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Pressure Gradient Scaling Method for Fluid Flow with Nearly Uniform Pressure*

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A method is described for increasing the efficiency of numerical calculations of compressible fluid flow problems in which the pressure field is nearly uniform in space. This condition is ordinarily satisfied at low Mach number. It is shown that in such problems, the pressure gradient in the momentum equation may be multiplied by a scaling factor $1/\alpha^2$ ($\alpha > 1$) without significant effect, provided that α is not too large and that the pressure inhomogeneities are not of interest. This scaling modification reduces the acoustic speed by a factor of α, thereby increasing the effective Mach number by the same factor. This reduces the disparity between the acoustic and convective time scales, which improves the computational efficiency of many numerical schemes for compressible flow. The relation between the present approach and the α-transformation of O'Rourke and Bracco is briefly discussed. The practical utility of the method is illustrated by sample calculations of combustion in ideal gas mixtures.

I. INTRODUCTION AND SUMMARY

Numerical calculations of compressible fluid flow have a notorious tendency to be inefficient at low Mach numbers, because of the wide disparity that then exists between the time scales associated with convection and the propagation of acoustic waves. In explicit schemes, the inefficiency occurs because the time steps needed to satisfy the Courant sound-speed stability condition are much smaller than those needed to satisfy the convective stability condition alone. To alleviate this difficulty, partially implicit schemes (such as the ICE [1, 2] and related methods) are frequently employed. Such schemes remove the sound-speed stability condition so that larger time steps may be taken. The inefficiency in question then manifests itself in the additional computational labor needed to solve the resulting implicit system of equations on each time step. The solution is usually performed by iterative techniques. In some formulations, the inefficiency is aggravated by a tendency for the iteration scheme to converge more slowly as the Mach number is decreased, at least over a certain range of Mach numbers. Moreover, pointwise iteration schemes such

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as the method of successive overrelaxation are inherently inefficient in problems where substantial changes in the overall pressure level occur, because long-wavelength errors relax very slowly.

These considerations lead one to contemplate the possibility of devising methods for artificially increasing the Mach number to somewhat larger values, while still keeping it small in an absolute sense. One such method, called the α-transformation, was described by O'Rourke and Bracco [3]. Our purpose here is to present a closely related, but not quite equivalent, method for achieving the same objective. The present method is considerably simpler than the α-transformation, both conceptually and operationally, and it has the further advantage of being somewhat more widely applicable. It can easily be incorporated into any existing computer program for compressible fluid flow, with only trivial modifications.

An obvious way to increase the Mach number is to reduce the acoustic speed c. The proper way to do so, however, is not immediately apparent. In the first place, c does not appear explicitly in the primitive form of the governing differential equations. By manipulating these equations in various ways, one can obtain various equivalent systems of equations in which c does appear explicitly, but they will no longer be equivalent if c is modified and it is not clear a priori which such formulation is to be preferred. And of course one is not simply free to arbitrarily select one of these formulations and reduce c therein; one is constrained by the requirement that the modification of c must not alter any of the solution features of interest.

In the present method, the governing equations are modified in a very simple way: the pressure gradient in the momentum equation is multiplied by a scaling factor $1/\alpha^2$, where $\alpha > 1$. We therefore refer to the method as the pressure gradient scaling, or PGS, method. One readily verifies that this modification has the desired effect of reducing the effective acoustic wave speed by a factor of α. However, it might at first be expected to affect the solution in other ways as well, and therefore to be unacceptable. In particular, since the pressure gradient has no way of distinguishing pressure inhomogeneities of acoustic origin from any other pressure inhomogeneities, one might expect to incur errors in accelerations, and hence in velocities, that are not merely acoustic in character. Fortunately, and perhaps surprisingly, this fear is not well founded. Physically, the saving grace is that the pressure gradients in a low Mach number flow are effectively determined by the velocity field, and not vice versa. The pressure gradients adjust themselves to whatever values are necessary for the velocity field to have the correct divergence (which in general is nonzero) [3, 4]. The presence of the factor $1/\alpha^2$ merely causes these gradients to become larger by a factor of α^2 in order to establish the same velocity field.

The preceding remarks do not, of course, provide a firm justification for the PGS method; they are merely a plausibility argument. A systematic derivation of the method is presented in Section II. This derivation shows that the basic condition for the PGS method to be applicable is not that the Mach number be low per se, but rather that pressure inhomogeneities be negligible. Ordinarily, of course, these two

conditions are closely related [3], but the latter is really the more fundamental in the present context and will henceforth supersede the former.

In contrast to the α-transformation of O'Rourke and Bracco [3], the PGS parameter α may be time dependent. It can therefore be adjusted during the course of a transient calculation to improve the overall efficiency. This adjustment is easily automated by monitoring the magnitude of the pressure inhomogeneities. One simply increases α when the pressure inhomogeneities are very small, and decreases α (subject to a lower bound of unity) when they threaten to become non-negligible. The automatic selection of α is discussed in Section III.

