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REACTION AND DIFFUSION IN TURBULENT COMBUSTION

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1 INTRODUCTION

The motivation for this project is the need to obtain a better quantitative understanding of the technologically-important phenomenon of turbulent combustion. In nearly all applications in which fuel is burned—for example, fossil-fuel power plants, furnaces, gas-turbines and internal-combustion engines—the combustion takes place in a turbulent flow. Designers continually demand more quantitative information about this phenomenon—in the form of turbulent combustion models—so that they can design equipment with increased efficiency and decreased environmental impact.

For some time the PI has been developing a class of turbulent combustion models known as PDF methods (see Pope 1985). These methods have the important virtue that both convection and reaction can be treated without turbulence-modelling assumptions. However, a mixing model is required to account for the effects of molecular diffusion. Currently, the available mixing models are known to have some significant defects. The overall motivation of the project is to seek a better understanding of molecular diffusion in turbulent reactive flows, and to develop a better mixing model.

The principal approach taken in the research is to use Direct Numerical Simulations (DNS) to study the coupled processes of reaction and molecular mixing in turbulent combustion. Because of inevitable computational limitations, it is impossible to simulate turbulent combustion in the parameter range of practical interest. Instead, our approach is 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 that are applicable to practical combustion devices.

The project objectives (as stated in the proposal) are:

1. To perform Direct Numerical Simulations of reaction in isotropic turbulence to simulate non-premixed combustion in different regimes.
2. To analyze the results of the simulations from both Eulerian and Lagrangian viewpoints, and hence to shed light on the interaction between reaction, molecular diffusion, and the local turbulence field.
3. To use the Lagrangian time series (and insights) obtained from the simulations to develop a stochastic model for mixing in reactive flows.
4. To study (theoretically and using DNS) relative molecular motion, and its relationship to stochastic mixing models. (This approach may establish a physical basis for the otherwise phenomenological stochastic mixing models.)

The following is a list of topics on which considerable progress has been made. The dates 1992 and 1991 indicate whether the progress was made (principally) this year or last year.

1. The development of two-variable ($\xi - y$) thermochemistry suitable for DNS studies (1991).
2. The determination of laminar flame properties based on this thermochemistry (1992).

3. Determination of the parameter range that can be accessed by DNS with good resolution (1991).
4. Implementation of the thermochemistry in the DNS code (1991).
5. Performance of exploratory simulations, and the development of techniques of relating Eulerian DNS data to turbulent combustion theories (1992).
6. Implementation of the DNS code on parallel and distributed computers (1992).
7. The study of relative molecular motion in turbulence (1992).

The items of progress in 1992 are described in the following sections.

2 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 ($\rho = 1$), and the molecular diffusivities Γ 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 $Y_e(\xi)$ which is determined by the specified stoichiometric mixture fraction ξ_s ($0 < \xi_s < 1$) and by the specified equilibrium constant K ($K > [\xi_s(1 - \xi_s)]^{-1}$). The equilibrium value $Y_e(\xi)$ can be determined from the relation

$$K = \frac{Y_e^2}{[\xi - \xi_s Y_e][1 - \xi - (1 - \xi_s)Y_e]} \quad (1)$$

In the numerator, Y_e represents the mass fraction of products, while in the denominator the two terms in square brackets represent the mass fractions of fuel and oxidant, respectively.

It can be deduced from Eq. (1) that the maximum value of $Y_e(\xi)$, $Y_{\max}$, is

$$Y_{\max} = \frac{1}{1 + 2/\sqrt{K}}, \quad (2)$$

which occurs at $\xi = \xi_{\max}$:

$$\xi_{\max} = \frac{\xi_s + K^{-1/2}}{1 + 2K^{-1/2}}. \quad (3)$$

As K tends to infinity it may be observed that $Y_{\max}$ tends to unity and $\xi_{\max}$ tends to ξ_s .

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 purposes of DNS it is desirable to define the thermochemistry for all values of ξ , and for negative values of Y . The specification given above leads to well-defined and sensible values of $Y_e(\xi)$ for all values of ξ .

