Technical Comments

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Comment on "Analytical Model for the Impulse of Single-Cycle Pulse Detonation Tube"

Matei I. Radulescu* and Ronald K. Hanson[†] Stanford University, Stanford, California 94305

Introduction

INTENBERGER et al. attempted to estimate the pressure history on the thrust wall of pulse detonation engines (PDE) to predict the generated impulse. In their model, they use the Chapman-Jouguet (CJ) state computed from equilibrium calculations as the starting point of the gas expansions. In their treatment, they assume that the isentropic index is equal to the heat capacity ratio γ , hence, tacitly implying that the chemical composition is chemically frozen. However, their choice of the isentropic exponent is inconsistent with the usage of the equilibrium CJ sound speed. Furthermore, in reality, during the expansion of the product gases, the gas composition continuously changes due to chemical recombination. For this reason, the approximation made by Wintenberger et al. is only valid for gases in which recombination effects are negligible, for example, for large dilutions with inert gas or low degrees of dissociation. In this comment, it is shown that, following their procedure, the performance of PDEs is underestimated by as much as 10%. Because the constant- γ approximation is widely used in PDE simulations and in gasdynamic calculations in general, we wish to comment on the proper choice of the isentropic exponent to model the expansions of gases under chemical equilibrium.

Isentropic Flow

For an isentropic flow, the one-dimensional unsteady motion of gases undergoing a process where the gases are either chemically frozen or follow a series of equilibrium states (infinite reaction rates) is described exactly by the invariance of the Riemann variables (see Ref. 2):

$$\int_{s=\text{const}} \frac{\mathrm{d}p}{\rho c_{f/e}} \pm u = \text{const}$$
 (1)

where p is pressure, ρ is density, u is particle velocity, c is the sound speed, and s the specific entropy. Equation (1) is valid along the two families of characteristics C_+ and C_- given by

$$\frac{\mathrm{d}x}{\mathrm{d}t} = u \pm c_{f/e} \tag{2}$$

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*Visiting Research Fellow, Mechanical Engineering Department. Member AIAA.

[†]Professor, Mechanical Engineering Department. Fellow AIAA.

The sound velocity c in Eqs. (1) and (2) is either the equilibrium value c_e or frozen value c_f , depending on whether the set of equations describe an equilibrium or a frozen flow. Clearly, both the equilibrium and frozen solutions are represented by the same set of equations, provided that the correct sound velocity is used and the integral in Eq. (1) is carried out on the chemically frozen isentrope or on the chemical equilibrium isentrope.

When the same initial state, for example, the CJ state for the PDE problem, is used, the frozen and equilibrium isentropes are different.³ The chemically frozen isentrope is given locally by $p\rho^{-\gamma_f} = \text{const}$, where γ_f is the ratio of specific heats. (The subscript f is used to emphasize that the chemical composition is frozen on the isentrope.) For a chemical equilibrium process, it can be shown empirically that the isentrope can be approximated very accurately by a power law of the same form,⁴ but with a different exponent, because the gas composition changes. We denote the isentropic exponent taken along the equilibrium isentrope as γ_e , which now takes the definition $\gamma_e \equiv (\partial \ln p / \partial \ln \rho)_s$. For further discussions on the usage of γ_e in perfect-gas models to approximate the behavior of real gases at equilibrium, the reader is referred to Refs. 5 and 6.

If one assumes that either of these two exponents is constant, the integrals in Eq. (1) are readily evaluated, yielding the more familiar form of the Riemann invariants:

$$[2/(\gamma_{f/e} - 1)]c_{f/e} \pm u = \text{const}$$
 (3)

Note that the same formulation is valid for a chemically frozen or a chemical equilibrium process, provided that the correct combination of isentropic exponent and sound velocity is used.

When applied to the PDE problem, the flowfield behind the detonation wave can be described by the preceding isentropic relations because each fluid particle of the reaction products generated at the detonation front is bound to the isentrope through the CJ point. The strength of the self-similar Taylor expansion wave propagating behind the detonation wave and bringing the gas to rest can be obtained by integration of Eq. (1) or Eq. (3) along a C_- characteristic until the gas velocity vanishes. This procedure was also used in Wintenberger et al. to compute the plateau pressure behind the Taylor wave, yielding

$$p/p_{\rm CJ} = \{(\gamma + 1)/2 - [(\gamma - 1)/2](V_{\rm CJ}/c_{\rm CJ})\}^{2\gamma/(\gamma - 1)}$$
 (4)

where $V_{\rm CJ}$ and $c_{\rm CJ}$ are the CJ detonation speed and sound speed obtainable from equilibrium calculations. Equation (4) can be used to determine the sensitivity of the solution to the choice of isentropic exponent. Because the difference between γ_e and γ_f is on the order of \sim 10% for fuel-oxygen mixtures, the error in substitution of γ_f for γ_e yields a plateau pressure lower by ~10%. For fuel-air mixtures, differences between the two indexes are on the order of \sim 1%, hence, very weakly affecting the plateau pressure. This is due to the large proportions of the diluent gas, lower temperatures, and smaller degrees of dissociation. Equation (4) can also be used to assess the accuracy of the use of a constant γ_e . Because γ_e changes by less than 1% from the CJ state to the plateau value in the ethyleneoxygen products,³ the plateau pressure is estimated to within an error of $\sim 1\%$ in Eq. (4). This was also verified by numerical integration of Eq. (1) on the C_{-} characteristics to obtain the plateau pressure.