The PGS method is suitable for use in conjunction with both explicit and implicit numerical schemes. The resulting gains in computational efficiency are more easily appreciated and estimated in the explicit case, where the time step is subject to the Courant sound-speed stability condition. The PGS method reduces the effective acoustic speed by a factor of α without changing the flow velocities. When the Mach number is small, therefore, the explicit time step may be increased by nearly a factor of α, and computational efficiency is thereby increased by the same factor. In implicit schemes, where the time step is not restricted by the acoustic speed, improvements in efficiency can also be substantial but will depend on the type of solution procedure used. In particular, point-relaxation schemes such as successive overrelaxation are in general expected to benefit significantly, as illustrated and discussed in Section IV and the Appendix.

The practical utility of the PGS method is illustrated in Section IV by presenting the results and computation times for two sample problems involving combustion in ideal gas mixtures. The numerical calculations were performed using the CONCHAS-SPRAY computer code [5] both with and without the PGS method.

After this work was completed, the related work of Lund [6] and Cundall [7] was brought to our attention. Lund has used a similar scaling in conjunction with an implicit numerical scheme for one-dimensional flow with chemical reactions, but he scales in the opposite direction. That is, he effectively sets $\alpha < 1$ to make the acoustic speed *larger* rather than smaller, so that acoustic waves are reduced in amplitude and pressure equilibration occurs more quickly. This is of course perfectly legitimate, provided that pressure inhomogeneities are small and that one's implicit scheme is constituted, as Lund's evidently is, in such a way that solution inefficiencies do not arise as the Mach number is decreased. However, Lund did not himself justify the procedure, which in our view requires one to show (as we do in Section II) that features other than pressure inhomogeneities are not sensibly altered by the scaling.

Cundall [7] has used a scaling procedure which seems similar in spirit to the PGS method, but in a rather different context. He is concerned with quasistatic problems in solid mechanics and fluid seepage. The scaling is applied to the density of the solid material and to the bulk modulus of the fluid. The procedure is heuristically motivated, but a systematic derivation analogous to that of Section II is not given.

Cundall's work illustrates the important point that scaling procedures analogous

to the PGS method are likely to prove useful in a variety of problems where widely different time scales exist. It must be emphasized, however, that a legitimate scaling procedure will not in general result from time step stability considerations alone, for one can easily construct incorrect scaling procedures which allow the use of larger time steps by doing violence to the features of interest. It is essential in every case to show that these features are preserved unchanged by the proposed scaling, and to confirm this behavior by direct numerical calculations.

II. Derivation of the Scaling

The governing equations for compressible fluid flow may be written in the form

$$\frac{D\rho_i}{Dt} = -\rho_i \nabla \cdot \mathbf{u} + R_i, \tag{1}$$

$$\rho \frac{D\mathbf{u}}{Dt} = -\nabla p + \mathbf{S}, \tag{2}$$

$$\rho \frac{De}{Dt} = -p\nabla \cdot \mathbf{u} + Q, \tag{3}$$

$$p = f(\{\rho_i\}, e), \tag{4}$$

where ρ_i is the partial mass density of chemical species i, ρ is the total mass density, $\mathbf{u}$ is the fluid velocity, p is the pressure, e is the thermal internal energy per unit mass, and $D/Dt = \partial/\partial t + \mathbf{u} \cdot \nabla$ is the convective derivative. The source terms Q, R_i, and $\mathbf{S}$ represent the effects of molecular transport and rate processes (e.g., viscosity, diffusion, and chemical reactions), as well as any external forces or heat and mass sources that may be present. Explicit forms for Q, R_i, $\mathbf{S}$, and the state function f will not be given, as they are immaterial for our purposes.

In what follows we shall consider various modifications of the above system of equations. None of these modifications will affect Eq. (1), so this equation will henceforth be omitted from consideration. It will simply be understood that Eq. (1) is to be included unchanged in any modified equation system to be considered below.

It is useful to define the spatially uniform average pressure level by

$$\bar{p}(t) = \frac{1}{V}\int_V d\mathbf{r}\, p(\mathbf{r}, t), \tag{5}$$

where the integration extends over the volume of the system under consideration. If the system is unbounded, the limit $V \to \infty$ is taken; $\bar{p}$ will then ordinarily reduce to the specified ambient pressure. The local deviation of the pressure from $\bar{p}(t)$ is

$$p'(\mathbf{r}, t) = p(\mathbf{r}, t) - \bar{p}(t), \tag{6}$$

whose volume average is zero. In terms of $\bar{p}$ and p', Eqs. (2)–(4) become

$$\rho \frac{D\mathbf{u}}{Dt} = -\nabla p' + \mathbf{S}, \tag{7}$$

$$\rho \frac{De}{Dt} = -(\bar{p} + p')\,\nabla \cdot \mathbf{u} + Q, \tag{8}$$

$$\bar{p} + p' = f(\{\rho_i\}, e). \tag{9}$$

We are concerned with problems in which $|p'|$ is everywhere much less than $\bar{p}$. Then provided that no interest attaches to the small pressure inhomogeneities themselves (or to the associated small variations in $\mathbf{u}$, e, and the ρ_i), p' may be neglected in comparison to $\bar{p}$ in any term to which both contribute. Therefore p' may be neglected in Eqs. (8) and (9), but not in Eq. (7). We thereby obtain the modified equation system

