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Large eddy simulation of turbulent diffusion flame combustion using a conserved scalar methodology

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Abstract: The present paper describes an LES prediction of turbulent diffusion flame combustion in a simplified axisymmetric combustor geometry. The calculations are carried out using a well tested finite volume incompressible LES code which has been modified to handle variable density and reacting flows. The basic mixture fraction conserved scalar method is used with the chemical state relationships described by fast chemistry. The turbulence chemistry interaction is modelled by a subgrid PDF method and the PDF is assumed to follow a Beta function shape. The LES predictions have been time averaged over 3.5 flow-through times to generate the mean radial profiles of mixture fraction, product mass fraction, temperature, axial velocity and axial rms. The agreement of the LES predictions with the experimental data is good for all the above quantities at four different axial positions with largest differences at the first measurement plane. The LES method also provides information on the unsteady nature of turbulent diffusion combustion. For turbulent reacting flows with large density ratio, it was found necessary to use a relaxation method in order to remove unphysical high frequency fluctuations and to maintain numerical stability.

Key words: large eddy simulation(LES); turbulent diffusion flame; conserved scalar methodology; relaxation method

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Nomenclature

α	relaxation factor
$\bar{\sigma}_{ij}$	resolved stress tensor
G_c	gain of the transfer function
p	hydrodynamic pressure
Sc	laminar Schmidt number
Sc_t	turbulent Schmidt number
S_{ij}	resolved strain rate tensor
t	time
T	static temperature
u_i	component of velocity vector in i direction
x	coordinate
Y_i	mass fraction of species i
Z	mixture fraction
Z'	variance of mixture fraction
ρ	density
μ	molecular viscosity,

μ_{sgs}	subgrid scale eddy viscosity
τ_{ij}	subgrid scale stress tensor
ϕ_c	phase angle of the transfer function
Δ	filter width
Γ_Z	diffusive coefficient of mixture fraction

Introduction

Understanding, and predicting accurately, combustion processes in a gas turbine combustor is crucial in further improving its design and performance, particularly in a low emissions context. The flows inside a gas turbine combustor are very complicated with highly swirling and recirculating unsteady flows, jets in cross flow, heat release, and turbulence combustion interaction. It is evident now that numerical solutions

via the RANS approach using a statistical turbulence model are unlikely to be capable of capturing complex, unsteady reacting flows sufficiently accurately. Large Eddy Simulation (LES) has proven to be superior to the RANS approach whenever flow development depends on detailed capture of the dynamics of the large scale motions which are responsible at high Reynolds number for controlling the rate of mixing. The present paper describes an LES simulation of unsteady nonpremixed combustion in a simplified gas turbine combustor like geometry.

The outline of the paper is as follows: a mathematical formulation for variable density flow, including a low Mach number approximation and a combustion model, will be presented in section 1. Numerical methods, including the solution procedure and a relaxation method for stabilizing a variable density flow will be introduced in section 2. The calculation results will be presented and discussed in section 3, and conclusions will be summarized in section 4.

1 Mathematical formulation

The mathematical description of nonpremixed combustion is based on a low Mach number approximation and a mixing controlled model for combustion.

1.1 Combustion model

A mixing controlled model^[1] has been adopted in the present study, based on the assumption that the rate of chemical reaction is much faster than the rate of mixing. The combustion is then described by the mixture fraction, Z , which obeys the transport equation:

$$\frac{\partial(\rho Z)}{\partial t} + \frac{\partial(\rho Z u_i)}{\partial x_i} = \frac{\partial(\rho Z)}{\partial x_i} \left(\Gamma_Z \frac{\partial Z}{\partial x_i} \right) \quad (1)$$

With the assumption of unity Lewis number and neglecting external heat losses due to thermal radiation or convective heat transfer, the energy equation for low Mach number flow and the transport equation for mixture fraction have the same boundary conditions and are linearly related. Therefore, the instantaneous temperature, density and all major species chemical compositions are unique functions of

the mixture fraction, Z ^[2].

$$Y_i = Y_i(Z); T = T(Z); \rho = \rho(Z) \quad (2)$$

Various reaction models have been proposed for use with the single conserved scalar approach: fast chemistry, chemical equilibrium and steady and unsteady laminar flamelets at various strain rates^[2-4]. In this paper, only the results from fast chemistry calculations are presented. The effects of more refined treatment of chemical kinetics will be discussed in a future paper.

For fast chemistry, all chemical reactions are assumed to be infinitely fast and irreversible. Therefore the chemical state relationships can be determined directly from the given reaction stoichiometry, requiring no information about reaction rates or chemical equilibrium information. The species mass fractions and the mixture fraction have simple straight line relationships as shown in Fig. 1 (for methane/air combustion at 3.8×10^5 Pa, $T_{\text{fuel}} = 300$ K, $T_{\text{air}} = 750$ K). The temperature and density as functions of mixture fraction are shown in Fig. 2.

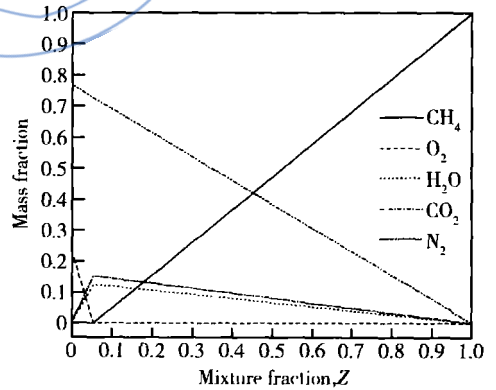


Fig. 1 Species mass fraction as functions of Z for fast chemistry (methane/air reaction)

