Evaluation of a Bounded High-Resolution Scheme for Combustor Flow Computations

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The present paper is concerned with the application of a high-resolution scheme for a finite volume discretization method. The capability of the chosen scheme is evaluated for the numerical simulation of three-dimensional flowfields. Special emphasis lies in the calculation of the processes in the mixing zone of gas turbine combustors. Thus, numerical results are compared with detailed measurements of velocity and temperature in a model mixing zone. The velocity field as well as the temperature field strongly depend on the scheme used for the discretization of the momentum and energy equations. The proposed high-resolution scheme and the well-known QUICK scheme yield similar results, which are superior to those obtained with the simple UPWIND scheme. For the simulation of turbulent transport, the standard k, ϵ model is employed. The effect of numerical diffusion caused by the usual UPWIND discretization of the convective transport of k and ϵ is assessed by the application of the high-resolution scheme of the discretization of the k and ϵ equations. As a result, it is found that the velocity and temperature fields are insensitive to the scheme that is applied for the discretization of the k and ϵ equations.

Nomenclature

A	= control-volume surface
a,b	= slopes of piecewise linear functions
D	= diameter
H	= duct height
J	= momentum flux ratio
k	= turbulent kinetic energy
S	= source term
s	= center-to-center distance between two jets
s	= slope of piecewise linear function
$\bar{T}$	= mean temperature
u,v,w	= Cartesian velocity components
V	= control volume
x,y,z	= Cartesian coordinates
Δx	= grid spacing in x direction
Γ_ϕ	= diffusion coefficient
ϵ	= dissipation rate of k
ρ	= density
ϕ	= dependent variable

Subscripts

B	= bottom wall
e,w	= control-volume interfaces in x direction
f	= control-volume interface
h,l	= control-volume interfaces in z direction
i,j,k	= grid indices
j	= jet entry
n,s	= control-volume interfaces in y direction
T	= top wall
∞	= inlet

Introduction

THE accurate prediction of the flow in gas turbine combustors requires the utilization of complex physical models as well as the consideration of three-dimensional effects. Thus, the numerical simulation of combustor flows requires both high computational time and large main storage. However, computational times as well as storage requirements, in general, are limited by the main storage region and the CPU time of the available computer. As a consequence, relatively coarse grids must be employed and consequently large discretization errors frequently arise. The acceleration of the efficiency of the solution procedure to permit finer mesh arrangements, as well as the augmentation of the accuracy of the applied discretization scheme, are a necessity for future computations of combustor flows.[1-5] The present study is devoted to the development of the finite volume discretization method for the numerical simulation of three-dimensional recirculating turbulent flows.

In recent years, in addition to the grid-adaption technique[6] for the discretization of the convective transport, a variety of so-called higher-order schemes has been developed. It is well-known that by the application of a higher-order scheme oscillations or under- and overshoots can arise. These under- and overshoots are often not obvious; however, in all cases where physical principles are evidently violated, higher-order schemes seem to be impracticable. In addition, over- and undershoots can induce large errors in all cases where the gradient of a flow quantity is of certain influence (e.g., the determination of local wall heat flux in the case of prescribed wall temperatures[6]). Over- and undershoots can even prevent convergence of calculations when nonnegative scalars (e.g., concentration or turbulent quantities like k and ϵ) become negative.

For a preliminary evaluation of the specific features of different discretization schemes, the propagation of a strictly conserved passive scalar in a stratified flow is computed. Figure 1 illustrates this simple test problem: The computational grid, consisting of 10×10 nodes and uniform control volumes, is arranged at an angle of 45° with respect to the flow direction. The velocity field is assumed to be homogeneous whereas at the inlet of the calculation field a stratification of a passive conserved scalar perpendicular to the flow is prescribed. In addition, it is assumed that no diffusive transport takes place, i.e., $\Gamma_\phi = 0$ [Eq. (1)]. Figure 2 shows for different discretization schemes the calculated distributions of ϕ over the direction s, i.e., perpendicular to the flow direction. Since $\Gamma_\phi = 0$ was assumed, no lateral exchange of ϕ can occur, and, therefore, the exact solution for ϕ jumps at $s/L = 0.5$ from $\phi = 0$ to $\phi = 1$.

