

Fig. 3 Drag reduction by the slip wall.

Acknowledgments

Funding for this project has been provided by the Deutsche Forschungsgemeinschaft and is gratefully acknowledged. In addition, we thank D. R. Noergel for his comments on the manuscript.

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Limitations of Traditional Finite Volume Discretizations for Unsteady Computational Fluid Dynamics

J. Russell Manson*

Bucknell University, Lewisburg, Pennsylvania 17837

Gareth Pender†

Glasgow University,

Glasgow G12 8LT, Scotland, United Kingdom

and

Steve G. Wallis‡

Heriot-Watt University,

Edinburgh EH14 4AS, Scotland, United Kingdom

Introduction

TRADITIONAL finite volume methods are popular in the field of refined subsonic flow simulation. Although a degree of confidence has been established in existing algorithms for accurate steady-state simulations (at least for laminar flows), a dubiety still pervades unsteady simulations.¹ The traditional finite volume approach is typified by Patankar's SIMPLE algorithm,² an approach and terminology for discretizing the equations of fluid flow, heat transfer, and associated transport processes. This methodology, although adequate for steady-state simulations, is ineffective for unsteady state problems with significant convective effects. This was

recognized over 15 years ago by Leonard,³ who describes two quite different methodologies for steady- and unsteady-state problems [QUICK (quadratic upstream interpolation for convective kinematics) and QUICKEST, respectively]. The computational fluid dynamics community has largely adopted Leonard's suggestion for steady subsonic flow modeling since Patankar's discretization can be readily "QUICK"ened by simply changing the interpolation functions for the face values. The same approach is not readily extendable to unsteady simulations. It performs progressively worse as the Courant number increases beyond 1, countering the only reason for using it in preference to the computationally cheaper explicit methods.

Advective Transport and Traditional Finite Volume Discretization

In one dimension unsteady convection (sometimes called advection) is represented in a conservative form by

$$\frac{\partial \phi}{\partial t} + \frac{\partial (u\phi)}{\partial x} = 0 \quad (1)$$

where ϕ is the convected variable and u the convecting velocity, taken here to be uniform, steady, and positive. Adopting the notation of Patankar, and referring to Fig. 1, the finite volume representation of Eq. (1) is given by integrating it over the control volume:

$$\int_w^e \left[\int_t^{t+\Delta t} \frac{\partial \phi}{\partial t} dt \right] dx = - \int_w^e \left[\int_t^{t+\Delta t} \frac{\partial (u\phi)}{\partial x} dt \right] dx \quad (2)$$

The discrete equation becomes

$$(\phi_p - \phi_p^0) \Delta x + \{ f[(u\phi)_e - (u\phi)_w] + (1-f)[(u\phi)_e^0 - (u\phi)_w^0] \} \Delta t = 0 \quad (3)$$

where f is a Crank-Nicolson temporal weighting factor. A stability analysis indicates that as long as $f \geq 0.5$, this discretization is unconditionally stable⁴; thus the choice of time step is not limited by stability considerations. In Eq. (3) the unknown values of ϕ at the future time have no superscript, whereas known values at the present time are given the 0 superscript. We may rearrange Eq. (3) as follows with all known quantities appearing on the right-hand side of the equation:

$$\phi_p + \frac{u\Delta t}{\Delta x} f(\phi_e - \phi_w) = \phi_p^0 - \frac{u\Delta t}{\Delta x} (1-f)(\phi_e^0 - \phi_w^0) \quad (4)$$

In Eq. (4), $u\Delta t/\Delta x$ is the Courant number. To complete the development, interpolation functions are required for the face values ϕ_e and ϕ_w in terms of the nodal values (ϕ_w , ϕ_p , ϕ_e , etc.). Perhaps the most intuitive interpolation for ϕ_e is given by

$$\phi_e = \frac{1}{2}(\phi_E + \phi_P) \quad (5)$$

whereas a more reasoned approach, which takes account of the physical argument that information travels downwind, is given by

$$\phi_e = \phi_p \quad (6)$$

Both of these simple interpolations are now widely discredited. The former method, termed central differencing, introduces too much artificial dispersion producing wiggles when individual Fourier components propagate at different celerities. The latter method, termed first-order upwinding, introduces too much artificial diffusion, which results in anomalously high spreading of initially sharp

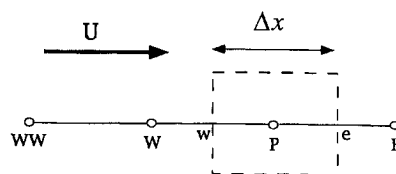


Fig. 1 Control volume for discretization.

