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NUMERICAL EXPERIMENTS ON TURBULENT MIXING(U) CORNELL
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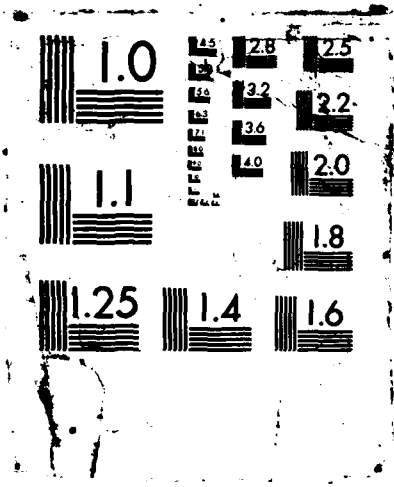
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<p>Mixing in simple turbulent flows has been investigated using (64)⁹ and (128)³ Direct Numerical Simulations. In turbulent combustion, mixing by molecular transport is an essential process that is not well understood. Because mixing occurs on the smallest length and time scales it is difficult to study experimentally. Instead, we have employed 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. The testing of a number of such particle tracking schemes has been completed with good results: accurate Lagrangian information can be extracted at a modest computational cost. In order to study processes in stationary turbulence, a forcing algorithm has been implemented. Tests on this scheme are complete, again with good results: the small scales are unaffected by the details of the forcing. Studies have been performed of: the mixing of a passive scalar; Lagrangian velocity, acceleration and dissipation statistics; and mixing and combustion problems viewed in terms of surfaces.</p>			
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INTRODUCTION

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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 to 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.

As well as looking at a scalar and its derivatives at a point, mixing and combustion can be usefully studied in terms of surfaces. For example, in a simple turbulent diffusion flame, reaction is concentrated around a constant property surface. In premixed turbulent combustion, the flame can form a highly wrinkled propagating surface. Surfaces are difficult to study experimentally since they are three-dimensional and encompass all scales.

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.

As is described in the following sections, we have performed a series of $(64)^3$ and $(128)^3$ direct numerical simulations of homogeneous isotropic turbulence. From the data obtained — both Eulerian and Lagrangian — we have been able to address several important questions in mixing and combustion theory.

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 the Cornell National Supercomputer Facility machines.
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.



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5. To study the mixing of a passive scalar, primarily through an examination of its pdf.
6. To study the Lagrangian statistics of velocity, acceleration and dissipation.
7. To use Lagrangian time series of the velocity gradient to address mixing and combustion issues in terms of line, surface and volume elements.

ACCOMPLISHMENTS

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 1 Mflops.

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 synchronous C i/o routines that have virtually eliminated this problem.

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

2. The Cornell National Supercomputer Facility operates two types of Supercomputer: FPS264's and an IBM 3090/600.

In the second year, most of our production runs were performed on the FPS264's. These machines have sufficient memory for us to perform $(16)^3$, $(32)^3$ and $(64)^3$ calculations, without explicit i/o. To perform $(128)^3$ calculations, would require either explicit i/o, or running 8 FPS264's in parallel. Because the i/o is too slow we did not pursue this route.

The IBM3090/600 is a very fast scalar machine with six vector processors that can be run in parallel. In the third year we adapted Rogallo's code to this machine, by recoding it to better exploit the vector and parallel features. Using six-way parallelism, and with the machine being lightly loaded, we can achieve computing speeds in excess of those on the Cray XMP.

With this latest (and hopefully final) version of the code we have performed $(128)^3$ simulations.

3. In order to extract Lagrangian time series from the computed 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 three types of more accurate schemes: Taylor series schemes; cubic splines; and, schemes in which the interpolation weights are optimized with respect to the turbulence spectrum.

A comparative testing of these schemes has been completed. Such testing is made quite difficult by the obvious lack of an analytic solutions for turbulent flow that can be compared directly with numerical results. We have performed four types of test: direct measurement of the interpolation error; determination of particle-tracking errors in a simple laminar flow for which an analytical solution exists; determination of

particle-tracking errors in a frozen turbulence field; and, determination of particle-tracking errors in forced isotropic turbulence.

The results show that the cubic spline scheme has the best overall performance. Using it, accurate Lagrangian time series can be extracted without unduly increasing the computational cost of the basic Eulerian code.

A paper describing the particle-tracking work (Yeung & Pope 1987b) has been submitted to the Journal of Computational Physics.

