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] in order to simplify the computation and develop analytic formulas for the impulse. Radulescu and Hanson (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, noting that we were aware of the significance of chemical reaction in the products, and our use of the frozen rather than equilibrium isentrope was an oversight on our part. We have recomputed our results[2] (see the tables and plots in the Errata accompanying this response) for all cases finding that the choice of frozen versus 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.

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[3,4] and comparing computed blast and expansion waves with experimental data. The thermochemical basis of this approximation has been examined[5–7] assuming "shifting" equilibrium in the products to compute the dependence of internal energy and molar mass on 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[6,7] between sound speed, pressure variation, and the polytropic exponents on the equilibrium isentrope are rather subtle and more involved than indicated in the

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[§] Professor, Aeronautics, Caltech MC 105-50, Pasadena, CA 91125, Member AIAA 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,[7,8] 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.,[8] 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 m to 5 m from the point of initiation at the closed end of the tube. Assuming small departures from chemical equilibrium, the species mass fractions are redefined as Y_i', where

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

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

$$DY'/Dt = \mathcal{J}Y' \ , \tag{2}$$

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 time scales to the flow time scale (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. The percentage of the total progress variables not in equilibrium by the end of the Taylor wave are plotted in Fig. 1.

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.

There are various possibilities for determining the effective polytropic exponent and we find that, in agreement with the detailed thermochemical considerations,[5,7] 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[9] 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.[10] 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 Errata. This is carried out by first numerically computing[9] the equilibrium isentrope with realistic thermochemistry. The pressure P_3 is found from the Riemann solution to the expansion flow by numerically integrating

$$\int_{P_3}^{P_2} \frac{dP}{\rho c} = u_2 \ , \tag{3}$$

where P_2 is the 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 polytropic exponent based on the equilibrium P-ρ relationship at the CJ point.

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

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 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[2] for the Errata, $\gamma = \gamma_e$ is used to calculate the parameter α; however, the exact choice is unimportant since 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 illustrated 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 illustrated in Fig. 3. The calculations based on equilibrium chemistry improve the agreement of our model prediction (164 s versus an original value of 151 s) with direct experimental impulse measurements[11] (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,[10] 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 since other non-ideal processes, such as heat transfer[10] 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.

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γ	C_2H_4+$3O_2$	C_2H_4+$3O_2$+$11.28N_2$
CJ frozen	1.236	1.253
CJ equilibrium	1.140	1.161
$P - \rho$ fit	1.134	1.164
$T - \rho$ fit	1.097	1.147

Table 1: Frozen and equilibrium values of γ evaluated at the CJ point for stoichiometric ethylene-oxygen and ethylene-air at 1 bar and 300 K initial conditions compared with results from fitting the equilibrium isentrope based on the polytropic relationship using pressure or temperature and density.

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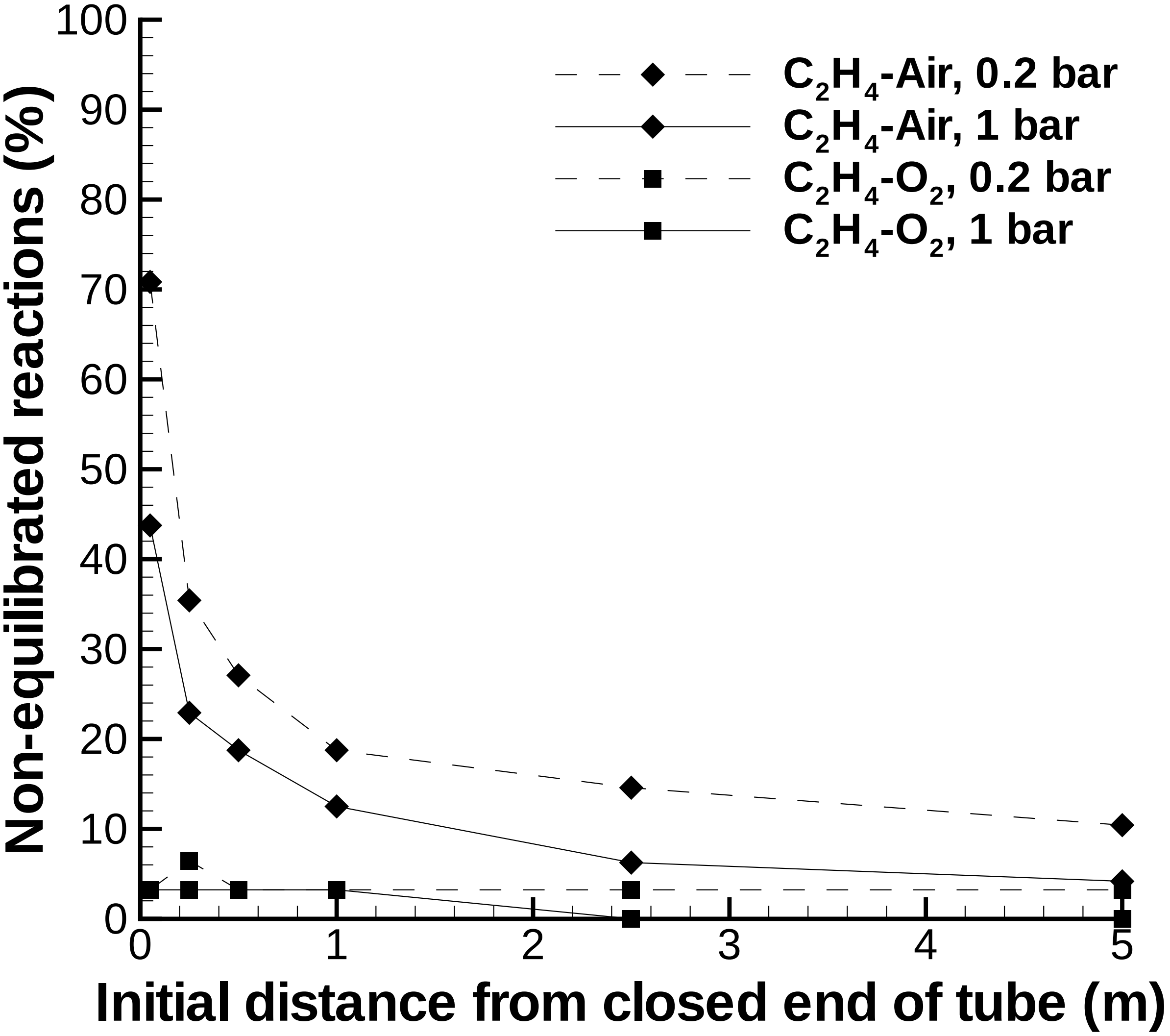

