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SOME CONDITIONAL STATISTICS IN REACTING NUMERICAL TURBULENCE

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INTRODUCTION

There has been a number of Direct Numerical Simulation (DNS) studies of nonpremixed turbulent reacting flows to understand different underlying physical phenomena (see Givi, 1989). In all of these studies, combustion was modeled using a single step irreversible reaction. This reaction was considered to be a global one. However, in reality the oxidation of fuel occurs through a number of elementary steps (Williams, 1985). Most of these elementary steps are reversible. Based on this observation, Bilger (1988) indicated that reaction zones would be thicker. Consequences, of this broadening effect on the structure of a turbulent nonpremixed reaction zone is investigated by Swaminathan *et al.* (1995). In this study, DNS field of Swaminathan (1994) has been investigated to obtain information on important statistics, like conditional strain rates, conditional probability density function (pdf) of reaction rates, and kinematics of reaction zones. Influence of reverse reaction on these statistics are elucidated.

NUMERICAL SIMULATION

The flow field considered is a homogeneous isotropic decaying turbulence with chemical reactions between two scalars. The scalars are spatially segregated initially. The reactants are assumed to be dilute so that the heat release effects on fluid dynamic fields are negligible. Chemical reactions are modeled by single irreversible and reversible reactions. A multistep mechanism having a reverse reaction and the same global reaction as in single step case is also considered (Swaminathan, 1994). Equations solved are continuity, Navier–stokes, and species conservation equations. Accurate solutions to these governing equations are obtained by a pseudospectral algorithm (Kerr, 1985) on different numerical grids. Aliasing errors are removed by using a 2/3rd rule. A third order Runge–Kutta method is used to time advance the discretized equations. Different parameters of numerical simulations are given in Table 1 with standard nomenclature. The rate constants (K's) are choosen based on resolution requirement. Scalar fields are initialized as alternating parallel slabs of fuel and oxidizer, whereas, the fluid dynamic fields are initialized by scaling a normally distributed random numbers to obtain a specified turbulent kinetic energy spectrum. The spectrum function is of the form $E(k,0) \propto k^4 \exp(-k^2)$, where k is the magnitude of three dimensional wavenumber vector.

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RESULTS AND DISCUSSION

Velocity derivative skewness (Kerr, 1985) reached a constant value of -0.45 after four eddy turn over times indicating the onset of self–similarity of small scales. The total turbulent kinetic energy decays with time according to a power law. Details on the behavior of fluid dynamic fields can be found in Swaminathan (1994). Time t in the following discussions and figures is made dimensionless by initial eddy turn over time. Above DNS fields are analysed at $t = 0.81, 5.36$ and 7.58. Pdf of a conderved scalar, mixture fraction, evolves from a double delta function to a Gaussian form.

Average reaction rate in turbulent reacting flows can be calculated as (Williams, 1985)

$$< \dot{\omega}_i >= -\frac{1}{2}\int_0^1 \int_0^\infty \rho \frac{d^2 Y_i}{dZ^2} \chi P_{\chi,Z}(\chi, Z) d\chi dZ. \quad (1)$$

It is a common practice to assume the scalar Z and its dissipation rate χ to be statistically independent. Conditional pdf $P(\chi|Z)$ calculated from the present simulation indicates that Z and χ are correlated which is consistent with experimental results of Starner *et al.* (1994). However, construction of conditional joint pdf $P(\chi, Z|\dot{\omega})$, conditional on reaction rate indicates that mixture fraction and its dissipa-

tion rate are conditionally independent. This result partially supports the assumption of statistical independence of mixture fraction and its gradient.

