Algorithmic Enhancements for Unsteady Aerodynamics and Combustion Applications

Sankaran Venkateswaran
University of Tennessee
Tullahoma, TN 37388

Summary of Research

1.0 Introduction

Research in the FY01 focused on the analysis and development of enhanced algorithms for unsteady aerodynamics and chemically reacting flowfields. The research was performed in support of NASA Ames' efforts to improve the capabilities of the in-house CFD code---OVERFLOW. Specifically, the research was focused on the four areas given below.

1. Investigation of Stagnation Region Effects. The preconditioning formulation, that is used for low speed aerodynamics computations in the OVERFLOW code, is known to be susceptible to instabilities in stagnation regions. In our research, we have employed perturbation analysis to shed light on the underlying causes of these instabilities. Specifically, it is evident that the instabilities are driven by the presence of large pressure fluctuations and it is necesary to modify the preconditioning formulation to account for such fluctuations. Based upon this insight, we have derived several modified preconditioning formulations and specific recommendations have been made for implementation in the OVERFLOW code.

2. Unsteady Preconditioning Dual-Time Procedures. We have aided NASA researchers in implementing the unsteady preconditioning algorithm into the OVERFLOW code. In addition, a multiple scales preconditioning formulation has been developed to address more complicated unsteady problems. This is also based upon using separate preconditioning formulations for the artificial dissipation terms and for the time-stepping. Detailed assessments of the enhanced algorithm need to be carried out and are currently underway.

3. Dissipation Formulation for Combustion. Various formulations for incorporating source terms into the artificial dissipation terms have been catalogued and evaluated. Appropriate forms for implementation into the OVERFLOW code have been identified.

4. Time-Stepping Methods for Combustion. We have assisted NASA researchers in the implementation of combustion capability in the OVERFLOW code. In addition, several methods of integrating the fluids equations with chemical source terms have also been evaluated. These include the fully implicit procedure, the Strang splitting method and the consistent splitting methods. The fully implicit procedure has been found to be efficient and accurate but lacks robustness. On the other hand, the Strang splitting procedure is robust and reasonably efficient, but it is inaccurate near the combustion region. Finally, the consistent splitting method is robust and accurate, but suffers from inefficiencies. However, it is readily adaptable to the diagonalized solution procedure that is the solution algorithm of choice in the OVERFLOW code. Thus, the latter approach appears to be a promising avenue. Further studies are necessary to verify these findings.

In the following sections, the specific research accomplishments in each of the above areas are discussed in greater detail. In addition, recommendations for further investigations are offered.

2.0 Stagnation Region Effects

Time-marching algorithms typically utilize preconditioning techniques to remain effective at low speeds or Mach numbers [1]. Although there are a wide variety of preconditioning techniques, all of them involve selective alteration or scaling of the physical time-derivatives in order to condition the system eigenvalues for all flow conditions. Specifically, all the methods essentially involve scaling of the pressure time-derivatives in the system by a term that is inversely proportional to the Mach-number squared. This scaling is crucial both for maintaining accuracy of the discrete formulation as well as for obtaining efficient convergence rates of the iterative solution procedure. However, in some instances such as in the stagnation region, this scaling has the adverse effect of loss of robustness. Although this problem has been widely recognized, it is not very well understood. In this section, we analyze the underlying causes for the loss of robustness and then use this insight to devise amelioratory procedures.

The preconditioning method utilized in the OVERFLOW code is a variant of the form orginally proposed by Choi and Merkle [2] and then later modified by Weiss and Smith [3]. It is closely related to the procedures utilized by Turkel [4], but it is different from that suggested by Van Leer et al. [5]. As mentioned above, in spite of their differences, all of these methods possess similar properties and all of them share a degradation in overall robustness for certain types of problems. To understand the reason for these difficulties, it is instructive to re-visit the derivation of the Choi-Merkle/Weiss-Smith formulation, which is based upon a perturbation analysis of the Euler equations. Here, we follow the procedure outlined by Venkateswaran and Merkle [1].

2.1 Perturbation Analysis

We start with the one-dimensional Euler equations for simplicity and note that a similar development is possible for the multi-dimensional Navier-Stokes equations as well. We write the equations in vector form as:

$$\Gamma \frac{\partial Q_p}{\partial \tau} + \frac{\partial E}{\partial x} = 0 \tag{1}$$

where:

$$Q_p = \begin{bmatrix} p \\ u \\ T \end{bmatrix} \qquad E = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ (e + p)u \end{bmatrix} \qquad \Gamma = \begin{bmatrix} \frac{\partial \rho}{\partial p} & 0 & \frac{\partial \rho}{\partial T} \\ u\frac{\partial \rho}{\partial p} & \rho & u\frac{\partial \rho}{\partial T} \\ h_0\frac{\partial \rho}{\partial p} - 1 & \rho u & \rho\frac{\partial h}{\partial T} + h_0\frac{\partial \rho}{\partial T} \end{bmatrix}$$

Here, we have written the equations using a primitive variables set. Although these are not necessarily the variables employed in the solution algorithm, we will see that the primitive variables set play a crucial role in the development of the preconditioning system. Note that the matrix Γ in Eqn. (1) represents the exact Jacobian of the variable transformation and the equations remain precisely equivalent to the standard physical system.

