DEVELOPMENT OF 3-D COMPUTER CODE TO STUDY AUTOIGNITION IN A TURBULENT MEDIUM

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Abstract

In this paper, the development and validation of 3-dimensional computer code to analyze autoignition in a non-premixed medium under isotropic and homogeneous turbulence is presented. During autoignition the density changes are considerable and hence the constant density assumption cannot be made. To include the effects of density fluctuations caused due to spatial inhomogeneities in temperature and species, a pressure based method is developed herein, which is a spectral implementation of the sequential steps followed in the predictor-corrector type of algorithms. The velocity and pressure field are solved in spectral space while the scalars are solved in physical space. The combustion is assumed to take place through a single-step irreversible reaction. Simulations are first validated for nonreacting turbulence without any scalars. Next, the decay of scalar variance has been studied which showed a power law decay as observed by the earlier researchers. Then the program is extended to analyze the reacting flow problems. The code has been parallelized using MPI calls to run it efficiently on IBM-SP machines. The details of the governing equations, solution methodology and comparison of present results with previous data are presented.

Nomenclature

A = Pre-exponential factor
c_p = Specific heat capacity
D = Fickian diffusion coefficient
D_a = Damkoler number
E = Turbulent kinetic energy per unit mass
E_a = Activation energy
$E(\underline{k},t)$ = Turbulent kinetic energy spectrum
F = Fourier transform
i = Unit vector in physical space
k = Turbulent kinetic energy per unit mass
$\underline{k}$ = Coordinate vector of wavenumber space
$\underline{k}_m$ = Wavenumber at which initial velocity spectrum peaks
L = Computational domain size
Le = Lewis number
p = Pressure
Re = Reynolds number based on Taylor scale
r_{st} = Stoichiometric ratio of fuel to oxygen
T = Temperature
T_a = Activation temperature of a reaction
u_{rms} = Root mean square value of velocity-fluctuations
W = Molecular weight
$\dot{w}_f'''$ = Chemical source term of fuel
Y = Species mass fraction
Z = Mixture fraction

Greek Letters

χ = Scalar dissipation rate
Φ = Viscous heat generation rate
$\hat{\phi}$ = Complex Fourier transform of ϕ
η = Sample space of mixture fraction
η_κ = Kolmogorov lengthscale
ι = Imaginary unity, $\sqrt{-1}$
κ = Thermal conductivity
λ = Taylor microscale
Λ = Integral lengthscale of velocity-field
Λ_z = Integral lengthscale of scalar-field
μ = Dynamic viscosity
ν = Kinematic viscosity
ρ = Mass density
σ_{ij} = Viscous stress tensor
τ_f = Characteristic eddy-turnover timescale

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Introduction

Autoignition is nothing but the initiation of combustion in a reactive substance, without the aid of any external source. An understanding of this is relevant from the perspective of practical equipment such as internal combustion engines (see, for example, Ref.[1]). In compression-ignition engines, autoignition takes place in an initially nonpremixed medium of fuel and air, while in spark-ignition engines, the undesirable knock is attributed to the autoignition of a premixed charge in the end-gas region. The present code is developed to address the effects of a 3-dimensional turbulence on the characteristics of autoignition in an initially nonpremixed, gaseous mixture of n-heptane and air.

Previous Fourier spectral simulations of turbulent combustion at low Mach numbers are limited to constant density flows with small heat release rates [2-3]. Autoignition is characterized by a short period of intense chemical activity accompanied by a large heat release rate. During this, it is expected that considerable spatial inhomogeneities in density will be created due to temperature and species fluctuations; in turn, this will cause changes in the velocity field; therefore the turbulence characteristics such as the energy spectrum will be quite different if the density is allowed to fluctuate. This aspect of combustion generated turbulence and its effect on the ignition characteristics have not been investigated previously. From experiments [4] and computations [5], it has been found that the ignition delay is quite dependent on the turbulence intensity in the medium, and therefore the effect of this additional turbulence on autoignition needs to be studied in detail.