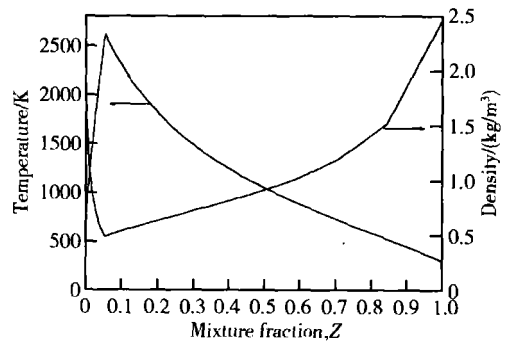


Fig. 2 Temperature and density as functions of Z for fast chemistry

1.2 Variable density flow equations

The compressible form of the governing flow equations for gaseous combustion processes contains vorticity, entropy, and acoustic modes^[5]. When the flow speed is much lower than the local speed of sound, the time scales of acoustic modes are much smaller than those of the other two modes, and there is thus no strong coupling of acoustic fluctuations with either vorticity or entropy modes. If the full compressible form of the governing equations is used, extremely small time steps have to be adopted to resolve the high-frequency acoustic waves. If a low Mach number approximation is adopted, acoustic interactions and compressibility effects are neglected, and it is assumed that the thermochemical variables such as density, temperature, enthalpy, and entropy can be decoupled from the local variations in static pressure whose spatial gradients are sources of momentum. The gas composition, temperature etc. is only related to a pre-specified background thermodynamically constant pressure field, p_0 . This implies that the speed of sound is nearly infinite. With this approximation, only p_0 is coupled to the thermodynamic variables and enters into the equation of state. For the open systems considered in this study it is also assumed that p_0 is uniform and constant. The change of density is only related to the changes in temperature and species composition.

With this low Mach number approximation, the governing equations for non-premixed reacting flow include the continuity equation, momentum equations, and a conserved scalar transport equation for mixture fraction. The instantaneous governing equations are spatially filtered by a grid filter (box filter). Mass weighted averaging similar to the Favre average in RANS modelling is used to reduce the terms arising from the filtering operation. The filtered governing equations can be written as^[3]:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_i}(\bar{\rho} u_i) = 0 \quad (3)$$

$$\frac{\partial \bar{\rho} u_i}{\partial t} + \frac{\partial}{\partial x_j}(\bar{\rho} u_i \tilde{u}_j) = - \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \bar{\tau}_{ij}}{\partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j} \quad (4)$$

$$\frac{\partial \bar{\rho} Z}{\partial t} + \frac{\partial}{\partial x_i}(\bar{\rho} u_i Z) = \frac{\partial}{\partial x_i}(\bar{D}_{z,i}) - \frac{\partial}{\partial x_i}(J_{z,i}) \quad (5)$$

in which $\bar{\rho}$ is the spatially-averaged resolved molecular stress tensor, and $\bar{D}_{z,i}$ is spatially-averaged resolved molecular diffusion flux for the conserved scalar Z in the i direction, τ_{ij} and $J_{z,i}$ are the residual or sub-grid scale fluxes of momentum and mixture fraction, respectively:

$$\tau_{ij} = \bar{\rho}(u_i u_j - \tilde{u}_i \tilde{u}_j) \quad J_{z,i} = \bar{\rho}(u_i Z - \tilde{u}_i Z) \quad (6)$$

The molecular properties in $\bar{\rho}$ (and $\bar{D}_{z,i}$) are considered constant and the fluxes are evaluated using linear relationships with the resolved scale

strain rate S_{ij} and scalar gradient $\frac{\partial Z}{\partial x_i}$:

$$\begin{aligned} \tau_{ij} &= 2\mu S_{ij} \quad S_{ij} = \frac{1}{2} \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) - \frac{1}{3} \delta_{ij} S_{kk} \\ \bar{D}_{z,i} &= \frac{\mu}{Sc} \left(\frac{\partial Z}{\partial x_i} \right) \end{aligned} \quad (7)$$

To close equations (4) and (5), gradient transport sgs models based on the standard Smagorinsky model^[6] and a constant turbulent Schmidt number have been used:

$$\begin{aligned} \tau_{ij} - \frac{1}{3} \delta_{ij} \tau_{kk} &= -2\mu_{sgs} S_{ij} = -2(\rho C_s \Delta)^2 |S_{ij}| S_{ij} \\ J_{z,i} &= -\frac{\mu_{sgs}}{Sc_t} \left(\frac{\partial Z}{\partial x_i} \right) \end{aligned} \quad (8)$$

In equation (8), $|S_{ij}|$ is the magnitude of the Favre averaged strain rate tensor ($\sqrt{2\tilde{S}_{ij}\tilde{S}_{ij}}$) and Δ is the filter width, assumed here to be the cube root of the local finite volume cell size. The sgs Prandtl/Schmidt number Sc_t is given the value 0.9.

Because of the non-linearity of the thermochemical relationships, the assumed PDF method was used to relate the instantaneous values in the chemical state relationships to filtered values required by the LES method. By presuming the subgrid scalar PDF of the mixture fraction, the filtered species mass fractions, density and temperature can be obtained:

$$\frac{1}{\bar{\rho}} = \int \frac{1}{\rho(Z)} \tilde{P}(Z) dZ \quad (9)$$

$$\tilde{Y}_i = \int Y_i(Z) \tilde{P} dZ \quad (10)$$

$$\tilde{T} = \int T(Z) \tilde{P}(Z) dZ \quad (11)$$

Cook and Riley^[17] proposed modelling $\tilde{P}(Z)$ by a Beta-function, parameterized via the resolved mixture fraction and its variance.

$$\begin{aligned} \tilde{P}(Z) &= \frac{Z^{a-1} (1-Z)^{b-1}}{\int_0^1 Z^{a-1} (1-Z)^{b-1} dZ} \\ a &= \tilde{Z} \left[\frac{\tilde{Z}(1-\tilde{Z})}{Z'^2_{sgs}} - 1 \right] \\ b &= (1-\tilde{Z}) \left[\frac{\tilde{Z}(1-\tilde{Z})}{Z'^2_{sgs}} - 1 \right] \end{aligned} \quad (12)$$

The sgs variance can be obtained from an equilibrium hypothesis:

$$Z'^2_{sgs} = C_V \Delta^2 \left(\frac{\partial \tilde{Z}}{\partial x_i} \right)^2 \quad (13)$$

where Δ is the filter width, and C_V is a constant set to 0.2 in the present simulations.