$$\rho \frac{D\mathbf{u}}{Dt} = -\nabla p' + \mathbf{S}, \tag{10}$$

$$\rho \frac{De}{Dt} = -\bar{p}\nabla \cdot \mathbf{u} + Q, \tag{11}$$

$$\bar{p} = f(\{\rho_i\}, e), \tag{12}$$

which will exhibit the same behavior as the original system of Eqs. (7)–(9) except with regard to the negligibly small variations,

In the modified system of Eqs. (10)–(12), the momentum equation is no longer coupled to the energy and state equations through p'. This decoupling changes the character of the system: the modified system of Eqs. (10)–(12) does not support acoustic waves. Since p' now appears only in Eq. (10), the determination of p' is now an elliptic problem. One may regard p' as being implicitly determined by Eq. (12), which is a local constraint on e and the ρ_i. This constraint is equivalent to a constraint on $\nabla \cdot \mathbf{u}$, as can be seen by applying D/Dt to Eq. (12) and combining the result with Eqs. (1) and (11) [3, 4]. Thus the pressure field appearing in the momentum equation is implicitly determined by a constraint on $\nabla \cdot \mathbf{u}$, just as in incompressible flow.

The modified system of Eqs. (10)–(12) has the peculiar feature that it appears to be underdetermined, since it contains the additional unknown function $\bar{p}(t)$ for which no determining equation appears. However, this difficulty is illusory; it is resolved by the realization that $\bar{p}(t)$ is effectively determined by the boundary conditions [3]. (The situation is closely analogous to parabolic flow in a closed duct, where the streamwise pressure variation is effectively determined by the boundary conditions on the duct walls [8–10]. These boundary conditions, however, are often disguised as an integral mass conservation condition [9, 10].) Indeed, the boundary conditions may be used to derive an explicit equation for $d\bar{p}/dt$ [3], but this will not be done here as we shall have no need for such an equation.

Equations (10)–(12) incorporate the simplification of neglecting p' in comparison to $\bar{p}$. However, the numerical solution of these equations necessitates the use of an implicit scheme to allow for the elliptic character, and this is usually quite time-consuming. It also requires the derivation and use of an explicit equation for $d\bar{p}/dt$ as discussed above. This can of course be done [11, 12], but it entails the development of a numerical scheme and computer program specifically tailored to the purpose, which then cannot be used for a wider class of compressible flow problems. We prefer to pursue a somewhat more flexible approach which can easily be implemented as an option in existing general purpose compressible flow numerical schemes and computer programs. To this end, we proceed to obtain a second modified system of equations which is closer in form to the original system and which can be solved by explicit techniques if desired. Alternatively, if an iterative implicit scheme is used, as in Section IV, the iteration convergence rate will frequently be substantially greater than that for a similar scheme applied to Eqs. (10)–(12) (see Appendix).

To obtain such a system, we further exploit the fact that $|p'|$ is everywhere much less than $\bar{p}$, but now we use this knowledge not to remove p' but to reintroduce it in a propitious way. Simply stated, the basic idea is that since p' is small, $\alpha^2 p'$ will also be small provided that α^2 is not too large. Therefore, for a certain range of α values, $\bar{p}$ may be replaced by $\bar{p}+\alpha^2 p'$ in Eqs. (11) and (12) with negligible effect. We thereby obtain a second modified equation system,

$$\rho \frac{D\mathbf{u}}{Dt} = -\nabla p' + \mathbf{S}, \tag{13}$$

$$\rho \frac{De}{Dt} = -(\bar{p}+\alpha^2 p')\,\nabla\cdot\mathbf{u} + Q, \tag{14}$$

$$\bar{p}+\alpha^2 p' = f(\{\rho_i\}, e). \tag{15}$$

Here α is taken to be independent of position, although it may still depend on time. The system of Eqs. (13)–(15) can be rewritten in a more convenient form by defining

$$\hat{p}(\mathbf{r}, t) = \bar{p}(t) + \alpha^2(t)\, p'(\mathbf{r}, t). \tag{16}$$

Thus $\nabla\hat{p} = \alpha^2\,\nabla p'$ and we obtain

$$\rho \frac{D\mathbf{u}}{Dt} = -\frac{1}{\alpha^2}\nabla\hat{p} + \mathbf{S}, \tag{17}$$

$$\rho \frac{De}{Dt} = -\hat{p}\,\nabla\cdot\mathbf{u} + Q, \tag{18}$$

$$\hat{p} = f(\{\rho_i\}, e). \tag{19}$$

We now observe that Eqs. (17)–(19) look just like the original Eqs. (2) – (4), except

that p is replaced by $\hat{p}$ (which is just a change of symbols) and a factor of $1/\alpha^2$ now appears in front of the pressure gradient in the momentum equation. We have therefore shown that, provided small perturbations such as acoustic waves are not of interest, a factor of $1/\alpha^2$ can be affixed to the pressure gradient with negligible effect. It is natural to refer to this modification as pressure gradient scaling (PGS).