In the earlier work [6], a pseudo-spectral code was developed which can handle variable density processes in turbulent medium. The program was limited to 2-dimensional flow only. However the real world the turbulence is 3-dimensional in nature. Due to the presence of *vortex-stretching* phenomenon in 3-dimensional turbulence, mixing process becomes different. Examples may be found in literature [7] where predictions including a 3-D flowfield seems to improve comparison with experimental data over that of the 2-D simulations. Thus the 3-D programs will enable DNS to simulate turbulence in a more realistic way. Furthermore, 3-D simulations provide more samples of the flame front for the statistical post processing and will therefore improve the quality of results, which led to the development of the code.

The most successful DNS have been performed with pseudospectral methods [8] because of the higher accuracy offered by the latter in comparison to the finite difference methods. However, spectral methods are more difficult to use for complex geometries and for programming. In this paper a numerical method is developed, in which the velocity and pressure are solved in spectral space while density and scalars are solved in physical space. The solutions are time-marched using a variant of the predictor-corrector scheme [9] which has been quite successful for modeling low Mach number, variable density combusting flows [10]. A requirement of the applicability of Fourier spectral method is that periodic boundary conditions (PBC's) must be enforced on all the flow variables. Such an idealized flow with homogeneous, isotropic turbulence serves as a suitable test-case to gather fundamental knowledge on the details of the process.

With the development of direct numerical simulation (DNS) technique as a research tool [11], many aspects of autoignition are beginning to be understood. Two-dimensional DNS studies pioneered by Mastorakos et.al [12] focused several interesting details of autoignition. Recently, this has been verified with respect to autoignition of an initially randomly segregated reactant field subjected to a homogeneous and isotropic turbulence [6]. An interesting result of the latter study was that the autoignition delay-time increased with increase in the turbulence intensity. A similar result was obtained previously from DNS of autoignition in a 2-D mixing layer [13]. Both Sreedhara et.al [6] and Im et.al. [13] attributed this variation to the increased strain rates and scalar dissipation rates caused by turbulence. On the other hand, experimental evidence [4,14,15] indicates that the delay-time decreases with an increase in turbulence intensity. This intriguing discrepancy needs to be resolved. In this paper, the 3-Dimensional code developed to study autoignition in a 3-D turbulent medium and its validation against previous results are discussed.

Description of the Problem and Governing Equations

A homogeneous, isotropic turbulence is the simplest turbulent flow configuration that could be simulated numerically. This standard problem has been examined by many researchers for turbulence modeling as well as for DNS. Such a flow exists in the downstream of a grid-generated turbulent flow. The computational domain considered here is a Fourier cube of length L into and out of which fluid flows. The flow inside the box is one of homogeneous, isotropic and decaying turbulence. The box initially

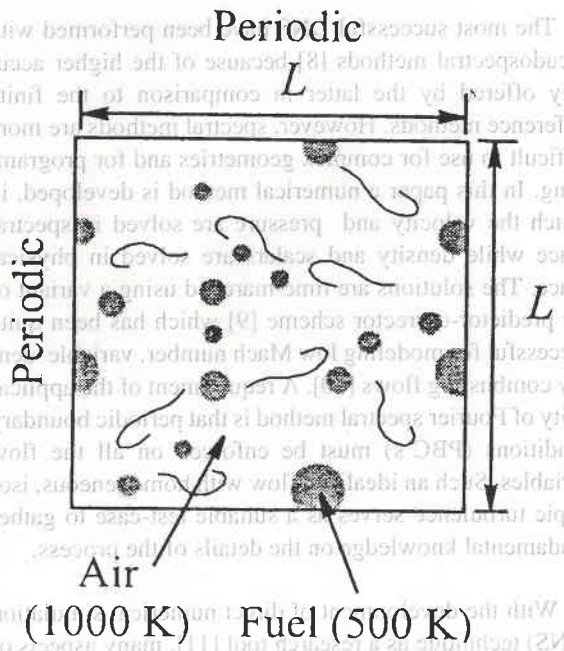

Fig. 1 A schematic of the computational region considered. The initial conditions on an arbitrary section normal to the z-axis is shown

consists of high pressure (4 Mpa), warm air, into which packets of gaseous fuel at lower temperature are randomly distributed. The fuel packets are all initially spherical but of different size, such that the overall air-fuel ratio is stoichiometric. As time advances, the air-fuel interface is distorted due to turbulence. Further, macroscopic packets of fluid with different scalar values are shifted to other regions, thus setting up new interfaces. Along the air-fuel interface, the gases become locally premixed due to molecular transport of heat and mass. Then exothermic chemical reactions begin depending upon the values of the local scalars. The initial size (hence the number) of fuel packets, and the initial turbulence intensity are varied in different simulations. The objective is to examine the time evolution of the flow variables such as the velocity and scalar fields.

