

Overview of the scalar transport/reacting flows group

This group conducted five projects aimed at developing improved modeling capabilities for turbulent flows with scalar transport or chemical reaction. Two projects used existing data bases selected from previous simulations of incompressible homogeneous flows, both with and without mean deformation; two modified the basic program for homogeneous incompressible turbulence to account for simple chemical reactions; and one modified the code to include a Boussinesq buoyancy term.

The invited participants were:

- Dr. William T. Ashurst (Sandia National Laboratories)
- Dr. Sherif El-Tahry (General Motors Research Laboratories)
- Prof. James C. Hill (Iowa State University)
- Mr. Mark J. Jennings (Illinois Institute of Chicago)
- Mr. Andrew D. Leonard (Iowa State University)
- Prof. Wolfgang Kollman (University of California, Davis)
- Dr. Thomas Morel (Integral Technologies)
- Mr. Masood Mortazavi (University of California, Davis)

The local participants were:

- Mr. Scott D. Abrahamson (Stanford University)
- Prof. Joel H. Ferziger (Stanford University)
- Prof. William C. Reynolds (Stanford University and NASA Ames)
- Dr. Robert S. Rogallo (NASA Ames)
- Dr. Michael M. Rogers (NASA Ames)
- Mr. Christopher J. Rutland (Stanford University)
- Mr. Kyle D. Squires (Stanford University)

The principal accomplishments of each project are summarized below.

Pressure gradient statistics in homogeneous shear

Using the data base for homogeneous shear, Kollman, Mortazavi, Squires and Rogers examined one-point probability density functions for the pressure gradient, conditioned on components of the fluctuating velocity and vorticity. The objective was to develop a firm basis for modeling quantities needed in pdf treatments of turbulent flows.

They found that the expectation value of the fluctuating pressure gradient, conditioned on a turbulence velocity component, is linear in the velocity component over the range of velocity where an adequate sample existed. In contrast, the expectation values of pressure gradient conditioned with vorticity were found to be very small, indicating that the pressure gradient is statistically independent of the vorticity. It thus appears that the conditioned pressure gradient term in homogeneous shear

flow can be modeled as $\langle (1/\rho)\partial p/\partial x_i | u_1, u_2, u_3, \omega_1, \omega_2, \omega_3 \rangle = \alpha_1 u_1 + \alpha_2 u_2$, where $\alpha_1 < 0$ and $\alpha_2 > 0$. This model is likely to be useful in pdf modeling of turbulence.

Modeling turbulent scalar transport

Morel, Jennings, and Abrahamson explored Morel's ideas for non-local modeling of turbulent scalar transport using integrals formed from two-point correlation functions. For homogeneous turbulent shear flow they examined quantity $I_{ij}(t) = \int Q_{kk}(\mathbf{r}, t) r_i r_j d^3 \mathbf{r}$ where $Q_{ij}(\mathbf{r}, t) = u_i(\mathbf{x}, t) u_j(\mathbf{x} + \mathbf{r}, t)$. Morel's conjecture was that the component of turbulent transport of a scalar ϕ in the i^{th} direction might be modeled as $T_{\phi_i} = C \Phi_{,j} I_{ij}$ where Φ is the mean scalar field. This is of the form $T_{\phi_i} = -D_{ij} \Phi_{,j}$ which Rogers *et al.* (1986) found fit their direct simulations of homogeneous turbulent shear flow. However, Morel's model gives a symmetric D_{ij} , whereas Rogers found that D_{ij} is non-symmetric. Thus, while Morel's model predicted the correct trends for the diagonal terms, it did not predict the off-diagonal terms. Further study of these ideas is planned by Morel and Jennings.

Buoyant convection

The Rogallo code for homogeneous turbulence was modified by Ashurst and Rogers to include a Boussinesq forcing term in the momentum equation. The objective was to study the effects of buoyancy on the relationships between vorticity and strain rate in homogeneous shear flow.

An unstable temperature gradient was imposed in the gravitational direction and the turbulence development was studied and compared to a zero gravity isotropic decaying case. A computational box that was twice as long in the gravitational direction as horizontal was employed to permit the simulation to be run longer before the flow structures were affected by the imposed periodic boundary conditions. The simulations were begun from developed initial isotropic fields at $Re_\lambda = 7.8$ and run on a $64 \times 32 \times 32$ grid. The Rayleigh number based on the Taylor microscale varied from 21 to 93, and the Prandtl number was 0.7.

