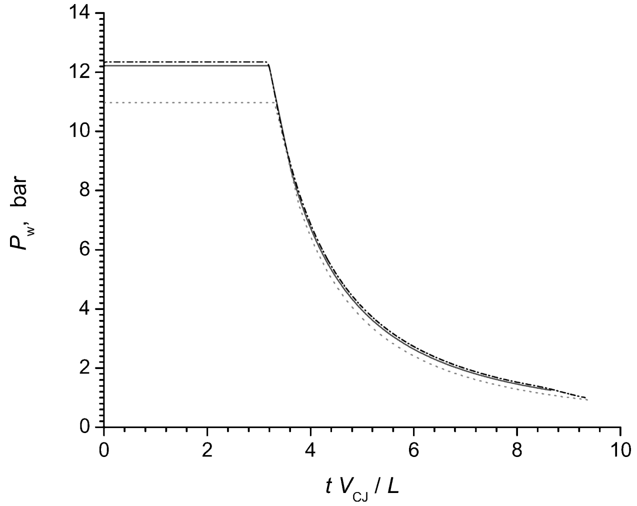

Fig. 1 Pressure history at the thrust wall of a smooth tube PDE computed via the method of characteristics for a C_2H_4 + $3O_2$ detonation, where the gas initial state is $p_0 = 1$ bar and $T_0 = 300$ K.

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.[1] 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 $c_{e,\mathrm{CJ}}$ and γ_f, as performed in Wintenberger et al.,[1] yields 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.[1] 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, ~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

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Response

WE used the polytropic approximation $P \sim \rho^\gamma$ to model the isentrope in the detonation products in our original study[1] to simplify the computation and develop analytic formulas for the impulse. Radulescu and Hanson[2] (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 results[3] 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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temperature and density for adiabatic flow. These studies demonstrate that there is a limited, but for our purposes useful, range of thermodynamic states over which the approximation of polytropic behavior is quantitatively reliable. The modest variations in density and temperature within the Taylor wave are favorable in this regard, but caution is indicated if a wider range of parameters will be considered. In addition, the relationships[8,9] between sound speed, pressure variation, and the polytropic exponents on the equilibrium isentrope are rather subtle and more involved than indicated in the comment of R&H. The energy exchange processes associated with the shifting composition influence the temperature on the isentrope in a way that is not consistent with the polytropic approximation based on fitting pressure–density data alone.

The extent of equilibrium in the detonation products has also been considered previously[9,10] and detonation products are not always in complete equilibrium for the spectrum of cases we considered in our study. In particular, as first noted by Borisov et al.,[10] there is a substantial difference between the cases of fuel–air and fuel–oxygen detonations, and the physical dimensions of the detonation region play an important role. We investigated this issue by numerically solving the species evolution based on detailed chemical kinetics and a prescribed pressure–time history approximated by the similarity solution[1] for the Taylor wave following a detonation propagating from the closed end of a tube. Results were obtained along different particle paths with starting positions of 0.05–5 m from the point of initiation at the closed end of the tube. When small departures from chemical equilibrium are assumed, the species mass fractions are redefined as Y_i', where

$$Y_i' = Y_i - Y_i^{\mathrm{eq}} \tag{1}$$

is the difference between the instantaneous mass fractions Y_i for species i and the equilibrium mass fractions Y_i^{eq}. Substituting Y_i' into the species conservation equation yields

$$\frac{\mathrm{D}Y'}{\mathrm{D}t} = \mathcal{J}Y' \tag{2}$$

where ρ is the density and the Jacobian matrix $\mathcal{J} = \partial\Omega_i/\partial Y_k$ specifies how the reaction rates Ω_i vary in response to changes in the mass fractions. The number of independent reaction progress variables is in most cases equal to the difference between the number of species and the number of atoms. The nonzero eigenvalues of matrix $\mathcal{J}$ are the reciprocals of the characteristic time required for the associated progress variables to relax to equilibrium after a disturbance. Comparison of these chemical timescales to the flow timescale (based on the rate of pressure decrease) is used to test the assumption of chemical equilibrium. Respective totals of 31 and 48 independent progress variables were considered for ethylene–oxygen and ethylene–air mixtures shown in Fig. 1 with initial pressures of 0.2 and 1 bar. The percentage of the total progress variables not in equilibrium by the end of the Taylor wave are shown as a function of initial distance from the closed end of the tube for the different particle paths analyzed.

Substantial nonequilibrium exists in fuel–air mixtures, especially for particles located near the closed end of the tube. The percentage of the total progress variables that have not equilibrated by the end of the Taylor wave increases as the initial mixture pressure decreases. In a 1-m tube, 20% of the progress variables have not reached equilibrium in the detonation products of a low-pressure ethylene–air mixture, whereas only 4% have not equilibrated in the products of a low-pressure ethylene–oxygen mixture. This means that ethylene–oxygen mixtures can be accurately modeled using the equilibrium flow assumption, but that significant departures from equilibrium are present for low-pressure ethylene–air mixtures, especially in short (<1 m) detonation tubes. Additional departures from equilibrium are expected if further flow expansion is obtained through a nozzle at the tube exit.