To analyze the behavior of the physical system under low Mach conditions, we employ perturbation expansions. We begin with the momentum equation, which we write in the noncon-servative form for simplicity,

$$\rho\frac{\partial u}{\partial \tau} + \rho u\frac{\partial u}{\partial x} + \frac{\partial p}{\partial x} = 0 \tag{2}$$

We next nondimensionalize the equations to facilitate order of magnitude comparisons between the terms. We introduce the following reference scales for the variables,

$$L, u_r, \tau_r, p_r, \rho_r, T_r$$

Here, L represents a characteristic length scale, u_r is the reference velocity and τ_r is the refer-ence time scale (to be defined later). p_r is the reference pressure, while ρ_r is the reference mix-ture density. The nondimensionalized version of Eqn. 2 is then given by:

$$\left(\frac{L}{u_r\tau_r}\right)\bar{\rho}\frac{\partial \bar{u}}{\partial \bar{\tau}} + \bar{\rho}\bar{u}\frac{\partial \bar{u}}{\partial \bar{x}} + \left(\frac{p_r}{\rho_r u_r^2}\right)\frac{\partial \bar{p}}{\partial \bar{x}} = 0 \tag{3}$$

where the overbars indicate nondimensional quantities.

We note that the coefficient of the pressure gradient term in the above equation becomes very large in the limit of low speed flows. To insure that the pressure gradient is always balanced by the convective terms, we define the small parameter,

$$\varepsilon = \frac{\rho_r u_r^2}{p_r} \tag{4}$$

and consider the limiting form of Eqn. 3 as this parameter goes to zero. We then expand the pres-sure in a power series,

$$\bar{p} = \bar{p}_0 + \varepsilon\bar{p}_1 + \ldots \tag{5}$$

and substitute it into Eqn. 3 to get

$$\left(\frac{L}{u_r \tau_r}\right)\bar{\rho}\frac{\partial \bar{u}}{\partial \bar{\tau}} + \bar{\rho}\bar{u}\frac{\partial \bar{u}}{\partial \bar{x}} + \frac{1}{\varepsilon}\frac{\partial(\bar{p}_0 + \varepsilon \bar{p}_1)}{\partial \bar{x}} = 0 \tag{6}$$

A more complete procedure would use analogous expansions for all the variables, but the results show that only the zeroth order quantities of the remaining variables appear in the final equations. Consequently, to minimize the algebra, we perturb only the pressure.

The purpose of the time-derivatives in a time-marching scheme is to drive the equations to the desired steady state solution. To insure that this process is efficient, we select the characteristic time-scale such that the time-derivatives are of the same magnitude as the convective terms. Specifically, in Eqn. 6, the coefficient of the time derivative must be of order unity so that $\tau_r = L/u_r$. This requirement clearly implies that the appropriate time scale is the convective time scale of the fluid particle. In that case, there remains no term to balance the $1/\varepsilon$ term in the pressure gradient term, leading us to conclude that,

$$\frac{\partial \bar{p}_0}{\partial x} = 0 \tag{7}$$

Moreover, for most problems, $\bar{p}_0$ is fixed by the boundary condition and, hence, this quantity can be taken to be independent of time as well. In other words, $\bar{p}_0$ is a constant and all changes in the pressure occur only in the first-order pressure. Note that this result makes an assumption on the size of the pressure fluctuations in the flowfield---i.e., the pressure fluctutions are of $O(\varepsilon)$. In fact, there may be situations wherein this stipulation may not hold, potentially leading to difficulties. We will discuss such exceptions later.

Using Eqn. 7, the zeroth order momentum equation therefore takes the form,

$$\bar{\rho}\frac{\partial \bar{u}}{\partial \bar{\tau}} + \bar{\rho}\bar{u}\frac{\partial \bar{u}}{\partial \bar{x}} + \frac{\partial \bar{p}_1}{\partial \bar{x}} = 0 \tag{8}$$

Note that the ε term in the pressure gradient has been cancelled by the $1/\varepsilon$ term that multiples it. All the terms in Eqn. 33 are clearly of order unity. In the time-marching framework, it is evident that this equation provides an adequate means of updating the velocity $\bar{u}$. However, the presence of the first-order pressure $\bar{p}_1$ implies that we must have a viable way of updating it from the continuity and energy equations. Accordingly, we consider these equations next.

To analyze the scaling of the continuity equation, we again non-dimensionalize and introduce the perturbation expansion,

$$\left(\frac{p_r}{\rho_r}\frac{\partial\rho}{\partial p}\right)\varepsilon\frac{\partial\bar{p}_1}{\partial\bar{\tau}} + \left(\frac{T_r}{\rho_r}\frac{\partial\rho}{\partial T}\right)\frac{\partial\bar{T}}{\partial\bar{\tau}} + \frac{\partial\bar{\rho}\bar{u}}{\partial\bar{x}} = 0 \tag{9}$$

The above equations has the time-derivative of the first-order pressure term present. However, this time-derivative become vanishingly small in the limit of $\varepsilon \to 0$. Thus, in this limit, there is no means of reliably updating the first-order pressure. In practice, the problem manifests itself in slow convergence of the time-marching procedure at low speeds. We further note that the situation is precisely the same as the singularity encountered in the incompressible limit.

One way of alleviating the singularity problem is to alter the time-marching system such that it remains well-conditioned at all speeds. In the present context, this may be achieved through the introduction of a pseudo-property term in the pressure time-derivative such that it becomes order unity. Thus,

$$\frac{\partial\rho'}{\partial p} = \frac{\rho_r}{p_r}\frac{1}{\varepsilon} = \frac{1}{u_r^2} \tag{10}$$

With this scaling, the time-dependent system is rendered suitable for time-marching computations at all flow speeds. This scaling procedure is generally referred to as preconditioning and, in the incompressible limit, it precisely corresponds to the artificial compressibility formulation [6].

