

Fig. 2 VSU percent survival summary.



Fig. 3 Photographs of posttest VSU samples illustrating survival dependence on shock overpressure.

is also pictorially demonstrated by the photograph in Fig. 3 of several posttest samples. These data, as well as companion Hy-Cam results, illustrate that, for shock ΔP greater than approximately 207–276 kPa, essentially all wheat vegetation was lofted within 2 ms of shock passage without root pull-up. Because stem shear stresses vary as a function of stem-length-to-diameter ratio, it is expected, however, that the noted breakoff threshold values will tend to increase with stem diameter and decrease with stem length. The airblast sweep-up experiments of Refs. 4 and 5 for grass vegetation samples, which indicate that minor vegetation lofting occurred, support this viewpoint.

Scale-up verification of the VSU results was made in Stanford Research Institute's (SRI's) 2.4-m shock tube⁴ upon completion of the VSU experiments. These large-scale tests were performed at shock overpressures of 207 kPa for decaying blast waves with long positive-phase durations (≈ 100 ms). Three tests were conducted with full-scale wheat samples mounted in planter beds (1.2–1.4 m in width) on floor-mounted pallets. Stalk spatial densities were comparable to the TRW shock tube values, and bed lengths varied from 1.2 to 4.9 m.

In general, the SRI experiments indicate that the primary removal mechanism for the wheat vegetation was similar to that for TRW's VSU tests, namely, stem rupture near the shock front without root pull-up. All broken and removed wheat stalks were pulverized by the shock impact process into small pieces, the largest of which were 2.5–10 cm in length. This shredding of vegetation debris was also typical of the TRW shock tube results.

Conclusion

Shock tube measurements have been made of the response of typical cropland vegetation to airblast flow conditions. Results demonstrate that, at shock overpressures greater than approximately 242 kPa, complete breakoff of vegetation stalks occurred without root pull-up within 2 ms of shock passage. Some additional testing may

be warranted, however, to complement these first-look results, with particular attention focused on the sensitivity of vegetation breakoff to stalk diameter, length, spatial density, etc.

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Limitations of a Reduced Model for the Simulation of Hydrogen/Air Combustion

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Introduction

PROBLEMS involving the combustion of hydrogen/air mixtures have received an increased amount of attention in recent years, mostly due to the drive toward the design of hypersonic airbreathing engines.¹ Numerous investigations in the kinetics of hydrogen burning in air have resulted in the development of several models for the detailed kinetic processes, which involve relatively large numbers of gaseous species and chemical reactions.^{2,3} Unfortunately, the practical utilization of large chemistry models for the simulation of reactive flows in realistic geometries is severely hindered, due to the extremely heavy computational requirements. (The most favorable estimate of the operation count for a simulation involving N gaseous species in chemical nonequilibrium is that it will scale as $N \ln N$; in addition, a significant amount of CPU time is typically spent evaluating chemistry source terms, which scale linearly with the number of chemical reactions.)

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The computational expense of large models has justified the search for reduced mechanisms that would accurately predict at least the bulk of the hydrogen/air combustion process; foremost among them is the model proposed by Rogers and Chinitz,⁴ which has gained significant popularity in the reactive flow simulation community.^{5,6} Note that reduced (also known as global) models are known to suffer from some inherent inaccuracies; in the case of the Rogers and Chinitz model the most notable one is the difficulty in correctly predicting ignition delays and temperature buildup. Adding more species and/or reactions usually alleviates these problems, although it results in more expensive models.

The purpose of this Note is to investigate the accuracy and overall validity of the Rogers and Chinitz model vis-à-vis more detailed (and expensive!) models for the combustion of hydrogen/air mixtures. The goal is to determine whether a very simple and inexpensive model can be used for combustion simulations without undue loss of accuracy and reliability. In the following, the two chemistry models utilized in this study are introduced, the numerical algorithm utilized for the simulations is summarized, and some relatively striking results are presented for what has become a popular test case for reactive flow simulations: the supersonic flow in a diverging nozzle section.⁵

Chemistry Models

Two chemistry models for the combustion of hydrogen in air have been considered in this study. The first one is a reduced model due to Rogers and Chinitz,⁴ which involves five gaseous species and only two chemical reactions. A more detailed chemistry model, due to Evans and Schexnayder,⁷ is used to assess the validity and accuracy of the reduced model; it involves 7 species and 28 chemical reactions. Diatomic nitrogen is assumed inert in both cases. Chemistry models that include nitrogen reactions are also available.^{2,3}

In this study, the forward reaction rates utilized in the simulations are obtained from the cited references. The backward rates are recovered from the knowledge of forward rates and equilibrium constants. A consistent set of equilibrium constants was obtained from the thermodynamic properties of the chemical species by minimization of the free energy. The details are reported in Ref. 8.