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 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 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.

The forcing scheme has been fully tested (Eswaran & Pope 1987a). It is found that statistically stationary turbulence is, indeed, achieved. A method of choosing the parameter in the Uhlenbeck-Ornstein processes has been established that allows turbulence of a specified Reynolds number to be generated. Because the numerical algorithm is based on a rectilinear grid in physical space, some anisotropy is introduced. Tests show that this is small: even the large-scale motions appear closely isotropic. Most importantly, it is found that the details of the forcing do not affect the small scales. Thus conclusions about microscale processes drawn from studies on forced turbulence have general applicability.

The paper describing this study (Eswaran & Pope 1987a) has been accepted for publication in Computers and Fluids.

5. Considering the importance of mixing to combustion, it is remarkable how ignorant we are of the details of the simplest mixing problem. To help remedy this situation we have performed Direct Numerical Simulations of a passive scalar in stationary turbulence.

Consider a passive scalar field $\phi(\underline{x}, t)$ which initially is composed of blobs of $\phi = -1$ and an equal amount of blobs of $\phi = 1$. Initially, then, the probability density function (pdf) of ϕ is a double-delta function distribution. As time progresses, due to mixing, the delta functions become smeared, and eventually the pdf becomes a Gaussian

centered on $\phi = 0$. This simple mixing problem is often taken as a test of mixing models — even though we have virtually no knowledge of how the pdf evolves between its initial and final stages.

We have simulated this flow and extracted joint pdf's of ϕ and its dissipation rate ϵ_ϕ , as well as conditional dissipation rates. The results are described in a paper (Eswaran & Pope 1987b) which has been accepted for publication in *Physics of Fluids*. In accord with experimental observations we find that the decay rate of the scalar depends strongly on the initial scalar length scale. But surprisingly, it is found that the shapes adopted by the pdf during its evolution appear to be independent of the initial condition.

These data will prove extremely valuable in the development of better mixing models.

6. A major emphasis of our work is to extract Lagrangian statistics. We have performed a study (Yeung & Pope 1987a) in which Direct Numerical Simulations are used to obtain Lagrangian time series of velocity, acceleration and dissipation. From these various statistics can be found.

Our numerical simulations have been successful in obtaining a wide-range of important Lagrangian velocity statistics, many of which, notably the cross-correlation between dissipation and acceleration, have apparently not been reported before. Numerical tests show that on 64^3 grids, the resolution is adequate to obtain accurate second-order velocity statistics up to R_λ at least 50. However, high-order statistics above R_λ about 30, in particular, high-order moments of velocity increments, may be underestimated. Nevertheless, several interesting physical conclusions can be drawn.

First, a Reynolds number of $R_\lambda = 50$ is not sufficient high for the Kolmogorov similarity hypotheses to apply. Second, Lagrangian velocity increments over short time intervals are observed to be intermittent and highly non Gaussian, the more so as Reynolds number increase. Third, the dissipation is found to be close to having a log normal distribution, especially for higher Reynolds numbers. Fourth, dissipation and acceleration are highly correlated, providing evidence of the close connection between dissipation fluctuations and the intermittency exhibited by the velocity increments. A transformation is time normalized by the local Kolmogorov scale yields more nearly Gaussian process.

7. Several important topics related to mixing and combustion have been addressed by studying the behavior of lines, surfaces and volume elements in turbulence. This is effected by extracting time series of the Lagrangian velocity gradient tensor.

It has long been recognized (at least since Batchelor 1954) that mixing is closely related to the deformation of infinitesimal material elements — lines, surfaces and volumes. For example, the stretching of material surfaces causes neighboring surfaces to approach each other, thus increasing gradients and mixing. Indeed in some cases (e.g. early times or large Schmidt numbers) the whole mixing problem can be posed in terms of the behavior of material surfaces.

Through DNS we have determined samples of the deformation tensor which completely describes the deformation of a material element. The wealth of information obtained is described by Girimaji and Pope (1988). As a simple example, we have studied the length of an infinitesimal line element. As can be shown analytically,

initially the length does not increase, because there is no alignment between the line and the rate-of-strain tensor. But eventually the length increases exponentially with time.

