Effects of numerical diffusion and mass conservation errors on turbulent transport of high Schmidt number scalars.

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Abstract: We investigate the negative effects of various transport schemes on turbulent mixing of low diffusivity passive scalars. We recommend new grid resolution criteria to account for these effects, and establish allowable error tolerances in order to reduce computational cost without sacrificing accuracy.

Keywords: Turbulent Mixing, High Schmidt, Numerical Diffusion, DNS

1 Introduction

Turbulent simulation of low diffusivity passive scalars (e.g.: soot) requires that numerical diffusivity of the transport scheme used be kept to a minimum to avoid contamination of transport characteristics. In addition, boundedness of scalar quantities, for example species mass fraction between 0 and 1, is essential to keep the simulations physically relevant. Unfortunately, these two properties often show mutually conflicting behavior. Ensuring the boundedness of Eulerian transport schemes (e.g. WENO, BQUICK) introduces significant numerical diffusion. Nonetheless, Eulerian schemes have traditionally been preferred over Semi-Lagrangian (SL) approaches with lower diffusion, since they ensure conservation. Numerical diffusion can be mitigated by using higher-order accurate methods, however the corresponding increase in computational cost is often significant. We present an analysis of the various effects that both numerical diffusion, and non-conservative transport have on high Schmidt number turbulent mixing.

2 Effects of transport schemes

The grid resolution required for fully resolving high Schmidt (Sc) number turbulent simulations is determined by the Batchelor scale (η_B). This necessitates the use of very fine grids to capture the physically important small scale structures. The need for high accuracy at these small scales makes the simulations extremely sensitive to numerical diffusion. Commonly used guidelines suggest that keeping $\kappa_{max}\eta \geq 1.5$, where κ_{max} is the largest wavenumber determined by the grid size (N) and η is the Kolmogorov length scale, ensures a fully resolved velocity field [1]. A similar criterion is currently used to suggest that setting $\kappa_{max}\eta_B \geq 1.5$ leads to a fully resolved scalar field [2]. However, resolving all the physically important scales does not necessarily guarantee that numerical diffusion will not have an appreciable adverse effect on the results. Using the scalar dissipation spectra plotted in Fig. 1, we can observe the considerable impact that numerical diffusion has on the smaller scales. The aforementioned grid resolution criteria are satisfied for $N = 256$. However, we see a large discrepancy (for $\kappa\eta \geq 4$) when we compare these Finite Volume results to those generated by a Spectral code. Refining the grid to $N = 512$ leads to better agreement, but at a cost increase of 16 times! These results clearly indicate that the currently established resolution criteria for ensuring physically accurate simulation of high Schmidt scalar transport may need to be revised. Hence, we propose new criteria for such flows, that account for dependence on numerical diffusivity of the scheme used.

In order to minimize numerical diffusion, we turn to a SL approach with MonotoneE - Cubic Hermite interpolation (MECH). This offers the advantages of a compact stencil and extremely faithful sub-cell reconstruction. Using this scheme substantially lowers numerical diffusion. However, ensuring both boundedness and conservation poses a significant challenge. We suggest that it is preferable to allow a minimal error in mass conservation, rather than to allow unphysical errors (e.g. negative mass fractions) to manifest, the effects of which can corrupt the entire computation. This approach is in essence identical to tolerating the numerical dissipation inherent to the discretization, i.e., the conservation error is treated to be the result of an unaccounted-for source term. In order to study the effect of numerical diffusion, we perform Direct Numerical Simulations (DNS) in Homogeneous Isotropic Turbulence configuration for various grid resolutions.

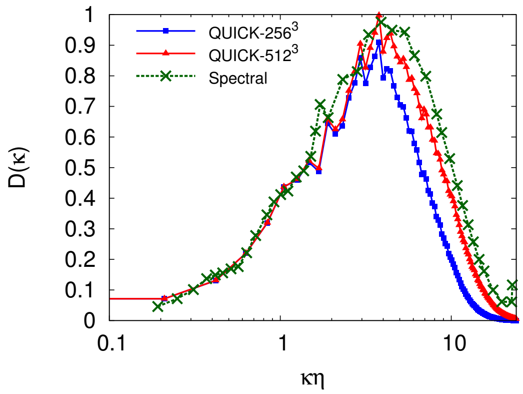

Figure 1: Normalized dissipation spectra showing the effect of numerical diffusion ($Re_\lambda \approx 8$, Sc$= 256$). “Spectral” data taken from [2].

3 Conclusion

We have established that numerical diffusion introduces appreciable error in simulation of high Schmidt number scalar transport. We recommend new grid resolution criteria that account for these errors. However, it is not always feasible to eliminate these errors by increasing grid resolution, due to the substantial rise in computational cost. An alternative in such cases is to use SL schemes with lower diffusion. These schemes introduce minor conservation errors. However, these errors do not seem to have a significant detrimental impact on the transport characteristics.

References

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