Of course, by introducing p' back into the energy and state equations we have restored acoustic waves to the system, but we have falsified their speed to our advantage. (At the same time, we have artificially increased their amplitude because the compressibility of the fluid has effectively been increased.) A conventional linearized analysis, with Q, R_i, and $\mathbf{S}$ taken to be zero, shows that the acoustic wave speed is artificially reduced by a factor of α, so that the effective Mach number is artificially increased by a factor of α. This increase is the desired effect of the PGS procedure, from which the increased computational efficiency results.

The preceding derivation is of a physical rather than a mathematical nature, and clearly does not constitute a rigorous proof that solutions of Eqs. (17)–(19) will be close to corresponding solutions of Eqs. (2)–(4). However, the derivation is fully satisfactory from a physical point of view, as it involves only the assumed negligibility of p' in comparison to $\bar{p}$. The expectation that PGS will not significantly alter the solution receives further support from the observation that solutions of the fluid dynamics equations in general appear to vary continuously with Mach number [13].

It should be noted that the quantity p' appearing in Eqs. (13)–(16) depends implicitly upon α, even though this has not been indicated by the notation. Thus p' in Eqs. (13)–(16) differs both from the original p' of Eqs. (2)–(4) and from the elliptic p' of Eqs. (10)–(12), although all of them may be expected to be of the same order of magnitude. These differences are of no concern, however, since p' is not itself of interest.

The fundamental condition for the validity of the PGS procedure is that $\alpha^2 p'$ be everywhere much less than $\bar{p}$. That is, the maximum absolute deviation of $\hat{p}$ from $\bar{p}$ should be much less than unity, say 0.01. This condition may be used to select $\alpha(t)$ automatically during the course of a calculation, as discussed in Section III. Of course, this requires evaluation of $\bar{p}$, which may be obtained from

$$\bar{p}(t) = \frac{1}{V} \int_V d\mathbf{r}\, \hat{p}(\mathbf{r}, t). \tag{20}$$

Strictly speaking, since p' now differs from the original p' its volume average need not be identically zero, and hence this $\bar{p}$ may differ slightly from the original $\bar{p}$. However, this difference is at most of order $\alpha^2 p'/\bar{p}$, and is therefore not significant.

The fact that the PGS method is implemented simply by affixing a factor of $1/\alpha^2$ to the pressure gradient in the momentum equation is a consequence of our use of a transport equation for the internal energy e rather than the total energy $E = e + \frac{1}{2}u^2$. Unlike the internal energy equation, the total energy equation contains a term involving the pressure gradient (namely, $\mathbf{u} \cdot \nabla p$), and strictly speaking the factor of

$1/\alpha^2$ should be affixed to this term as well. (This can be seen either by repeating the above development with Eq. (3) replaced by the total energy equation, or equivalently by combining the final PGS equations (17) and (18) to obtain the PGS equation for E.) In practice, however, this modification is not really necessary, because at low Mach number $\frac{1}{2}u^2 \ll e$ so that $E \cong e$. This in turn implies that the term $\mathbf{u} \cdot \nabla p$ in the total energy equation is negligible compared to the other terms and therefore need not be scaled. (The same conclusion emerges from a more formal similarity analysis of the transport equation for E, along the lines of Ref. [3]. Such an analysis shows that the term $\mathbf{u} \cdot \nabla p$, when expressed in terms of the appropriate dimensionless variables, appears with a coefficient of the Mach number squared and therefore vanishes as the Mach number tends to zero.) Thus, even when the transport equation for E is used instead of that for e, the PGS method may effectively be implemented by scaling ∇p in the momentum equation only.

We have mentioned that the PGS method is closely related, but not quite equivalent, to the α-transformation of O'Rourke and Bracco [3]. The precise relation between the two methods may be established as follows. In the α-transformation, the calculation of interest is performed with each independent and dependent variable ϕ replaced by a corresponding scaled variable ϕ^*. The scaled and unscaled variables are connected by simple relations involving α, which are given in Eq. (20) of Ref. [3]. The relation for p^* deserves special mention because $\bar{p}$ and p' are scaled differently: $\bar{p}^* = \bar{p}$ whereas $p'^* = \alpha^2 p'$, so that $p^* = \bar{p} + \alpha^2 p'$. After the calculation is completed, the resulting ϕ^* are converted back to the desired ϕ by use of the scaling relations.

