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NUMERICAL EXPERIMENTS ON TURBULENT MIXING(U) CORNELL  
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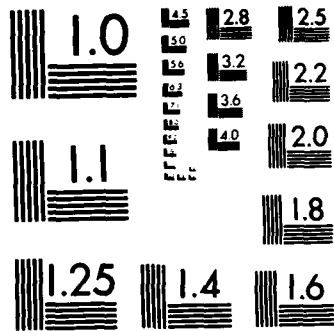
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In turbulent combustion, mixing by molecular transport is an essential process that is not well understood. Because mixing occurs on the smallest length and time scales it is difficult to study experimentally. Instead, we are starting a study based on the direct numerical simulation of turbulence, initially for a conserved passive scalar in homogeneous isotropic turbulence. The Eulerian velocity and scalar fields are calculated from the exact evolution equations, and both Eulerian and Lagrangian statistics are deduced from the computed fields. A particle-tracking scheme, needed to extract Lagrangian information, has been implemented and is undergoing testing. In addition, in order to study processes in stationary turbulence, a forcing algorithm has been developed and implemented, and is being tested.

## INTRODUCTION

Nearly all flows of technological importance are turbulent. In most combustion devices, turbulence plays a vital role in promoting fluid mixing and hence accelerating combustion rates. While experimental techniques are making significant progress, there are unanswered fundamental questions concerning turbulent mixing that remain beyond the reach of experimentalists. These unanswered questions are an obstacle to the development and testing of statistical models of turbulence. Answers are needed so that these models can be developed into reliable design tools.

The objective of this work is to answer fundamental questions concerning turbulent mixing, through numerical simulations of turbulent flows.

The details of the mixing process are difficult to study experimentally because the smallest length and time scales must be resolved. Further, it is not sufficient just to measure the value of the scalar (e.g. composition or temperature) at a point: rather its first two derivatives in each direction are the prime quantities of interest. That mixing is a microscale process compounds experimental difficulties, but it provides grounds to hope for universality. That is (according to classical theory), at high Reynolds number, the details of the mixing process are determined by a few macroscale quantities, but are otherwise independent of the large scales of the flow.

These considerations show that the direct numerical simulation of turbulence provides a good means of studying turbulent mixing. All scales are resolved, and any quantity of interest can be determined since the fields are known for all positions and times. In view of the universality of the small scales, it is sufficient to simulate just a few flows - the most easily computed being homogeneous turbulence.

## RESEARCH OBJECTIVES

1. To adapt Rogallo's direct numerical simulation code to run on a MASSCOMP minicomputer, and to check the veracity of the adaptations.
2. Similarly, to adapt the code to run on Cornell's Production Supercomputer Facility.
3. To develop, test and implement a numerical algorithm for tracking fluid particles through the simulated flow field.
4. To develop, test and implement a forcing procedure so that stationary isotropic turbulence can be studied.
5. To perform an Eulerian study of scalar mixing. Primary quantities of interest are the joint statistics of the passive scalar and its rate of dissipation.
6. Similarly, to perform a Lagrangian study of turbulent mixing. Here Lagrangian time series of the scalar are the prime quantities of interest.

## CURRENT STATUS

1. We have translated Rogallo's code into FORTRAN and checked the results in detail against Rogallo's calculations. The MASSCOMP has a built-in array processor capable of a peak rate of 5 Mflops. It is extremely difficult to achieve this peak rate, and we are content to have achieved an overall rate of about 1Mflops.

At one stage in the development of the code, the i/o was taking twice as long as the computation time. However, with the aid of MASSCOMP personnel, we incorporated asynchronous C i/o routines that have virtually eliminated this problem.

On this dedicated minicomputer we can perform  $(64)^3$  simulations in 1 day.

2. Rogallo's code has also been run on the Cornell Production Supercomputer Facilities machines - both FPS264's and the IBM3084. On the FPS264, because of storage limitations and slow i/o, only  $(32)^3$  calculations are possible. On the IBM3084  $(64)^3$  calculations have been performed in about 10 hours. We are ready to take advantage of the IBM 3090/400 due to arrive Fall 1986. This will be faster than the 3084 by at least a factor of 10 and will allow  $(128)^3$  calculations.
3. In order to extract Lagrangian time series from the computer flow field, a fluid particle tracking algorithm is required. One has been developed that uses a second-order Runge-Kutta scheme in time, consistent with Rogallo's code. On each Runge-Kutta step, interpolation is used to evaluate the fluid particle velocity from the velocities at the grid nodes in physical space. Initially simple (second-order accurate) linear interpolation was used. But numerical tests showed that this is insufficiently accurate. We have developed two types of more accurate schemes: Taylor series schemes; and, schemes in which the interpolation weights are optimized with respect to the turbulence spectrum. A comparative testing of these schemes is in progress. These tests are hindered by the obvious lack of exact solutions for particle paths in turbulence.
4. Lagrangian time series are most easily analyzed if the turbulence is stationary. This can be achieved by forcing. That is, energy is artificially added to the large-scale motions. The assumption underlying the use of this artifice is that the small-scale structures in the turbulent field are statistically independent of the large scale flow and the details of the forcing, being confined to low wavenumbers and large scales, do not, therefore, substantially alter the values of the small-scale quantities. This postulate is a reasonable one for high Reynolds-number flows and it follows from the Kolmogorov hypotheses. But, at the moderate Reynolds-numbers characteristic of direct numerical simulations, the postulate is less certain since the energy-containing and the dissipation regions in the energy spectrum may overlap. We are in the process of testing the validity of the postulate.

We have developed a forcing scheme which is different from the previous methods of Siggia and of Kerr. Briefly stated, the scheme involves adding a random forcing term to the momentum equations. The Fourier coefficients of this term are Uhlenbeck-Ornstein processes having a specified time scale and standard deviation. This forcing is restricted to the low wavenumber modes. The energy input occurs due to the correlation of the Fourier coefficients of the forcing and the velocity. By choosing the time scale and the standard deviation of the forcing we can control the time scale and average magnitude of the energy input.

Using this method we achieve statistically stationary turbulent fields in our numerical simulations. Our preliminary results show that, indeed, for a range of forcing time scales some high wavenumber quantities remain unchanged as long as the relevant flow parameters (e.g. the Reynolds number) are kept fixed. We tentatively conclude, then, that the small-scale statistics are, by and large, independent of the details of the forcing over a range of the forcing parameters. Testing of the forcing procedure is still in progress.

5.- Work on these two research objectives has yet to start.

6.

#### PUBLICATIONS

Under this research contract, the P.I. has written two papers concerned with turbulent combustion:

Pope, S.B. (1986) "The Evolution of Surfaces in Turbulence" submitted to Phil. Trans. Roy. Soc. Lond.

Pope, S.B. (1987) "Turbulent Premixed Flames" to appear in Annual Reviews of Fluid Mechanics, Vol. 19.

In addition, within the next six months we expect to submit two papers to the Journal of Computational Physics: one on particle-tracking, one on forcing.

#### PERSONNEL

Prof. S.B. Pope	P.I.	15%
Dr. V. Eswaran	Post-doctoral Research Associate	50%
Mr. P.K. Yeung	Ph.D. student	100%
Mr. S. Girimaji	Ph.D. student	summer only

#### INTERACTIONS

A presentation on this work was made at the AFOSR contractors meeting, Caltech 1985.

INVENTIONS

No inventions or patent disclosures have stemmed from the research effort.

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