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IV. The small scales mixing group

The study of direct numerical simulations of turbulence has significantly added to the understanding of many turbulent flows. Originally such simulations concentrated on examination of the turbulent velocity and vorticity fields, studying both statistics and the structure of the instantaneous flow fields. More recently there has been increased interest in using direct numerical simulations to examine the ability of turbulence to mix scalar quantities (such as temperature or concentration of a chemical species). This stems partly from the desire to extend the predictive capabilities of direct numerical simulations to chemically reacting flows.

The interaction of turbulence with a chemically-reacting flow field remains one of the most complex and least understood problems of engineering interest. In typical combustion applications the large heat release associated with the chemical reaction can significantly alter the local hydrodynamics. In addition the turbulence can dramatically alter the distribution of the reactant (and product) species. In many practical applications the rate of reaction is controlled primarily by the ability of the turbulence to mix reactant species. By examining the turbulent mixing of a passive scalar quantity (one which does not alter the hydrodynamic flow field) the mixing capability can be studied without the added complications associated with heat-release-induced alterations of the flow field. Such direct numerical simulations of passive scalar mixing thus lend themselves directly to the study of mixing by realistic turbulence, ignoring complex reaction kinetics and the effects of heat release.

In many practical combustion applications the reaction occurs in free shear flows, *e.g.* fuel jets, flame-holder wakes. Perhaps the simplest such free shear flow is the plane mixing layer and it is thus often used as the prototypical free shear flow for the study of turbulent mixing. The development of three-dimensionality and small-scale turbulence in such a plane mixing layer is of crucial importance to its mixing capabilities. Three of the four projects summarized below were directed at studying small-scale turbulence and scalar mixing in this flow. The fourth is more general in nature, directed towards elucidating the basic mechanisms of scalar mixing.

Recent direct numerical simulations have shed substantial insight into the early evolution of plane mixing layers. Despite this, no general theory is available to predict the layer evolution for disturbances that are too large for the results of linear theory to be valid. The fact that this flow is sensitive to slight changes in initial conditions underscores the need for such a model. Daniel Riahi, Bob Moser and Fabian Waleffe investigated various possible weakly-nonlinear theories in an effort to complement the direct numerical simulation results. This proved to be more difficult than initially anticipated due primarily to the time-evolving nature of the base flow under consideration.

Very large direct numerical simulations have just recently been able to simulate through the mixing transition (sudden increase in mixing due to proliferation of small-scale motions) in the plane mixing layer. It is of great interest to ascertain whether this transition resembles that seen in experiments. Yitshak Zohar, Bob Moser, Jeff Buell and Chih-Ming Ho extensively compared the post-transition numerical simulation velocity and vorticity fields with data taken in experimental mixing layers by Zohar and Ho. They found a high degree of correspondence between the two, with both indicating that the most probable length scale of the small-scale eddies corresponds to the scale associated with the peak of the energy-dissipation-rate spectrum and that the small-scale strains are comparable to the global strain associated with the velocity difference across the layer and the streamwise separation between eddies.

The mixing transition discussed above is associated with development of small-scale three-dimensional eddies by vortex stretching and thus presumably could not occur in a two-dimensional simulation. Javier Jiménez examined passive scalar mixing in very high Reynolds/Peclet number two-dimensional mixing layers to study the mixing behavior in the absence of the three-dimensional structures described above. He found that while a mixing transition of the kind seen in three-dimensional simulations was not observed, there was a definite increase in the complexity of the "reaction sheet" separating two chemical species (as measured by its fractal dimension). This increase was found to occur during the first pairing of the primary Kelvin-Helmholtz rollers and subsequent pairings did not further increase the dimension. The observed fractal dimensions, both before and after the pairing, have been explained in terms of two model structures. The simulations of Jiménez and Martel also confirm that the Peclet number (product of flow Reynolds number and scalar Schmidt number) is the relevant parameter for quantifying the mixing characteristics. Simulations with identical Peclet numbers (but different Reynolds and Schmidt numbers) were found to yield virtually identical scalar mixing behavior.

The final project in the small scales mixing group was a more general examination of the small-scale mixing behavior of a passive scalar quantity in homogeneous isotropic turbulence. In particular Carl Gibson, Mike Rogers, Jeff Chasnov and John Petresky sought to determine by numerical simulation whether the small-scale strain rate is relevant in determining the nature of the scalar field for Prandtl/Schmidt numbers much less than unity. Batchelor has proposed that the small-scale strain (primarily due to scales much smaller than the smallest scalar scales) would be irrelevant to the scalar behavior and predicted a $k^{-17/3}$ (k being the magnitude of the wavevector) decay of the scalar spectrum beginning from the Corrsin-Oboukhov scale. Gibson proposed mechanisms in which the small-scale strain rate is relevant and predicted an intermediate k^{-3} decay of the scalar spectrum between the Corrsin-Oboukhov scale and the Batchelor scale. Results from forced direct numerical simulations were found to scale in the manner proposed by Gibson, but this may be due to the low Reynolds numbers of the simulations. Higher-Reynolds-number simulations, obtained by using a subgrid-scale turbulence model for the velocity field, support the ideas of Batchelor; however it may be that the subgrid-scale model is not accurate enough to account for the small-scale strain-related mechanisms suggested by Gibson.

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