PROGRESS REPORT

DOE/ER/14128--1

DE92 006684

DEPARTMENT OF ENERGY

Grant DE-FG02-90ER14128

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REACTION AND DIFFUSION IN TURBULENT COMBUSTION

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October 2, 1991

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INTRODUCTION

The primary objective of the research is to use Direct Numerical Simulations (DNS) to study turbulent non-premixed combustion. In DNS, the fluid mechanical and thermochemical conservation equations are solved by an accurate numerical method, without any averaging or turbulence modelling. In principle, then, DNS could be used to study a turbulent diffusion flame, for example. In practice, however, computational limitations severely restrict the flows that can be simulated.

For non-reacting flows, DNS is restricted to simple geometries and moderate Reynolds number. For reacting flows there are severe restrictions on the thermochemistry. Indeed, DNS is a misnomer since simplifying assumptions are made about the chemical kinetics and molecular transport processes. It is completely out of the question to account for the 50 species and 200 reactions that typically occur in a turbulent flame.

What then is the use of DNS for turbulent combustion? Our approach is to use DNS to study very simple turbulent reactive flows, that contain qualitatively the same phenomena as real flames. Based on the insights and information gained, statistical models will be developed and tested. These models are then applicable to the turbulent flames of practical importance.

Most of the effort in the first year of this grant has been in developing a suitable thermochemical model and in determining the parameter range that can be simulated. This is described in the next two sections.

THERMOCHEMISTRY

We consider the simplest possible thermochemistry that allows the study of finite-rate kinetic effects in non-premixed combustion. Accordingly, the density is taken to be constant, and the molecular diffusivities are taken to be equal and constant. The mixing is then completely characterized by the mixture fraction ξ . A one-step reaction is considered, with Y being the reaction progress variable.

We have carefully developed a simple thermochemical model in terms of ξ and Y which is suitable for DNS, and yet retains as much of the essential ingredients as possible. At equilibrium, Y adopts the value $Y_e(\xi)$. This function Y_e is defined by the stoichiometric mixture fraction ξ_s and by the equilibrium constant K . It is normalized to have a maximum value of unity. Figure 1 shows $Y_e(\xi)$ for $\xi_s = \frac{1}{2}$ and a range of K , while Fig. 2 shows the second derivative $Y_e''(\xi)$. Different fuels can be simulated by different choices of ξ_s and K .

For a real flame both ξ and Y lie between zero and unity. However, for the current purposes it is desirable to define the thermochemistry for all values of ξ , and for negative values of Y . It may be seen from Figs. 1 and 2 that the specifications described above lead to sensible $Y_e(\xi)$ for all ξ .

Rather than the reaction progress variable, we consider its perturbation from equilibrium

$$y \equiv Y_e(\xi) - Y$$

Then, the reaction rate is of the form:

$$S_y(\xi, y) = f(y)g(\xi)/\tau_c,$$

where f and g are normalized functions, and τ_c is the specified reaction time scale. Figure 3 shows the chosen forms of f , g and S_y . These functions are defined for all ξ and y , although negative values of y are unphysical.

The parameters in the thermochemical model can be chosen to encompass a broad range of conditions—slow or fast reactions, high or low activation energy, small or large equilibrium broadening etc. An important parameter (which can be controlled) is the characteristic width of the reaction zone in mixture fraction space, $\Delta\xi_r$.

NUMERICAL RESOLUTION

In DNS, it is very important to understand the demands of numerical resolution, not only to ensure accurate simulations, but also so that the broadest parameter range can be investigated. The three most important non-dimensional parameters are the Reynolds number R_λ , the Damkohler

number Da , and $\xi'/\Delta\xi_r$ —the ratio of the r.m.s. to the reaction zone thickness (in mixture fraction space).

Using numerical forcing, we study stationary homogeneous isotropic turbulence. The use of forcing not only facilitates the analysis and interpretation of the results, but it also allows higher Reynolds numbers to be obtained compared to the case of decaying turbulence. For non-reacting flows, the resolution issues are well understood: on a $(128)^3$ grid $R_\lambda \approx 90$ can be obtained.

In practice, the resolution requirements connected with the Damkohler number are simple to satisfy. The requirement is that the time step Δt be small compared to the reaction time scale τ_c . Other considerations already limit Δt to be small compared to the Kolmogorov time scale τ_η . Hence the fast-chemistry limit ($\tau_c/\tau_\eta < 1$) can be approached without penalty.

The resolution requirement connected to the parameter $\xi'/\Delta\xi_r$, on the other hand, is extremely restrictive. Considerable time has been spent in understanding and quantifying the requirement. Using the same spectral method used in the DNS code, calculations have been performed of simple one-dimensional laminar flames. The fundamental conclusion from this study is that about 6 grid nodes are needed in the reaction zone in order to provide adequate resolution.

For the 3D turbulence simulations, the resolution requirements have been quantified in terms of the number of wave numbers K_m required in the spectral representation as a function of R_λ and $\xi'/\Delta\xi_r$. (For a simulation on an N^3 grid, K_m is approximately equal to $\frac{1}{2} N$.) For the non-reacting case ($\xi'/\Delta\xi_r = 0$), as R_λ increases, so does K_m , because more wavenumbers are needed to represent the broadening turbulence energy spectrum. At fixed R_λ , increasing $\xi'/\Delta\xi_r$ corresponds to decreasing the thickness of the reaction zones. As these zones become thinner, in order still to maintain 6 grid nodes across them, the total number of wavenumbers must increase.

The quantitative results are contained in Fig. 4 which is a contour plot of K_m as a function of R_λ and $\xi'/\Delta\xi_r$. In a 128^3 simulation the wavenumber range is 60. Consequently, the parameter range for which well-resolved 128^3 simulations are possible lies below and to the left of the $K_m = 60$ contour on Fig. 4. For example, while $R_\lambda \approx 100$ can be obtained in the non-reacting

case, for the quite small value $\xi'/\Delta\xi_r = 1$, the maximum R_λ that can be resolved is little more than 30.

CURRENT STATUS AND OUTLOOK

In the DNS code, the extensions have been made to incorporate the conservation equations for ξ and y . All numerical issues appear to have been resolved. The first set of simulations (on a relatively small 32^3 grid) are now in progress. These results will be fully analyzed and visualized before we proceed to the full-scale 128^3 runs.

As described in the proposal, we will also study mixing in terms of molecular motion. The DNS code is being extended in order to facilitate the tracking of molecules. Results can be expected in the next year.

EXPENDITURES

The expenditures have been close to those budgeted. No financial problems exist or are foreseen. A Silicon Graphics workstation has been purchased. This provides excellent color graphics as well as four powerful CPU's. We have been very pleased with its performance.

Fig.1 .

Equilibrium curves $Y_e(\xi)$, $\xi_s = 0.5$ (A: $K=100$; B: $K=500$; C: $K=1000$)

Fig.2 .

Second derivative of $Y_e(\xi)$, $\xi_s = 0.5$ (A: $K=100$; B: $K=500$; C: $K=1000$)

Fig.3

Reaction rate $S_y(\xi, y) = f(y)g(\xi)/\tau_c$

($\xi_s = 0.5$, $K = 400$, $B = 15$, $\tau_c = 0.1$)

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Fig.4 Contour plot of K_m .

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