It is well known that the effect of so-called numerical diffusion is large for coarse grid spacings and high-flow velocities

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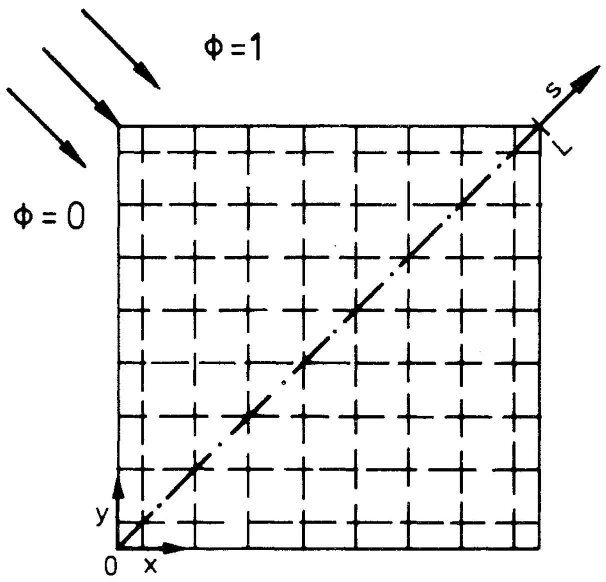

Fig. 1 Test case.

when the flow vectors are oblique to the control-volume faces. Therefore, in the test case presented, a flattening of the profile is predicted by the UPWIND scheme. In contrast to the UPWIND scheme, the higher-order schemes give better approximations to the exact solution. However, these schemes lead to unrealistic results that become obvious in Fig. 2 since in this test case ϕ must lie in the range [0,1]. QUICK[7] as well as the so-called linear-upwind scheme LINUP[2] result in over- and undershoots; the central-difference scheme leads to oscillations. Figure 2 also shows the results of two other schemes that do not suffer from boundedness problems; the clipped central-difference scheme and the MLU scheme. The present paper is focused on the derivation and evaluation of these schemes.

For the suppression of oscillations, a variety of procedures based on the increase of the effective viscosity has been developed. Besides the direct inclusion of additional (artificial) diffusivity in the original transport equations, the so-called flux-blending methods represent procedures increasing the local diffusion.[8] A very simple flux-blending method is the well-known HYBRID scheme. In that scheme, depending on the local Peclet number $Pe = (\rho u \Delta x)/\Gamma$, the UPWIND or the central-difference scheme is taken for the discretization of convection. Thus, the numerical diffusion of the UPWIND discretization guarantees the solution to be in the range of physical bounds. However, since the numerical diffusion is proportional to the Peclet number, the HYBRID scheme often suffers from large discretization errors. This is particularly true in the calculation of the complex flows in gas turbine combustors.

The idea of combining various discretization schemes of different order of accuracy in the sense of truncation error was used to derive a variety of more sophisticated flux-blending methods.[10] An interesting example for such a flux-blending method is the method proposed by Peric.[8] For each control volume, Peric derives a linear combination of two discretization schemes of different order, such that the final solution lies within the physical bounds. However, flux-blending procedures can considerably augment the computation costs. In addition, they often are unable to provide the desired "optimum" accuracy.

High-Resolution Schemes

In parallel with the development of higher-order schemes and the associated flux-blending methods, the construction of so-called high-resolution (HR) schemes[11-17] has taken place in recent years. These schemes are at least of second-order accuracy in smooth regions of the calculated flow. They do not generate spurious oscillations and do not need any explicitly added artificial diffusion. A comprehensive survey and a comparison of such discretization schemes originally derived for the finite difference discretization of one-dimensional hyperbolic flow problems is given by Munz[17]. The so-called TVD schemes (see Harten[14]) form a special group of the HR schemes. Principles for the derivation of TVD discretization are reported by Van Leer,[13] Osher and Chakravarthy,[15] and Harten and Osher.[16]

To avoid oscillations the HR schemes, in general, switch to the UPWIND interpolation whenever local extremes are encountered. Thus, local extremes are clipped, and oscillations in the final solution resulting from a higher-order scheme are excluded. Unfortunately, this clipping cannot be restricted to spurious oscillations; this approach also dampens meaningful extremes. An impressive example of the suppression of oscillations is given in Fig. 2 where, for the calculation of the previously mentioned stratified flow, the results obtained by a conjunction of the clipping step and the central-difference scheme are shown.

However, the clipping of local extremes is a highly nonlinear procedure that can prevent convergence. Therefore, special attention must be focused on the construction of discretization schemes suitable for a stable connection with the clipping step. For the finite difference formulation, a variety of such schemes is given in the literature.[17] Contrary to simple test cases, there is very little experience with the performance and the application of HR schemes for calculations of three-dimensional complex recirculating flows. Therefore, in the present study one promising scheme was adopted for flow calculations based on finite volume discretization, and the performance of the selected scheme was examined in the calculation of complete three-dimensional combustor flows.