Received Aug. 4, 1995; revision received Oct. 4, 1995; accepted for publication Nov. 10, 1995. Copyright © 1995 by the American Institute of Aeronautics and Astronautics, Inc. All rights reserved.

*Assistant Professor of Civil Engineering, Department of Civil Engineering.

†Lecturer in Civil Engineering, Department of Civil Engineering.

‡Lecturer in Civil and Offshore Engineering, Department of Civil Engineering and Offshore Engineering.

features. Both, these interpolation practices were popular in the seventies, and computational fluid dynamics (CFD) codes developed to accommodate them.

Because of the inadequacy of these simpler interpolations, Leonard³ introduced the idea of QUICK. In practice, this gives rise to interpolating functions of the form

$$\phi_e = \frac{1}{2}(\phi_E + \phi_P) - CF(\phi_E - 2\phi_P + \phi_W) \quad (7)$$

where CF is a curvature correction factor that Leonard originally suggested to be constant with value 0.125. Recent work suggests that for optimum performance CF should not be a constant but should be some function of the ϕ profile.⁵ Notice that QUICK interpolation is equivalent to central differencing with an additional upwinded curvature correction factor.

Leonard³ also derived an unsteady version called QUICKEST. This scheme may be derived in a number of different ways⁶; however, in one sense it requires that a higher-order temporal differencing be used. Regrettably, this idea was not taken on board by the CFD community, perhaps because QUICKEST is only conditionally stable. Most CFD codes for unsteady subsonic flow therefore adopt QUICK interpolation for the face values within the context of traditional temporal differencing as suggested by Patankar.²

When these interpolation functions are incorporated into Eq. (4), the result is a formula for ϕ_P in terms of ϕ_{WW} , ϕ_W , and ϕ_E :

$$a_P \phi_P = f \sum_{nb} a_{nb} \phi_{nb} + (1-f) \sum_{nb} a_{nb}^0 \phi_{nb}^0 + a_P^0 \phi_P^0 \quad (8)$$

where the subscript nb indicates a neighboring node to node P (i.e., E , W , and WW). Equation (8) is written for each node and the resulting equations may be assembled into the solution matrix. A proper implementation of the QUICK interpolation would result in an unsymmetrical quadridiagonal matrix structure, whereas the simpler central or first-order upwinding produces a tridiagonal matrix structure. Because existing CFD codes were already developed to exploit fast tridiagonal solvers, it seemed desirable to simplify QUICK differencing to produce only a tridiagonal matrix. This can be achieved by taking the curvature terms at the present or known time level as follows:

$$\phi_e = \frac{1}{2}(\phi_E + \phi_P) - CF(\phi_E^0 - 2\phi_P^0 + \phi_W^0) \quad (9)$$

This practice, known as transferring the curvature terms to the source, will limit the maximum time step that can be used for an unsteady analysis. This becomes particularly restrictive for pure advection.⁴ Boundary conditions are required to solve the system. At the inlet, the value of ϕ was specified. In theory, no boundary condition is required at the outlet, for pure advection. In practice, a zero gradient boundary condition is often employed.

Example Runs

For the present purposes a simple test case will suffice. In this problem the initial condition is taken to be $\phi(x, 0) = \alpha e^{-X^2}$, where $X = (x - \mu)/\sigma$. This represents a Gaussian profile, with maximum value given by α , the standard deviation given by σ , and the location of the peak at μ . In the present study, α takes the value 0.51, μ takes the value 8000.0 mm, and σ is assigned the value 388.0 mm. This is a severe test case because the numerical method must resolve the difference between maximum and zero over about four grid spacings. The spatial resolution, defined as $(4\sigma/\Delta x)$, is 7.76. The velocity is 0.45 mm/s, Δx is 200 mm, and the time step Δt is chosen to give Courant numbers $(u\Delta t/\Delta x)$ of 0.45 and 6.45. Two values of the time weighting factor f are investigated: 0.5 and 1.0. Only the strict QUICK interpolation, Eq. (7), has been tested here. The simulation time of 20,000.0 s allows the profile to translate 9000.0 mm downwind. Figure 2a shows the results of the runs with f equal to 1.0, the value recommended by Patankar.¹ Figure 2b shows the results with f set to 0.5. In both figures the exact solution is shown as a continuous line, whereas the numerical solutions are shown as broken lines.