To avoid the PDF convolution at run time, the integrations can be pre-calculated and stored in look-up tables as a so-called interpolation library. For adiabatic flows, the table has two dimensions: mixture fraction and its variance. To facilitate linear interpolation of the look-up table, the variance of mixture fraction is normalized as:

$$Z'_s = \frac{Z'^2_{sgs}}{0.25 \cdot Z(1-Z)} \quad (14)$$

The density and temperature data in the fast chemistry library are shown in Figures (3) and (4) respectively.

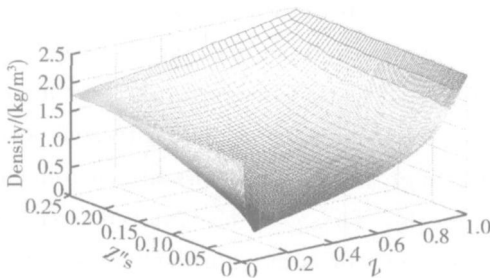


Fig. 3 Density profiles in fast chemistry library

2 Numerical method

The LULES code used as the basic constant

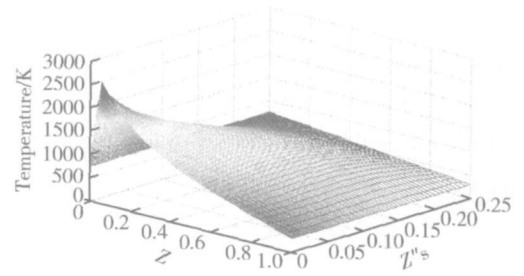


Fig. 4 Temperature profiles in fast chemistry library

density LES methodology adopted at the outset of the present work is a finite volume code based on body-fitted, orthogonal curvilinear coordinates. In curvilinear coordinates, velocity may be decomposed into its contravariant components. One difficulty encountered when using contravariant velocity components is due to the additional body force terms which arise because of grid line curvature. These additional terms cause memory requirement and accuracy problems which can be quite serious in three-dimensional applications^[8]. In addition, the attraction of orthogonal coordinates is that grid staggering may be used to avoid checkerboard oscillations and the necessity for any added smoothing. However, the geometry complexity for which 3D orthogonal grid can be generated is restricted. To avoid these problems, the body-fitted curvilinear grid generation in the present code is limited to only the x - y plane and in the third dimension, z , the grid is either translated or rotated. Although this is somewhat restrictive, many cylindrical or fully annular gas turbine related combustor geometries can be easily represented by this approach.

2.1 Spatial discretization

The spatially filtered transport equations described above are discretised using the finite volume method on a staggered grid. For the momentum equations, spatial derivatives for both convective and diffusive terms are calculated using a second order central differencing scheme. For the scalar transport equation, a central differencing scheme is used for the diffusion term while a second-order TVD scheme is used for convection discretization^[9].

2.2 Solution procedure

The governing equations are solved using an Explicit Adams-Bashforth predictor/corrector scheme in the following sequence:

(1) The subgrid eddy viscosity is calculated using the Smagorinsky model.

$$\mu_{\text{sgs}}^{n+1} = \mathcal{P}(C_s \Delta)^2 |\tilde{S}_{ij}^n| \quad (15)$$

(2) The density weighted value, $\tilde{\rho}z$, is solved at the $(n+1)$ time step, using velocities and density at the (n) and $(n-1)$ time steps.

$$(\tilde{\rho}z)^{n+1} = (\tilde{\rho}z)^n + \Delta t \cdot$$

$$\left[\frac{3}{2} \left[\begin{array}{c} \bullet (\tilde{\rho} u^n \tilde{z}^n) - \\ \Delta \left[\left(\frac{\mu^n}{Sc} + \frac{\mu_{\text{sgs}}^n}{Sc_t} \right) \tilde{z}^n \right] \end{array} \right] \right. \\ \left. - \frac{1}{2} \left[\begin{array}{c} \bullet (\tilde{\rho} u^{n-1} \tilde{z}^{n-1}) - \\ \Delta \left[\left(\frac{\mu^{n-1}}{Sc} + \frac{\mu_{\text{sgs}}^{n-1}}{Sc_t} \right) \tilde{z}^{n-1} \right] \end{array} \right] \right] \quad (16)$$

(3) Intermediate values of mixture fraction and its variance are calculated to find the density at $(n+1)$ time step.

$$\tilde{z}^* = \frac{(\tilde{\rho}z)^{n+1}}{\tilde{\rho}^n} \quad (17)$$

$$\tilde{Z}_{\text{sgs}}^{2*} = C_v \Delta^2 |\tilde{\Delta} \tilde{z}^*|^2 \quad (18)$$

(4) After obtaining predictor value of $\tilde{z}^*$ and $\tilde{Z}_{\text{sgs}}^{2*}$, these are used as entries into the fast chemistry library to calculate an estimated value of density at the $(n+1)$ time step.

$$\tilde{\rho}_{\text{est}}^{n+1} = \left[\int \frac{1}{\tilde{\rho}(\tilde{z}^*)} \tilde{P}(\tilde{z}^*) d\tilde{z}^* \right]^{-1} \quad (19)$$

(5) For combustion with large density variations, a relaxation method, which will be described in detail in the next section, has to be applied for density to guarantee computational stability. After updating the density at the $(n+1)$ time step using this relaxation method, mixture fraction has to be updated accordingly in order to retain consistency.

$$\tilde{\rho}^{n+1} = (1 - \alpha) \tilde{\rho}_{\text{est}}^{n+1} + \alpha \tilde{\rho}^n \quad (20)$$

$$\tilde{Z}^{n+1} = \frac{(\tilde{\rho}z)^{n+1}}{\tilde{\rho}^{n+1}} \quad (21)$$

(6) After correcting mixture fraction for the $(n+1)$ time step using equation (21), its variance is updated for the $(n+1)$ time step. The species mass fractions and temperature are then

evaluated from the fast chemistry library using $\tilde{Z}^{n+1}$ and $\tilde{Z}_{\text{sgs}}^{2*}$ as entries.

$$\tilde{Z}_{\text{sgs}}^{2*} = C_v \Delta^2 |\tilde{\Delta} \tilde{Z}^{n+1}|^2 \quad (22)$$

(7) The momentum equations are solved for the $(n+1)$ time step to get an the intermediate velocity field, using the Adams-Bashforth scheme expressed as follows:

$$\tilde{\rho}^{n+1} \tilde{u}_i^* = (\tilde{\rho} u_i)^n + \Delta t \left[-\frac{1}{2} (\text{adv.} + \text{diff.})^n + \frac{1}{2} \frac{\partial \tilde{p}^{n-1}}{\partial x_i} \right] \quad (23)$$

A convective outflow boundary condition is applied after solving equation (23).