Monotonized Linear-Upwind Scheme

The time-averaged transport equation of a physical flow quantity ϕ can be cast in the following form:

$$\operatorname{div}(\rho c \phi) = \operatorname{div}(\Gamma_\phi \cdot \operatorname{grad}\phi) + S_\phi \qquad (1)$$

For the discretization of such a partial differential equation, various methods are known. In applying the finite volume discretization, the differential equation is integrated over control volumes. Thus, with the assumption of a homogeneous distribution of ϕ over each of the control-volume faces enclosing grid node i,j,k the convective terms are approximated by

$$\int_V \operatorname{div}(\rho c \phi)\, \mathrm{d}V = \int_A \rho c \phi \, \mathrm{d}A = (\rho u \phi A)_{i+\frac{1}{2},j,k} - (\rho u \phi A)_{i-\frac{1}{2},j,k} + (\rho v \phi A)_{i,j+\frac{1}{2},k} - (\rho v \phi A)_{i,j-\frac{1}{2},k} + (\rho w \phi A)_{i,j,k+\frac{1}{2}} - (\rho w \phi A)_{i,j,k-\frac{1}{2}} \qquad (2)$$

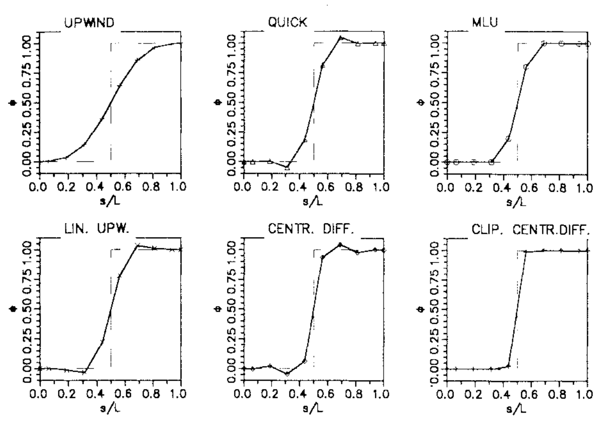

Fig. 2 Results from different discretization schemes ($Pe = \infty$, $|v/u| = 1.0$).

Various discretization schemes are derived from different interpolation rules for the determination of ϕ at the control-volume interfaces. The conservation of the integral balances requires that the flux across a common interface area must be the same for each of both adjacent volumes (consistency of fluxes). Thus, for each interface area of two adjacent control-volumes, a sole interpolation rule must hold. In general, this is achieved by the shifting of the interpolation schemes for a flow quantity ϕ in the upstream direction (UPWIND shifting, UPWIND weighting).

Well-known examples of this approach are the QUICK scheme and the so-called linear-upwind scheme (LINUP).[2] The QUICK scheme uses a parabolic interpolation function fitted to the ϕ values at three adjacent grid points: two upstream and one downstream of the considered interface (cf. Fig. 3). With the LINUP scheme, ϕ at an interface is extrapolated out of the straight line connecting the two ϕ values upstream of the interface (Fig. 3). In using this rule $\phi_{i-½}$ at the control-volume interface, $i-½$ is determined by

$$\phi_{i-½} = \phi_{i-1} + \frac{x_i - x_{i-1}}{2} \cdot \frac{\phi_{i-1} - \phi_{i-2}}{x_{i-1} - x_{i-2}} \quad \text{for } u_{i-½} > 0 \tag{3a}$$

$$\phi_{i-½} = \phi_i - \frac{x_i - x_{i-1}}{2} \cdot \frac{\phi_{i+1} - \phi_i}{x_{i+1} - x_i} \quad \text{for } u_{i-½} < 0 \tag{3b}$$

As mentioned before, the QUICK as well as the LINUP scheme can cause over- and undershoots in the final solution, which is particularly true for flow regions with steep gradients.