Table 1 Frozen and equilibrium values of γ compared with results from fitting the equilibrium isentrope (1 bar and 300 K initial conditions)

γ	$C_2H_4 + 3O_2$	$C_2H_4 + 3O_2 + 11.28N_2$
CJ frozen	1.236	1.172
CJ equilibrium	1.140	1.161
P–ρ fit	1.134	1.164
T–ρ fit	1.097	1.147

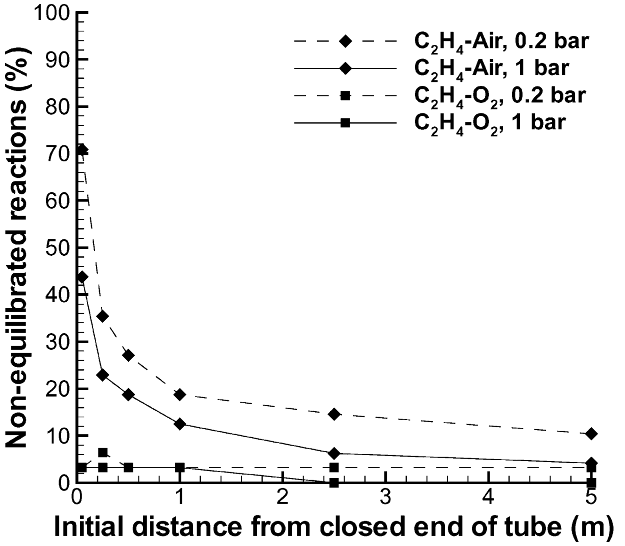

Fig. 1 Percentage of independent reaction progress variables in nonequilibrium by the end of the Taylor wave in ethylene-oxygen and ethylene-air mixtures.

There are various possibilities for determining the effective polytropic exponent, and we find that, in agreement with the detailed thermochemical considerations,[7,9] a unique value does not exist. We have examined the possible range of values by fitting polytropic forms, $T \sim \rho^{\gamma-1}$ and $P \sim \rho^{\gamma}$, to the numerically computed[11] equilibrium isentrope based on realistic thermochemistry. The approximate value of γ obtained depends on the thermodynamic variables selected for the fit (Table 1). The values shown are obtained with a least-squares procedure based on at least 50 points equally spaced in pressure between states 2 and 3.

Note that the range of values for γ shown in Table 1 are larger for the fuel–oxygen than the fuel–air case, consistent with the greater extent of dissociation in the former. The pressure–density fit underestimates the temperature variation, which is consistent with the observations of Radulescu et al.[12] As the pressure decreases through the Taylor wave, the shift in composition associated with the recombination reactions releases energy, increasing the temperature over the value obtained if the composition was frozen. This results in a value of γ closer to one, indicating a more nearly isothermal process.

The parameter γ is used in two ways in our paper. First, it is used to compute the value of the plateau pressure P_3 [Eq. (13) of Ref. 1]. Second, it is used to compute the factor α [Eq. (19) of Ref. 1] associated with the acoustic transit time of the first signal (characteristic) from the detonation interaction with the open end of the tube.

The most accurate method to compute the plateau pressure is to avoid using a polytropic approximation altogether. This is how we have proceeded in our new computations given in the Erratum.[4] This is carried out by first numerically computing[11] the equilibrium isentrope with realistic thermochemistry. The pressure P_3 is found from the Riemann solution to the expansion flow by numerically integrating

$$\int_{P_3}^{P_2} \frac{\mathrm{d}P}{\rho c} = u_2 \tag{3}$$

where P_2 is the Chapman–Jouguet (CJ) pressure and u_2 is the flow velocity behind the detonation wave. We have compared this to our original approximation [Eqs. (12) and (13) of Ref. 1] using a

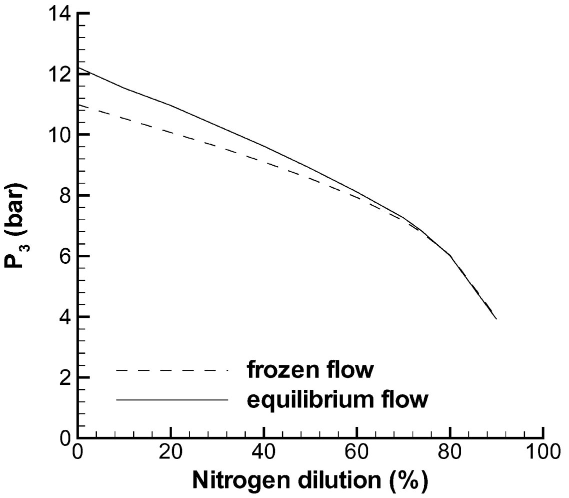

Fig. 2 Influence of assumption of frozen vs equilibrium flow in Taylor wave on the plateau pressure P_3 for stoichiometric ethylene–oxygen mixtures diluted with nitrogen at 1 bar and 300 K initial conditions.