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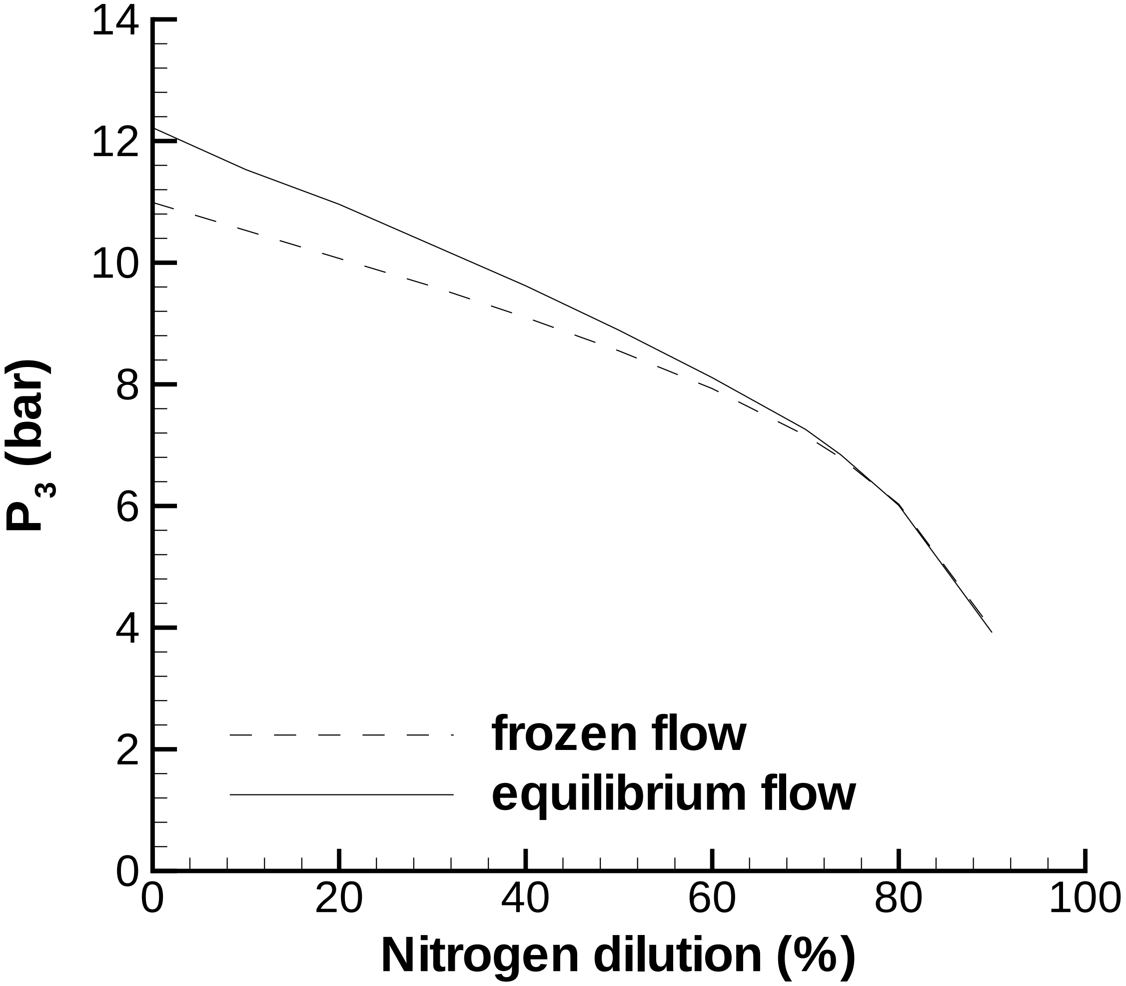