One promising scheme examined by Munz[17] is the so-called monotonized central-difference scheme originally proposed by Van Leer.[13] From this scheme, the slope of s of a piecewise linear distribution between two adjacent grid points i and $i-1$ is assumed as

$$s_{i-½} = \text{minmod } [(a+b)/2,\ 2 \cdot \text{minmod } (a,b)] \tag{4}$$

The minmod-function is defined as

$$\text{minmod}(a,b) = \begin{cases} a \text{ for } |a| \le |b| \text{ and } a \cdot b > 0 \\ b \text{ for } |a| > |b| \text{ and } a \cdot b > 0 \\ 0 \text{ for } \quad a \cdot b \le 0 \end{cases} \tag{5}$$

where a and b represent slopes of piecewise linear functions. For the cell boundary at $i-½$, the slope a is defined as

$$a = \frac{\phi_i - \phi_{i-1}}{x_i - x_{i-1}} \tag{6a}$$

In contrast to the determination of a, the specification of the slope b and of $\phi_{i-½}$, depends on the sign of the contravariant velocity component $u_{i-½}$:

$u_{i-½} > 0$:

$$b = \frac{\phi_{i-1} - \phi_{i-2}}{x_{i-1} - x_{i-2}} \tag{6b}$$

$$\phi_{i-½} = \phi_{i-1} + s_{i-½} \cdot \frac{x_i - x_{i-1}}{2} \tag{6c}$$

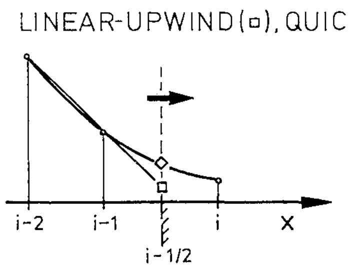

Fig. 3 QUICK, linear-upwind scheme (LINUP).

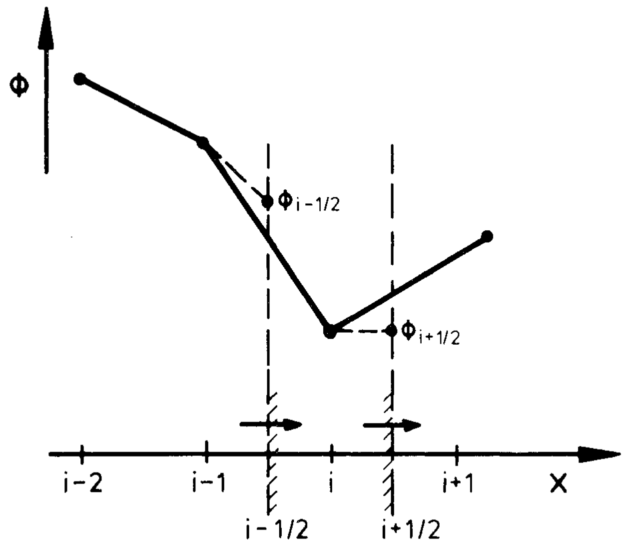

Fig. 4 MLU interpolation.

$u_{i-½} < 0$:

$$b = \frac{\phi_{i+1} - \phi_i}{x_{i+1} - x_i} \tag{6d}$$

$$\phi_{i-½} = \phi_i - s_{i-½} \cdot \frac{x_i - x_{i-1}}{2} \tag{6e}$$

This approach is illustrated in Fig. 4, where positive velocities are assumed. For the application of the finite volume discretization, the UPWIND shifting represents a major element. Therefore, the presented scheme in the following will be referred to as the monotonized linear-upwind scheme (MLU). The MLU scheme is of second-order accuracy whenever $a \cdot b > 0$ [see Eq. (5)], i.e., in smooth regions of the flow. At local extremes it degenerates to first-order accuracy. The results obtained by the application of this scheme for the calculation of the stratified flow are shown in Fig. 2. For this simple test case the gradients of ϕ at $s/L = 0.5$ achieved by QUICK, LINUP, and MLU do not differ. However, only the results of the MLU scheme lie within the physical bounds.

Nonisothermal Jet Mixing

In evaluating the relative merits of the suggested MLU scheme under practical conditions, this scheme was implemented in the computer program EPOS (Elliptic Package on Shear Flows), developed at the Institute for Thermal Turbomachinery of the University of Karlsruhe. EPOS can be used to solve the three-dimensional transport equations for recirculating turbulent flows with chemical reaction based on a finite volume discretization. A generalized conjugate gradient iterative procedure for the solution of the system of equations formed by the difference equations is employed. For the calculation of the velocity field, the Navier-Stokes equations are solved on a nonstaggered grid. The coupling of velocity and pressure fields is taken into account by a SIMPLE-like[18] procedure. Turbulent transport is simulated by the well-known standard k, ϵ-model. For the prediction of combustion processes, various combustion models are available.