(8) A multigrid solver (see [8]) is used to solve a Poisson equation to get the pressure field at the $(n+1)$ time step.

$$\frac{\partial^2 \tilde{p}^n}{\partial x_i \partial x_i} = \frac{2}{3 \Delta t} \left[\frac{\partial (\tilde{\rho}^{n+1} \tilde{u}_i^*)}{\partial x_i} + \frac{\partial \tilde{\rho}^{n+1}}{\partial t} \right] \quad (24)$$

where

$$\frac{\partial \tilde{\rho}^{n+1}}{\partial t} = \frac{\tilde{\rho}^{n+1} - \tilde{\rho}^n}{\Delta t} \quad (25)$$

(9) The intermediate velocity field is then updated using the new pressure field to get the velocity at $(n+1)$ time step. A convective outflow boundary condition is again applied.

$$\begin{aligned} \tilde{u}_i^{n+1} &= \frac{1}{\tilde{\rho}^{n+1}} \left[\tilde{\rho}^{n+1} \tilde{u}_i^* - \frac{3 \Delta t}{2} \frac{\partial \tilde{p}^{n+1}}{\partial x_i} \right] \\ &= \tilde{u}_i^* - \frac{3 \Delta t}{2 \tilde{\rho}^{n+1}} \frac{\partial \tilde{p}^{n+1}}{\partial x_i} \end{aligned} \quad (26)$$

2.3 Relaxation method

In flows with strong density gradients (due to intense heat release and expansion), because of the use of spatial discretization in the transport equations using a non-diffusive central scheme, high frequency errors are introduced to all quantities. These can be removed from density by relaxation in time in order to achieve a stable scheme^[10]. The relaxation of density is the classical relaxation scheme:

$$\tilde{\rho}^{n+1} = (1 - \alpha) \tilde{\rho}_{\text{est}}^{n+1} + \alpha \tilde{\rho}^n \quad (27)$$

where α is the relaxation factor which is defined as:

$$\alpha = e^{-\Delta t/T} \tag{28}$$

in which $\Delta t = t^{n+1} - t^n$ is the time step and T is the relaxation time.

The relaxation method above is in the form of a recursive operation of a convolution, i. e., discrete integration of $\bar{\rho}^*(t)$ with an exponential decaying weighting function.

$$\rho^{n+1} = \int_{-\infty}^{t^{n+1}} \bar{\rho}^*(t) \frac{e^{-\frac{t^{n+1}-t}{T}}}{T} dt \tag{29}$$

The density is averaged over the relaxation time with a weighting function that decays exponentially backwards in time. This is a filtered convolution by a lowpass filter, with $\bar{\rho}^*(t)$ the signal being filtered. The convolution kernel or filter kernel is:

$$h(t) = \frac{1}{T} e^{-\frac{t^{n+1}-t}{T}} \phi(t) \tag{30}$$

in which $\phi(t)$ denotes the Heaviside unit step function, i. e.,

$$\phi(t) = \begin{cases} 1, & t \geq 0 \\ 0, & t < 0 \end{cases} \tag{31}$$

The transfer function of this low-pass filter in the frequency domain can be evaluated via a Laplace transform of the impulse response:

$$H(s) = L\{h(t)\} = G_c e^{j\phi_c} = \frac{1}{\sqrt{1 + (\omega T)^2}} e^{j\arctan(-\omega T)} \tag{32}$$

where $G_c = 1/\sqrt{1 + (\omega T)^2}$ is the gain of the transfer function and $\phi_c = \arctan(-\omega T)$ is the phase angle. The Power Spectral Density of the low-pass filter kernel with different characteristic relaxation times is shown in Fig. 5.

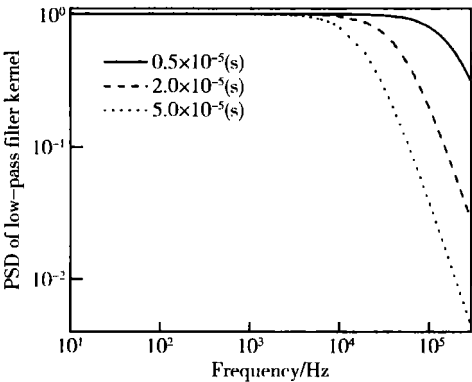


Fig 5 Power spectrum density of the low-pass filter kernel

The Fourier transform of ρ^{n+1} is equal to the multiplication of the Fourier transform of $\bar{\rho}^*(t)$ and the low-pass filter kernel, i. e.,

$$L\{\rho^{n+1}(t)\} = L\{\bar{\rho}^*(t)\} \times L\{h(t)\} \tag{33}$$

After knowing the frequency spectrum of $\rho^{n+1}(t)$, we can derive the frequency spectrum of $\bar{\rho}^*(t)$. However, since there is a feedback between density and the other variables in the system, the derived frequency spectrum of $\bar{\rho}^*(t)$ with different relaxation time will be similar but not precisely the same.