As noted earlier, the preconditioning scaling of Eqn. 10 is contingent upon the assumption inherent in Eqn. 7. In problems involving pressure variations that are larger than $O(\varepsilon)$, one may therefore expect difficulties. By enforcing the requirement that p_0 is a constant, the first order pressure p_1 may become unnaturally large. In turn, the preconditioning scaling of the time-derivative in the continuity equation may render this term large rather than of order unity (as it is designed to do). As a result, unstable solution behaviour may be encountered, leading to the observed lack of robustness. A common situation wherein this probem is encountered is in flows where the pressure level is not known *a priori*. For instance, in choked nozzle flows, the mass flow is often specified as an inflow boundary condition and the chamber pressure is determined as a

result of the solution. In such cases, large transients in the thermodynamic pressure (p_0) may occur, contributing to potential instability when the standard preconditioning scaling (in Eqn. 10) is adopted. Stagnation point flows are likewise associated with strong local pressure gradients, leading to pressure fluctuations, which may trigger local instabilities.

2.2 Mitigating Procedures

The perturbation analysis sheds light into the fundamental mechanics of the instabilities that arise due to large pressure fluctuations. Further, this insight suggests various avenues for mitigating the problem. We discuss three potential methods below.

2.2.1 Update Equation for the Zeroth Order Pressure

The fundamental problem arises because of the assumption of a constant zeroth order pressure. This suggests that a possible solution would be to allow p_0 to be time-varying. Of course, this means that an additional equation has to be introduced to provide a means of updating p_0, independent of p_1. A temporal equation for the mean pressure level in a chamber can be obtained by treating the region as a zero-dimensional volume (i.e., by using a lumped mass assumption). Using global conservation of mass, we get,

$$\frac{\partial \rho}{\partial p} V \frac{dp_0}{d\tau} = \dot{m}_{in} - \dot{m}_{out} \tag{11}$$

Augmenting the preconditioned system with the above equation for the thermodynamic pressure allows the first order pressure to represent only the dynamic pressure. Thus, large pressure changes are handled by Eqn. 11, while small pressure fluctuations are handled by the conventional preconditioned continuity equation, Eqn. 10. This formulation is very simple to implement; however, its disadvantage is that it is a global "fix" and not a local one. Thus, it is well equipped to handle problems wherein the base pressure level is not known at the start of the computation, but it is not designed to deal with local pressure disturbances such as those encountered in stagnation regions.

2.2.2 Modified Preconditioning Scaling

A second approach is to modify the scaling of the pressure time derivtaive in the continuity equation to account for the size of the local pressure fluctuation. In other words, the scaling suggested in Eqn. 10 is altered in such a manner that the pressure update is order unity for all magnitudes of Mach number *and* pressure fluctuation. Thus,

$$\frac{\partial \rho'}{\partial p} = Min\left(Max\left(\frac{1}{u_r^2}, \frac{\rho_r}{\Delta p_r} \right), \frac{\partial \rho}{\partial p} \right) \tag{12}$$

Here, when the pressure fluctuations are large, they are used to select the scaling of the time-derivative, until a point is reached, wherein the physical property derivative is itself well-conditioned. At that juncture, the system is no longer preconditioned. The advantage of this formulation is that it can be implemented on a local basis and is therefore be particularly effective for problems involving stagnation regions. In fact, other researchers [3, 5] have successfully employed similar procedures for stagnation point flows.

2.2.3 Linearized Preconditioning Procedures

Yet another approach may be devised by making the observation that the instability arising from preconditioning scaling in the presence of large pressure fluctuations is fundamentally non-linear in nature. Therefore, a simple but effective way of handling the problem is to perform the preconditioning scaling *after* linearization rather than at the non-linear level. Thus, linear convergence is ensured even if the local pressure fluctuations are large. The linearized preconditioned scheme takes the following algorithmic form,

$$\Gamma_p \frac{\partial Q_p}{\partial \tau} + \left(\frac{\Gamma}{\Delta t} + \frac{\partial A}{\partial x} \right) \Delta Q_p = -\left(\frac{\partial E}{\partial x} \right)^n \tag{13}$$

Note that the formulation has been cast in a dual-time framework, wherein Δt is the non-linear time step and τ is the linear time step. The preconditioning scaling is introduced only in the linear time-level, while the physical time-derivatives are retained in the non-linear level. Note that this formulation is completely general. In practice, it would be often possible to select the non-linear

time-step to be infinity, thereby leading to a single-time-step scheme. More details on the linearized preconditioning scheme is given in Ref. [1]. These studies and additional results will also be summarized in a forthcoming article to be presented at the AIAA Fluid Dynamics Conference [7].

3.0 Unsteady Preconditioning Formulation

Low Mach number and other stiff problems require the use of preconditioning scaling, which alters the form of the time-derivatives used in the time-marching algorithm. This means that the system is no longer time accurate. Unsteady computations therefore need to be performed within a dual time-stepping framework, similar in form to that presented in the previous section (Eqn. 13). The equations are marched in physical time and, at each physical time-step, the pseudo-time derivative is used to iterate the solution to convergence. The pseudo-time derivative may be altered or preconditioned to maximize convergence and accuracy. We point out that the preconditioning may be introduced at either the non-linear or the linear level, but we use the former procedure because it is customary to do so [1,8].

The OVERFLOW code has dual-time iterative capability for unsteady computations as well as preconditioning capability for steady problems. However, the original version of the code did not possess the ability to apply preconditioning for unsteady computations. The major task of this research was to provide NASA researchers with guidance regarding the implementation of a preconditioned dual-time procedure for unsteady computations. The main challenge in this regard is the tailoring of the dual time procedure to the diagonalized algorithm that is used in the OVERFLOW code. We have followed the procedure of Merkle and Buelow [9] to accomplish this task. Secondly, the unsteady preconditioning procedure [1,8,9] was orginally devised for handling problems, characterized by a single unsteady time scale. However, this is inadequate for complex problems, wherein multiple local time scales may co-exist in a single problem. Accordingly, a second aspect of the research is to adapt the preconditioning strategy to handle multiple time scales. In the following sub-sections, we describe the two aspects of the research.