For the inclusion of the MLU scheme in the momentum and energy equations, the following approach is adopted: The convective flux across an interface f of a control volume at a grid point i,j,k is expressed in terms of the UPWIND flux

$$(\rho c A)_f \phi_f^{\text{MLU}} = (\rho c A)_f \phi_f^{\text{UPW}} - (\rho c A)_f \Delta\phi_f$$

$$f = e, w, n, s, h, l \tag{7}$$

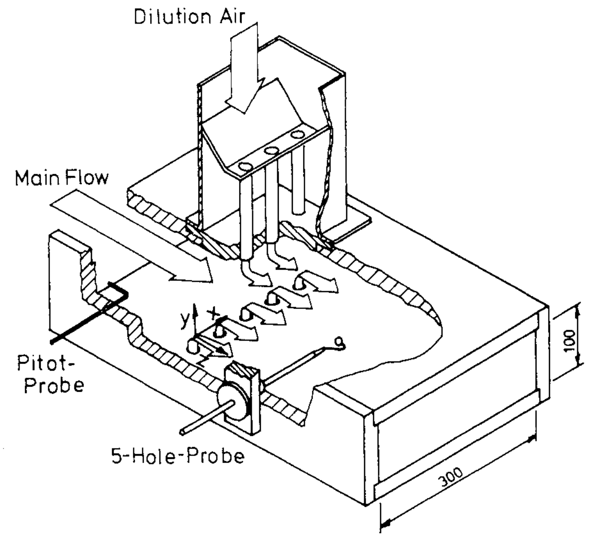

Fig. 5 Test section.

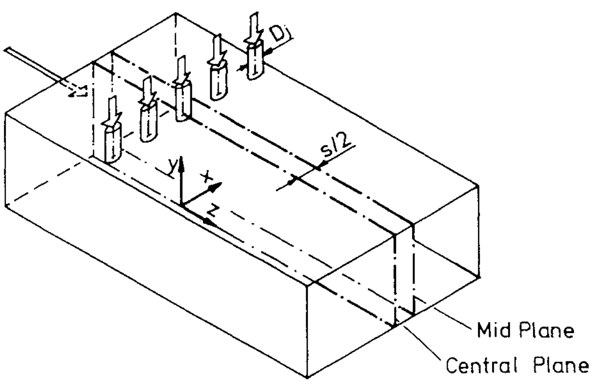

Fig. 6 Calculation field.

The differences $(\rho c A)_f \Delta\phi_f$ are added to the constant part of the source term $S = S^\circ - S'$ of the difference equations

$$S^{\circ *} = S^\circ + \sum_f [(\rho c A)_f \Delta\phi_f] \qquad f = e,w,n,s,h,l \tag{8}$$

The presented MLU scheme was found to be a very efficient discretization procedure in a number of practical applications. With emphasis on the computation of combustor flows, one special test case was selected for presentation in the present context.

Flow in the Combustor Mixing Zone

Operation at elevated turbine inlet temperatures imposes stringent limitations on the quality of the combustor exit temperature profiles, which should be matched carefully to the blade stress levels. The temperature profile at the combustor exit depends decisively on the mixing of cooling air jets with the combustion products in the mixing or dilution zone. The penetration and mixing characteristics of rows of cooling jets injected into a hot confined crossflow, therefore, have been subject to several experimental studies.[19-22] For the validation of a program for the numerical calculation of three-dimensional elliptic flows, detained measurements of the velocity, as well as of the appropriate temperature fields, for various nonisothermal jet mixing flows were accomplished.[1] The test section employed for these measurements is shown in Fig. 5. Air from a compressor is subdivided into primary and mixing air flow. The primary air flow can be heated up to 350°C before it enters the test section of a 300 × 100 mm cross-sectional area. The cold mixing air is led into secondary air chambers, where the air is injected through pipes with a length to diameter ratio of 10 mounted in the top and bottom walls of the test section. Measurements of the velocity and temperature were accomplished by means of a calibrated five-hole probe with a sphere diameter of 2.9 mm and by calibrated NiCr-Ni thermocouples. At seven discrete measurement planes, it is possible to attach a probe-transversing mechanism. A detailed description of the whole instrumentation of the test facility can be found in Ref. 1. Due to the symmetry of the flow, it is sufficient to restrict the measurements, as well as the numerical simulation to the region, between two adjacent planes of symmetry, i.e., between the central plane at $x/s = 0$ and the midplane at $x/s = 0.5$ (see Fig. 6).

The test conditions of a series of experiments are specified in Table 1. Whereas the velocity profiles were nearly homogeneous at the channel inlet, the temperature varied over the channel height with a maximum deviation of about ±2%, related to the average value $\bar{T}_\infty$.