To see what equations are effectively being solved by this procedure, it is simply necessary to replace each variable ϕ in the governing Eqs. (1)–(4) by its corresponding ϕ^*, and then to algebraically eliminate the ϕ^* in favor of the ϕ by means of the scaling relations. In order to do this, the explicit forms of the source terms Q, R_i, and $\mathbf{S}$ must be specified. If these terms are taken to have the forms given in Ref. [3], one finds that the equations which are effectively being solved by use of the α-transformation are identical to our Eqs. (1) and (13)–(15), except that the viscous dissipation term in Q is multiplied by a factor of α^2. Thus the α-transformation has the same effect on acoustic waves and pressure inhomogeneities as the PGS method, but it has the additional effect of artificially increasing the viscous dissipation rate by a factor of α^2. However, viscous dissipation is ordinarily negligible at low Mach number [3], so this difference is expected to be unimportant in practice.

The α-transformation and the PGS method will therefore produce essentially equivalent results for the same fixed value of α, but they are significantly different in regard to convenience and generality. In both respects the PGS method is to be preferred. It is simpler to use because it eliminates the need to scale and unscale variables, and it is more general in that it allows the use of a time-dependent scaling parameter α. Moreover, it is somewhat more widely applicable by virtue of the fact that its validity does not depend on the form of the source functions Q, R_i, and $\mathbf{S}$.

We remark parenthetically that the PGS method can readily be extended to cer-

tain situations in which the pressure is significantly nonuniform but differs only slightly from a known nonuniform pressure p_0 whose gradient is balanced by a term in S. The obvious example of such a situation is low-speed flow in a gravitational field, where p_0 may be identified with the hydrostatic pressure. A straightforward generalization of the present development shows, as one would intuitively expect, that only the deviation of ∇p from ∇p_0 should be scaled by $1/\alpha^2$. That is, the proper implementation of the PGS method in such problems is to replace ∇p by $\nabla p_0 + (1/\alpha^2)\nabla(p - p_0)$ in the momentum equation. The result of course reduces to Eq. (17) when p_0 is uniform.

The PGS method can also be extended to certain flows at low Mach number in which an essential role is played by pressure inhomogeneities of an elliptic rather than an acoustic character. Examples of such flows are low-speed flows driven by a pressure drop, or pressure drag on an obstacle immersed in a low-speed flow. Such pressure inhomogeneities are clearly represented correctly in the intermediate elliptic equations (10)–(12). Their relation to the PGS pressure field may be inferred by examining the elliptic approximation to the PGS equations (17)–(19), which is obtained by replacing $\hat{p}$ with $\bar{p}$ in Eqs. (18) and (19). Comparison with Eqs. (10)–(12) then shows that the elliptic pressure inhomogeneities in $\hat{p}$ are simply α^2 times the true elliptic pressure inhomogeneities. The PGS method can therefore be applied in problems where such pressure inhomogeneities are significant simply by scaling the pressure differences by a factor of α^2. For example, the appropriate pressure drop to impose as a boundary condition on a PGS calculation would be α^2 times the physical pressure drop. Similarly, the physical pressure drag on an obstacle would be $1/\alpha^2$ times the pressure drag calculated using PGS.

III. Automatic Selection of α

Since α is allowed to depend on time in the PGS method, it is natural to try to devise an automatic selection algorithm which will appropriately adjust α in accordance with the pressure inhomogeneities that are found to exist at different times during a calculation. This of course requires an arbitrary decision as to the value of $\alpha^2 |p'|/\bar{p}$ above which the pressure inhomogeneities are no longer considered small. For purposes of discussion we shall take this value to be 0.01, but we emphasize that this is a subjective decision to be made by the user in the context of the particular problem under consideration.

Based on Eq. (16) and a cutoff value of 0.01, an obvious prescription for selecting α would be

$$(\alpha^{n+1})^2 = (\alpha^n)^2 \frac{0.01\,\bar{p}}{\max |\hat{p} - \bar{p}|}, \tag{21}$$

where the "max" operation is performed with respect to all cells of the finite difference mesh, and the superscripts n and $n+1$ refer to the time level as usual. (It is

understood, of course, that any such prescription is subject to a lower bound of unity for α^{n+1}.) However, this prescription does not limit the amount by which α^{n+1} differs from α^n, and in the absence of such a limit α may develop artificial oscillations in time. The naive prescription of Eq. (21) is therefore not recommended.

A better prescription results from the idea that α should *relax toward* the value given by Eq. (21) with a relaxation time that is not allowed to become too short. This idea may be implemented by writing

$$\frac{\alpha^{n+1}-\alpha^n}{\Delta t} = -\frac{\alpha^n - \alpha_0^{n+1}}{\tau}, \tag{22}$$

where α_0^{n+1} denotes the value of α^{n+1} that would be obtained by the naive prescription of Eq. (21), Δt is the time step $t^{n+1}-t^n$, and the relaxation time τ has yet to be specified. It seems natural to identify τ with the pressure equilibration time for the system, which may be estimated as the round-trip transit time for an acoustic wave to traverse the length L of the region of interest. We therefore set $\tau = 2L\alpha^n/c$, where c is a representative *true* (unscaled) sound speed. Equation (22) then becomes

$$\frac{\alpha^{n+1}-\alpha^n}{\Delta t} = \frac{c}{2L}\left[\left(\frac{0.01\,\bar{p}}{\max|\hat{p}-\bar{p}|}\right)^{1/2} - 1\right], \tag{23}$$

which again is subject to a lower bound of unity for α^{n+1}. This prescription has been found to work well in practice, and was used in the sample calculations to be discussed in the next section.

