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MONTE CARLO CALCULATIONS OF

TWO-DIMENSIONAL COMBUSTOR FLOWS

Final Report

Stephen B. Pope

4/12/82

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Progress has been made in developing a computational procedure to calculate the properties of two-dimensional turbulent reactive flow fields appropriate to gas turbine combustors. The flow field is calculated by a standard finite-difference technique while a Monte Carlo method is used to solve the transport equation for the joint pdf of the species mass fractions. In the course of this project, a more accurate and efficient grid-free Monte Carlo method has been devised and an improved model of turbulent mixing has been developed. For plane constant-density flows, the Monte Carlo method has been implemented in a computer program.

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FOREWORD

"Monte Carlo Calculations of Two-Dimensional Combustor Flows" was originally a two-year research program being performed at the Massachusetts Institute of Technology. Since the principal investigator left MIT at the end of 1981, the contract was terminated, and the research is being continued at Cornell University under contract number DAA929-82-K-0017. This final report is for the one-year period 1/13/81 - 1/12/82.

Problem Statement

The objective of this work was to develop and demonstrate a combined Monte Carlo/finite-difference procedure for calculating the properties of two-dimensional combustor flows.

It is a formidable theoretical problem to calculate the turbulent reacting flow properties in a gas turbine combustor. Added to the well-known problems of calculating any turbulent flow, are the difficulties caused by the highly non-linear combustion reactions. An approach that goes a long way to overcoming the problems caused by the non-linear reactions is to describe the turbulent reacting flow field in terms of the joint probability density functions (pdf) of the species mass fractions. The transport equation for the joint pdf of the species contains an exact term pertaining to reaction. That is, irrespective of the complexity and non-linearity of the reaction scheme, in the joint pdf equation the reaction term does not have to be modelled. For this reason, several authors have used this equation to calculate turbulent reactive flows: Dopazo (1975), Janicka, Kolbe and Kollmann (1979) and Pope (1981a).

By standard techniques (e.g. finite-differences), the joint pdf equation would be extremely expensive to solve numerically (if, ineeed, it were possible), except in simple cases. However, by using a Monte Carlo method, the equation can be solved at a reasonable cost for situations of practical complexity. The basic Monte Carlo method is described by Pope (1981b).

The Monte Carlo solution of the joint pdf equation deals only with the species fields. The mean velocity and turbulence fields are calculated by a standard finite difference procedure using the k-ε turbulence model.

Results

In the Monte Carlo method described by Pope (1981b), the joint pdf is represented by ensembles of elements at discrete grid nodes. There is both a truncation error and a statistical error associated with the discretization of physical space. An improved method has been developed in which the elements are distributed throughout the flow field — not just at discrete nodes. This method resembles a Lagrangian particle tracking procedure with a random walk to simulate turbulent diffusion. The numerical error is greatly reduced, and hence the computational economy is improved. The method is described by Pope (1982a).

This method has been implemented for plane, constant-density flows. The two major tasks were to treat the boundaries correctly and to develop the necessary least-squares cubic spline procedures. The cubic splines are used to extract information about mean quantities from the elements randomly distributed through the flow field. At the end of the contract, the code had been developed and testing was under way.

One of the components of the Monte Carlo method is a model of turbulent mixing. Most investigators use Curl's (1963) model or a variant of it (Dopazo, 1979; Janicka, Kolbe and Kollmann, 1979). In the course of this investigation it was found that these models have serious defects. Specifically, when the models are applied to the simple case of decaying fluctuations they should predict a Gaussian pdf. However, the predicted pdf is far from Gaussian and, in fact, its fourth and higher even moments are infinite. Because of this observed defect, a new class of mixing models has been developed that overcomes this problem (Pope, 1982b). The improved models result in approximately Guassian pdf's, and a consequent gain in accuracy is expected in the pdf calculations.

Personnel and Publications

The principal investigator Stephen B. Pope and the graduate student Babak Minaie have worked on the project throughout 1981. The following papers have been prepared for publication:

"An Improved Turbulent Mixing Model," by S. B. Pope, to be published in Comb. Sci. Technol., 1982.

"PDF Methods in Turbulent Reactive Flows," by S. B. Pope (in preparation), to be published in Prog. Energy Comb. Sci., 1982.

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