Numerical Algorithm

A finite volume numerical code that can simulate the flow of arbitrary mixtures of thermally perfect gases in local chemical equilibrium^{9,10} was modified to allow for simulation of mixtures in chemical nonequilibrium. The inviscid (Euler) equations were solved for this study. The finite volume discretization, time-integration algorithm (based on an approximate factorization scheme), and space discretization (based on an approximate Riemann solver of the Roe type, with second-order accuracy in space, and using the Van Leer limiter) follow the approach discussed by Whitfield et al.¹¹ and Cinnella and Grossman.¹² More details are available in Ref. 8, as well as the references already mentioned.

Nozzle Results

The steady inviscid flow in the diverging portion of a nozzle was simulated using both chemistry models. The circular cross-sectional area of the nozzle A is given by the following function of the distance along the axis x :

$$A(x) = (\pi/16)[1 + \sin(\pi x/2L)]^2 \quad (1)$$

where L is the nozzle segment length, which was taken to be equal to 2 m. This geometry has been widely used as a test case for chemical nonequilibrium simulations.^{5,6,8}

At the nozzle segment inlet, a temperature of 1884.3 K and a pressure of 8.0263×10^4 N/m² were prescribed. The inlet velocity was taken to be 1245 m/s, and the equivalence ratio (defined as the ratio of hydrogen mass fraction to oxygen mass fraction, divided by the stoichiometric ratio) was 0.29841, which corresponds to a lean mixture. The mass fraction of the inert nitrogen was 0.7551.

To ensure grid-independent results, a grid refinement study was attempted. Figure 1 shows the temperature profile in the nozzle obtained by using three (axisymmetric) grids, ranging from a coarse

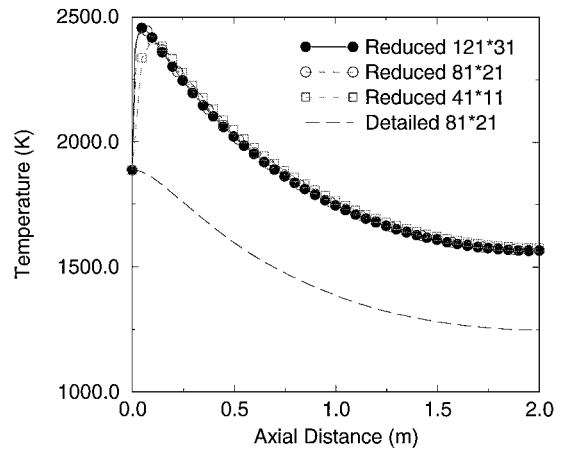


Fig. 1 Area-averaged temperature for reduced and detailed chemistry models. Also shown is a grid convergence study for the reduced model.

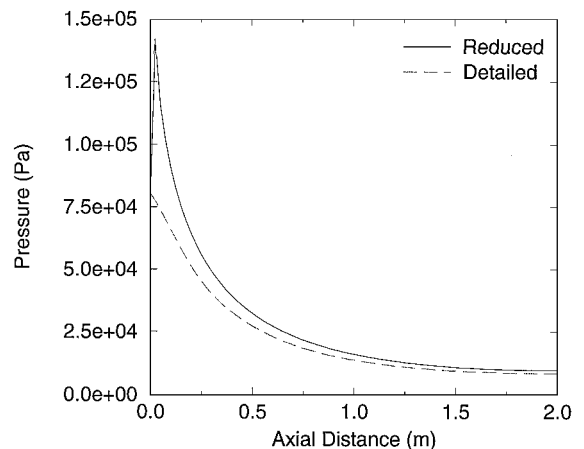


Fig. 2 Area-averaged pressure for reduced and detailed chemistry models.

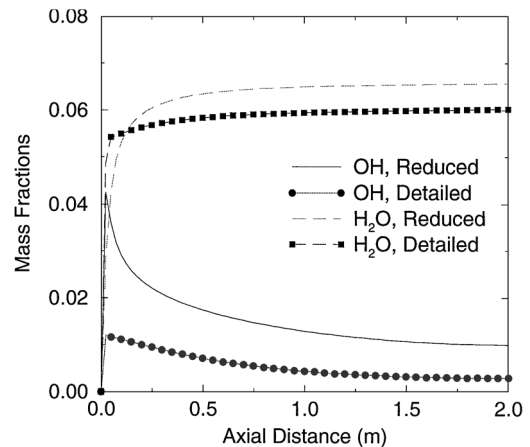


Fig. 3 Area-averaged OH and H₂O mass fractions for reduced and detailed chemistry models.