In turbulent flows, isoscalar sufraces are stretched and compressed by the most extensive and compressive strain rates. The most compressive strain rate γ amplifies the scalar gradient by bringing the isoscalar surfaces together thereby forming fine scale structures. These structures are smeared out by the molecular diffusion process. The above fluid dynamic process increases scalar dissipation rate and hence the mixing of scalar fields. In mixing controlled reacting flows, hence, the behavior of γ is of great interest. Instantaneous realtionship between reaction rate and scalar dissipation rate (produced by γ) is derived by Bilger (1976) and Peters (1984) for infintely fast and finite rate chemistry respectively. Leonard (1989) oberved a good correlation of γ with reaction rate. A similar result is shown in figure 1 from the present study. We find that γ to be the most dominant one inside the reaction zone. It is also oberved that intense reaction surfaces are orientated along the direction of γ. However, these correlations are reduced in the presence of a reverse reaction. Conditional expectation of γ conditional on reaction rate is shown in figure 2. This figure indicates a reduced correlation between the strain rate and reaction rates in the presence of a reverse reaction. Conditional expectation of orientation of intense reaction surfaces with γ indicate that they are orientated at about 58° unlike in single step irreversible case. This reduced correlation of reaction rate with γ gives a poor correlation of reaction rate with scalar dissipation rate. This is shown in figure 3, where conditional pdf of scalar dissipation rate conditioned on reaction rate is plotted at $t = 5.36$.

Conditional pdf of reaction rate conditioned on scalar dissipation rate of specific scalar (denoted by the subscript) is shown as contours in figure 4. Figures 4a-d are from simulation R4 with multistep chemistry, whereas, figure 4e is from single step case R2. Time of these snap shots are also given. Contours lying along (or closer to) a straight line $\omega_A = \chi_{Z \text{or} I}$ indicates a perfect (or better) correlation of these two quantities. This can be seen in figure 4e for singlestep case. However, the behavior of this pdf with multistep chemistry shown in figure 4c and 4d, at the same time ($t = 5.36$) as in single step case, indicates that the reaction rate correlates better with the dissipation rate of an intermediate species than with mixure fraction dissipation. At later time ($t = 7.58$) the correlation of reaction rate with χ_Z becomes better. These behavior in multistep chemistry indicates that there are history associated effects. Implications of these results on model development for turbulent reacting flows will be discussed. Effects of turbulence–chemistry interaction on the kinematics of reaction zones will also be presented.

Table 1: SIMULATION CHARACTERISTICS

Run	Mesh	R_{λ_o}	K_f	K_B	ν	Sc	Da_o
R1	64^3	35.6	1.0	0.0	0.01	1.0	0.038
R2	64^3	35.6	20.0	0.0	0.01	1.0	0.757
R2a	128^3	35.6	20.0	0.0	0.01	1.0	0.757
R3	64^3	35.6	20.0	20.0	0.01	1.0	0.757
		K_{1f}	K_{1b}	K_2	K_3	ν	Sc
R4	64^3	2.0	4.0	15.0	20.0	0.01	1.0
R4a	128^3	2.0	4.0	15.0.	20.0	0.01	1.0

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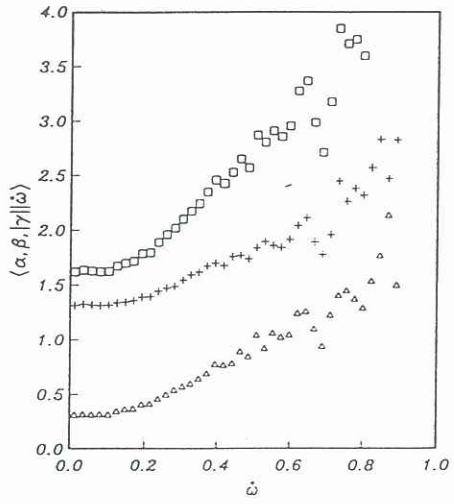


Figure 1: Conditional expectation of magnitude of unnormalised principal strain rates from simulation R2 at $t = 5.36$, $\triangle - \beta$, $+ - \alpha$, and $\square - \gamma$.