IV. Sample Calculations

The PGS method has been proof-tested in a number of calculations using the CONCHAS–SPRAY computer program [5]. In this section we describe the pertinent features of CONCHAS–SPRAY and how we have modified the program to include the PGS method. Then we describe the results of one- and two-dimensional calculations performed with and without the PGS method. Large computational time-savings were realized using the PGS method because the number of iterations was reduced for a given value of the computational time step. The reason for this reduction is analyzed in the Appendix. Acceptably accurate results were obtained using a value of 0.01 for the allowable ratio of pressure fluctuation amplitude to mean pressure.

CONCHAS–SPRAY solves the two-dimensional, unsteady equations of motion for a chemically reacting mixture of ideal gases interacting with a vaporizing, single-component fuel spray. The program utilizes the ICE method [1, 2], in which those terms associated with acoustic wave motion are differenced implicitly. These are the pressure gradient terms in the momentum equations, and the term associated with

dilatation ($\nabla \cdot \mathbf{u} \neq 0$) in the mass (and, if desired, energy) equation. A pointwise iterative method similar to successive overrelaxation is used to solve the implicit finite difference equations. Use of the ICE method obviates the need to observe the Courant sound-speed stability condition, and CONCHAS–SPRAY computes its time step internally based on convective and diffusional stability criteria, on a maximum growth factor per cycle, and on the number of iterations required for convergence of the iteration procedure. If the number of iterations on a given cycle excedes a parameter ITMIN (usually taken to be twenty) then the time step is not allowed to increase on the next cycle. If the number of iterations exceeds a parameter ITMAX (usually taken to be fifty) then the time step on the next cycle is reduced by a factor of 0.75.

To implement the PGS method in CONCHAS–SPRAY, we simply updated the value of α using Eq. (23) and then divided the finite difference approximations to the pressure gradient terms in the momentum equations by α^2. The time step criteria based on the number of iterations were retained using the values ITMIN = 20 and ITMAX = 50.

Both test problems involve the calculation of premixed flames. A flame, or deflagration, is a wave or front in which there are exothermic chemical reactions and which propagates subsonically relative to the fluid ahead of it [14]. The pressures are nearly uniform in flame propagation problems, which therefore serve as excellent test cases for the PGS method. In describing the test problems we will give in detail only those computational parameters and results that relate to the use and validation of the PGS method.

The first test problem was to compute the flame speed of a steady, one-dimensional, hydrogen–air flame. An initial guess was made for the flame structure, consistent with the known conditions far upstream and downstream of the flame, and the steady state was then computed as the long-time limit of a transient process. The flame was kept stationary by adjusting the prescribed inflow velocity upstream of the flame so that the mass flow rate of reactant equaled its rate of consumption in the flame. The value of this inflow velocity is the computed flame speed. At the downstream outflow boundary, the pressure was prescribed. The heat and mass diffusivities were taken to be constant and a single-step global chemical reaction was used to represent hydrogen oxidation.

Using the standard CONCHAS–SPRAY program, a calculated flame speed of $17.21 \pm .02$ cm/sec was obtained after 15 sec of problem time. This required 16.3 min of computer time on a CRAY-1 computer. The calculated flame speed exhibited small oscillations about the mean value, and the above error bounds were inferred from the most recent maximum and minimum values prior to termination of the calculation. The final computational time step was limited to a value of 1.04×10^{-3} sec by the ITMIN parameter.

When the same problem was run with the PGS method, a calculated flame speed of $16.95 \pm .68$ cm/sec was obtained after 15 sec of problem time and 1.20 min of computer time. The oscillations in the flame speed here were larger than in the standard calculation because of the higher-amplitude acoustic waves. The final time step