3.1 Diagonalized Unsteady Preconditioning Formulation

The preconditioned dual-time scheme may be expressed as:

$$\Gamma\frac{\partial Q}{\partial \tau} + \frac{Q^{n+1} - Q^n}{\Delta t} + \frac{\partial E^{n+1}}{\partial x} + \frac{\partial F^{n+1}}{\partial y} = 0 \tag{14}$$

where Γ is the preconditioning matrix. This matrix premultiplies the pseudo-time derivative, while the other time-derivative retains its physical form. At each physical time-level, the preconditioned time-iterative procedure is exercised until a specified "convergence" level is attained. At that point, the solution is advanced to the next physical time level and the iterative procedure starts over. The choice of the preconditioning matrix is therefore decided as per the requirements of convergence and accuracy of the pseudo-iterations. The importance of accuracy is due to the dependence of the form of the artificial dissipation terms on the preconditioning matrix and will be addressed in greater detail in the following sub-section.

The preconditioned implicit ADI version of the dual-time scheme may be written as:

$$\left(S + \Delta\tau\frac{\partial}{\partial x}A^k\right)S^{-1}\left(S + \Delta\tau\frac{\partial}{\partial y}B^k\right)(Q^{k+1} - Q^k) = -\Delta\tau\left(\frac{Q^k - Q^n}{\Delta t} + \frac{\partial E^k}{\partial x} + \frac{\partial F^k}{\partial y}\right) \tag{15}$$

where

$$S = \Gamma + \frac{\Delta\tau}{\Delta t}I$$

As mentioned earlier, the main solution algorithm in the OVERFLOW code is the diagonalized ADI procedure. Equation 15 thus needs to be adapted to the diagonalized procedure. Following Buelow and Merkle [9], we get the following algorithm:

$$\left(I + \Delta\tau S^{-1}A\frac{\partial}{\partial x}\right)\left(I + \Delta\tau S^{-1}B\frac{\partial}{\partial y}\right)(Q^{k+1} - Q^k) = -\Delta\tau S^{-1}R^k \tag{16}$$

where

$$R^k = \frac{Q^k - Q^n}{\Delta t} + \frac{\partial E^k}{\partial x} + \frac{\partial F^k}{\partial y}$$

Now, introducing the modal matrices, we may diagonalize the LHS operators:

$$M_x\left(I + \Delta\tau\Lambda_x\frac{\partial}{\partial x}\right)M_x^{-1}M_y\left(I + \Delta\tau\Lambda_y\frac{\partial}{\partial y}\right)M_y^{-1}(Q^{k+1} - Q^k) = -\Delta\tau S^{-1}R^k \quad (17)$$

The extension to 3D is straightforward and is not given here.

3.2 Multiple Scales Preconditioning Strategy

The definition of the preconditioning matrix for unsteady computations depends not only on the flow Mach number but also the choice of physical time scales. The choice is reflected in the precise definition of the pseudo-property term in the preconditioning matrix, which takes the following form [1]:

$$\frac{\partial\rho'}{\partial p} = Min\left(Max\left(\frac{1}{u_r^2}, \frac{(\pi\Delta t)^2}{l^2}\right), \frac{\partial\rho}{\partial p}\right) \quad (18)$$

It can be observed that for low-frequency problems, the standard choice of the inverse-velocity squared is employed. However, for high frequency problems, a new unsteady velocity scale is used in the definition of the preconditioning parameter.

The unsteady velocity scale in Eqn. 18 is computed from a global length scale and the physical time step size and is therefore a global velocity scale. Thus, it is appropriate only for problems that are characterized by a single unsteady frequency. In complex physical problems, multiple unsteady scales may be present. In such cases, the above definition needs to be modified in some fashion. However, one must bear in mind that preconditioning influences both the efficiency and accuracy of the computation and, in unsteady computations, the appropriate choice of preconditioner for efficiency is often different from the appropriate choice for accuracy.

To accomodate such conflicting demands, we propose a multi-scales preconditioning strategy that is based upon employing different sets of preconditioners for the time-derivative and the artificial dissipation terms. Thus, we have

$$\Gamma_I \frac{\partial Q}{\partial \tau} + \frac{Q^{n+1} - Q^n}{\Delta t} + \frac{\partial E^{n+1}}{\partial x} = \frac{\Delta x}{2} \frac{\partial}{\partial x} \Gamma_{II} \left| \Gamma_{II}^{-1} A \right| \frac{\partial Q}{\partial x} \tag{19}$$

where Γ_I is the time-derivative preconditioner chosen for efficient convergence properties and Γ_{II} is the dissipation preconditioner chosen for accuracy of the flux formulation. The selection of the pseudo-properties in the two preconditioning matrices will depend upon the specific constraints for achieving efficiency and accuracy. Accordingly,

$$\left.\frac{\partial \rho'}{\partial p}\right|_I = Min\left(Max\left(\frac{1}{u_r^2}, \frac{(\pi \Delta t)^2}{l^2} \right), \frac{\partial \rho}{\partial p} \right) \qquad \left.\frac{\partial \rho'}{\partial p}\right|_{II} = Min\left(Max\left(\frac{1}{u_r^2}, \frac{t_s^2}{l_s^2} \right), \frac{\partial \rho}{\partial p} \right) \tag{20}$$

Note that the time-derivative preconditioner has the *same* form as in Eqn. 18, while the dissipation preconditioner uses difrerent local scales to dertemine the unsteady velocity scale. Exactly how this scale should be defined on a local basis remains a research issue, although it would appear that local length and time scales could be prescribed *a priori* from a knowledge of overall physics of the flow. Additionally, it is possible that the scheme may be more readily implemented using an AUSM-style dissipation procedure as described in Ref. 10.