In the theory of turbulent diffusion flames (e.g. Bilger 1989), the quantity

$$Y_e''(\xi) \equiv \frac{d^2 Y_e(\xi)}{d\xi^2}, \quad (4)$$

plays an important role. Figure 1 shows a plot of $Y_e''(\xi)$ for $\xi_s = 0.1$ and different values of K .

A central quantity in the present formulation is y —the departure from equilibrium of the reaction progress variable:

$$y = Y_e(\xi) - Y. \quad (5)$$

The pair of variable (ξ, y) contains the same information as (ξ, Y) . The perturbation y is zero for equilibrium, and otherwise positive.

The reaction rate S is defined as the rate of creation of Y . It is specified by

$$S_V(\xi, Y) = S(\xi, y) = f(y)g(\xi)/\tau_c, \quad (6)$$

where τ_c is a specified time scale,

$$f(y) = B y \exp(1 - By), \quad (7)$$

$$g(\xi) = \exp[-B(Y_{\max} - Y_e(\xi))], \quad (8)$$

and B is a specified parameter—related to the activation energy. Both f and g are positive, with maximum values of unity. Figure 2 shows $f(y)$ for different values of B , while Fig. 3 shows $g(\xi)$ for $K = 100$. The make-up of the reaction rate is summarized for one set of parameters on Fig. 4.

Several derived quantities play an important role. The lean and rich limits of the reaction zone in mixture-fraction space (ξ_l and ξ_r) are defined to be the lower and upper values of ξ at which $g(\xi)$ equals e^{-1} . Then, the reaction zone thickness in mixture-fraction space is defined to be

$$\Delta\xi_r = \xi_r - \xi_l. \quad (9)$$

The quantity $S_0(\xi)$ is defined by

$$S_0(\xi) = \left[\frac{\partial S(\xi, y)}{\partial y} \right]_{y=0} = g(\xi)/\tau^*, \quad (10)$$

where

$$\tau^* \equiv \tau_c/(Be). \quad (11)$$

The significance of S_0 is that for small values of y the reaction rate is approximately $yS_0(\xi)$. At $\xi_{\max}$, for small y the reaction rate is y/τ^* , and hence we take τ^* to be the characteristic reaction time scale.

3 LAMINAR FLAME PROPERTIES

The flamelet model of non-premixed turbulent combustion (see e.g. Peters 1984) is expected to be accurate for high Damkohler number and thin reaction zones (i. e. small τ^* and $\Delta\xi_r$

for fixed turbulence conditions). In order to make comparisons between DNS results and the flamelet-model, we have made careful calculations of the strained *laminar* flames given by the chosen thermochemistry. The calculations pertain to a steady one-dimensional opposed-flow diffusion flame, with imposed strain rate a . The governing equations are

$$ax \frac{d\xi}{dx} + \Gamma \frac{d^2\xi}{dx^2} = 0, \quad (12)$$

$$ax \frac{dY}{dx} + \Gamma \frac{d^2Y}{dx^2} + S_Y(\xi, Y) = 0, \quad (13)$$

where Γ is the molecular diffusivity, and the boundary conditions are

$$\xi(-\infty) = 0, \quad \xi(\infty) = 1, \quad Y(-\infty) = Y(\infty) = 0. \quad (14)$$

Equation (12) admits a simple analytic solution $\xi(x)$, with ξ increasing monotonically with x . This allows Eq. (13) to be transformed with ξ replacing x as the independent variable. The resulting equation is approximated by a centered finite-difference scheme, and the resulting set of non-linear equations is solved by Newton's method. Arc-length continuation (see e.g. Chan 1984) is used to obtain solutions for all values of a —even those corresponding to physically unstable states.

There is a maximum strain rate a_q for which the equations admit a solution. For the conditions $\xi_s = 0.5$, $K = 400$, $B = 15$, this is found to be

$$a_q \tau^* = 5.312 \times 10^{-3}. \quad (15)$$

The maximum value of Y , Y_m , which occurs at ξ_s decreases with increasing a . Figure 5 shows Y_m against a_q/a for the stated conditions. For very small values of a (not shown) Y_m approaches $Y_{\max} \approx 0.909$. The upper branch ($Y_m > Y^* = 0.8292$) corresponds to stable solutions, and the lower branch ($Y_m < Y^*$) to unstable solutions.