The Fluid Dynamics Model

The instantaneous velocity components averaged over all points within the box are always zero. The fluid density and pressure are considered to be variable, but the thermophysical properties namely, conductivity, specific heat, diffusivity and viscosity are considered to be constants. The molecular transport of momentum, heat and mass follow Newton's, Fourier's and Fick's laws respectively. Radiation heat transfer is not considered. The fluid is assumed to be a perfect gas. Body forces are neglected. The value of Lewis number is tentatively taken as unity for the simulations reported herein although the formulation is valid for arbitrary, constant values. However, differential diffusional effects (Le ≠ 1) could be important when rapidly diffusing radical species e.g., monatomic hydrogen (H) are present.

The results reported in the foregoing refer to the non-reacting, passive scalar mixing problem, and hence any combustion model is not yet used. In the scalar mixing problem, initially the box consists of a species A (say air) at some temperature T_A and another species B at some other temperature T_B is dispersed randomly in it. As time advances, the two species mix due to turbulence and molecular transport. Here, the goal is to compute the temporal evolution of the distribution of concentrations and temperature field within the box.

The next step will be to introduce chemical reaction source terms into the species and energy equations, and hence a combustion model will be required. Herein, the combustion model used is same as that used in earlier 2-D simulations [6].

The Combustion Model

The fuel is taken as n-heptane at 500 K, while the oxidizer as air at 1000 K, the overall mixture being stoichiometric. In reality, autoignition chemistry is complex and prevailed by several elementary chain-branching steps which are crucial to a proper modeling of the thermochemical dynamics. As the objective of this work is to study the fluid dynamical effects, herein the chemical kinetics is modeled using a relatively simple, single-step, irreversible reaction

$$n\text{-}C_7H_{16} + 11 \times (O_2 + 3.762\, N_2) \rightarrow 8\, H_2O + 7\, CO_2 + 11 \times 3.762\, N_2 + \text{Heat}$$

The rate of fuel consumption is assumed to follow a global law given by

$$\dot{w}_f''' = -\frac{A\rho^2}{W_{ox}} Y_f Y_{ox} \exp\left(\frac{-T_a}{T}\right) \quad (1)$$

Suffixes f and ox stands for fuel and oxidizer. The initial mean pressure of the mixture is taken as 4 Mpa.

For a gaseous mixture undergoing a single-step chemical reaction at a finite rate, instantaneous and local mass fractions of all the species (with equal diffusivities) may be described in terms of linear relations between two scalars, e.g. a mixture fraction Z and the temperature T [5].

The Governing Equations

Herein, the governing equations are solved using a pseudospectral method, and hence the corresponding continuity and momentum equations are written in the Fourier spectral space. In this, the independent variables are the wavenumber vector ($\boldsymbol{k} = k_1, k_2, k_3$) and time ($t$). However, the balance equations for enthalpy and species are written in the physical space ($\boldsymbol{x} = x_1, x_2, x_3; t$) as these contain nonlinear source terms which are difficult to handle with the spectral method. Then the conservation equations for variable density, chemically reacting, Navier-Stokes flow are :

Continuity (spectral):

$$\frac{d}{dt}\hat{\rho}\,(\boldsymbol{k}, t) + i\,k_j\,\hat{\rho u_j}\,(\boldsymbol{k}, t) = 0 \tag{2}$$

Momentum (spectral):

$$\frac{d}{dt}\left[\hat{\rho u_i}\,(\boldsymbol{k}, t)\right] + F\left\{\frac{\partial\,\rho\,u_i\,u_j}{\partial\,x_j}\right\}_k = -\,i\,k_j\,\hat{p}\,(\boldsymbol{k}, t) + F\left\{\frac{\partial\,\sigma_{ij}}{\partial\,x_j}\right\}_k \tag{3}$$