2.4 Test case and computational setup

The experimental test case used for validation of the LES simulation was the coaxial jet combustor configuration of Owen et al.^[11] which has been used previously as an LES validation test case in [12, 13]. The configuration has a low velocity (0.93 m/s) central fuel jet, and a higher velocity (20.6 m/s), annular non-swirling air jet. The Reynolds number based on air stream outer radius (R) and the inlet bulk velocity of the air (U) is 10^4 . The computational domain was chosen to extend from $2R$ upstream of the combustor mixing plane to $8.5R$ downstream of this plane. The calculations used $200 \times 64 \times 64$ grid points in the axial, radial and azimuthal directions, respectively. A coarse mesh with $100 \times 32 \times 32$ grid points was also used for a grid-dependence study (Note that the predictions of [12, 13] used a grid size 3 time denser than the finer grid used here). The coarse mesh is shown in Fig. 6. No random noise was imposed at inlet and uni-

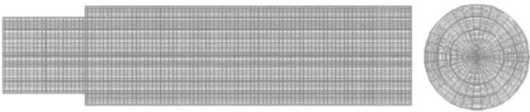


Fig.6 Schematic of grid used for the simulations

form velocity profiles were applied, because the flow conditioning devices were located only a short distance upstream of the jet orifice. Pierce^[13] used fully developed inflow condition, even though the experimental arrangement properly did not allow this. Convective outflow boundary conditions were specified at the outlet. All the solid boundaries, including the annular

splitter plate, were assumed to be adiabatic and impermeable.

3 Results and discussion

3.1 Energy spectrum

Three calculations have been carried out with the same time step ($dt=0.0026\text{ ms}$), but different relaxation time T , i.e., 0.005 ms , 0.02 ms , and 0.05 ms . The predicted density and axial velocity power spectral densities at a point ($x/R=0.77$, $y/R=0.85$, $\theta=\pi/2$, with centre of the mixing plane as the origin) are shown in Fig 7.

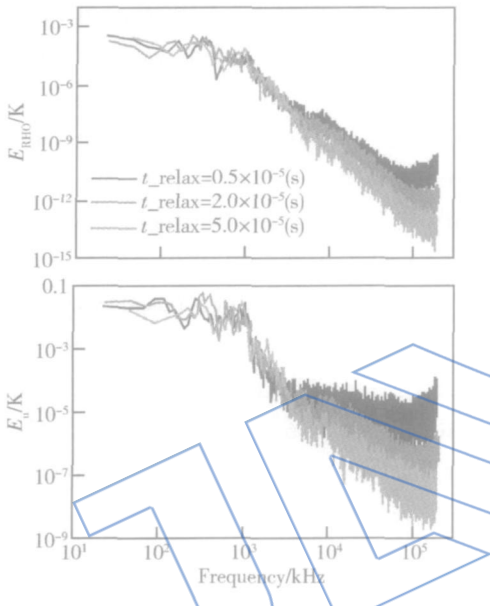


Fig. 7 Energy spectrums of density and axial velocity at point ($x/R=0.77$, $y/R=0.85$, $\theta=\pi/2$, with centre of the mixing plane as the origin)

It is shown that the predicted energy spectra are different only in the high frequency range where the energy levels have fallen by around 3 orders of magnitude, with longer relaxation time providing stronger damping of high frequencies, while the low frequency range remains unaffected. Compared with the results for relaxation time 0.005 ms , results for relaxation time 0.02 ms show noticeable additional decay only after about 4000 Hz , while those for relaxation time 0.05 ms show noticeable extra decay after about 1500 Hz . This is consistent with the predictions of the low-pass filter theory introduced above. It also demonstrates that the relaxation method is able to promote numerical stability without undermin

ing the simulation accuracy. Note the increase in energy at high frequency obtained with the smallest relaxation time ($5\times10^{-6}\text{ s}$); it is the growth in these high frequency fluctuations which would make the calculation catastrophically unstable if left undamped.

3.2 Analysis of the mean flow field

The time averaged axial velocity and mixture fraction fields for predicted diffusion flame combustion are shown in Fig. 8, in comparison with results from a pure mixing (nonreacting) calculation.

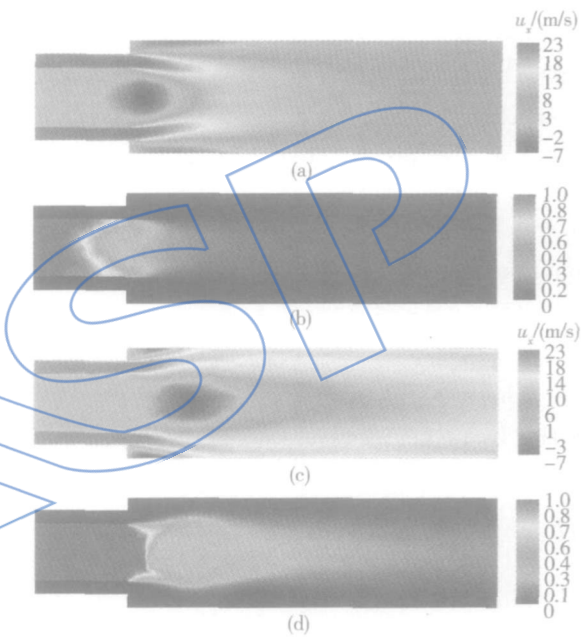


Fig. 8 Time averaged fields of axial velocity and mixture fraction, (a) axial velocity, mixing, (b) mixture fraction, mixing, (c) axial velocity, reacting, (d) mixture fraction, reacting

In the mixing case, the high axial velocity of the annular air jet decays quickly. The flow field includes a large, strong central recirculation region which enters the fuel jet supply and a long, flat recirculation region near the corner of the step. The fuel and air mix very efficiently and the potential core of the fuel jet is short. The mixing begins well inside the fuel inlet port. In the reacting case, heat release forces the flow to accelerate. The high axial velocity regions continue until the outlet. Since the reacting fluid expands, the high speed annular air jet is pushed outward to the wall. The central recirculation region is

shifted downstream and is elongated as the flow accelerates, while the recirculation region near the step corner becomes much smaller. The mixing efficiency of fuel and air is substantially reduced compared with the nonreacting case, and there is an identifiable potential core of fuel downstream of the fuel inlet.