Figure 6 shows y against ξ for different strain rates. These values will be used to compare DNS results with flamelet theory.

4 DIRECT NUMERICAL SIMULATIONS OF NON-PREMIXED COMBUSTION

4.1 Governing Equations

The governing equations for velocity, ξ and y are solved by a pseudo-spectral method on an N^3 grid. Artificial forcing is added to the Navier-Stokes equations to yield statistically-stationary homogeneous turbulence. The way this is done, and the properties of the resulting turbulence, are fully described by Eswaran & Pope (1988a) and Yeung & Pope (1989). The turbulence is characterized by the turbulent kinetic energy k , the mean dissipation rate $\langle \epsilon \rangle$ and the kinematic viscosity ν . Important derived quantities are the Kolmogorov length scale η , the Taylor-scale Reynolds number R_λ , and the eddy turnover time T_e .

The equation

$$\frac{D}{Dt} \hat{\xi} = \Gamma \nabla^2 \hat{\xi}, \quad (16)$$

is solved for the conserved passive scalar $\hat{\xi}$. It is known that after some time $\hat{\xi}$ becomes self-similar, with a one-point one-time distribution that is close to Gaussian (Eswaran & Pope 1988b).

Let $[\hat{\xi}]$ denote the volume average of $\hat{\xi}$, and let $\sigma_{\hat{\xi}}$ be

$$\sigma_{\hat{\xi}}^2 = [(\hat{\xi} - [\hat{\xi}])^2]. \quad (17)$$

Then the quantity

$$\tilde{\xi} = (\hat{\xi} - [\hat{\xi}])/\sigma_{\hat{\xi}}, \quad (18)$$

has volume average mean zero and variance unity. Based on this variable, the mixture fraction is defined by

$$\xi(\mathbf{x}, t) = \langle \xi \rangle + \xi' \tilde{\xi}(\mathbf{x}, t), \quad (19)$$

where $\langle \xi \rangle$ and ξ' are the specified mean and standard deviation.

The mixture fraction defined by Eq. (19) is not conserved. Instead its evolution equation contains a deterministic forcing term (linear in ξ) that is required to make ξ statistically stationary.

The equation solved for y is

$$\frac{Dy}{Dt} = \Gamma \nabla^2 y - \frac{1}{2} \chi Y_e''(\xi) - S(\xi, y), \quad (20)$$

where

$$\chi \equiv 2\Gamma \nabla \xi \nabla \xi, \quad (21)$$

is the scalar dissipation. This equation results from the definition of $y(y = Y_e(\xi) - Y)$ and from the equations $D\xi/Dt = \Gamma \nabla^2 \xi$ and $DY/Dt = \Gamma \nabla^2 Y + S$. (In fact, the forcing terms implicit in the equation for ξ used lead to additional terms in the equation for y . These are not included: their omission corresponds to a forcing in the Y equation.)

4.2 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 $\xi'/\Delta\xi$,—the ratio of the r.m.s. to the reaction zone thickness (in mixture fraction space). (The Damkohler number is $Da = T_\xi/\tau^*$, where T_ξ is the decay time scale of the variance of $\hat{\xi}$.)

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 (Yeung & Pope 1989).

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^* . Other considerations already limit Δt to be small compared to the Kolmogorov time scale τ_η . Hence the fast-chemistry limit ($\tau^*/\tau_\eta < 1$) 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. 7 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. 7. For example, while $R_\lambda \approx 100$ can be obtained in the non-reacting case, for $\xi'/\Delta\xi_r = 1$, the maximum R_λ that can be resolved is little more than 30.

4.3 Performance and Analysis of Exploratory Simulations

In order to develop the methodology, several simulations have been performed at the relatively low Reynolds number $R_\lambda \approx 20$. This allows reasonably large fluctuations ($\xi'/\Delta\xi_r \approx 0.8$) to be investigated in 64^3 simulations, while with small fluctuations ($\xi'/\Delta\xi_r \leq 0.25$) 32^3 suffices (see Fig. 7). In both cases a range of Damkohler number has been investigated.

At present, an analysis of the results is being performed which will lead to sufficient understanding to plan a systematic investigation. Here—in a non-systematic way—we illustrate the type of results obtained.