As expected, the Boussinesq term eventually caused the velocity fluctuations and length scales in the gravity direction to grow. The relationship between the vorticity and the eigenvectors of the strain-rate tensor in the buoyant fields was qualitatively similar to that observed in incompressible homogeneous shear flow and isotropic decaying turbulence studied previously (Ashurst *et al.* 1987). Specifically, the vorticity has a large probability of aligning with the intermediate strain-rate eigenvector direction and at large strains this intermediate strain-rate is extensional. This direction has a low probability of being aligned with the gravitational direction. The temperature field also behaves like the passive scalar fields in incompressible shear flow in that the local temperature gradient is most likely to be aligned with the most compressive eigenvector of the strain-rate tensor. In addition, the scalar dissipation (conditioned on the kinetic energy dissipation) resembles the behavior in incompressible shear flow, exhibiting a near linear dependence at large values. These results should be useful to developers of models for buoyant turbulent convection.

Premixed flame in homogeneous turbulence

El-Tahry, Rutland, Ferziger, and Rogers modified the Rogallo code for homogeneous turbulence to study premixed turbulent flames in decaying isotropic incompressible turbulence. The objective was to determine the effect of turbulence on flame structure and speed over a range of Damkohler number. The results, though preliminary, are of interest to combustion modelers.

They considered the reaction $A \rightarrow B$, where A denotes premixed reactants and B denotes products. A temperature-dependent reaction rate was used, with the Arrhenius parameters adjusted to yield a flame width of about ten gridpoints (to resolve the structure) and a 15°C temperature rise across the flame (to allow treatment as incompressible). In order to keep the flame thin compared to the turbulence scales and still resolve the flame structure, the Reynolds number had to be kept small, and the Taylor microscale Reynolds number was only about 5 in their simulations. The Damkohler number was approximately 1.5. A $128 \times 128 \times 128$ grid was employed, with a uniform initial chemical distribution (premixed reactants) and a Gaussian temperature distribution sufficient to ignite the reaction. A purely laminar case was run for reference purposes.

The resulting flame front exhibited the characteristics of a wrinkled laminar flame; the local flame structure was everywhere similar to that of a laminar flame, with isotherms approximately parallel at about the same spacing as in the laminar case. The wrinkling of the instantaneous flame front appeared well correlated with the local velocity fluctuations and resulted in a mean flame thickness of about twice the local (laminar) flame thickness. The increased reaction area led to turbulent flame speeds about 20% larger than the laminar flame speed. As the flame propagated through the decaying hydrodynamic field it slowed due to the decaying turbulence intensity (decreasing roughly linearly with the rms turbulence intensity) and thickened slightly, perhaps due to the increasing turbulent length scales.

The probability distribution of the mean reactant mass fraction at different positions through the mean flame location agrees with the wrinkled laminar flame model of Bray and Moss (1977), consisting of two delta functions representing pure reactant and pure product joined by a region of low probability proportional to the inverse of the reactant mass fraction gradient.

Diffusion flame in homogeneous turbulence

Hill, Leonard and Rogers modified Rogallo's code to begin a study of a simple diffusion chemical reaction in incompressible homogeneous turbulence. The objective was to determine the influence of vorticity and strain rate on the structure and propagation of the reaction zone (flame).

They considered a simple irreversible chemical reaction $A + B + C \rightarrow P + C$ occurring in isotropic turbulence with the reaction rate proportional to the product of the local concentrations of non-premixed reactants A and B through a constant reaction rate coefficient. P denotes the product, and C is an inert diluent. The mass fractions of the four species were computed along with the hydrodynamic field on a $64 \times 64 \times 64$ grid. The initial chemical composition consisted of alternating slabs

of pure reactants $A + C$ and $B + C$. The Schmidt number was unity for all species. Two runs with different reaction rates resulted in Damkohler numbers based in the initial mean reactant concentration, turbulence intensity, and integral velocity scale of 2 and 10.

The instantaneous reaction front appeared more convoluted in this study than in the premixed flame calculation described previously, presumably due at least in part to the higher Reynolds number of this simulation. The structure of surfaces of constant reactant concentration appear to be well correlated with the local velocity field. The simulation indicates that the dissipation microscale of the concentration fields is not greatly affected by the Damkohler number, suggesting that the diffusive effects can be treated reasonably well by correctly modeling an equivalent non-reacting flow.

These observations may be helpful in reaction for modeling. Hill and Leonard are continuing this work, and plan to study the effects of mean strain and shear on the flames, variation of the reactant Schmidt numbers, sensitivity to initial conditions and non-stoichiometric mixtures.

W.C. Reynolds, M. M. Rogers

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