Figure 2: **Influence of the assumption of frozen versus equilibrium flow in the Taylor wave on the plateau pressure P_3 for stoichiometric ethylene-oxygen mixtures diluted with nitrogen at 1 bar and 300 K initial conditions.**

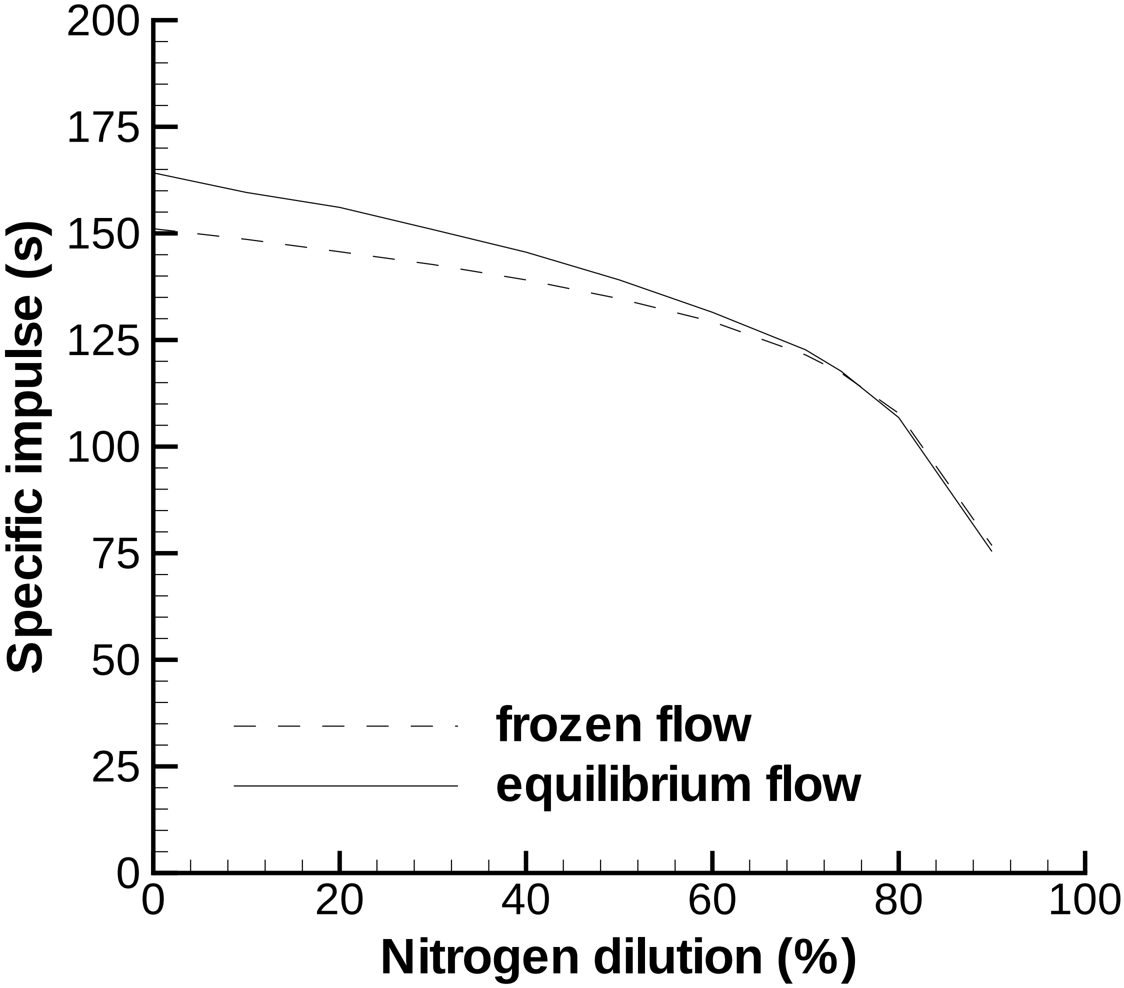

Figure 3: **Influence of the assumption of frozen versus equilibrium flow in the Taylor wave on the mixture-based specific impulse for stoichiometric ethylene-oxygen mixtures diluted with nitrogen at 1 bar and 300 K initial conditions.**