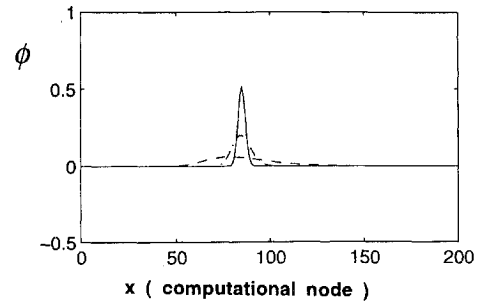


Fig. 2a QUICK scheme, $f = 1$: —, analytical; ---, Courant number = 0.45; and - · -, Courant number = 6.45.

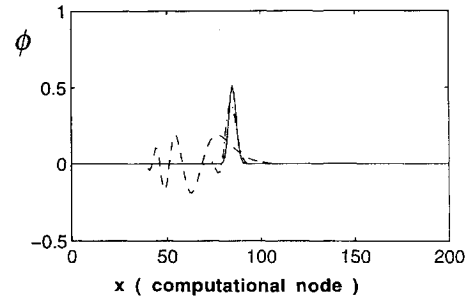


Fig. 2b QUICK scheme, $f = 0.5$: —, analytical; ---, Courant number = 0.45; and - · -, Courant number = 6.45.

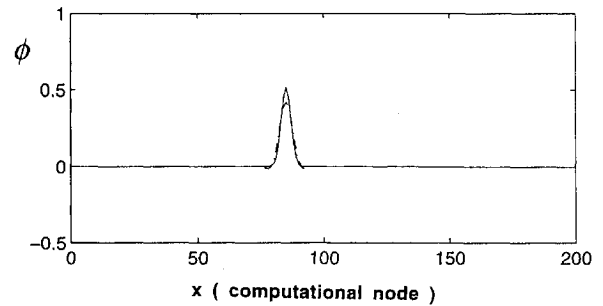


Fig. 3 QUICKEST scheme: - · -, analytical and —, numerical. Courant number = 0.45.

Results

Qualitatively, Fig. 2a shows that with $f = 1$ for Courant numbers less than 1, the numerical solution is highly overdiffused. No wiggles appear, but the accuracy is low. For Courant numbers in excess of 1, the results are so diffused as to consider not including the advection terms in the model. Figure 2b shows that if the Courant number less than 1, the numerical solution is much more accurate than when $f = 1$. Although a small wiggle appears at the trailing edge, overall the agreement is better. Considering the severity of the test case, the method has performed well. Unfortunately, $f = 0.5$ is not the recommended practice. When the Courant number is greater than 1, the method is again very poor, developing wiggles that completely destroy the solution.

Conclusions and Recommendations

Traditional implicit finite volume formulations for transport equations do not work for unsteady simulations to any greater Courant number than do explicit methods when the convective terms are significant. If practitioners do use QUICKened traditional finite volume codes for unsteady simulations, then the time step should be chosen to satisfy a Courant condition to achieve physical realism. Although tolerable results may be obtained⁴ with Courant numbers up to about 2, time steps should be chosen to give Courant numbers less than 1. For unsteady simulations a value of 0.5 should be used for f for time accuracy, and solutions should always be shown to be independent of Δt . Trying to demonstrate grid independence for unsteady simulations will be difficult since each time the grid is refined (if Δt remains the same) the Courant number will increase correspondingly. For high accuracy in unsteady simulations practitioners should adopt a QUICKEST-type differencing¹⁰ and accept

the Courant limitation on the choice of time step for stability. The results for the same test case using a QUICKEST scheme are shown in Fig. 3. Although only one severe test case has been studied in this short work, the study is being extended to cover a wide range of spatial resolutions and also to include the effects of a diffusion term. Finally, recent work by Manson and Wallis⁷ (DISCUS), Roache⁸ (FBMMOC), and Leonard et al.⁹ (NIRVANA) may suggest ways to achieve unconditionally stable unsteady simulations.

Acknowledgment

The authors wish to thank B. P. Leonard for his helpful comments on an earlier draft of this paper.

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Simulating Heat Addition via Mass Addition in Variable Area Compressible Flows

W. H. Heiser,* W. B. McClure,[†] and C. W. Wood[‡]
U.S. Air Force Academy, Colorado 80840-6222

Introduction

THE authors recently demonstrated the striking and potentially useful similarity between the influence of heat addition and mass addition (injected normal to the flow with the same total temperature and composition) on constant area compressible duct flows.¹ This was primarily accomplished by means of closed-form, mathematical solutions for flows involving a single forcing function (e.g., heat or mass addition), commonly known as simple flows.² The analyses were primarily based on the classical one-dimensional model of the steady, frictionless, constant throughflow area flow of a calorically perfect gas.² The similarities were also found to exist when wall friction is present, including the estimated point of boundary-layer separation in supersonic flow. This article extends the prior results to incorporate the influence of throughflow area variation.