Enthalpy (physical):

$$\frac{\partial\,(\rho\,c_p\,T)}{\partial\,t} + \frac{\partial\,(\rho\,u_j\,c_p\,T)}{\partial\,x_j} = \kappa\,\frac{\partial^2 T}{\partial\,x_j\,\partial\,x_j} + \Phi + \frac{D\,p}{D\,t} - Q_f\,\dot{w}_f''' \tag{4}$$

Mixture fraction (physical):

$$\frac{\partial\,(\rho\,Z)}{\partial\,t} + \frac{\partial\,(\rho\,u_j\,Z)}{\partial\,x_j} = \rho\,D\,\frac{\partial^2 Z}{\partial\,x_j\,\partial\,x_j} \tag{5}$$

where usual notation is followed to indicate x_1, x_2 and x_3-directional values. The heat of combustion of the fuel is denoted by Q_f. Equations (2-5) must be supplemented by (i) an equation of state :

$$\rho = \frac{p\overline{W}}{RT}\,;\ \overline{W}\left(\sum_{\alpha}\frac{Y_\alpha}{W_\alpha}\right)^{-1} \tag{6}$$

(ii) expressions for viscous stress tensor σ_{ij} and viscous heat generation rate Φ (for which relations for a Newtonian fluid are assumed), and (iii) an expression for the species chemical source term $\dot{w}_f'''$.

The mixture fraction Z is evaluated with the standard definition,

$$Z(\boldsymbol{x}, t) = \frac{\beta\,(\boldsymbol{x}, t) - \beta_1}{\beta_2 - \beta_1} \tag{7}$$

where $\beta = (Y_F - r_{st}\,Y_{O2})$ is a conserved scalar for the single-step mechanism, and $r_{st} = (1/3.52)$ for n-heptane-air system. Then $Z = 0$ for pure air and $Z = 1$ for pure fuel respectively. The scalar dissipation rate is defined as

$$\chi\,(\boldsymbol{x}, t) = 2D\,\frac{\partial Z}{\partial x_i}\,\frac{\partial Z}{\partial x_i} \tag{8}$$

Boundary Conditions

For the problem just described, periodic boundary conditions (PBC's) are valid. That is, $\phi\,(\boldsymbol{x}) = (\boldsymbol{x} + i\boldsymbol{L})$, where $\phi = \{\rho\,,\ \rho\,u_j,\ p,\ T,\ Z\}^T$. It is generally commented that PBC's are not a proper choice for reacting turbulent flows. This is due to the reason that with PBC's, it is not possible to maintain a thermochemically steady state in the presence of heat release. However, in the present work, the objective is to compute the temporal evolution of the flow, and not the steady state. And when the steady state is eventually attained, the heat release would have been complete. Therefore, the PBC's are imposed, which are the natural ones for the Fourier spectral space. PBC's for the mass flux vector ρu_j imply that the total mass within the control volume remains constant. For a constant-volume box, this in turn implies that the mean density $<\rho>$ (or its zeroth wavenumber component, $\hat{\rho}_0$) remains constant in time.

Initial Conditions

The initial fields for velocity and scalars including density variations is generated by a procedure due to Erlebacher, et.al [16] and could be summarized as follows:

1. First, the density is kept constant and uniform, and a random velocity field is generated using a standard method such that the mass continuity is satisfied (see for e.g.., p.115 of Ref.[17]). These random velocities are scaled to satisfy a realistic turbulence kinetic energy spectrum. The spectrum previously used for autoignition [18] having the form $E\,(\underline{k},0) = u_{rms}^2\,(\underline{k}/\underline{k}_m^2)\,\exp\,(-\underline{k}/\underline{k}_m)$ with its maxi-

mum at $\underline{k}_m$ is chosen with u_{rms} represents the RMS velocity of turbulent fluctuations.

2. Next, the initial pressure field is computed from the Poisson equation with a constant density.

3. At this stage, the initial fields for scalars (Z,T) are generated by the method developed by Eswaran and Pope [19].

4. Using the local pressure and scalars, the initial density field is computed from Eq.(6).

5. The initial fields generated this way do not yet satisfy the continuity with variable density, Eq.(2). So, the entire simulations without chemical reactions are carried out until the continuity is satisfied, typically in about 10-12 steps.