The predicted central plane velocity and temperature profiles for the three discretization schemes UPWIND, QUICK, and MLU are compared with the appropriate measurements in Fig. 7 for test case no. 6, Table 1. The employed calculation field consists of 10 × 30 × 33 grid nodes in x, y, and z directions, respectively. In the calculations shown in Fig. 7, the UPWIND scheme was employed to discretize the convective transport of k and ϵ. This is common practice,[23] and is justified by the assumption that the source terms in the k and ϵ equations are dominant. This assumption, which is also a presupposition for the standard k, ϵ model, can be applied particularly well in high-shear regions, e.g., the jet entrance

Table 1 Test conditions of experiments

No.	s/D_j	H/D_j	J_T	J_B	$\bar{T}_\infty$	T_j	w_∞	$\bar{T}_T$	$\bar{T}_B$
1	2.5	12.5	41.7	—	422.5	314.3	15.7	385	400
2	0.0	20.0	17.6	—	426.5	314.3	14.8	380	400
3	0.0	20.0	24.1	—	449.6	315.2	15.5	395	415
4	5.0	12.5	—	51.5	435.0	314.9	17.8	415	416
5	2.5	12.5	—	34.2	443.6	310.2	15.8	420	425
6	2.5	12.5	30.3	31.6	460.1	308.5	13.7	420	390
7	2.5	12.5	52.5	53.6	486.1	311.8	15.8	438	405
8	2.5	12.5	17.8	36.1	450.3	304.6	14.7	405	381
9	2.5	12.5	29.8	30.6	444.9	308.8	15.7	407	365
10	2.5	12.5	—	44.0	482.7	312.3	17.3	450	450

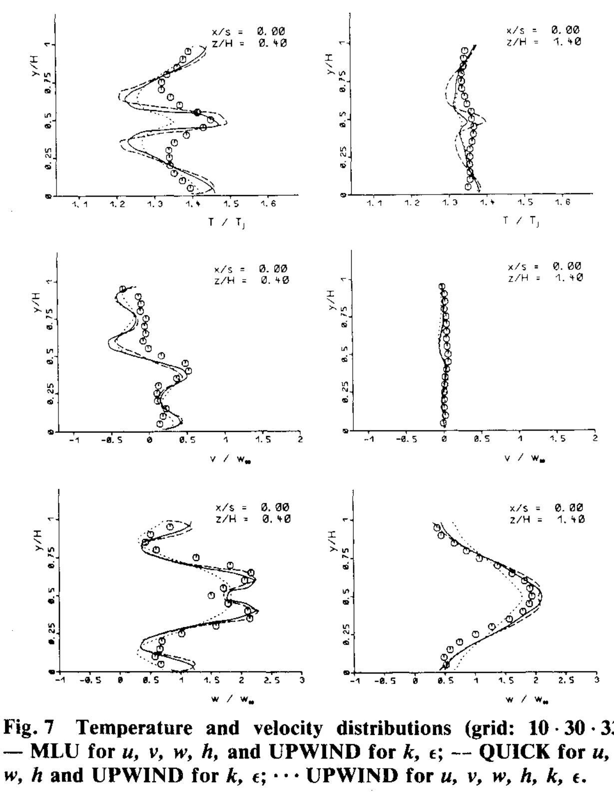

Fig. 7 Temperature and velocity distributions (grid: 10 · 30 · 33): — MLU for *u, v, w, h,* and UPWIND for *k, ε*; -- QUICK for *u, v, w, h* and UPWIND for *k, ε*; ··· UPWIND for *u, v, w, h, k, ε*.

region of the considered mixing flow. This will be demonstrated later.

The calculated profiles of the axial velocity component w, as well as of the temperature T, clearly reflect the characteristic deficiency of the UPWIND scheme: the smearing of gradients. The other two schemes delivered remarkably better results whereby the QUICK scheme yields the slightly steeper gradients. Similar tendencies were found in the computation of a three-dimensional swirling flow that, for instance, can be found in combustor primary zones, where a combination of vortex-controlled flame stabilization and jet stabilization is applied.[1-3]