3.3 Mean profiles

After reaching statistically steady state, calculations with different relaxation times provided essentially the same time-averaged results. The

mean profiles from calculation with relaxation time 0.02 ms were used to compare against the experimental data. Calculation results using the initial coarse mesh were compared with those of the finer mesh to study the grid-dependence. The profiles of mixture fraction, temperature, product mass fraction, axial mean velocity and rms along the centreline of the combustor are shown in Fig. 9. The profiles along the lipline of the splitter plate between central fuel jet and annular air stream are shown in Fig. 10.

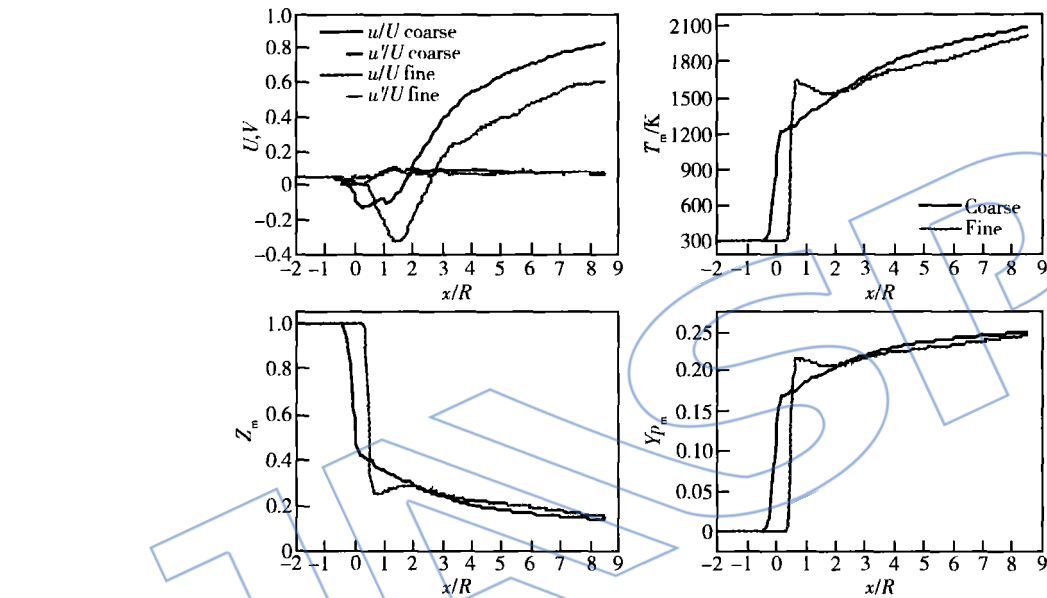


Fig. 9 Axial profiles of time-averaged mixture fraction, temperature, products mass fraction, axial velocity and its rms along the centerline of the combustor

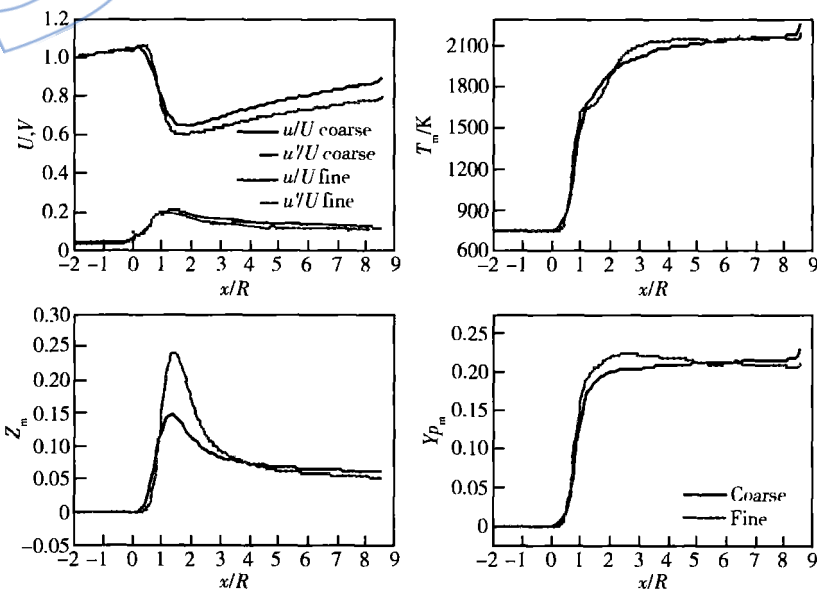


Fig. 10 Axial profiles of time-averaged mixture fraction, temperature, products mass fraction, axial velocity and its rms along the lipline

Both Figures 9 and 10 show that when the mesh is refined, the calculation results in general agree fairly well. The main changes occur in a small region near the inlet port. In Fig. 9, it is shown that the fine mesh calculation results for mixture fraction (and thus the temperature and product mass fraction predictions) show a steeper gradient at fuel jet exit than in the coarse mesh, and this zone is shifted slightly downstream. The resolved central recirculation zone is also stronger than that predicted with the coarse mesh. In Fig 10, the fine mesh and coarse mesh results are in close agreement, showing that the mixing across the jet annular shear layer is reasonably well resolved with a higher mixture fraction predicted in the first two radii downstream. The fine mesh results are used to compare with the experimental data.

Since density, temperature and species mass fractions all depend on mixture fraction, it is important to predict mixture fraction profiles accurately. Fig 11 shows the radial profiles of time averaged mixture fraction compared with the experimental data at four different axial locations.

The LES results of Pierce^[12] with fast chemistry are also shown for reference. It is found that the present simulation is in good agreement with Pierce's results at all axial positions. The results agree with the experimental data better as axial distance increases. At axial position $x/R=0.21$, the simulation results agree poorly with the experimental data by predicting unburnt mixture. This was also shown in Pierce's^[12] calculations. Pierce^[12] considered that the difference may be caused by specification of fully-developed inlet conditions, but this was not used here and the results are essentially the same. It is believed that the difference is due to the very rapid changes which taken place in the axial direction and the invalidity of the simple chemistry model used here to cope with these. It is also noticed that, in the mid and far downstream region, the calculated mixture fraction is higher than that of the experimental data. This is believed to be caused by the fast chemistry model, which over predicts the heat release rate and thus leads to a lower mixing rate.