4.0 Artificial Dissipation Formulation for Combustion Problems

There is currently an effort to bring in multi-species combustion capability into the OVERFLOW code. We are closely working with NASA researchers in this endeavour. Further, we are focusing on the new challenges associated with source terms, particularly those arising from stiff chemistry. Overall, the research is focused on two areas---namely, artificial dissipation formulation and time-stepping schemes. In the present section, we address techniques to modify the artificial dissipation formulation to account for dominant source terms. Specificially, we catalog various approaches that have been proposed by researchers in the field. Time-stepping issues are dealt with in the following section.

The design of artificial dissipation terms in source-dominated computations may be controlled by two sets of circumstances, namely, *well-resolved* sources and *under-resolved* sources.

In the former instance, all the gradients induced by the presence of source terms are well-resolved by the computational grid. In this case, the artificial dissipation terms should be selected so as to provide the *minimal* amount of damping that is necessary to suppress odd-even oscillations in the flowfield. The second instance arises when the computational grid is too coarse to resolve the source-induced gradients in the flowfield. Such problems arise frequently in chemically reacting flows, wherein some of the chemical time scales are extremely small, leading to very rapid relaxation of the solution (or part of the solution) to equilibrium. In such cases, it is typically impractical to fully resolve the source terms and, therefore, the computational solution is characterized by a discontinuity that separates two equilibrium states. The formulation of the artificial dissipation function must then be to capture these discontinuities accurately, i.e., they must ensure the correct location of the discontinuity, the correct equilibrium states on either side of it and solution monotonicity in its vicinity.

The situation is similar to shocks, that arise from the solution of the Euler equations of compressible flow. In the absence of source-terms, several well-known methods have been devised to capture such discontinuities. These include the artificial dissipation methods of Jameson and Turkel [11], the flux-vector splitting methods of Steger and Warming and Van Leer, the approximate Riemann methods of Roe [12] as well as the more recent AUSM method of Liou [13]. The adaptation of these methods to account for the presence of source terms has been considered by several researchers in different contexts. This includes some early work by Roe [14], and the more recent contributions of Pember [15], Bermudez and Vasquez [16], Jin and Levermore [17], Mohanraj et al. [18], Yu and Chang [19] and Sussman [20]. While some of these papers are concerned primarily with under-resolved flows, many consider the well-resolved situation as well. At any rate, we believe that the two sets of circumstances are closley related and cannot be studied in isolation. Many of these proposals are related and, in general, they all point to the need for a distributed treatment of the source terms. However, differences remain in the flavor and form of the implementation, and there is no general consensus amongst the authors. We will therefore review several of these contributions in this report with the aim of determining the right direction to pursue for further development.

4.1 Modifications to the Roe Scheme

Roe has proposed at least three different variants of his flux-differencing procedure to

accommodate the presence of source terms in the system of equations [12,14]. All three modifications are somewhat related, but vary in the precise details.

In Ref. 12, Roe considers quasi-1D flow with area variation. This corresponds to the source term vector being defined as:

$$H = \begin{bmatrix} 0 \\ -p\frac{\partial A}{\partial x} \\ 0 \end{bmatrix} \tag{21}$$

The characteristic form of the quasi-1D Euler equations now becomes:

$$\frac{\partial W}{\partial t} + \Lambda\frac{\partial W}{\partial x} = M^{-1}H = S \tag{22}$$

In the steady state, these characteristic equations yield solutions that satisfy scalar equations of the form:

$$\frac{\partial w_k}{\partial x} = \frac{s_k}{\lambda_k} \tag{23}$$

Roe's approach is to define a new Riemann variable based upon the above equation such that:

$$\delta w_k' = \delta w_k - \frac{s_k \delta x}{\lambda_k} \tag{24}$$

and to re-define the flux-differencing procedure in terms of this new variable. The interfacial flux is then defined as:

$$\hat{E}_{i\pm\frac{1}{2}} = \frac{1}{2}(E(Q_L) + E(Q_R)) - \frac{1}{2}\sum|\tilde{\lambda}_k|\delta w_k' \vec{m}_k \tag{25}$$

In other words, the above procedure modifies the wave-strengths to account for the presence of source terms in the characteristic equations.

The second approach used by Roe has been summarized by Barth [21]. The scheme appears similarly motivated---that is, it is modified to admit locally stationary solutions to account for the presence of the source term---but it is expressed in a different fashion. The numerical flux at the interface is modified to include the source term in the following fashion:

$$\hat{E}_{i+\frac{1}{2}} = E(Q_L) - \frac{\delta x}{2}|\tilde{A}|\tilde{A}^{-1}\overline{H}(Q_L, Q_R) \tag{26}$$

which can, in turn, be written as:

$$\hat{E}_{i\pm\frac{1}{2}} = \frac{1}{2}(E(Q_L) + E(Q_R)) - \frac{1}{2}|\tilde{A}|(Q_R - Q_L) - \frac{\delta x}{2}|\tilde{A}|\tilde{A}^{-1}\overline{H}(Q_L, Q_R) \tag{27}$$

Although Eqn. 27 is closely related to Eqn. 25, it is much easier to implement in practice. Also, note that the average source term may be computed by a trapezoidal rule integration. Further, Barth [21] makes the point that if the source discretization is *carefully* chosen, the overall scheme may be rendered higher-order accurate.

For a first-order scalar system, it is instructive to examine Eqn. 25 further. Using simple averaging of the source term flux, we can write the full first-order discrete scheme as:

$$\frac{\partial q}{\partial t} + \frac{e_{i+1} - e_{i-1}}{2\delta x} = h_i + \frac{\delta x}{2}|\lambda|\frac{\partial^2 q}{\partial x^2} + \frac{\delta x}{2}\frac{\partial h}{\partial x} \tag{28}$$

which involves an additional dissipation term, characterized by the source term.