Below a critical Damkohler number, the overall reaction rate is insufficient to maintain a statistically-stationary reacting state. Instead y increases with time, and after a while the reaction rate becomes negligible (see Fig. 4). Figure 8 shows $\langle y \rangle$ as a function of time for $Da = 4.1$ and $\xi'/\Delta\xi_r = 0.8$ (curve B). For comparison, curves A and C show the corresponding results (y_L and y_H) for $Da = 0$ and $Da = \infty$, respectively. It may be seen that for $Da = 0$ and $Da = 4.1$, $\langle y \rangle$ increases linearly with time, whereas with $Da = \infty$ a stationary state is achieved. (The quantity y_s used for normalization is defined below, Eq. 23.)

Next we describe the results of a simulation with high Damkohler number ($Da = 36.3$) and low mixture fraction fluctuations ($\xi'/\Delta\xi_r = 0.0625$). For these conditions we expect to observe QEDR (Quasi-Equilibrium Distributed Reactions, Bilger 1989). This is characterized by a balance of the last two terms in Eq. (20) (for ξ in the reaction zone). We define $y_H(\xi, \chi)$ to be the value of y that pertains to QEDR, with the further assumption that y is sufficiently

small for S to be expanded in a Taylor series. Thus

$$y_H(\xi, \chi) \equiv -\frac{1}{2}\chi Y_e''(\xi)/S_0(\xi), \quad (22)$$

where S_0 is defined in Eq. (10). We further define

$$y_s = y_H(\xi_s, \langle \chi \rangle), \quad (23)$$

to be a reference value of y .

Figure 9 shows the means of y/y_s and y_H/y_s against time. It is clear that the two quantities are essentially coincident, and that they are statistically stationary.

A very direct test of the QEDR approximation is provided by the scatter plots shown on Fig. 10. Figure 10a shows a scatter plot of y/y_s and ξ . The conditional mean and rms of y/y_s are both approximately unity, and values over 9 are observed. Figure 10b shows the scatter plot of $(y - y_H)/y_s$. The conditional mean is close to zero; the r.m.s. is of order 0.1; and the maximum absolute value is about 1. This confirms that the QEDR approximation $y \approx y_H$ is accurate under these conditions.

4.4 Implementation on Parallel and Distributed Computers

While DNS calculations are quite common nowadays, they remain one of the most computationally-demanding scientific computations routinely performed. With three benefits in mind, we have started to implement the DNS code on two parallel machines at the Cornell National Supercomputer Facility. The benefits are: access to a wider parameter range (larger R_λ and $\xi'/\Delta\xi_r$); better statistics through the performance of multiple simulations; and, enhanced research productivity brought about by shorter turnaround times.

We are collaborating with personnel from Kendall Square Research to implement the DNS code on the KSR1 machine at Cornell. This is a scalable architecture which appears to the user as a shared memory machine, which simplifies implementation. It is hoped to achieve over 2Gflops (e.g. 128 processors at 16Mflops each). Such speeds allow 256^3 computations to be performed, and provide excellent turnaround for 128^3 simulations.

On a single node, the DNS code has been implemented and tested on grids from 16^3 to 128^3 . Parallel execution has been successful on small grids with a small number of processors. Further development work is underway to extend this capability.

A second approach being taken is to use a cluster of 16 IBM RS6000-560 workstations to perform *multiple independent simulations*.

A DNS simulation should be viewed as a single realization of a random phenomenon—the randomness entering (mainly) through the probabilistic specification of the initial conditions. Run-to-run variations can be quite large. For example, Fig. 11 (taken from Yeung & Pope 1992) shows a correlation coefficient as a function of time obtained from 11 realizations of a DNS simulation. For each of the 11 runs the physical and numerical parameters are identical—only the random number sequence is different. Clearly the statistical variability is quite large, and it is difficult to draw firm conclusions from these results. The correct way to deal with this situation is to perform a statistical analysis of such multiple independent simulations. For example, Fig. 12 (also from Yeung & Pope 1992) shows similar results

to Fig. 11, but now the quantity plotted is the mean over many simulations together with the 90% confidence intervals. Only when the confidence intervals have been quantified can legitimate conclusions be drawn.