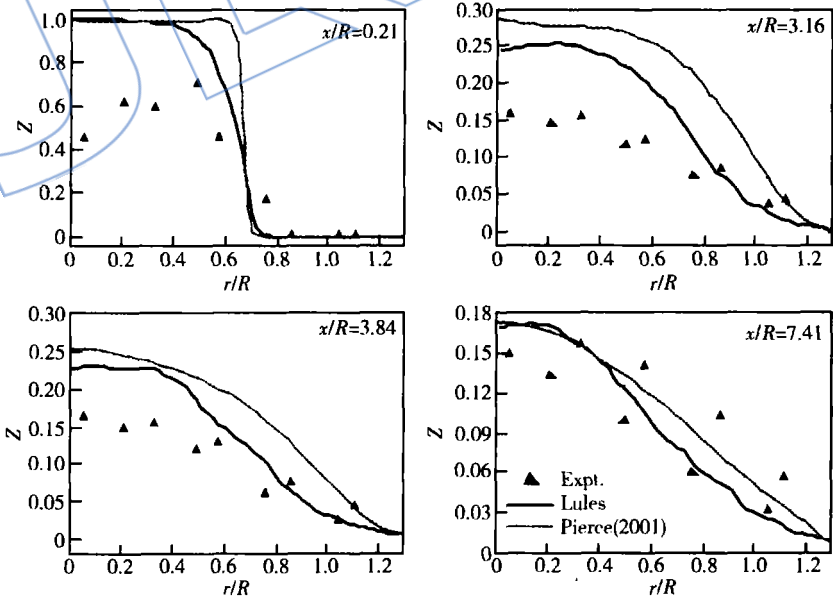


Fig. 11 Radial profiles of time averaged mixture fraction

Fig. 12 shows radial profiles of time averaged product mass fraction compared with the experimental data at four axial locations. The product mass fraction is defined as the sum of

the mass fractions of CO_2 and H_2O . It can be seen that the simulation provides good results at three downstream axial positions. The discrepancy between the prediction and the experimental

data at the $x/R = 0.21$ location is consistent with that of the mixture fraction and can be explained by the steep gradient shown in Fig. 9. Near the inlet, the product mass fraction is due mainly to recirculation of products from reactions happening downstream. It is also apparent that the fast chemistry model consistently overpredicts the levels of product concentration in the inner regions.

The radial profiles of time-averaged temperature at four different axial locations are shown in Fig. 13. The results show fair agreement with

the experimental data. It seems that the prediction of temperature profiles is generally better than those for the product mass fraction; however, it has to be pointed out that the temperature profiles are measured at four axial positions which are different and further downstream than those for product mass fraction measurements. The radial profiles of time-averaged axial velocity and axial fluctuation intensity are shown in Fig. 14. The agreement between the simulation and experiment is good, except for an under prediction in the inner region near the fuel outlet.