A third approach is outlined by Roe and Arora [14], where the authors adopt a more involved characteristics integration strategy to define the inteface fluxes. The method appears to be similar to the earlier approaches in principle and is not discussed further here.

4.2 Bermudez and Vazquez Source Term Discretization

Bemudez and Vazquez [16] find in their analysis of source-dominated flows that point representations of the source term have more limited stability and positivity constraints. They present a formal derivation to obtain a numerical source function, that parallels the development of the numerical inviscid fluxes that arise in flux-difference schemes. We summarize their development here.

The overall discrete scheme is expressed as follows:

$$\frac{\partial Q}{\partial t} + \frac{\hat{E}_{i+\frac{1}{2}} - \hat{E}_{i-\frac{1}{2}}}{\delta x} = \hat{H}_i \tag{29}$$

where the numerical fluxes $\hat{E}_{i\pm\frac{1}{2}} = \hat{E}_{i\pm\frac{1}{2}}(Q_L, Q_R)$, while the numerical source function,

$\hat{H}_i = \hat{H}_i(x_{i-1}, x_i, x_{i+1}, Q_{i-1}, Q_i, Q_{i+1})$. The numerical fluxes are defined as given before for the Roe scheme, while the authors provide the following prescription for the numerical source function:

$$\hat{H}_i(x_{i-1}, x_i, x_{i+1}, Q_{i-1}, Q_i, Q_{i+1}) = H_L(x_{i-1}, x_i, Q_{i-1}, Q_i) + \hat{H}_R(x_i, x_{i+1}, Q_i, Q_{i+1}) \quad (30)$$

where

$$\hat{H}_L(x_{i-1}, x_i, Q_{i-1}, Q_i) = \frac{1}{2}[I + |\tilde{A}|\tilde{A}^{-1}]\overline{H}(x_{i-1}, x_i, Q_{i-1}, Q_i)$$

$$\hat{H}_R(x_i, x_{i+1}, Q_i, Q_{i+1}) = \frac{1}{2}[I + |\tilde{A}|\tilde{A}^{-1}]\overline{H}(x_i, x_{i+1}, Q_i, Q_{i+1})$$

Note the close similarity to Eqn. 26 of Roe's second method. Bermudez and Vazquez recommend one of the following expressions for the average source values:

$$\overline{H}(x_{i-1}, x_i, Q_{i-1}, Q_i) = \frac{1}{2}[H(x_{i-1}, Q_{i-1}) + H(x_i, Q_i)] \quad (31)$$

$$\overline{H}(x_{i-1}, x_i, Q_{i-1}, Q_i) = H\left(\frac{x_{i-1} + x_i}{2}, \frac{Q_{i-1} + Q_i}{2}\right) \quad (32)$$

Substituting these expressions into Eqn. 30, we would obtain an averaged representation of the source terms.

4.3 Other Approaches

Jin and Levermore [17] offer two approaches to handle source term effects. Both methods are closely related to Roe's approaches in that they seek to include the source term in the definition of the interface numerical flux. The difference between the two approaches, in fact, lies in where the Taylor expansion is centered. In the piecewise steady method, similar to Roe, the Taylor expansion is performed about the nodal values, while in their so-called modified upwind scheme, the Taylor expansion is centered about the interface point. This subtle difference leads to philosophically related but distinct expressions for the source fluxes. Jin and Levermore prove that both their methods preserve proper solution behavior in the asymptotic limits of small, intermediate and large source terms.

Mohanraj *et al.*[18] adopt a two-pronged strategy in addressing source term effects. They adopt Roe's first strategy (Eqn. 25) and augment it by further using a distributed source represen-

tation similar to that suggested by Bermudez and Vasquez. They report improvements for several source-dominated flows. Further, they catalog higher-order source term discretizations as well in their paper.

Finally, Yu and Chang [19] use the so-called space-time methodology to construct fluxes in the presence of source terms. They argue that unlike conventional flux-difference methods, the space-time method naturally introduces a distributed evaluation of the source term, which yields the correct physical behavior for source-dominated flows.

5.0 Time-Stepping Schemes for Combustion Problems

Over the years, several methods have been employe by researchers to compute reacting flow fields. Overall, we may classify the methods as being direct methods or splitting methods. In direct methods, the source term is treated fully implicitly, while in splitting methods, typically, the source term is treated using an ODE solver, while the convection-diffusion terms are treated in a conventional manner using a PDE solver. The most popular splitting method is the one due to Strang, but many variants are possible, among which we consider one that we refer to as the consistent splitting method.

5.1 Direct or Fully Coupled Scheme

In direct or fully coupled methods, the chemical source terms and the transport terms are solved simultaneously. In one dimension, the direct scheme may be written as:

$$\left[I + \Delta\tau D + \Delta\tau\frac{\partial A}{\partial x}\right]\Delta Q = -\Delta\tau\left(\frac{\partial E^n}{\partial x} - H_r^n\right) \tag{33}$$

where the residual R contains the convection diffusion terms, while the source term vector H contains the chemical source terms.

Direct methods are often considered the best method because of its unconditional stability. In fact, this statement is not strictly true as discussed in detail in Ref. 22. Direct or implicit treatment of negative sources (or sinks) is unconditionally stable; however, implicit treatment of positive sources is only conditionally stable. In combustion computations, it is normal to encounter

positive source terms during the initial non-linear stages of the computation, while, in the later linear stages, only sink terms are encountered. Thus, full implicit treatment may lead to instabilities initially, but is asymptotically stable in the linear convergence process.

A further difficulty of direct schemes is that they are not ideally suited for implementation in diagonalized implicit schemes. This is due to the fact that the source term Jacobian cannot be readily diagonalized. Thus, it is customary to solve the species equations (that contain the source terms) uncoupled from (or, more precisely, loosely coupled to) the fluids equations, which in turn may lead to additional loss of robustness and efficiency. For these reasons, we will consider the properties of the Strang splitting and consistent splitting schemes next.

