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Analysis of non-premixed turbulent reacting flows

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Studies of chemical reactions occurring in turbulent flows are important in the understanding of combustion and other applications. Some situations, hypersonic reacting flows for example, are difficult to study experimentally and will benefit from direct numerical simulations. Current numerical methods are limited in their applications due to the numerical resolution required to completely capture all length scales but, despite the fact that "realistic" combustion cannot be solved completely, numerical simulations can be used to give insight into the interaction between the processes of turbulence and chemical reaction (Jou and Riley, 1987).

The objectives of this work were (1) to investigate the effects of turbulent motion on the effects of chemical reaction to gain some insight on the interaction of turbulence, molecular diffusion and chemical reaction to support modeling efforts, and (2) to develop efficient strategies for evaluation of multi-point probability density functions (pdfs) and develop other post-processing tools. For lack of time, only the first objective was actually addressed.

A direct turbulence simulation spectral code (Rogallo 1981) was modified to include the effects of chemical reaction and applied to an initial value problem of chemical reaction between non-premixed species. Preliminary results show the dissipation microscale of the scalar variance to be independent of Damkohler number. The influence of hydrodynamics on the instantaneous structure of the reaction was investigated.

The specific problem under consideration is the isothermal, irreversible chemical reaction of two initially segregated species, of the type

$$A + B \rightarrow P \tag{1}$$

occurring in a decaying homogeneous isotropic turbulent flow. The concentration of one reacting species follows the mass conservation equation

$$\frac{\partial A}{\partial t} + \mathbf{u} \cdot \nabla A = D_A \nabla^2 A - KAB \tag{2}$$

and the turbulent velocity field obeys the Navier-Stokes equations

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u} \, . \tag{3}$$

The reaction-rate coefficient, K, is constant, and so the situation can be thought of as an isothermal diffusion flame. The turbulent velocity and the concentration of

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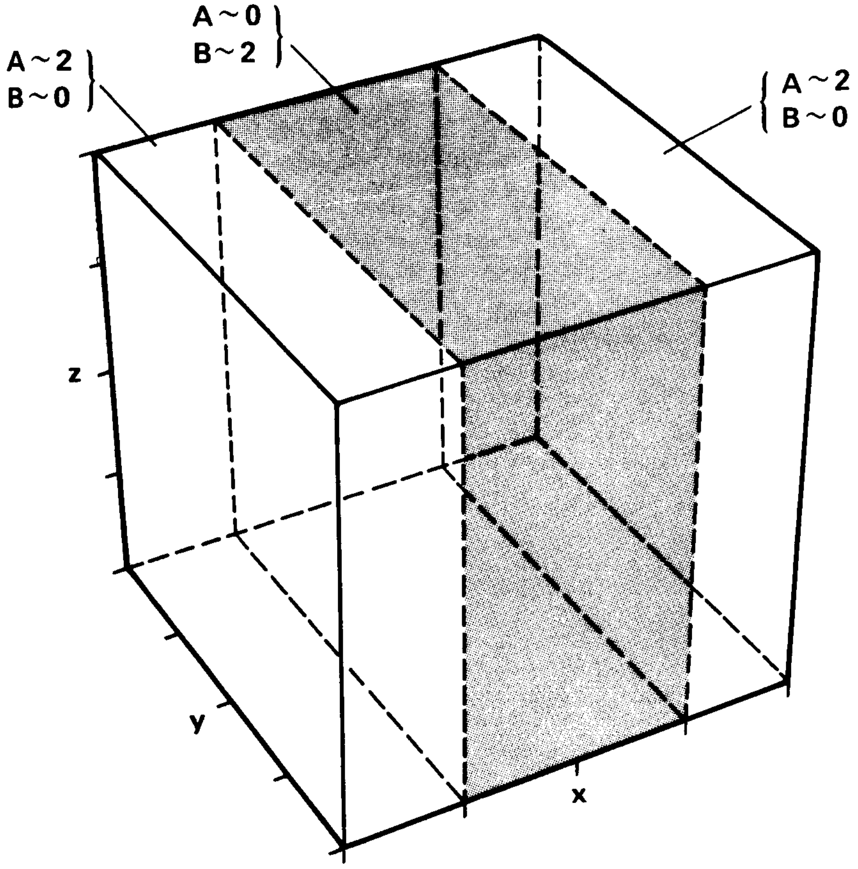

FIGURE 1. Schematic diagram of initial conditions for reactants A and B.

chemical species were all calculated using direct numerical simulation. A pseudospectral method was used with aliasing errors removed. It was necessary to add the term for chemical reaction in equation (2) to an existing program for the direct simulation (Rogallo 1981; see also Lee and Reynolds 1985). The Courant-Freidricks-Lewy stability criterion was appropriately modified to include the effect of reaction on the scalar field equation, and some modifications were needed to obtain diagnostics for the scalar field.