At the Cornell National Supercomputer Facility there is a cluster of IBM RS6000-560 workstations, with the number of workstations slated to increase with time from 7 to 16 to 64 etc. Each workstation is capable of performing a 64^3 simulation. Hence it is simple to use the cluster to perform multiple independent simulations.

The PI has implemented this strategy on the IBM cluster in a different context (Pope 1992), and it is currently being implemented for the DNS code.

5 MOLECULAR MOTION IN TURBULENCE

Ultimately, molecular mixing is due to the motion of molecules relative to each other. We have used DNS to study the motion of molecules in homogeneous turbulence.

Direct numerical simulations have been used previously (Yeung & Pope 1989) to determine Lagrangian statistics by following an ensemble of N fluid particles. Let $\mathbf{X}(t)$ denote the position of one such particle. We now also track an ensemble of N molecules, with position denoted by $\mathbf{Y}(t)$, from coincident initial conditions (i.e. $\mathbf{Y}(0) = \mathbf{X}(0)$). This is achieved by numerically integrating the stochastic differential equation for $\mathbf{Y}(t)$, which involves the molecular diffusion coefficient $D = \nu/Sc$ (where ν is the kinematic viscosity and Sc is the Schmidt number).

From the N time series of $\mathbf{X}(t)$ and $\mathbf{Y}(t)$ we have extracted many statistics on the dispersion of molecules (e.g. $\langle \mathbf{Y}(t) \cdot \mathbf{Y}(t) \rangle$) and on the relative dispersion between molecules and fluid particles (e.g. $\langle (\mathbf{Y} - \mathbf{X}) \cdot (\mathbf{Y} - \mathbf{X}) \rangle$). It is found that these statistics are in good agreement with the theory of Saffman (1961). For example, the theory predicts (to order t^3)

$$\langle Y(t)^2 \rangle = \langle X(t)^2 \rangle + 2Dt - \frac{1}{9}Dt^3/\tau_\eta^2,$$

where τ_η is the Kolmogorov time scale. The term that is linear in t gives the direct additive contribution of molecular diffusion. The term that is cubic in t gives, interestingly, a decrease in molecular dispersion with an increase in the molecular diffusivity, which is due to a decorrelation of the fluid velocity following a molecule. Figure 13 shows $\langle Y(t)^2 \rangle$ plotted in such a way as to reveal terms higher than linear in t . Excellent agreement with Saffman's theory is evident for all Schmidt numbers investigated.

Higher-order statistics are also being investigated. Figure 14 shows the flatness factor of the relative displacement $\mathbf{Y}(t) - \mathbf{X}(t)$. For low Schmidt number ($Sc = 0.1$) this is close to the Gaussian value of 3 for all time; whereas for $Sc = 10$, it rises above 10 before decreasing. For this case it is found that (to a good approximation) the pdf of $|\mathbf{Y} - \mathbf{X}|$ is log-normal.

6 CURRENT STATUS AND OUTLOOK

The status of the project can be characterized as follows: we have spent about two years assembling and honing the tools to be applied to the problem. Because of this extensive

groundwork, we believe that the results of our study will have greater lasting significance than most DNS studies reported.

In the next year, our major goals are:

1. To complete a DNS study of non-premixed combustion, and report the results as a paper in a premier journal.
2. To complete a paper on the study of molecular motion in turbulence.
3. To implement the DNS code on the parallel and distributed machines available at Cornell.
4. Based on the results of 1-3, to plan and initiate further DNS studies to achieve the overall objectives of the project.

7 PUBLICATIONS

Thus far, no papers have been prepared for submission for publication. This we regard as quite appropriate to a new project of this level of technical complexity. We have invested our time in developing tools which, in the next year, will lead to significant novel results worthy of publication.

To reassure the reader that the PI is productive in terms of quality publications once a project has reached maturity, an abbreviated list of articles published in 1990 and subsequently follows.

R.S. Cant, S.B. Pope and K.N.C. Bray (1990) Twenty-Third Symposium (International) on Combustion, pp. 809-815.

S.S. Girimaji and S.B. Pope (1990) Physics of Fluids A, **2**, 242-256.