5.2 Strang Splitting Scheme

In splitting methods, the integration of the equations are carried out in two steps, namely a chemistry integration, which requires the use of an ODE solver, followed by a transport integration, which utilizes a conventional PDE solver. In fact, since the transport step does not contain the source term Jacobian, it is well suited for use with a diagonalized implicit solver. We may express the Strang scheme in the following fashion:

$$\frac{Q^* - Q^n}{\Delta\tau} = \frac{1}{\Delta\tau}\int_{\Delta\tau} H_r(\tau)d\tau \tag{34}$$

$$\frac{Q^{n+1} - Q^*}{\Delta\tau} + \frac{\partial E^{n+1}}{\partial x} = 0 \tag{35}$$

where we have first carried out a chemistry integration step followed by a transport-step.

The Strang scheme is robust because the ODE solver automatically adapts the integration time-step according to the stability constraints of the problem. In other words, for positive sources, the ODE solver reduces the time-step size to insure stability and gradually increases it as the sink terms become dominant. Further, the procedure is efficient because it allows the use of the diagonalized algorithm for the transport step. However, the Strang splitting scheme does have

the disadvantage of compromising the accuracy of the computation. This is readily seen when the scheme is written in delta form in the "sink" limit:

$$[I + \Delta\tau D]\left[I + \Delta\tau\frac{\partial A}{\partial x}\right]\Delta Q = -\Delta\tau\left(\frac{\partial E^n}{\partial x} - H_r^n - \Delta\tau D\frac{\partial E^n}{\partial x}\right) \tag{36}$$

It is evident that, upon convergence, the RHS operator retains a splitting error in the final solution. In fact, this error is proportional to the source term Jacobian. Because of the relatively large magnitudes of the source term eigenvalues, this error term can be large, leading to serious inaccuracies in the converged result. Example computations showing the effect of this inaccuracy are given in Ref. 23.

5.3 Consistent Splitting Scheme

It is desirable to combine the robustness of the splitting method with the accuracy of the direct method. This is accomplished in the following manner:

$$\frac{Q^* - Q^n}{\Delta\tau} = \frac{1}{\Delta\tau}\int_{\Delta\tau}\left[H_r(\tau) - \frac{\partial E^n}{\partial x}\right]d\tau \tag{37}$$

$$\frac{Q^{n+1} - Q^*}{\Delta\tau} + \frac{\partial E^{n+1}}{\partial x} = H_r^* \tag{38}$$

Note all terms in the governing equation are present in both chemistry and transport steps. In the chemistry step, the source term is advanced, while the transport terms are lagged. In the transport step, the transport terms are advanced, while the source term is evaluated at the intermediate "*" level. For this reason, this scheme is referred to as the consistent splitting method.

The general accuracy of the formulation is readily verified by writing the scheme in the delta form:

$$[I + \Delta\tau D]\left[I + \Delta\tau\frac{\partial A}{\partial x}\right]\Delta Q = -\Delta\tau\left(\frac{\partial E^n}{\partial x} - H_r^n\right) \tag{39}$$

Note that there are no splitting errors introduced into the residual and, therefore, upon convergence, the scheme will converge to the proper solution. Further the consistent splitting scheme preserves the robustness property in the same manner as the Strang splitting scheme. However, there is a new source of concern, *viz.*, the splitting error on the LHS. This error is akin to the approximate factorization error in ADI schemes and introduces a time-step limitation. By itself, the splitting error does not materially impact the choice of the time-step. However, when the consistent splitting scheme is combined with the ADI (or other factorization) method for the transport operator, the combined effect of the splitting error can introduce a significant limitation of the time-step size.

The optimal time-step selection of the ADI scheme is well understood [24]. The presence of the source term operator however introduces further complexity. Detailed investigation of these effects are summarized in Ref. 23 and are not given here. The final optimal time-step selection is given as follows:

$$NDT = 2ndLargest(CFL_x, CFL_y, CFL_z, STN) \tag{40}$$

where NDT stands for non-dimensional time-step size and is usually around 10, $CFL_{x,y,z}$ stand for the CFL numbers and have their usual definitions, and STN is the source term number, defined using the largest eigenvalue of the source Jacobian. Thus, the optimal time-step should be based upon the second largest non-dimensional time-step in the problem, rather than the maximum or the minimum. While this result is general, its implementation in a coupled system is not always straightforward and further studies are necessary to refine it.

6.0 Summary

Research in FY 2001 has touched on a wide array of topics. The major goal has been to assist NASA researchers in the implementation of unsteady preconditioning and combustion capability in the OVERFLOW code. Further, research has been pursued in areas related to the above implementation. Specifically, the research falls into four categories:

1. Stagnation Region Effects. Perturbation analysis of the low Mach number limit of the Euler equations has been carried out to shed light on the underlying causes of difficulties. In particular, the analysis has revealed that large pressure fluctuations can lead to unstable behavior in the presence of preconditioning. It is believed that this is the fundamental reason for the cause of instabilities near stagnation regions. The perturbation analysis has also pointed to several mitigating procedures, namely, updating the zeroth order pressure independently, using a modified preconditioning choice and applying preconditioning at the linear level. Of these, the modified preconditioning choice which considers the magnitudes of the local pressure fluctuations appears to be the most promising procedure. Implementation and testing in the OVERLFOW code are in progress.

2. Unsteady Preconditioning Formulation. A diagonalized preconditioning formulation has been implemented in the OVERFLOW code by NASA researchers and is currently being evaluated for a variety of aerodynamic problems. In addition, we have developed a multiple scale preconditioning formulation, which is a refinement of the present method. Following further testing and verification, the improved method will be incorporated into the OVERFLOW code.