The Numerical Method for DNS

A computer program has been recently developed to simulate autoignition in a 2-D turbulent medium [6]. In this, the classical pseudospectral approach [8] is taken to obtain a highly accurate solution. Velocities and pressure are solved in spectral space, while density and scalars are solved in physical space. The spatial gradients of scalars are first computed in spectral space and then back transformed into physical space. The computer package ESSL is employed to extract the Fourier transforms and their inverse of dependent variables. The standard 2/3rd procedure is adopted for de-aliasing to remove spectral errors. Effects of periodic boundary conditions are minimized by selecting the integral scale smaller than the computational domain size. The ratio L/Λ was about 5 in most of the present simulations. The numerical resolution is usually indicated by the value of $\eta\, k_{max}$, which was around 1.6 at early times during the simulations and further increases with time. A second order Runge-Kutta technique is used for time marching after confirming that a fourth order Runge-Kutta method hardly affect the results. A variant of the predictor-corrector procedure due to Issa [9] is employed to advance the solutions in time. Further details of the solution procedure may be found in Ref.[6]. The same code has been upgraded for solution of the 3-dimensional problem. As the required computational resources greatly increase, the code was modified with MPI calls so as to run on a parallel processing computer (IBM-SP system with sixteen processor). Before using this code for turbulent combustion, it was extensively validated for nonreacting turbulence, first with only velocity field and then including a passive scalar. The results are summarized in the next section.

Results and Discussion

Selection of Parameters; Numerical Accuracy

Several simulations were carried out using different sets of parametric values, which are summarized in Tables-1 and 2. With the available computational resources, a maximum of 64^3 grids could be employed for each simulation. It is to be noted that only representative, and not realistic values of the thermophysical and chemical properties of the fluid could be used so that numerically accurate results are obtained. The resolution of 64^3 grids

Table-1 : Values of the parameters common for all the present simulations. All runs employed a 64^3 mesh

Property	Value
Computational space, L	6.28 mm
Prandtl number, Pr	0.66
Lewis number, Le	1.0
Numerical Mesh width, Δx	0.09813 mm
Numerical timestep, Δt	1 ms

Table-2 : Values of the various parameters used in typical simulations. Initial lenthscale ratio Λ/Λ_z was 0.8, 1.25 and 5 for runs C,D and E respectively. Typical computational time taken with 3-processors on IBM-SP machine is around 40 CPU hours

Run	$\tau_{f,0}$ (s)	Reλ	Λ_0 (mm)	λ_0 (mm)	η_0 (mm)	ν (mm^2/s)
A	0.514	43.01	0.514	0.418	0.036	0.01189
B	1.01	132.96	1.033	0.4544	0.045	0.008
C	0.1045	44.12	0.8363	0.667	0.051	0.0586
D	0.1939	43.90	1.2603	1.000	0.076	0.0586
E	0.1939	43.90	1.2603	1.000	0.076	0.0586

is comparable to that of contemporary DNS work in turbulent combustion [21,22].

Comparison with Results from Theory and Previous DNS

In Fig.2, the time-evolved values of several quantities computed using present code are compared with that of Local-Energy-Transfer (LET) theory by McComb and Shanmugasundaram [20]. For this purpose, a decaying turbulence with an initial energy spectrum in the form of $E(\underline{k},0) = c_1 \underline{k}^{c2} \exp(-c_3 \underline{k}^{c4})$ (spectrum I in Ref.[20]), was considered without any scalars. While the evolution of the total kinetic energy of turbulence $E(t)$ and the turbulent Reynolds number $\mathrm{Re}_\lambda(t)$ compares well, there is a small difference in the evolution of skewness factor $S(t)$ between theory and the present DNS. However, the predicted $S(t)$ compares well with the original DNS data of Orszag and Patterson [21]. Shown in Fig.3 is the evolution of energy spectrum at different instants of time. This is also found to compare well the predictions of the LET theory. The results obtained using new DNS code also satisfy the self-preservation condition for the spectrum which is shown in Fig.4 (similar to Fig.11 of Ref.[20]).