From Fig. 7 it is difficult to decide whether the results gained by the QUICK discretization or the results of the MLU scheme are more accurate. Therefore, a further calculation of the mixing flow computed on a refined computational mesh of $14 \times 57 \times 65 = 51870$ nodes was made, based on the MLU scheme. The results of the fine-grid computation are compared with the corresponding measurements in Fig. 8. As shown in Figs. 7 and 8, the measured and calculated velocity components are in excellent agreement for the QUICK as well as for the MLU scheme. In contrast, considerable discrepancies occur between measured and calculated temperatures. The analysis for the flow under consideration reveals that, particularly in the jet entrance region, the pressure gradient term in the momentum equations is significantly larger than the terms comprising the turbulent transport processes. Thus, the turbulence model is only of reduced influence on the velocity field. Since, conversely, the energy equation does not possess a source term in the absence of radiation, the temperature field tends to uncover any shortcomings of the turbulence model employed. However, one reason for the discrepancies can also lie in the assumption of dominant source terms in the k, ϵ equations. If this assumption does not hold, the UPWIND discretization of the convective transport of k and ϵ can lead to conspicuous discretization errors. On the other hand, the application of an accurate discretization scheme for k and ϵ can change substantially the results only in those cases where the convective terms of k and ϵ are important compared with the source terms.

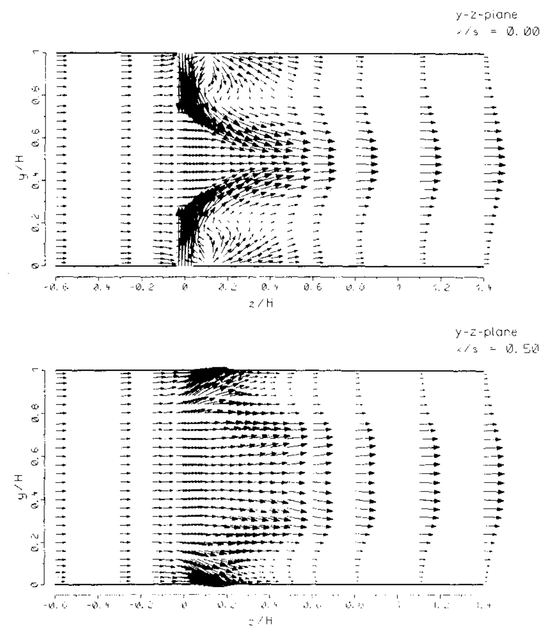

Fig. 10 Calculated velocity distributions.

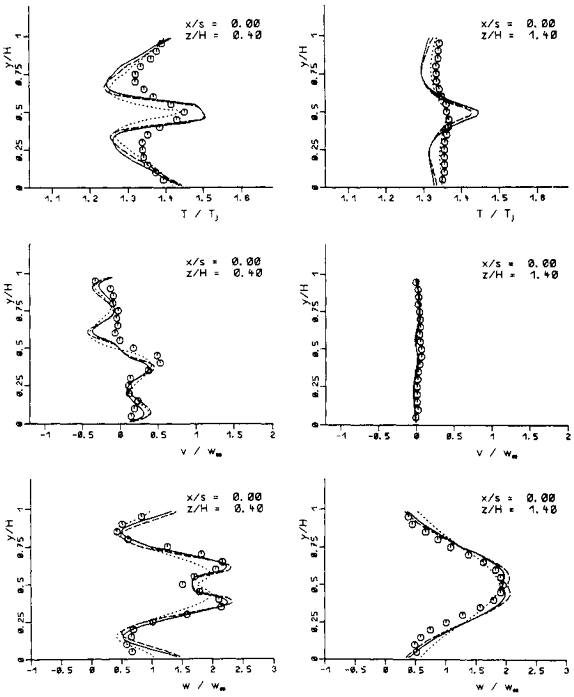

Fig. 8 Temperature and velocity distributions (grid: 14 · 57 · 65): — MLU for *u, v, w, h, k, ε*; -- MLU for *u, v, w, h*, and UPWIND for *k, ε*; ··· UPWIND for *u, v, w, h, k, ε*.

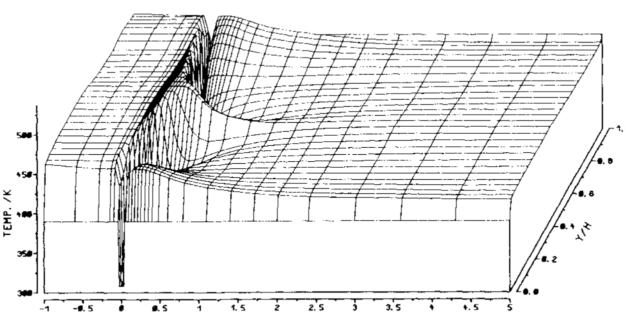

Fig. 9 Calculated temperature distribution (central plane *x/s* = 0; MLU).