Two calculations were performed on a mesh of 64x64x64 points. Three velocity components and four scalar components were calculated in each simulation, including the reactant species (denoted as A and B), the product species (denoted as P) and the non-reacting species (denoted as C). Two different values of the reaction-rate coefficients were used in the study. The Damkohler numbers (dimensionless reaction-rate coefficients) based on the initial mean reactant concentration, turbulence intensity and the integral velocity length scale were 10 and 2 for the two runs. The Schmidt number for all species was unity. The initial conditions for the reactant species are illustrated in Figure 1. Initial values of A and C were identical. The turbulence was freely decaying from an arbitrarily chosen initial energy spectrum.

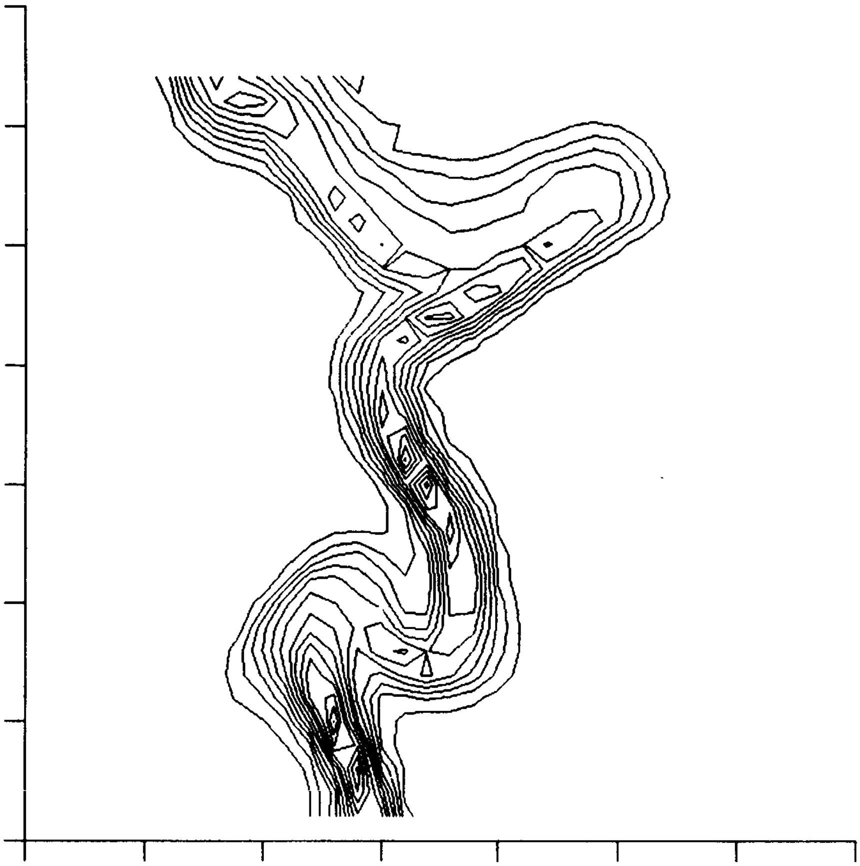

FIGURE 2. Reaction term in equation (2), KAB, for $t = 1.1$ and $Da = 10$. The contour interval is 0.2.

The initial Reynolds number based on the Taylor microscale was 24. Velocity fields were initialized using random numbers scaled to fit a given energy spectrum that was nearly Gaussian in form. The simulations were carried out for 400 steps for the case with the higher reaction rate and for 300 steps for the case with the lower reaction rate.

Modification of the program, small-scale calculations to verify the changes, and running the 64x64x64 calculations required three weeks to complete. Several data sets were saved with the full set of Fourier coefficients for the scalar and velocity fields, so that the IRIS workstation and interactive graphics programs could be used to examine the spatial dependence of the fields in physical space at a single value of time. Many of the results are only qualitative at this writing.