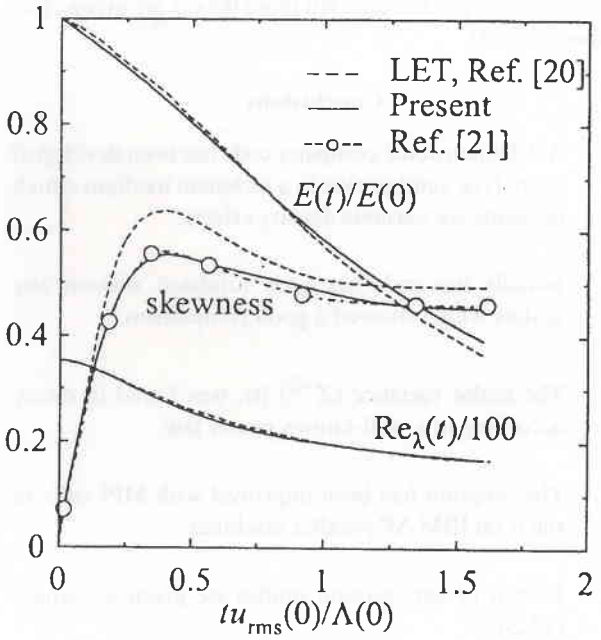

Fig. 2 Validation of the 3-dimensional DNS code for the passive scalar mixing problem. Comparison of predicted fluid dynamical quantities with theoretical results of McComb and Shanmugasundaram [20] and DNS data of Orszag and Patterson [21]. E(t)=total kinetic energy of turbulence. (Run A)

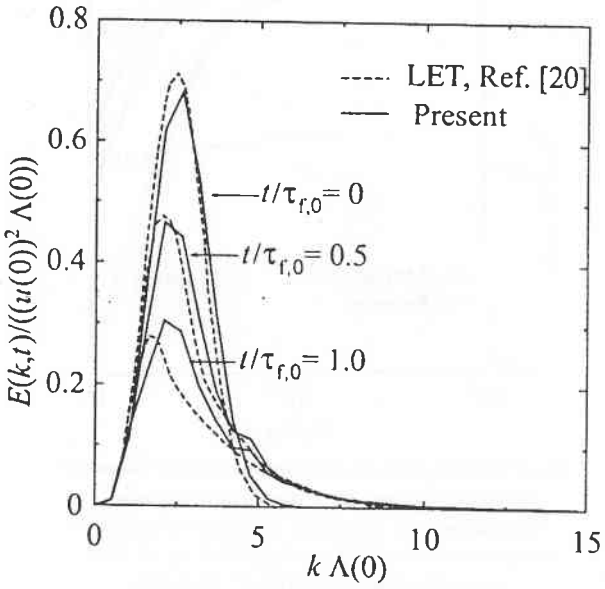

Fig. 3 Results from the simulations without chemical reactions: the passive scalar mixing problem. Comparison of predicted evolution of energy spectrum with theoretical results for code-validation. (Run A)

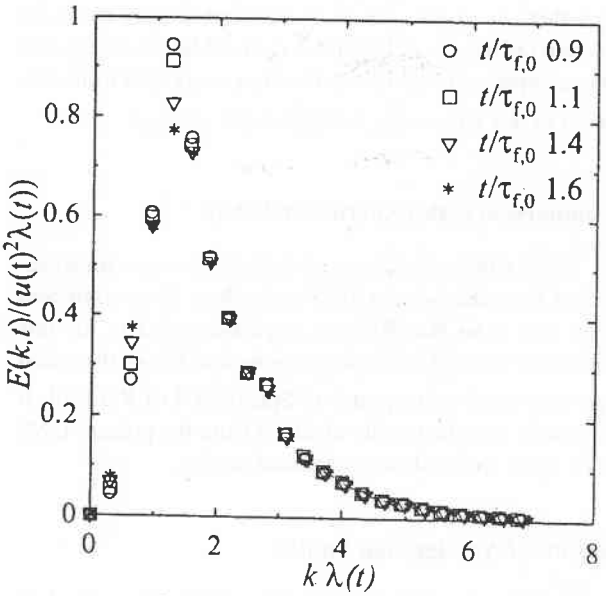

Fig. 4 Validation of the 3-dimensional DNS code for the passive scalar-mixing problem. Comparison of predicted turbulence kinetic energy spectrum at different instants of time. Note that the results exhibit a self-similarity. (Run A).

