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Navier-Stokes Solutions for Chemical Laser Flows: Cold Flows

Ajay P. Kothari* and John D. Anderson Jr.† *University of Maryland*, *College Park*, *Md*.

COMPUTATIONAL fluid dynamics is growing rapidly as a new third dimension in aerodynamics, complementing both laboratory experiment and pure analysis. ^{1,2} Work is advancing on both numerical methods and applications to practical engineering problems. The present paper straddles both categories. In particular, the present authors have been developing finite-difference solutions for the Navier-Stokes equations applied to the chemically reacting viscous flow in chemical lasers. ³ In the process of calculating such flows, several different finite-difference techniques for solving the Navier-Stokes equations have been examined and tested. The purpose of this paper is to describe some numerical experiments dealing with these techniques; these results have impact on the numerical solution of the Navier-Stokes equations in general.

The physical problem is illustrated in Fig. 1. A stream of partially dissociated fluorine is mixed tangentially with a stream of H₂; both streams are diluted with He. Characteristic of many chemical lasers, the Reynolds number is assumed low enough that laminar flow prevails in the mixing region. The ensuing chemically reacting flow downstream of the nozzles in a chemical laser is described precisely by the complete, two-dimensional Navier-Stokes equations including multicomponent diffusion and finite-rate chemical reactions. However, for the present numerical experiments, the chemical kinetics have been "switched off" artificially in order to examine the purely fluid-dynamic behavior of the solution. Thus, the following results do not contain the influence of chemical reactions. Such "coldflows" are purely artificial because in nature H₂ and F₂ are hypergolic. However, such results are quite appropriate for the present investigation.

These equations, without the chemical production terms, can be cast into the form

$$\partial U/\partial t = -(\partial F/\partial x) - (\partial G/\partial y) \tag{1}$$

where U, F, and G are one-dimensional vectors. The vector U contains elements such as ρ , ρu , ρv , ρE and ρ_i (standard nomenclature), and F and G contain these, as well as the viscous terms involving x and y derivatives of u, v, T and ρ_i . The full equations are given in detail in Ref. 3.

The finite-difference schemes used to solve these equations are of the predictor-corrector type patterned after the thoughts of MacCormack.⁴ A time-dependent solution is

used to calculate the complete flowfield in steps of time, starting from arbitrarily assumed initial conditions and eventually approaching the steady-state flow at large values of time. This steady state is the desired result, and the time-dependent solution is simply a means to that end. The predictor-corrector procedure is to obtain the flowfield at time (n+1) from

$$U_{n+1} = U_n + (\partial U/\partial t)_{\text{av}} \Delta t \tag{2}$$

where $(\partial U/\partial t)_{av}$ is an average of the values obtained from Eq. (1) evaluated first from the known flow at time n (the predictor), and then from the predicted flow at time n+1 (the corrector). The flow conditions at the nozzle exits (x=0 in Fig. 1) are specified and held fixed, invariant with time. The use of time-dependent solutions for chemically reacting flows is well documented, e.g., Refs. 5 and 6.

In Eq. (1), the spatial derivatives $\partial F/\partial x$, $\partial G/\partial y$, and the x and y derivatives of u, v, T, etc., are obtained from finite differences. Herein lies the essence of the four different techniques examined in the present paper as follows:

- 1) Central differences: central differencing for F, G, ρ , T, u, v, and ρ_i everywhere, at all times.
- 2) Partial MacCormack: forward and backward differencing for F, G for predictor-corrector steps, respectively, while using central differencing for ρ , T, u, v, and ρ_i .
- 3) Full MacCormack: predictor step-forward for F, G, and forward for ρ , T, u, v, ρ_i ; corrector step-backward for F, G, and backward for ρ , T, u, v, ρ_i .
- 4) Modified MacCormack: predictor step-forward for F, G, and backward for ρ , Tu, v, ρ_i ; corrector step-backward for F, G, and forward for ρ , T, u, v, ρ_i .

The use of these four schemes for the spatial differencing leads to some striking comparsions in the numerical flowfield results, as described below. Consider again the physical picture in Fig. 1. Imagine a fixed point in the flowfield at x/h = 10 and y/h = 0.5. The temporal behavior of the pressure at this point is shown in Fig. 2, as calculated from the four schemes. Note that schemes 2 and 4 yield the proper asymptotic approach to a steady flow at large times, whereas scheme 1 is oscillatory. For this particular problem, scheme 3 was observed to be unstable, as also shown in Fig. 2.