The application of the QUICK scheme for the discretization of the k and ϵ equations in general fails because over- and undershoots can cause negative values of k or ϵ. Negative values for k or ϵ lead to negative values of the eddy viscosity and thus prevent convergence. Since the final solution based on the MLU scheme lies within the physical bounds, this scheme is suitable for the discretization of the k and ϵ transport equations. However, since the MLU scheme is highly nonlinear, its boundedness is not guaranteed for all intermediate stages of the solution. Therefore, even with the MLU scheme, negative values for k and ϵ can arise during the iterative solution process. Since, in this case the source term corrections for the application of the MLU scheme are negative, a remedy is found in modifying the linearized part rather than the constant part of the source term:

$$S_i^* = S' - \frac{1}{\phi_{i,j,k}} \cdot \sum_f [(\rho c A)_f \Delta\phi_f] \qquad f = e,w,n,s,h,l \tag{9}$$

Thus, the values of k and ϵ cannot fall below zero.

Figure 8 compares the results obtained on the finer grid for the "pure" UPWIND discretization, the "mixed" UPWIND/MLU discretization (see Fig. 8) and the "pure" MLU discretization (i.e., including the application of the MLU scheme for k and ϵ). The results clearly indicate that even for the relatively fine grid the UPWIND results suffer from numerical diffusion, whereas the other two calculations differ only slightly. Since the velocity field is well predicted from the latter observation, it can be concluded that, as expected, in the presented mixing flow the source terms of the k and ϵ equa-

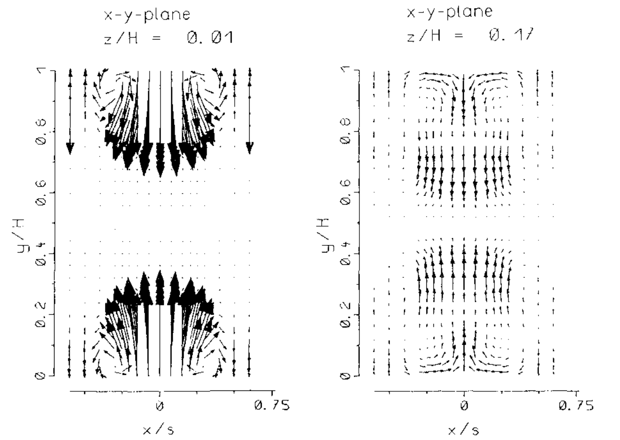

Fig. 11 Calculated velocity distributions (cross-sectional *x*, *y* planes).

tions are dominant and that the employed standard k,ϵ turbulence model is responsible for the discrepancies found between measured and calculated temperatures.

Although the results obtained for the temperature show visible differences between measurements and calculations, important characteristics of the considered flow are clearly reflected by the calculations. Figure 9 illustrates the whole temperature field in the central plane calculated by the MLU scheme on the coarser grid. Obviously, high temperatures arise in the flow region just behind the jet entrance at $z/H = 0$. The temperature rise behind cold air jets is also observed in the measurements (cf. Fig. 7). The temperature indicates a transport process that is typical for three-dimensional jet mixing flows. An explanation is given in Figs. 10 and 11, where the spatial properties of the flow are elucidated. Figure 10 shows the projections of calculated velocity distributions for a central as well as for a midplane, whereas Fig. 11 gives velocity projections on two cross-sectional $x\,y$ planes. It is evident from these figures that each jet induces a lateral movement of air into the wake of the jet, and, thus, behind the mixing jets two counterrotating vortices are formed. Therefore, part of the hot core of the flow in a real combustor can arrive at the near field of the wall. For the protection and cooling of the flame tube in practical arrangements, cooling air films are often applied. These films are destroyed by the vortices induced by the mixing jets. Thus, the combustor wall immediately behind the jet entrances often shows very hot regions. Since, in addition, large gradients of the wall temperature arise, flame tubes are highly strained immediately behind jet entrances.

Summary

The comparison between measurements and calculations confirms the well-known fact that, in general, reliable numerical predictions of complex three-dimensional flows require the application of proper discretization schemes. This was also found for a relatively fine grid consisting of $14 \times 57 \times 65$ nodes. The analysis for the flow considered, which is typical for the mixing zone of gas turbine combustors, reveals, that in the jet entrance region where strong streamline curvature is present the turbulence model has only a minor influence on the predicted velocity field. In contrast to the examination of the calculated velocity field, the comparison between measured and calculated temperature distributions reveals certain shortcomings of the employed standard k,ϵ model. However, it was found that, in contrast to the discretization of the convection of momentum and energy, the discretization of the convective transport of k and ϵ has only a minor influence on the calculated velocity and temperature distributions.

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