The flamelet model of turbulent diffusion flames is currently quite popular even though several of its key premises remain untested. For example, it is assumed that scalar dissipation χ is uniquely related to the rate of strain γ normal to the stoichiometric surface; and further it is assumed that there is but a small probability of γ being positive (corresponding to the surface being compressed in its own plane). We have tested these hypotheses. With mild assumptions, a stoichiometric surface is well approximated by a material surface. For this case we find that there is no unique relationship between χ and γ , and that γ is positive about 30% of the time.

A useful model of premixed turbulent flames is that, at any instant, the flame can be regarded as a surface separating reactants from products (Pope 1987a,b, Pope & Cheng 1988). This surface propagates normal to itself at a speed w relative to the fluid. (To a first approximation w is the laminar flame speed.) When w is small (compared to the turbulence intensity, say) it has been assumed that the propagating surface remains close to the material surface on which it originated. This is certainly true when w^* (w normalized by the Kolmogorov velocity scale) is small; and then z^* (the distance between the surfaces, normalized by the Kolmogorov length scale) is simply proportional to w^* . From DNS we have computed the pdf of z^*/w^* . From this we can deduce, for example, that even for $w^* = 1$ there is a significant probability that the surfaces will separate by 15 Kolmogorov scales. (Once this occurs, the linear analysis used breaks down, and the surfaces are likely to separate yet further.)

PUBLICATIONS

V. Eswaran and S.B. Pope (1987a) "An examination of forcing in direct numerical simulations of turbulence," *Computers and Fluids* (to be published).

V. Eswaran and S. B. Pope (1987b) "Direct numerical simulations of the turbulent mixing of a passive scalar," *Physics of Fluids* (to be published).

S. Girimaji, S. and S. B. Pope (1988) "Deformation of infinitesimal material elements in turbulence," in preparation.

S. B. Pope (1987a) "Turbulent premixed flames," *Annual Reviews of Fluid Mechanics*, 19, 237-70.

S. B. Pope (1987b) "The evolution of surfaces in turbulence," *International Journal of Engineering Science* (to be published).

S. B. Pope and W. K. Cheng (1988) "The stochastic flamelet model of turbulent premixed combustion," submitted to *Twenty-Second Symposium (International) on Combustion*.

P. K. Yeung and S. B. Pope (1987a) "Lagrangian velocity statistics obtained from direct numerical simulations of homogeneous turbulence," *Sixth Symposium on Turbulent Shear Flows*, Toulouse.

P. K. Yeung and S. B. Pope (1987b) "An algorithm for tracking fluid particles in numerical simulations of homogeneous turbulence," submitted to Journal of Computational Physics.

PERSONNEL

Prof. S.B. Pope	Principal Investigator	15%
Awards D. Sc. (Eng.), University of London, May 1986		
Dr. V. Eswaran	Post-doctoral Research Associate	50%
Mr. P.K. Yeung	PhD student (degree expected 8/88)	100%
Mr. S. Girimaji	PhD student (degree expected 8/89)	30%

INTERACTIONS

The P.I. participated in the workshop on Research Directions and Funding in Fluid Mechanics, held in Savannah, September 17-20, 1986. He contributed to the group report on Chemically Reacting/Combustion Flows.

Meetings Attended (1986-87)

S.B. Pope, Seminar UTRC, Hartford, CT, May 1986.

S.B. Pope, Twenty-First Symposium on Combustion, Munich, August 1986.

S.B. Pope, Society of Engineering Science, Annual Meeting, Buffalo, NY, August 1986.

S.B. Pope, American Physical Society, Fluid Dynamics Division Annual Meeting, Columbus, OH, November 1986.

V. Eswaran, Tenth Symposium on Turbulence, Missouri-Rolla, September 1986.

S.B. Pope, A.I.Ch.E. Annual Meeting, New York City, Invited lecture, November 1987.

S.B. Pope, SIAM. San Francisco, Invited lecture, January 1987.

S.B. Pope, Rouen, France (Workshop), Invited talk, July 1987.

S.B. Pope, U.C., Davis (Workshop), Invited talk, April 1987.

S.B. Pope, General Motors Research Laboratories, (Workshop), October 1987.

S.B. Pope, APS/DFD Meeting, Eugene, Oregon, November 1987.

P.K. Yeung, APS/DFD Meeting, Eugene, Oregon, November 1987.

S.B. Pope, Yale, Invited Seminar, October 1987.

P.K. Yeung, Sixth Symposium on Turbulent Shear Flows, Toulouse, France, September 1987.

INVENTIONS

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

END

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