polytropic exponent based on the equilibrium P–ρ relationship at the CJ point,

$$\gamma_e = \frac{\rho}{P}\left(\frac{\partial P}{\partial \rho}\right)_{Y_i^{\mathrm{eq}},S} \tag{4}$$

This method predicted the values of c_3 within 1% and the values of P_3 within 2% of the exact method based on Eq. (3) for all of the mixtures studied in our paper.[1] However, larger differences were found in some cases for the impulse, up to 6% at low initial pressures. In our new computations[3] for the Erratum,[4] $\gamma = \gamma_e$ is used to calculate the parameter α; however, the exact choice is unimportant because α varies less than 1.6% for $1.05 < \gamma < 1.25$.

The influence of the assumption of equilibrium flow in the Taylor wave on the pressure P_3 behind the Taylor wave is shown in Fig. 2 for ethylene–oxygen mixtures diluted with nitrogen. Our original calculation was with a constant value $\gamma = \gamma_f$, based on the frozen isentropic P–ρ relationship and evaluated at the CJ point. The revised calculation using Eq. (3) and the equilibrium isentrope yields higher pressure values than the frozen calculation because of the additional energy released by exothermic recombination reactions during the expansion process. This difference increases with decreasing nitrogen dilution due to the increasing CJ temperature and additional dissociation. As observed by R&H, the pressure P_3 for stoichiometric ethylene–oxygen is 10% lower when assuming frozen flow rather than equilibrium flow, but we note that it is only 0.7% lower for ethylene–air.

These differences translate into the predicted specific impulse being between 8% lower (for ethylene–oxygen) and 0.4% lower (for ethylene–air) for the frozen model than for the equilibrium model, as shown in Fig. 3. The calculations based on equilibrium chemistry improve the agreement of our model prediction (164 s vs an original value of 151 s) with direct experimental impulse measurements[13] (171 s) for stoichiometric ethylene–oxygen at an initial pressure of 1 bar. R&H calculate a value of 176 s using a code, based on the method of characteristics,[12] and integrating the pressure–time history at the thrust wall until the pressure decays to ambient. Because our model accounts for the contribution of the negative overpressure region following the pressure decay,[1] we expect their value to be higher than ours. At the present level of modeling, it is difficult to distinguish between these specific impulse values because other nonideal processes, such as heat transfer[12] and two-dimensional flow, have comparable effects on the impulse. Further improvement on the agreement between models, computations, and experiments will require a more sophisticated approach than used in Ref. 1.

The difference in impulse between using the frozen and equilibrium isentropes for the stoichiometric fuel–air mixtures investigated in our paper[1] at 1-bar initial pressure is less than 1.3%, whereas the difference for stoichiometric fuel–oxygen mixtures at 1-bar initial pressure can be up to 9.5%. These differences increase with decreasing initial pressure. For computing impulse, accounting for the difference between frozen and equilibrium processes is important only in fuel–oxygen mixtures and makes a negligible difference for high-pressure fuel–air mixtures. This is not the case for species or temperature predictions, and computations based on realistic thermochemistry and, possibly, reaction kinetics are needed to obtain accurate estimates for these quantities.

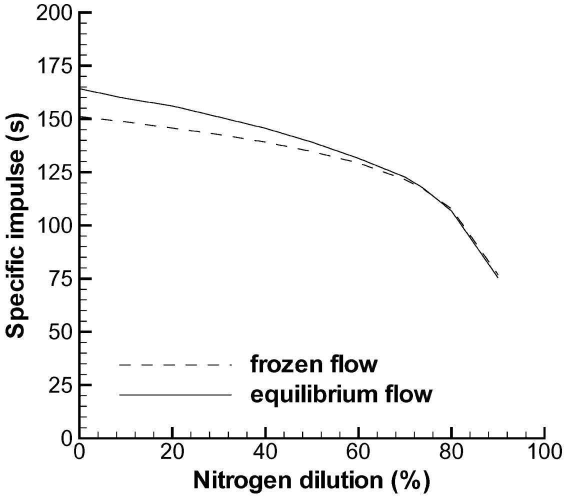

Fig. 3 Influence of assumption of frozen vs equilibrium flow in Taylor wave on the mixture-based specific impulse for stoichiometric ethylene–oxygen mixtures diluted with nitrogen at 1 bar and 300 K initial conditions.

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