S.S. Girimaji and S.B. Pope (1990) Journal of Fluid Mechanics **220**, 427-458.

S.S. Girimaji and S.B. Pope (1992) Journal of Fluid Mechanics **234**, 247-277.

U.A. Maas and S.B. Pope (1992) Combustion and Flame, **88**, 239-264.

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S.B. Pope (1990) Invited Plenary Lecture, Twenty-Third Symposium (International) on Combustion, The Combustion Institute, pp. 591-612.

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S.B. Pope and Y.L. Chen (1990) *Physics of Fluids A*, **2**, 1437-1449.

P.K. Yeung, S.S. Girimaji and S.B. Pope (1990) *Combustion and Flame* **79**, 340-365.

8 EXPENDITURES

The expenditures have been close to those budgeted. No financial problems exist or are foreseen.

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Fig.1. Second derivative of $Y_e(\xi)$ with $\xi_s = 0.1$ for various equilibrium constants. (A, $K=100$; B, $K=500$; C, $K=1000$)

Fig.2. Shape of $f(y) = By \exp(1 - By)$ with various values of B .
(A, $B=1$; B, $B=5$; C, $B=10$; D, $B=15$)

Fig.3. Shape of $g(\xi) = \exp[B(Y_e - Y_{max})]$ with $\xi_s = 0.5$, $K = 100$, and various B . (A, $B=1$; B, $B=5$; C, $B=10$; D, $B=15$)

Fig.4. Reaction rate $S_y(\xi, y) = f(y)g(\xi)/\tau_c$; (a) Contour plot of $S_T(\xi, Y)$ together with equilibrium curve $Y_e(\xi)$; (b) Contour plot of $S_Y(\xi, y)$. Points on the line $y = 0$ represent equilibrium states; (c) $f(y)$; (d) $g(\xi)$.
 ($\xi_s = 0.5$, $K = 400$, $B = 15$, $\tau_c = 1$)

Fig.5. The maximum value of Y versus a/a_q for the strained laminar flame.
 ($\xi_s = 0.5$, $K = 400$, $B = 15$, $\tau_c = 1$)

Fig.6. Perturbation of progress variable at various a/a_q for the strained laminar flame. (A, $a/a_q = 1/3$; B, $a/a_q = 2/3$; C, $a/a_q = 1$)

Fig.7. Contour plot of the wavenumber range K_m required for a well-resolved simulation as a function of R_λ and $\xi'/\Delta\xi_r$.

Fig.8. Evolution of the spatial means of y_L/y_s (A), y/y_s (B), and y_H/y_s (C) for $Da = 4.1$ and $\xi'/\Delta\xi_r = 0.8$.

Fig.9. Evolution of the spatial means of y/y_s (A) and y_H/y_s (B) for $Da = 36.3$ and $\xi'/\Delta\xi_r = 0.0625$.

Fig.10. Scatter plots for $Da = 36.3$ and $\xi'/\Delta\xi_r = 0.0625$. (a) y/y_s and ξ .
 (b) difference between DNS and QEDR approximation.

Fig.11. Evolution of the correlation coefficients between the $Sc = 0.25(\phi_1)$ and $Sc = 1.0(\phi_3)$ scalars shown in normalized time. Each solid line represents a different realization. The dashed line represents the average over all (11) realizations, and the vertical bars indicate one standard deviation above and below the mean.

Fig.12. Evolution of the correlation coefficients between different scalars taken in pairs : $Sc = (0.25, 0.5)(\Delta)$, $Sc = (0.25, 1.0)(\circ)$, and $Sc = (0.5, 1.0)(\square)$, shown in normalized time. The lines shown are averages over multiple realizations. Vertical bars denote bounds of 90% confidence intervals (calculated using Student's t distribution because sample size is small) for the respective ensemble averages.

Fig.13. Difference between molecular and fluid-particle dispersion in isotropic turbulence. A, $Sc = 0.1$; B, $Sc = 1.0$; C, $Sc = 10.0$. Solid line, Saffman's theory $\frac{1}{9}(t/\tau_\eta)^3$.

Fig.14. Flatness factor of relative distance between molecules and fluid particles for the simulations of Fig.13.

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