Center for Modeling of Turbulence and Transition
Research Briefs - 1990

The Study of PDF Turbulence Models in Combustion

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1. Motivation and Objectives

1.1 Motivation

The accurate prediction of turbulent combustion is still beyond reach for today's computation techniques. It is the consensus of the combustion profession that the predictions of chemically reacting flow were poor if conventional turbulence models were used. The main difficulty lies in the fact that the reaction rate is highly non-linear, and the use of averaged temperature, pressure and density produces excessively large errors. The probability density function (pdf) method is the only alternative at present time that uses local instant values of the temperature, density, etc., in predicting chemical reaction rate, and thus is the only viable approach for turbulent combustion calculations.

1.2 Objectives

The present work aims at the development and implementation of the the pdf turbulence models in solving realistic combustion problems. The fact that the pdf equation has a very large dimensionality renders finite difference schemes extremely demanding on computer memories and thus impractical, if not entirely impossible. A logical alternative is the Monte Carlo scheme, which has been used extensively in statistical physics. However, the use of Monte Carlo scheme to solve both the flowfield and the chemical reaction is very time consuming. Further more, since CFD has reached a certain degree of maturity as well as popularity, it seems less beneficial to abandon CFD completely and opt for Monte Carlo schemes. Therefore, we propose the use of a combined CFD and Monte Carlo scheme in the present study. The scheme would use the conventional flow solvers when calculating the flowfield properties such as velocity, pressure, etc., while the chemical reaction part would be solved using Monte Carlo solvers.

2. Works Accomplished

2.1 Code development.

A parabolic code with $k-\epsilon$ turbulence models have been developed in the past months. Three different $k-\epsilon$ models have been tested with satisfactory numerical results.

A grid dependent Monte Carlo scheme is being explored. This scheme discretize the pdf equation on a given grid and write, for parabolic flows:

$$\tilde{P}_{x+dx,j} = \alpha_j \tilde{P}_{x,j+1} + \beta_j \tilde{P}_{x,j} + \gamma_j \tilde{P}_{x,j-1} \tag{1}$$

and we require

$$\alpha_j + \beta_j + \gamma_j = 1 \tag{2}$$

Using a very simple test case of a convection/diffusion process with two scalars, it was found that the previous scheme does not conserve mass fractions due to re-contamination. It is found that in order to conserve the mass fractions absolutely, one needs to add further restriction to the scheme, namely

$$\alpha_j + \gamma_j = \alpha_{j-1} + \gamma_{j+1} \tag{3}$$

A new algorithm was devised and is currently being tested. Again using the simple test case of two scalars with assumed constant coefficients in the pdf equation, the new algorithm is shown to conserve the mass fractions perfectly in cases of uniform flows or pure diffusion problems. Deficiencies such as directional bias and re-contamination that were found in the previous algorithm are completely eliminated.

2.2 Applications.

The code developed has been validated by solving a heated turbulent jet. The temperature is treated as a conserved passive scalar and solved using the pdf Monte Carlo simulation while the flow field is obtained using a conventional CFD solver. The mean temperature profile and RMS of the temperature fluctuation were compared with experimental data.

As a first application to combustion problems, the non-premixed flame of hydrogen and fluorine is being studied. A comparison between primary results from the present study and experimental data show that the present scheme predicts the mean flame temperature accurately.

3. Future Plans

1. Further investigate the case of hydrogen-fluorine reaction.
2. Study finite rate calculation of the same non-premixed flame.
3. Study the interaction between mixing and chemical reaction.
4. Study compressibility effects.

4. Publications

1. Hsu, A.T., "The Study of PDF Turbulence Models in Combustion," 9th National Aero-Space Plane Technology Symposium, November 1-2, 1990.

2. Hsu, A.T., " On Recontamination and Directional Bias Problem in Monte Carlo Simulation of PDF Turbulence Models," NASA CFD Conference, April 12-14, 1991, Moffett Field,California.

3. Hsu, A.T., "Progress in the Development of PDF Turbulence Models for Combustion," 10th National Aero-Space Plane Technology Symposium, April 23-25, 1991, Monterey, California.

4. Hsu, A.T., "The Study of PDF Turbulence Model in Nonequilibrium Hydrogen Diffusion Flames" AIAA Paper 91-1780, Honolulu, Hawaii, June, 1991.