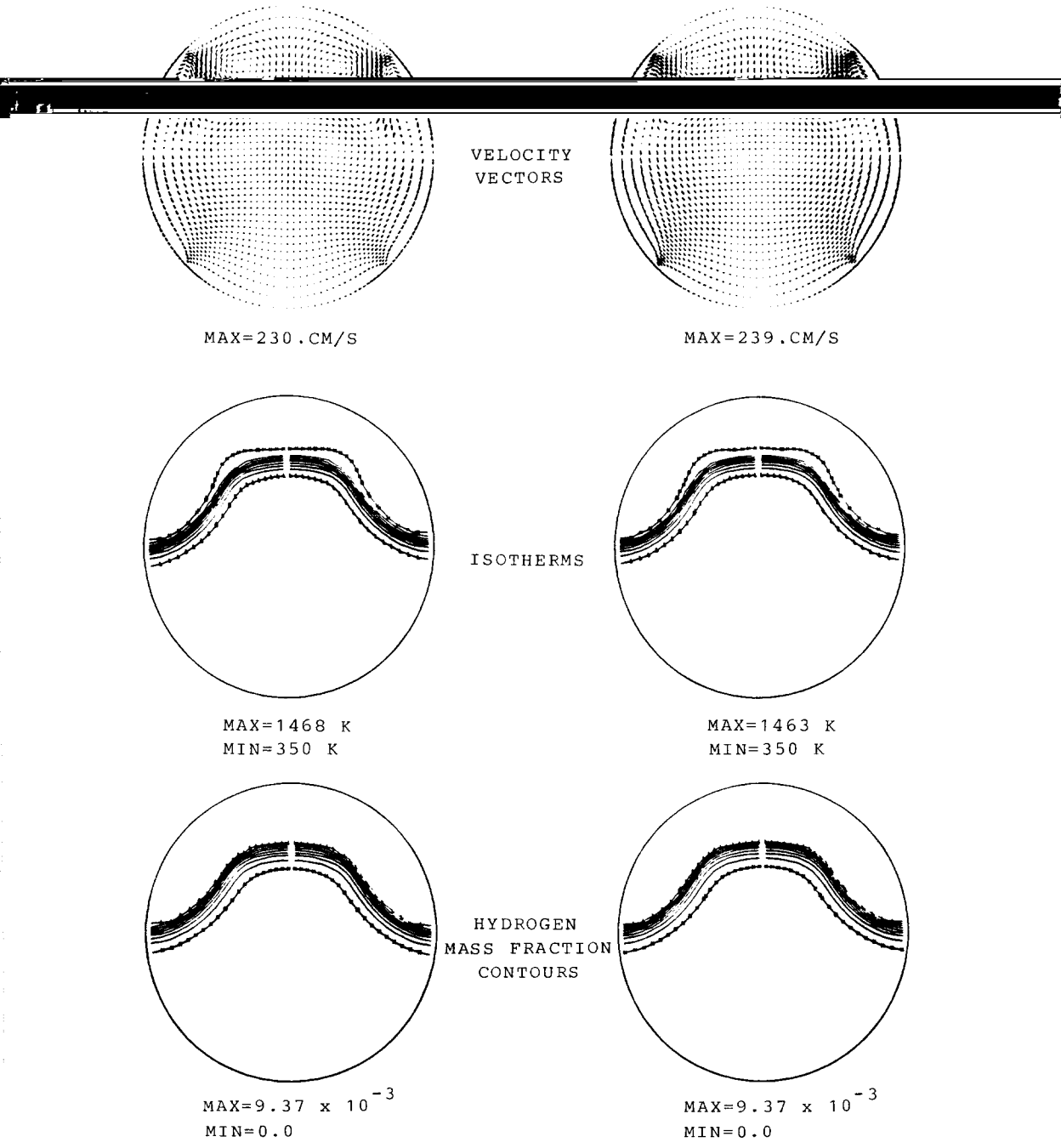

FIG. 1. Computer-generated plots of velocity vectors, hydrogen mass-fraction contours, and isotherms in the CONCHAS-SPRAY (left) and PGS (right) calculations.

of 1.06×10^{-2} sec was determined by the diffusional stability condition. This was an order of magnitude larger than in the standard calculation. The steady value of α in this calculation was 120.

In order to reduce the amplitude of the computed acoustic waves in the previous problem, we repeated the calculation changing only the maximum allowed ratio of the pressure fluctuations to the mean pressure. This ratio was lowered from 0.01 to 0.002. A computed flame speed of $16.89 \pm .06$ cm/sec was then obtained after 15 sec of problem time and 1.25 min of computer time. The time step was again 1.06×10^{-2} sec and the steady value of α was 60.0. Lowering the allowed pressure inhomogeneities reduced the flame speed oscillations without significantly changing the computational time, which was still more than an order of magnitude smaller than in the standard CONCHAS–SPRAY calculation. The resulting flame speed differed by two percent from the value obtained in the standard calculation, probably because of the truncation errors associated with the use of a larger time step in the PGS calculation.

The second test problem was a two-dimensional calculation of the unsteady burning of a hydrogen–air mixture in a closed, spherical volume. Again we give only the computational parameters and results that are relevant to the use and validation of the PGS method. A more detailed description of some related problems is given elsewhere [15].

Use of the PGS method reduced the computer time for this test problem by more than a factor of two. The standard CONCHAS–SPRAY calculation took 37.0 min of CRAY-1 computer time, while the PGS calculation took 15.9 min. The ratio of allowed pressure fluctuations to the mean pressure in the PGS calculation was 0.01. In both calculations the time step was limited by ITMIN, but in the PGS calculation this limitation did not occur until the time step was a factor of two or

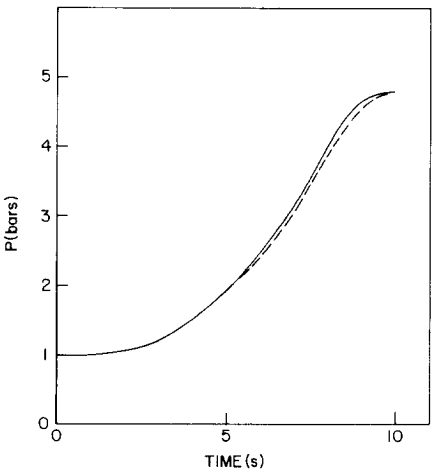

FIG. 2. Pressure histories obtained in the two-dimensional CONCHAS–SPRAY (solid line) and PGS (dashed line) calculations.

more larger than in the standard calculation. The value of α in the PGS calculation varied considerably in response to the changes in the dynamic state of the fluid.

