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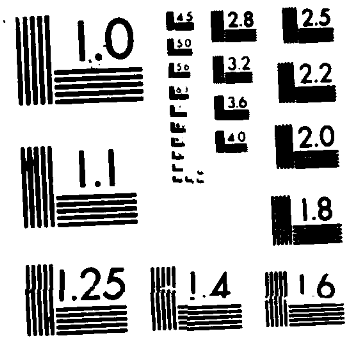

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PDF Calculations of Premixed Combustion

Final Report

S.B. Pope

April 8, 1987

U.S. Army Research Office

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The PDF method has been further developed and used to calculate the detailed structure of turbulent premixed flames. For one-dimensional flames, combustion generated turbulence and counter-gradient diffusion are observed. The Monte Carlo method used to solve the PDF equation has been refined in several respects. In particular an accurate cross-validated cubic smoothing spline algorithm has been developed and tested.

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PROBLEM STATEMENT

This research project is concerned with applying PDF methods to premixed turbulent flames. The method is used to calculate the detailed structure of two types of flame: the stationary, one-dimensional, plane flame; and, the rod-stabilized V-flame. In addition, numerical aspects of the Monte Carlo method used are refined.

IMPORTANT RESULTS

The principal results are itemized below. Full details are presented in the papers and theses referenced.

1. A comprehensive set of calculations were performed for the variable-density, plane, one-dimensional premixed flame. Counter-gradient diffusion and large energy production are observed, in accord with experimental observations and with the Bray-Moss-Libby model.

2. Pdf calculations have been performed of turbulent premixed V-flames, and the results have been compared to the measurements of R.K. Cheng. For two reasons, this comparision reveals shortcomings in the modelling approach used. First, in the flames considered, the laminar flame speed is of the same order as the turbulence intensity, whereas in the calculation it is assumed to be negligible. Second, the calculations essentially invoke the boundary-layer assumptions which are inaccurate because of the significant heat release and volume expansion. Because of these deficiencies the quantitative comparison of calculations and experiments is poor. However, many important quantitative features are predicted.

3. An essential component of the Monte Carlo method is an algorithm for approximating the mean of a function, given sample values with large random fluctuations. This is a classic problem that arises in many different contexts. For some years we have been using a method (developed by us) based on cubic smoothing splines using cross-validation. This method works extremely well, but until recently its performance had not been quantified. Since the method is successful, and has wide applicability, we have described it in a paper (Pope & Gadh 1987) and demonstrated its excellent performance.

4. Two contributions have been made to our understanding of the pressure field in turbulent premixed flames. First, it has been shown that the complete neglect of the fluctuating pressure field can lead to dramatic errors, since it is tantamount to ignoring the fluid-mechanical effect of acceleration reaction. Second, it has been shown that in the flame-sheet regime the pressure field can be decomposed into five contributions due to: velocity gradients in the uniform-density reactants and products; the velocity of the flame sheet; the acceleration of the flame sheet; and a boundary contribution that is of no consequence. An interesting observation is that the pressure field due to the flame sheet velocity causes no acceleration of the products.

5. A formalism has been developed for the statistical treatment of surfaces in turbulence. Since in many circumstances flames can be approximated as surfaces, this formalism can form the basis of a new statistical approach to modelling combustion in the flamelet regime.

LIST OF PUBLICATIONS, REPORTS AND THESES

1. S.B. Pope (1985) "PDF methods for turbulent reactive flows," Prog. Energy Combust. Sci., 11, 119-192.

2. M.S. Anand and S.B. Pope (1987) "Calculations of premixed turbulent flames by pdf methods," Combust. Flame 67, 127-142.

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

4. S.B. Pope (1986) "The evolution of surfaces in turbulence," submitted for publication to Int. J. Eng. Sci..

5. S.B. Pope and R. Gadh (1987) "Fitting noisy data using cross-validated cubic smoothing splines, " submitted to SIAM J. on Scientific and Statistical Computing.

6. M.S. Anand (1986) "Probability density function (pdf) calculations for premixed turbulent flames" Ph.D. Thesis, Cornell University.

7. R. Gadh (1987) "Numerical aspects of Monte Carlo methods as applied to turbulent premixed flames, " M.S. Thesis, Cornell University.

SCIENTIFIC PERSONNEL SUPPORTED AND DEGREES AWARDED

Professor S. B. Pope, D. Sc. (Eng.)
University of London, 1986

Dr. M.S. Anand, Ph.D.
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Mr. R. Gadh, M.S.
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END

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