ, is close to 150 (Chevillard *et al.*, 2008); Re_λ changes in proportion to $\tau_\eta{}^{-1}$. When needed, the molecular diffusivity is given by $D = \mathrm{Sc}^{-1}\nu$ – with ν the kinematic viscosity – and assuming that $\tau_\eta = (\nu/\varepsilon)^{1/2}$ is changed keeping the mean energy dissipation rate, ε, constant. Then, since $\varepsilon = \nu\langle S_{\alpha\beta}S_{\beta\alpha}\rangle/2$ and, from the model results, $\langle S_{\alpha\beta}S_{\beta\alpha}\rangle$ is found to scale as τ_η^{-2} for τ_η smaller than 0.15, ν must scale as $\nu \sim \tau_\eta^2$ for small to moderate values of τ_η – i.e. for moderate to large Reynolds number.

The numerical method uses a second-order predictor-corrector scheme (Welton & Pope, 1997) to solve Eqs. (8)-(10). The calculation is run for $2\times10^5 T$ with time step $0.1\tau_\eta$ and the statistics of the variables under study are derived from their respective stationary time signals.

RESULTS

The variance of the scalar gradient grows linearly with the Schmidt number (Fig. 2) which makes the mean scalar dissipation, $\langle\chi\rangle = D\langle G^2\rangle$, Schmidt number independent, as expected. Figure 3 shows that the scalar gradient variance also closely follows a Re_λ^2-law.

The model underpredicts the kurtosis of scalar gradient components, $K = \langle G_1^4\rangle/\langle G_1^2\rangle^2$ (Fig. 4); at $\mathrm{Re}_\lambda = 150$, for instance, K should be around 10 at least (Warhaft, 2000). Even so, the kurtosis, has no Schmidt number dependence and duly grows with the Reynolds number. Its rise is milder than the mean power-law that can be derived from the data gathered by Warhaft (2000) ($\sim \mathrm{Re}_\lambda^{0.25}$ *vs* $\mathrm{Re}_\lambda^{0.38}$); the universal nature of this Reynolds-number dependence, however, is not firmly shown.

Figure 5 shows that the p.d.f of scalar dissipation departs from lognormality. Deviations from lognormal statistics have already been found both experimentally (Su & Clemens, 2003) and numerically (Schumacher & Sreenivasan, 2005). The p.d.f in Fig. 5 is plotted for $\mathrm{Sc} = 2$ and $\mathrm{Re}_\lambda = 150$, but is robust for other values of the Schmidt and Reynolds numbers. It is worth noticing that this p.d.f, with a rather fat tail for low dissipation values and a steep fall for large values, is clearly reminiscent of the p.d.f's computed by Schumacher & Sreenivasan (2005).

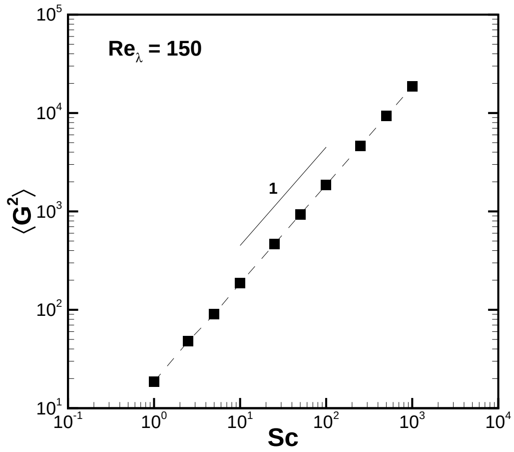

Figure 2. Variance of the scalar gradient *vs* Schmidt number for $\mathrm{Re}_\lambda = 150$.

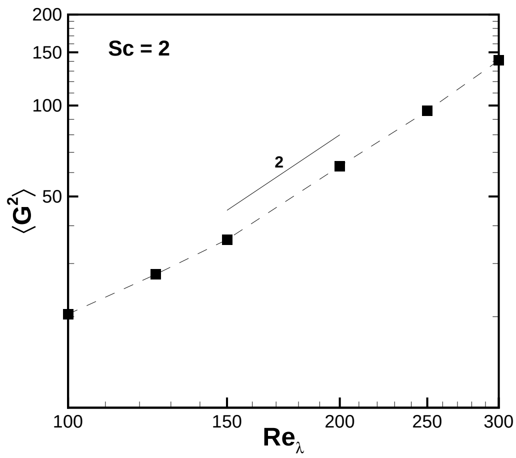

Figure 3. Variance of the scalar gradient *vs* microscale Reynolds number for $\mathrm{Sc} = 2$.

CONCLUSION

The physics of stretched scalar layers has been used to include the effect of large Schmidt number in a stochastic Lagrangian model for the scalar gradient. Modelling molecular diffusion of the scalar gradient through a friction term, an equation for the diffusive damping rate is derived from the behaviour of the scalar gradient in stretched layers. Interestingly, the latter is itself a non-linear damping equation which ensures that the diffusive rate responds to instantaneous compressional and extensional effective strain rates experienced by the scalar gradient.

First results regarding the statistics of scalar dissipation are consistent with the physics of isotropic scalar turbulence. In agreement with previous studies, the model also predicts departure from lognormality. However, the kurtosis of the scalar gradient components which indicates the level of intermittency is not quite satisfactory; although an increase with the Reynolds number is duly predicted, the level of intermittency is underestimated and the Reynolds-number dependence is rather mild. The model has thus to be checked further to address a more complex physics such

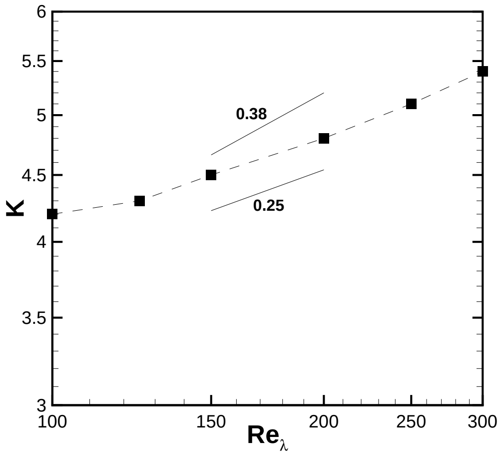

Figure 4. Kurtosis of one component of the scalar gradient, $K = \langle G_1^4 \rangle / \langle G_1^2 \rangle^2$, *vs* microscale Reynolds number; 0.38 is the mean slope derived from the data gathered by Warhaft (2000).

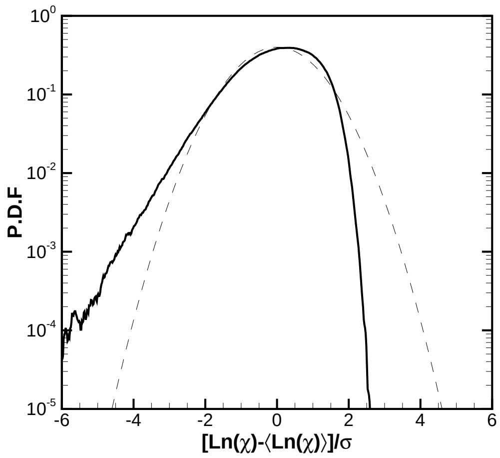

Figure 5. Probability density function of $(\ln\chi - \langle \ln\chi \rangle)/\sigma$ with σ the standard deviation of $\ln\chi$; the dashed line is the lognormal distribution with the same standard deviation.

as anisotropic forcing of the scalar field.

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