The computational results agreed very closely. Shown in Fig. 1 are computer-generated plots of velocity vectors, hydrogen mass-fraction contours, and isotherms at an intermediate time in both calculations. Given below the plots are the computed maximum fluid speeds and the highest and lowest hydrogen mass-fractions and temperatures. It can be seen that none of the comparable values differ by more than four percent. Similar agreement was seen at other times in the calculations. Figure 2 shows the pressure histories obtained in the two calculations; the differences in pressure are seen to be less than four percent at any given time.

Appendix

Here we analyze the effect of PGS on the convergence rate of successive overrelaxation (SOR) in a simple one-dimensional problem with Dirichlet boundary conditions. The analysis is worked out in some detail, thereby explicitly exhibiting the increase in asymptotic convergence rate as a function of α. Similar results can also be derived in more than one dimension and for different boundary conditions. The SOR scheme considered here is essentially the same as that used in CONCHAS–SPRAY [5]; the only difference is that the implicit equations solved iteratively in CONCHAS–SPRAY are actually weakly nonlinear, and this nonlinearity is neglected here.

The asymptotic rate of convergence R^∞ of an iteration scheme is defined by $R^\infty = -\ln \rho(G)$, where $\rho(G)$ is the spectral radius of the iteration matrix G associated with the scheme [16]. The rate R^∞ is approximately the reciprocal of the number of iterations required to reduce the solution error by a factor of e^{-1}. Thus better iteration schemes have larger values of R^∞.

An examination of the CONCHAS–SPRAY iteration scheme [5] for a one-dimensional problem with Dirichlet boundary conditions, in which the density and sound speed are uniform, shows that the linearized system being solved is $Ax = b$, where A is the symmetric tridiagonal matrix with elements $A_{ii} = 1 + 2/\varepsilon^2$ and $A_{i,i+1} = A_{i+1,i} = -1/\varepsilon^2$, all other elements being zero, $\varepsilon = \alpha\, \Delta x/c\, \Delta t$, Δx is the cell width, Δt is the time step, and c is the true (unscaled) sound speed; the source vector b is immaterial for present purposes. The associated Jacobi iteration matrix G^{J} is [16] $G^{\mathrm{J}}_{i,i+1} = G^{\mathrm{J}}_{i+1,i} = (2+\varepsilon^2)^{-1}$, all other elements being zero, and its eigenvalues are [16] $\mu^{\mathrm{J}}_i = 2(2+\varepsilon^2)^{-1} \cos(i\pi a)$ $(i = 1,..., N)$, where $a = (N+1)^{-1}$ and N is the number of computational cells. The spectral radius of G^{J} is therefore $\rho_{\mathrm{J}} = 2(2+\varepsilon^2)^{-1} \cos(\pi a)$. The corresponding spectral radius for Gauss–Seidel iteration is [16] $\rho_{\mathrm{GS}} = \rho_{\mathrm{J}}^2$, while that for SOR with optimal relaxation factor is [16] $\rho_{\mathrm{SOR}} = (1-r)/(1+r)$, where $r = (1-\rho_{\mathrm{J}}^2)^{1/2}$.

Unfortunately, however, one rarely uses SOR with the optimal relaxation factor, so it would be unfair to evaluate R^∞ using ρ_{SOR}. It is reasonable, however, to suppose that R^∞ lies between the values it would have for Gauss–Seidel iteration and

optimal SOR iteration. These values are readily obtained from ρ_{GS} and ρ_{SOR} above, and when ε and a are small we obtain

$$R_{GS}^{\infty} = 2\ln(1+\tfrac{1}{2}\varepsilon^2) + \pi^2 a^2$$

and

$$R_{SOR}^{\infty} = 2(\varepsilon + \pi a).$$

Two interesting observations may now be made. First, as α increases so does ε, and the convergence rates R_{GS}^{∞} and R_{SOR}^{∞} increase accordingly. This exhibits the improvement in convergence rate that occurs when the PGS method is used in the present context. Second, we note that a decreases as N increases, so that the convergence rates worsen as the resolution is increased. However, they do not worsen below the positive lower bounds obtained by setting $a=0$. (Ordinarily Δt will vanish at least as rapidly as Δx, so ε will remain constant or perhaps even increase as $N \to \infty$.) In contrast, as $N \to \infty$ ($a \to 0$) in an incompressible calculation, where $\varepsilon = 0$, the convergence rates tend to zero.

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