3. Dissipation Formulation for Combustion. Methods of modifying the artificial dissipation to account for dominant chemical source terms have been reviewed. Overall, the different approaches are related. They essentially involve two aspects, namely the modification of the interface numerical flux formulas and the representation of an *averaged* source term. Further, the derivation of higher order representations of the system including the source term needs to be studied further. The most promising approaches will then be compared and evaluated for implementation in OVERFLOW.

4. Time-Stepping Schemes for Combustion. Three different time-integration techniques for combustion problems have been compared and contrasted. The direct (or fully implicit) scheme has been observed to be efficient and accurate but lacks robustness. The Strang splitting scheme is robust and efficient, but is inaccurate under some circumstances. Finally, the consistent splitting scheme is robust and accurate, but is inefficient under some circumstances. Nevertheless, it appears that the consistent splitting scheme is well-suited for implementation within a diagonalized framework. Therefore, it shows promise for implementation in OVERFLOW. Moreover, it may be possible to combine the method with schemes that are already used in OVERFLOW.

7.0 References

1. Venkateswaran, S. and C. L. Merkle, Analysis of preconditioning methods for the Euler and Navier Stokes equations, *VKI Lecture Series 1999-03*, von Karman Institute for Fluid Dynamics, Rhode Saint Genese, Belgium (1999).

2. Choi, Y.-H. and C. L. Merkle, The application of preconditioning to viscous flows, *J. Comp. Phys.*, **105**, 207-223 (1993).

3. Weiss, J. and Smith, W., Preconditioning Applied to Variable and Constant Density Flows, *AIAA Journal*, Vol. 33, pp. 2050-2057, 1995.

4. Turkel, E., Preconditioning techniques in computational fluid dynamics, *Annu. Rev. Fluid Mech.*, **31** (1999).

5. Darmofal, D. and Van Leer, B., Local Preconditioning: Manipulating Mother Nature to Fool Father Time, *Computing the Future II: Advances and Prospects in Computational Aerodynamics*, M. Hafez and D. Caughey, eds. John wiley and Sons, 1998.

6. Chorin, A. J., A numerical method for solving incompressible viscous flow problems," *J. Comp. Phys.*, **2**, 12 (1967).

7. Venkateswaran, S. and Merkle, C. L., Influence of Large Scale Pressure Changes on Preconditioned Solutions at Low Speeds, Submitted to the 32nd AIAA Fluid Dynamics Meeting, 2002.

8. Venkateswaran, S. and Merkle, C., Dual Time-Stepping and Preconditioning for Unsteady Computations, AIAA Paper 95-0078, 33rd Aerospace Sciences Meeting and Exhibit, Reno, NV, 1995.

9. Buelow, P., Schwer, D., Feng, J., Merkle, C. and Choi, D., A Preconditioned Dual-Time Diagonalized ADI scheme for Unsteady Computations, AIAA Paper 97-2101, 13th CFD Conference, Snowmass, CO, June, 1997.

10. Venkateswaran S. and Merkle, C., Efficiency and Accuracy Issues in Contemporary CFD Algorithms, AIAA Paper 2000-2251, Fluids 2000 Conference, Denver, CO, 2000.

11. Jameson, A., Schmidt, W. and Turkel, E., "Numerical Solution of the Euler Equations by Finite Volume Methods using Runge-Kutta Time-Stepping," AIAA Pap., 81-1259.

12. Roe, P. L., "Characteristic Based Schemes for the Euler Equations," Ann. Rev. Fluid Mech., 18 (1986), pp. 337-65.

13. Liou, M.-S. and Steffen, C., "Development of a New Flux Splitting Scheme," AIAA 91-1611.

14. Arora, M. and Roe, P., "Issues and Strategies for Hyperbolic Problems with Stiff Source Terms," Barriers and Challenges in Computational Fluid Dynamics, V. Venkatakrishnan et al., Editors, Kluwer Academic Publishers, (1998), pp. 139-154.

15. Pember, R., "Numerical Methods for Hyperbolic Conservation Laws with Stiff Relaxation II. Higher-Order Godonov Methods," SIAM J. Sci. Comput., 14, No. 4, (1993), pp. 824-859.

16. Bermudez, A. and Vazquez, E., "Upwind Methods for Hyperbolic Conservation laws with Source Terms," Computers and Fluids, 23 (1994), pp. 1049-1071.

17. Jin, S. and Levermore, D., "Numerical Schemes for Hyperbolic Conservation Laws with Stiff Relaxation Terms," Journal of Comp. Phys., 126 (1996), pp. 449-467.

18. Mohanraj, R., Neumeier, Y. and Zinn, B., "Characteristic-Based Treatment of Source Terms in Euler Equations for Roe Scheme," AIAA Journal, Vol. 37, No. 3, March, 1999.

19. Yu, S. T. and Chang, C. H., "Reacting Flow Computations using the Space-Time Method," AIAA Paper.

20. Sussmann, M., "Source Term Evaluation for Combustion Modeling," AIAA 93-0239.

21. Barth, T., "Implicit Linearization Procedures for Upwind Algorithms," (unpublished).

22. Venkateswaran, S., Deshpande, M. and Venkateswaran, S., Computation of Turbulent and Reacting Flows Using Time-Marching Methods, *CFD Journal*, Vol. 8, No. 2, pp. 220-231, 1999.

23. Schwer, D. and Venkateswaran, S., Comparison of Methods for Comuting Reacting Flows, in preparation.

24. Buelow, P., Venkateswaran, S. and Merkle, C., Stability and Convergence Analysis of Implicit Upwind Schemes, *Computers and Fluids,* Vol. 30, pp. 961-988, 2001.