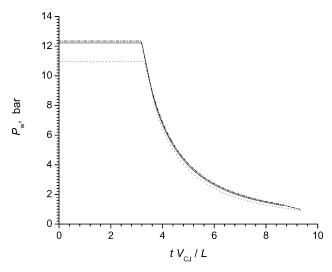


Fig. 1 Pressure history at the thrust wall of a smooth tube PDE computed via the method of characteristics for a $C_2H_4 + 3O_2$ detonation, where the gas initial state is $p_0 = 1$ bar and $T_0 = 300$ K.

To estimate the performance of PDEs, the pressure distribution at the thrust wall of a PDE was evaluated numerically by integration of the characteristic equations for the non-simple region of the flowfield. The details of the numerical code are described elsewhere.³ The solution is initialized with the CJ state behind the detonation wave computed with the CEA equilibrium code.⁴ The results obtained for stoichiometric ethylene-oxygen detonations are shown in Fig. 1. The two computations shown are obtained with either the equilibrium isentropic exponent or the ratio of specific heats, as performed in Ref. 1. The two exponents are assumed constant and fixed at the CJ value. Also shown is the pressure profile obtained via finite kinetic rate simulations with realistic thermodynamic data obtained in Ref. 3 for a case where the kinetic timescales are a few orders of magnitude shorter than the fluid timescales, that is, when the equilibrium assumption is adequate. The pressure plateau of the equilibrium model is found to lie 1% below the finite rate model, within the accuracy of the constant isentropic exponent approximation. However, the results in Fig. 1 also show that the combination of $c_{e,CJ}$ and γ_f , as performed in Wintenberger et al., vields an underestimation of the plateau pressure by approximately 10% in this typical example of fuel-oxygen detonations.

Conclusions

For the example considered, the specific impulse was estimated by integration of the pressure time history in Fig. 1 until the pressure decays to ambient. (Note in Fig. 1 that the abscissa is the nondimensional time where L is the tube length; the continuous line is obtained with the equilibrium model by the use of the isentropic exponent γ_e : The dotted line is obtained with the Wintenberger et al. incorrect assumption by the use of the equilibrium CJ sound speed and frozen isentropic exponent; the dash-dotted line is obtained from finite rate simulations in a PDE with L = 1.6 m.) The equilibrium model yields a specific impulse of 176 s, \sim 1% less than the impulse estimated from the finite rate simulation. However, using the Wintenberger et al. combination of parameters, we obtain only 158 s, 10% lower than the ideal value. By inspection of the pressure time histories obtained at the thrust wall under these different assumptions (Fig. 1), this difference is directly associated with the differences in pressure plateau values.

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Reply to Comment on "Analytical Model for the Impulse of Single-Cycle Pulse Detonation Tube" by M. I. Radulescu and R. K. Hanson

E. Wintenberger,* M. Cooper,† F. Pintgen,‡ and J. E. Shepherd§

California Institute of Technology,

Pasadena, California 91125

Response

We assume the polytropic approximation $P \sim \rho^{\gamma}$ to model the isentrope in the detonation products in our original study¹ to simplify the computation and develop analytic formulas for the impulse. Radulescu and Hanson² (R&H) point out that, for the stoichiometric ethylene—oxygen case, an equilibrium approximation to the isentrope is more realistic than the frozen approximation that is implied by our choice of polytropic exponent. We appreciate their observation and note that we were aware of the significance of chemical reaction in the products and that our use of the frozen rather than equilibrium isentrope was an oversight on our part. We have recomputed our results³ and find for all cases that the choice of frozen vs equilibrium isentrope makes less than a 10% difference in the impulse in the most extreme cases, at most a 1.3% difference for fuel—air cases, and changes none of the qualitative conclusions of our study. (See the tables and plots in the Erratum, Ref. 4.)

Their comment raises three issues that we did not address in our original study. 1) Is the polytropic approximation reliable for equilibrium detonation products? 2) To what extent are the detonation products in equilibrium within the Taylor wave? 3) What is the appropriate choice for the polytropic exponent γ in our model?

The polytropic approximation has been used extensively for studying the nonsteady flow in equilibrium detonation products^{5,6} and comparing computed blast and expansion waves with experimental data. The thermochemical basis of this approximation has been examined^{7–9} assuming shifting equilibrium in the products to compute the dependence of internal energy and molar mass on

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^{*}Postdoctoral Scholar, Aeronautics, Caltech MC 205-45. Member AIAA.
†Graduate Student, Mechanical Engineering, Caltech MC 205-45, Member AIAA.

[‡]Graduate Student, Applied Physics, Caltech MC 205-45.

[§]Professor, Aeronautics, Caltech MC 105-50, Member AIAA.