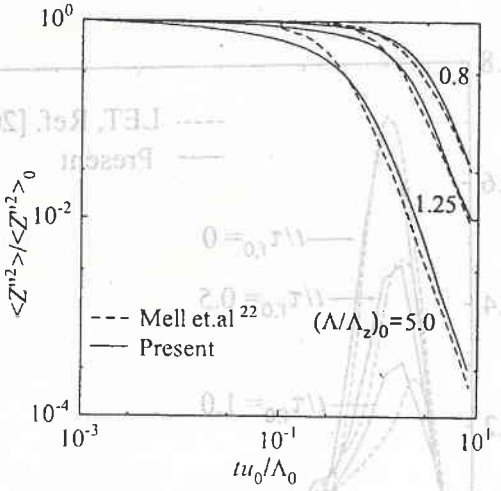

Fig. 5 Results from the simulations without chemical reactions: the passive scalar mixing problem. Comparison of predicted evolution of scalar variance with the DNS results of Mell, et. al. [22] for code-validation. (Runs C, D and E)

Next, the mixing of passive scalars was examined by varying the initial ratio of integral scale of velocity to that of scalars (Λ/Λ_Z at t = 0) as a parameter. In each case, the scalar variance (Z''^2) (t) was found to decay according to the power-law, which is evident from the lines with constant slopes in the loglog plot. It may be seen from Fig.5 that there is good agreement between results from the present DNS code and the DNS data of Mell et.al [22]. For this comparison, the initial kinetic energy spectrum was taken as $E(\underline{k},0) = u_{rms}^2 (k/\underline{k}_m^2) \exp(-k/\underline{k}_m)$.

Comparison with Experimental Data

In Fig.6 the one-dimensional dissipation spectrum predicted from the present DNS code (Run B) is compared with that from the different experimental data. In this result, the value of initial Re_λ was around 40 and the initial spectrum used corresponds to Spectrum 4 of Ref.[20]. It is evident that the results obtained from the present DNS code agree well with experimental results.

Results of Autoignition Studies

Further, the 3-D code developed has been used to investigate the effects of a fully 3-D turbulence on autoignition characteristics. Topological features of the evolving autoignition spots are examined by (1) finding the conditions of the mixture fraction and of scalar dissipation rate at the ignition sites, and (2) locating these sites with

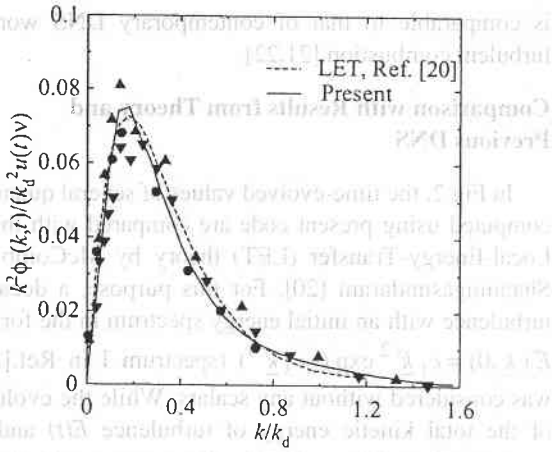

Fig. 6 Results from the simulations without chemical reactions: the passive scalar mixing problem. Comparison of predicted one-dimensional dissipation spectrum with experimental results for code-validation. Symbols refer to different experimental data whose references are compiled by McComb [20]

respect to the core/edge of the small-scale vortical structures. Also, the effect of turbulence intensity on the delay time is studied by carrying out simulations with different values of the initial eddy-turnover time. Comparisons are made between the results of 2-D and 3-D simulations for identical flow parameters. All these details are given elsewhere [23,24].

Conclusions

1. A 3-Dimensional computer code has been developed to analyze autoignition in a turbulent medium which accounts for variable density effects.
2. Initially the code has been validated without any scalars which showed a good comparison.
3. The scalar variance (Z''^2) (t), was found to decay according to a well-known power law.
4. The program has been improved with MPI calls to run it on IBM-SP parallel machines.
5. Results of autoignition studies are given elsewhere [23,24].

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