Our proposal was to examine the local scalar dissipation rates and the local reaction rates to determine the influence of vorticity or rate of strain on the reaction and the structure of the scalar field. Consequently, the region where the reaction occurs was the focus of attention. The location of this region is marked by the value of the term KAB in equation (2) and is clearly shown in Figure 2. The region was

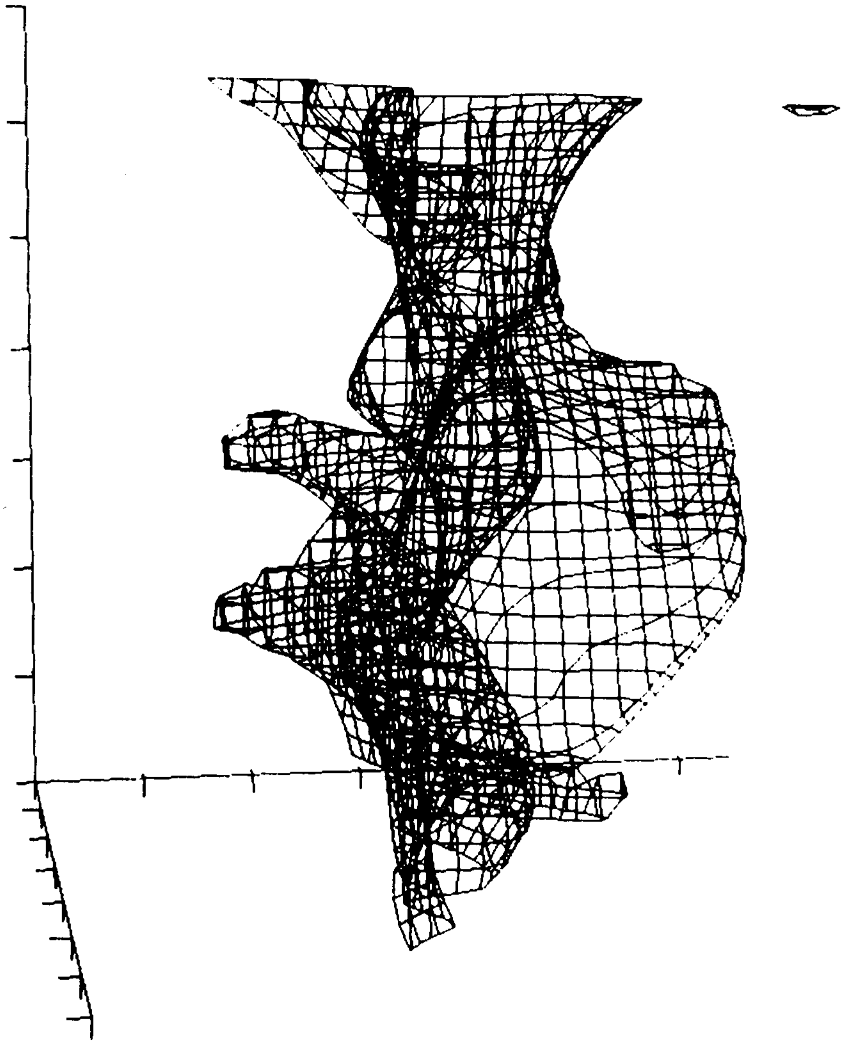

FIGURE 3. Surface where the conserved scalar $A - B$ equals zero.

also marked by the product species concentration and high values of the magnitude of the gradients of reactant species concentrations as the reaction was nearly diffusion limiting, due to the high reaction rates. The reactant species, therefore, remain highly segregated over the course of the reaction with sharp gradients in the reaction zone. The thickness of the zone is about four grid points at the higher Damkohler number. The reaction zone is distorted by the turbulent motion and the reaction rate and product concentrations are not uniform within the reaction zone. The regions of high reaction rate correlate only roughly with regions of high product concentration.

An attempt was made to determine the influence of the hydrodynamics on the structure of the reaction zone. Surfaces at which the concentration of the conserved scalar $A - B$ equals zero appear to be good indicators of the location of the reaction