41×11 mesh to a fine 121×31 mesh, for the Rogers–Chinitz chemistry model. The numerical predictions are grid independent within plotting accuracy starting with a medium 81×21 mesh. A similar grid refinement study was conducted for the detailed chemistry model, with essentially the same outcome. In the following, all of the calculations presented are the ones obtained with the medium grid.

Figures 1–3 show a comparison between the predictions obtained by the Rogers–Chinitz model and those obtained by the detailed model. Area-averaged values of temperature, pressure, and mass fractions of OH and H₂O are shown. The reduced-model results predict an overshoot of temperature and pressure near the inlet (corresponding to a spike in the hydroxyl production), followed by a

decrease caused by the nozzle expansion. The overall water vapor production is not affected by the near-inlet behavior. However, the detailed-model predictions do not show anything comparable in the near-inlet region: The production of hydroxyl peaks there (see Fig. 3) but at much more moderate values. Overall, the hydroxyl levels are lower, and this corresponds to significantly reduced values of both temperature and water vapor. The values of pressure downstream of the nozzle are not dramatically affected by these discrepancies in the thermodynamic behavior of the gas mixture (a result consistent with the mechanical nature of pressure¹³). Overall, the detailed model seems to predict a process of hydrogen combustion significantly different from that of the reduced model, with profound ramifications on the thermodynamic state of the gas mixture.

Both the rate of convergence and the overall CPU time requirements are very different for the two models: The Roger-Chinitz calculation achieves a residual reduction of over six orders of magnitude in about 400 iterations; the detailed-model simulation reaches a residual reduction of three orders of magnitude only after over 2000 iterations, with four orders of magnitude reached at about 4000 iterations. The cost per iteration of the full model is over five times that of the reduced model (73 s per iteration vs 13 on an R8000 microprocessor).

Conclusions

Is a reduced hydrogen combustion model a viable alternative to more detailed and expensive models? Based on computational requirements, it is tempting to answer "yes." However, the possible penalty in physical accuracy might force the scientist to reconsider. Probably the answer is strictly problem dependent: If global values such as pressure levels and velocity are the most important pieces of information required, then a reduced chemistry model is a good alternative; on the other hand, reliable thermodynamic information can be gleaned only from more detailed (and expensive!) calculations.

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Higher-Order Subiteration-Free Staggered Algorithm for Nonlinear Transient Aeroelastic Problems

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I. Introduction

A NONLINEAR transient aeroelastic problem can be formulated as a three-field coupled problem, the fluid, the structure, and the dynamic mesh that is often represented by a pseudostructural system, governed by the following coupled semidiscrete equations¹:

$$\frac{d}{dt}(AW) + F^c(W, x, \dot{x}) = R(W, x) \quad (1)$$

$$M \frac{d^2 u}{dt^2} + Ku = f^{\text{ext}}[W(x, t), x], \quad \tilde{M} \frac{d^2 x}{dt^2} + \tilde{D} \frac{dx}{dt} + \tilde{K}x = 0$$

where a dot denotes a time derivative, x is the displacement or position vector of the moving fluid grid points; W is the fluid state vector; A results from the finite element/volume discretization of the fluid equations; $F^c = F - \dot{x}W$ is the vector of arbitrary Lagrangian Eulerian (ALE) convective fluxes; F is the vector of convective fluxes; R is the vector of diffusive fluxes; u is the structural displacement vector; M and K are, respectively, the finite element mass and stiffness matrices of the structure; f^{ext} is the vector of external forces acting on the structure; and \tilde{M} , \tilde{D} , and \tilde{K} are fictitious mass, damping, and stiffness matrices associated with the moving fluid grid and constructed to control its motion. For example, $\tilde{M} = \tilde{D} = 0$ includes as particular cases the spring analogy and continuum-mechanics-based mesh motion schemes advocated by many investigators.

For simple and small-scale structural problems, for example, for an airfoil with one or two vibrational degrees of freedom (DOFs), the second of Eqs. (1) can be efficiently recast in first-order form so that the fluid and the structural equations of motion can be combined into a single formulation (for example, see Ref. 2). In such a case, a monolithic fully explicit or fully implicit treatment of the coupled fluid/structure equations of motion is possible. However, for more complex structural systems, the simultaneous solution of Eqs. (1) by a monolithic scheme is, in general, computationally challenging, mathematically and economically suboptimal, and software-wise unmanageable.

Alternatively, Eqs. (1) can be solved by a partitioned procedure where the fluid and structure subproblems are time discretized by different methods tailored to their different mathematical models, and the resulting discrete equations can be solved by a staggered, segregated, or time-lagged algorithm.^{1,3-7} Such a strategy simplifies explicit/implicit treatment, subcycling, load balancing, software modularity, and replacements as better mathematical models and

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