Received Feb. 1, 1995; accepted for publication Nov. 20, 1995. This paper is declared a work of the U.S. Government and is not subject to copyright protection in the United States.

*Professor, Department of Aeronautics. Fellow AIAA.

[†]Associate Professor, Department of Aeronautics. Senior Member AIAA.

Multiple Combined Effects

Versatile though it may be, one-dimensional flow analysis cannot provide closed-form solutions for arbitrary distributions of several independent parameters. This applies in particular to the important case of heat (or mass) addition in a duct of varying throughflow area, for which the distribution of both is crucial to the outcome [i.e., the exit conditions depend on more than the total heat (or mass) addition and throughflow area change]. This case is important because it is the essence of dual-mode ramjet/scramjet combustor operation, where choking during ramjet operation results from the cooperation between the chemical energy release that drives the local Mach number up to 1 (hence the term thermal choking) and the throughflow area increase that continues the acceleration beyond Mach 1.^{3,4}

A simple numerical procedure was therefore developed to explore cases and design experiments with arbitrary axial distributions of heat addition, mass addition, wall friction, and/or throughflow area. Although the code permits other variations, all of the following discussions of mass addition refer only to the case of injection normal to the duct axis of a gas with the same total temperature and composition as the inlet flow. The algorithm is based on the one-dimensional unsteady Euler equations, cast in a conservative finite volume form and solved using a first-order flux-vector splitting scheme.⁵ The working fluid was modeled as a calorically perfect gas with a fixed ratio of specific heats. The duct wall friction force was included in the control volume momentum balance and was modeled via a local wall friction factor. For cases with the inlet Mach number $M_i > 1$, the exit pressure was set low enough to prevent shock wave formation within the duct. For cases with $M_i < 1$, the exit pressure was iteratively adjusted to be compatible with the inlet conditions. The code was run on a Sun SparcStation with 35 megabytes of memory. Initial conditions in the duct were arbitrarily set based on M_i . A typical run of 100,000 global time steps over 100 equally spaced cells took about 15 min. Residual error, quantified as the average absolute fractional change of the local momenta between successive time steps, was of the order of 10^{-7} .

Please note that the differences in the manner in which the fluxes are calculated for supersonic and subsonic cells result in artificial property discontinuities at the transonic transitions (i.e., the sonic point and shock waves). The impact of these discontinuities can be minimized by using a fine grid in such regions, as was done in this study to achieve derivatives of satisfactory accuracy.

Before moving on to the results of computations, it should be noted that closed-form analytical solutions again made an important contribution by providing three useful benchmarks for the development of the code. First, numerical analyses reproduced all of the results described in Ref. 1. Second, generalized one-dimensional flow analysis furnishes the unique position of the choking or sonic point should it occur, as well as the corresponding Mach number axial gradients, even for combined effects, through the well-known "special conditions at the sonic point."^{2,3} The algebraic results of this analysis for the typical contemporary dual-mode combustor case of parabolic heat (or mass) addition and linear area distribution are compiled in Table 1, where T_t is the total temperature; \dot{m} is the mass flow; α , τ , and μ are constants of area variation, heat, and mass addition, respectively; A is the local throughflow area; L is the axial length of the duct; M is the local Mach number; γ is the ratio of specific heats; ξ is the dimensionless axial coordinate x/L ; the subscript i designates the inlet conditions; and the subscript c indicates the choking or sonic point. The numerical analyses reproduced these results whenever the flow choked. Third, inspection of the complete one-dimensional compressible flow differential equations of Ref. 2 reveals that adding either heat or mass alone should produce identical Mach number, static pressure, and total pressure axial distributions for specified inlet conditions and duct geometry provided only that

$$\frac{d\dot{m}}{\dot{m}} = \frac{1}{2} \frac{dT_t}{T_t} \quad \text{or} \quad \frac{\dot{m}}{\dot{m}_i} = \sqrt{\frac{T_t}{T_{ti}}} \quad (1)$$

The axial distributions of other flow properties, such as density, velocity, and static temperature, are not identical but can easily be found from the Mach number axial distribution and the "useful integral relations" of Ref. 2. The numerical analyses of the axial