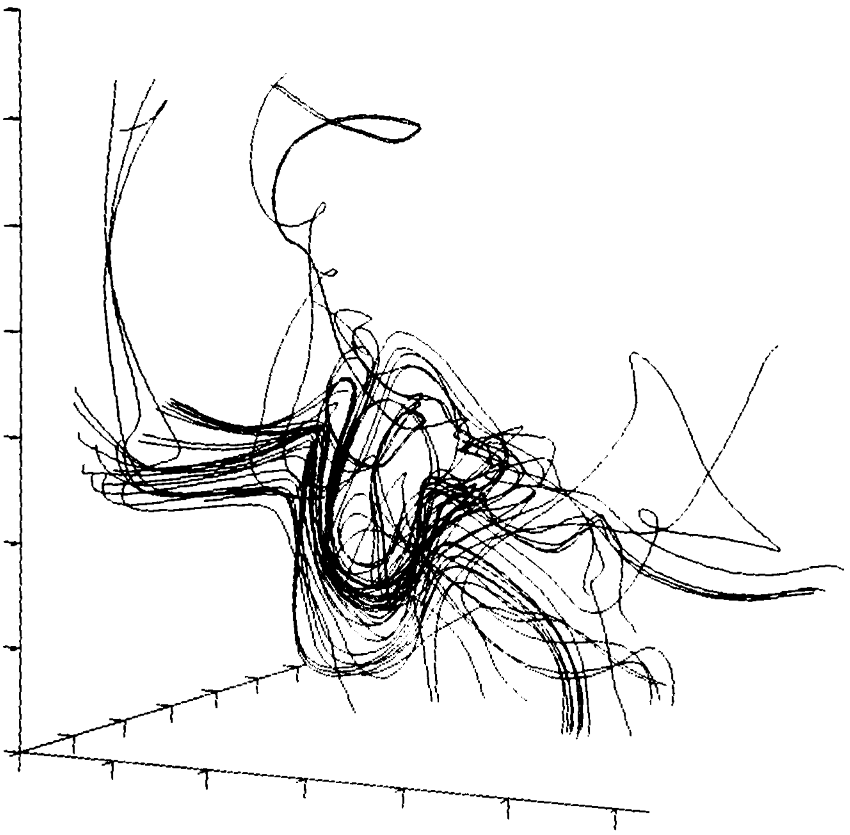

FIGURE 4. Vortex lines passing through points near one of the finger-like structures in Figure 3.

zone. These surfaces show fingers of reactant pushing into the reaction zone (Figure 3). Vortex lines passing through a group of points located near one of the fingers are shown in Figure 4. The vortex lines are suggestive of the idea that a vortex ring is producing the finger by eduction, but the evidence is inconclusive and needs more extensive investigation.

The results of the simulations supported earlier findings (Leonard and Hill, 1987) that the dissipation microscale of the concentration fields is not greatly affected by the Damkohler number (Table 1). Modeling the effects of dissipation is a weakness of some theories, as the process is not local. These findings suggest that diffusive effects can be treated reasonably well by correctly modeling an equivalent non-reacting flow.

The work done at the summer program was a beginning of an effort to look closely at the influence of hydrodynamics on the instantaneous structure of the reaction. Previous work (Leonard and Hill, 1987) had looked primarily on volume-averaged quantities to test closure theories (Toor 1969; Patterson, 1981). The effect of strain rate on the reaction has yet to be investigated. Further work is planned for analysis

Da	λ_A $t_e = 0$	λ_A $t_e = 1$
0	1.46	1.02
2	1.46	1.00
10	1.46	0.94

$$Da = K\overline{A_0}u_0'/L_0 \qquad \lambda_A^2 = 6\overline{a^2}/\overline{|\nabla a|^2} \qquad t_e = L_0/u_0'$$

Table 1. Effect of Da on dissipation microscale of reactant A.

of the simulations performed during the CTR summer program and for additional simulations to study the effects of parameters such as different molecular diffusivities for reactant species, non-stoichiometric ratio of reactant concentrations, steady (forced) turbulence, external mean shear or strain, and different initial velocity conditions.

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REFERENCES

JOU, W.-H. & RILEY, J. J. 1987 On Direct Numerical Simulations of Turbulent Reacting Flows. *AIAA-87-1324*.

LEE, M. J. & REYNOLDS, W. C. 1985 Numerical Experiments on the Structure of Homogeneous Turbulence. *Dept. Mech. Eng. Report TF-24*. Stanford University, Stanford, California.

LEONARD, A. D. & HILL, J. C. 1987 Direct Numerical Simulation and Simple Closure Theory for a Chemical Reaction in Homogeneous Turbulence. *U.S.-France Joint Workshop on Turbulent Reactive Flows,* Rouen, France.

PATTERSON, G. K. 1981 Application of Turbulence Fundamentals to Reactor Modelling and Scaleup. *Chem. Eng.Commun.* **8**, p 25.

TOOR, H. L. 1969 Turbulent Mixing of Two Species With and Without Chemical Reaction. *Ind. Eng. Chem. Fundam.* **8**, p655.

ROGALLO, R. S. 1981 Numerical Experiments in Homogeneous Turbulence. *NASA TM-81315*.