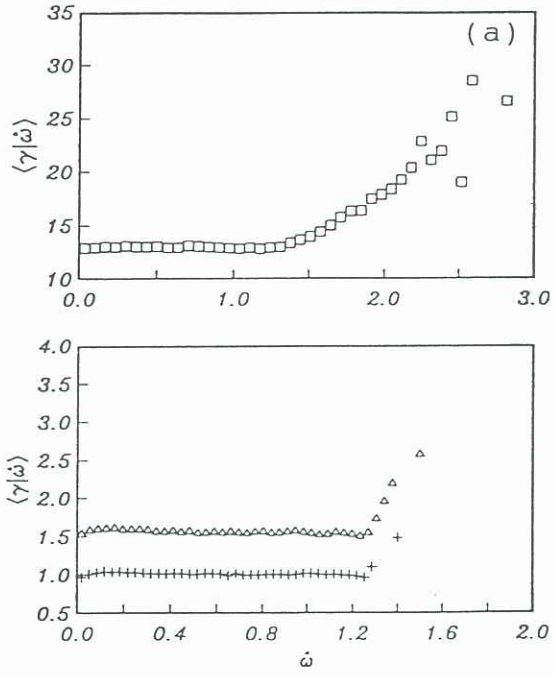
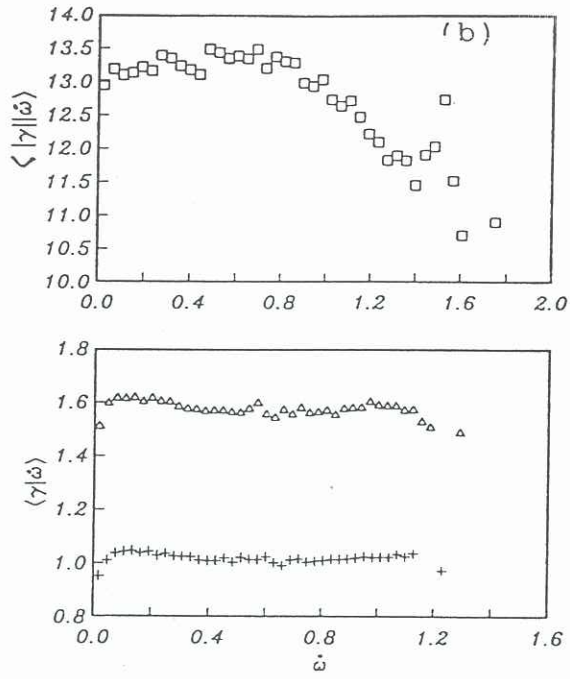


Figure 2: Conditional expectation of $|\gamma|$ conditioned on (a) forward rate, (b) backward rate contributions from simulation R3 at $t = 0.81(\square), 5.36(\triangle), and 7.58(+)$.



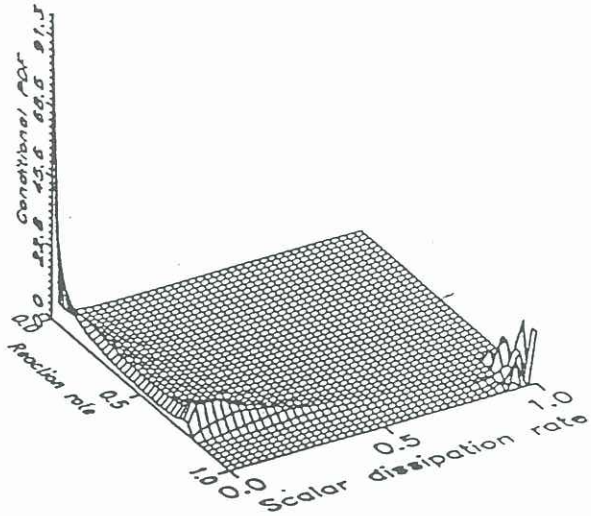


Figure 3: Conditional pdf of χ conditioned on reaction rate from simulation R3 at $t = 5.36$.