Consider now the final steady-state flowfield at x/h = 10. Figures 3-5 illustrate the velocity, F₂ density, and pressure profiles, respectively, across the flowfield, as calculated from the different schemes. Note that the use of central differences leads to wiggles in the profiles, whereas the modified Mac-Cormack approach (scheme 4) yields perfectly smooth profiles. The wiggles introduced by central differences are evident particularly in the pressure profile shown in Fig. 5. These results clearly demonstrate the superiority of the modified MacCormack approach. This superiority is substantiated further by Griffin, who has obtained identical comparisons for a completely different application, namely, the solution of the Navier-Stokes equations for the flow inside an internal combustion reciprocating engine. Moreover, the experience of the present authors is in line with suggestions from Hankey, 8 obtained after the present work was finished. For further details, see Ref. 3.

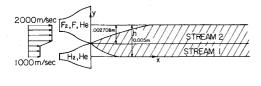
A comment is made on the boundary conditions at y=0 and y=h. Symmetry conditions hold at these boundaries, as can be seen from Fig. 1, which models a segment of the multinozzle flow characteristic of many chemical lasers; i.e., $\partial u/\partial y = \partial p/\partial y = \partial \rho_i/\partial y = v=0$ at y=0 and y=h. In the present finite-difference scheme, the reflection principle is used which is an accurate representation of boundary conditions on a line of symmetry; i.e., $P_{j+1} = P_{j-1}, T_{j+1}T_{j-1}, v_{j+1} = -v_{j-1}$, etc., where j is an index in the y direction, and j lies on the boundary itself. Examining the results in Figs. 3-5, straight lines are drawn between each grid point. For this reason, the gradients shown at the boundary are deceptive and

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^{*}Graduate Research Assistant, Department of Aerospace Engineering.

^{*}Professor and Chairman, Department of Aerospace Engineering. Associate Fellow AIAA.



	STREAM I	STREAM 2
P n/m²	500	500
T ºK	150	150
ρ Kg/m³	8.I6I9×10 ⁻⁴	3.7214×10
PF ₂ Kg/m²	_	1.8282×10 ³
ρ# ₂ Kg/m³	8.00136×10 ⁻¹	
P _F Kg/m		0.6094×10 ⁻³
P _R Kg/m		
P _{Me} Kg/m	1.6048×10 ⁻⁵	1.2838×10 ⁻³

Fig. 1 Nozzle configuration and downstream mixing flow in a chemical laser. Nozzle exit conditions are given.

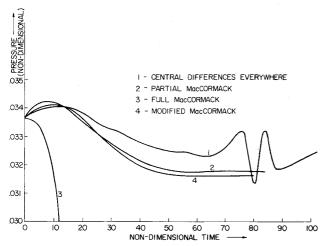


Fig. 2 Pressure vs time at x/h = 10 and y/h = 0.5. Reference pressure $p_r = \rho_r U_r^{\ 2} = 1.49 \times 10^4 \text{ kg/m-sec}^2$. Also, one nondimensional time is equivalent to 2.5×10^{-6} sec.

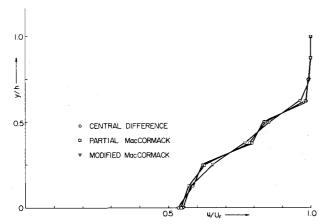


Fig. 3 Velocity profile at x/h = 10.0. Reference velocity $U_r = 2000$ m/sec.

do not always appear to have a zero value; however, the zero values are included correctly in the finite-difference solution, as discussed previously. As an additional comment, for the present results the cell Reynolds numbers (based on v and Δy) are less than 3: within the safe limits for accuracy and stability as discussed by Roache. ¹

The main conclusion of the present paper is to discourage the use of central differences in finite-difference solutions of

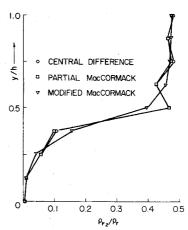


Fig. 4 Flourine density profile at x/h = 10.0. Reference density $\rho_r = 3.72 \times 10^{-3} \text{kg/m}^3$.

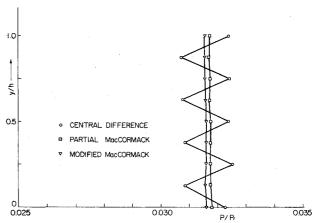


Fig. 5 Pressure profile at x/h = 10.0. Reference pressure $p_r = \rho_r U_r^2 = 1.49 \times 10^4 \text{ Kg/m-sec}^2$.

the Navier-Stokes equations, at least for mixing flows, and to encourage the use of the modified MacCormack differencing, as given in scheme 4. Moreover, it is anticipated that the present experience should be useful to other investigators attempting to solve numerically the Navier-Stokes equations for other types of applied problems.

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