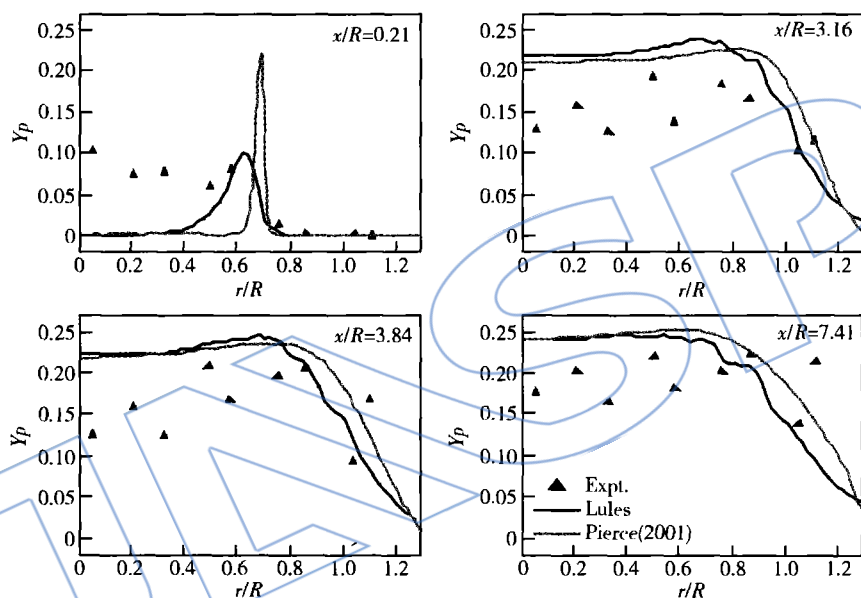


Fig. 12 Radial profiles of time-averaged product mass fraction

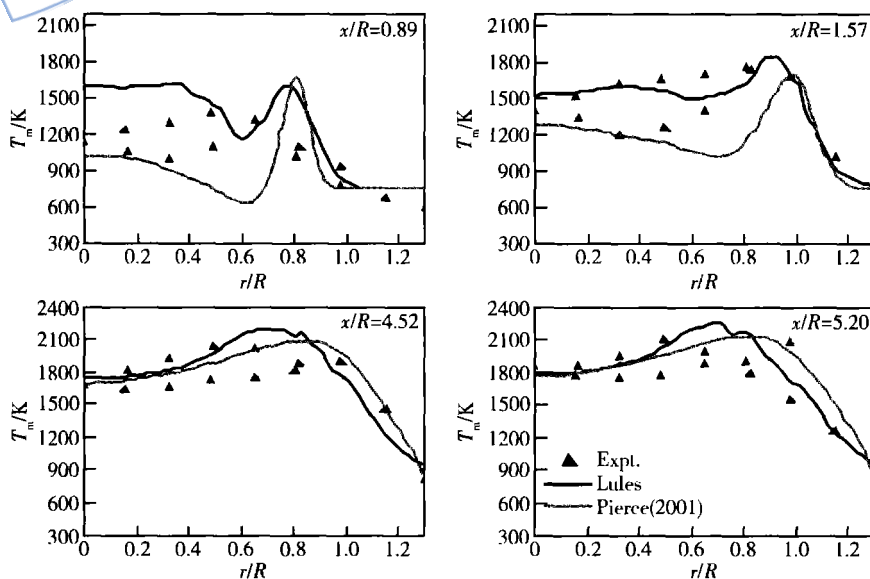


Fig. 13 Radial profiles of time-averaged temperature

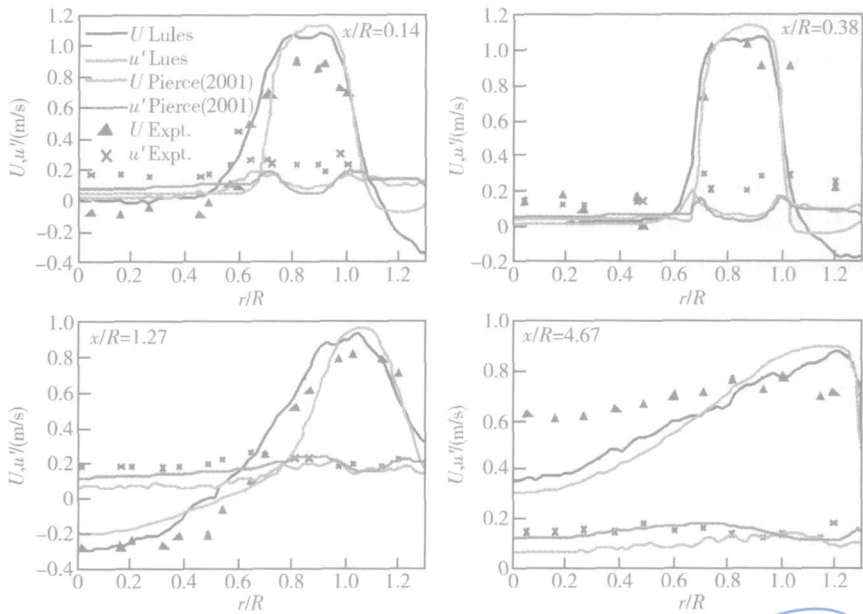


Fig. 14 Radial profiles of time-averaged axial velocity and axial fluctuation intensity

The simulation successfully captures the peaks of axial fluctuation intensity within the shear layer between the fuel and air streams. However, the predicted turbulence level is lower than in the experimental results.

3.4 Flame structures

A snapshot of the predicted instantaneous temperature field is shown in Fig 15, which serves to illustrate the flame structures. The high temperature regions represent the location

of the flame. It is seen that the annular air stream is pushed out forwards the wall and creates a lower temperature layer surrounding the inner higher temperature reacting region. This layer gradually disappears as the axial distance increases. The diffusion flame is found to be lifted and composed of separate high temperature zones within the circular region of the fuel air shear layer. Near the inlet, the size of the high temperature zones is small. As the axial distance increases, the high temperature zones become larger and begin to connect. Near the outlet, the high temperature zones become fully connected and occupy the whole azimuthal direction.

4 Conclusions

A finite volume incompressible variable density Large Eddy Simulation code has been developed for low Mach number nonpremixed combustion. The mixture fraction method is used with the chemical state relationships described by fast chemistry. The turbulence chemistry interaction is modelled by a sub-grid PDF method and the PDF is assumed to be a Beta function.

An explicit Adams-Bashforth scheme is used for the temporal integration, with the Poisson equation for pressure being solved by a multigrid method. The code is validated against ex-

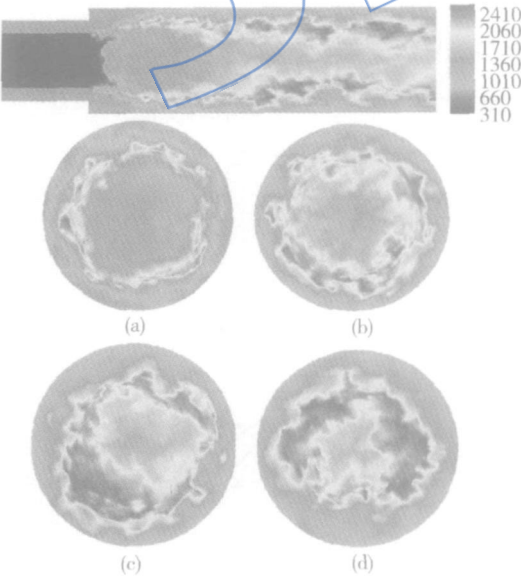


Fig. 15 Instantaneous temperature fields;
Top: meridional plane; Bottom: radial cross
Sections (a) $x/R=1.5$, (b) $x/R=3.0$,
(c) $x/R=4.5$, (d) $x/R=6.0$

perimental data from [11] and Pierce's LES predictions^[13]. The LES predictions have been averaged over 3.5 flow-through times to generate mean radial profiles of mixture fraction, product mass fraction, temperature, axial velocity and axial fluctuation intensity. The agreement of the LES predictions with the experimental data is good for all profiles at four different axial positions considering that only a simple subgrid model and a simple combustion model have been employed. The effects of heat release on mixing have been illustrated by comparing with the results of a nonreacting calculation. It is found that the strong heat release during combustion considerably decreases the mixing rate of fuel and air. The LES method is also shown to be capable of revealing the unsteady nature of turbulent diffusion flame combustion. For turbulent reacting flows with large density ratio, it was found necessary to use a relaxation method in order to remove unphysical high frequency fluctuations and to maintain numerical stability. The relaxation method (following [10]) is found to perform like a low-pass filter in the frequency domain, and helps to remove the high frequency oscillations and keep the calculations stable, while at the same time leaving the low frequency energy containing components unaffected, thus allowing high accuracy of LES calculation.

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