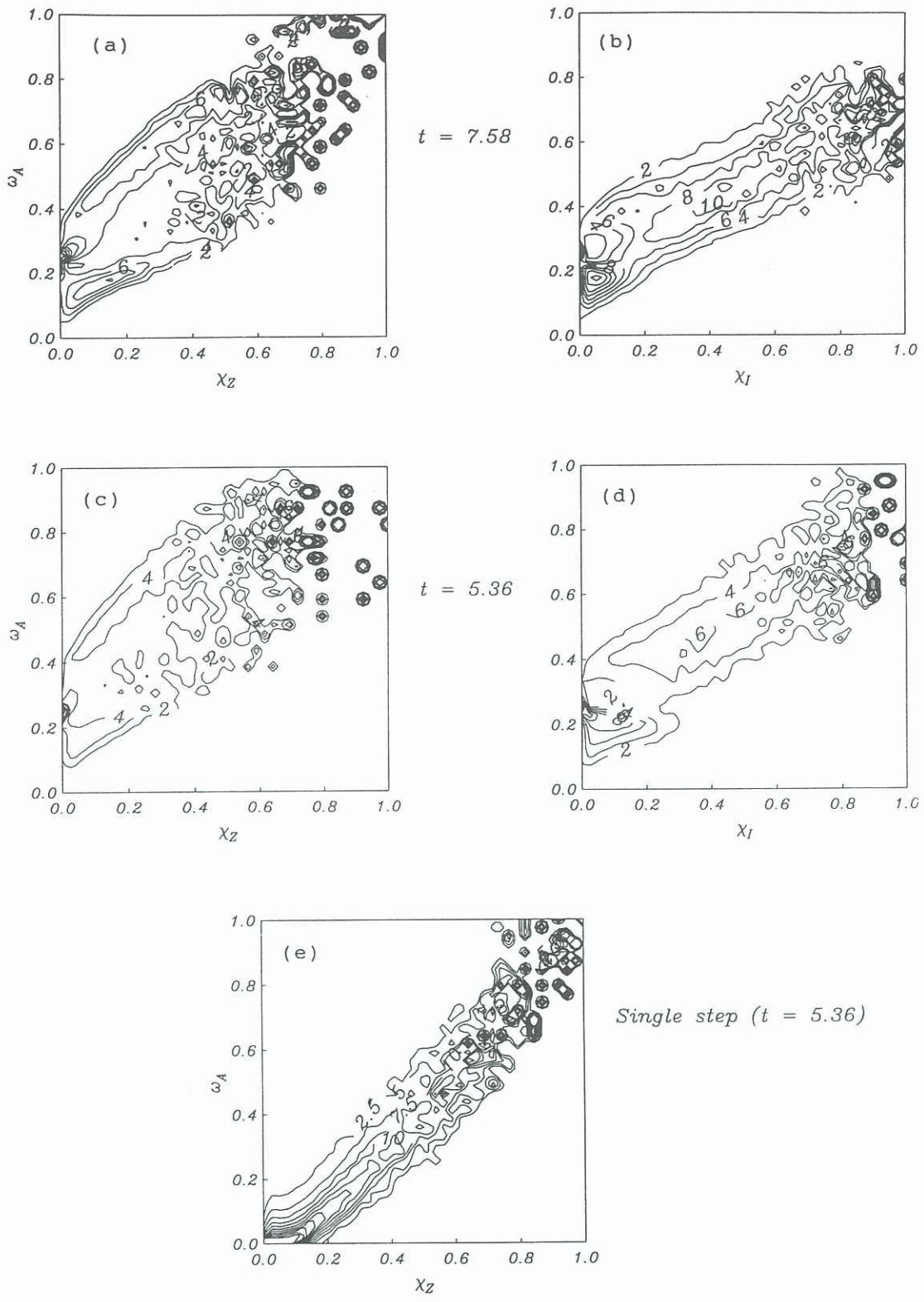


Figure 4: Conditional pdf of reaction rate conditioned on χ from simulation with (a)–(d) multistep and (e) singlestep chemistry.