Determining Detonation Velocity for O_3 assuming O_2 and O as products

Unknowns: u_1, u_2, T_2, P_2, $X_{O,2}$, $X_{O2,2}$ (6 unknowns)

Equations:

$$\rho_1 u_1 = \rho_2 u_2$$

$$P_1 + \rho_1 u_1^2 = P_2 + \rho_2 u_2^2$$

$$h_1 + \frac{1}{2}u_1^2 = h_2 + \frac{1}{2}u_2^2$$

$$P_2 = \rho_2 \frac{R_u}{M_2} T_2$$

$$M_2 = 32 X_{\mathrm{O}_2,2} + 16 X_{\mathrm{O},2}$$

$$K_p(T_2) = \frac{X_{\mathrm{O}_2,2}}{X_{\mathrm{O},2}^2}\frac{P_{\mathrm{ref}}}{P_2}$$

Knowns: T_1, P_1, h_1, ρ_1

<u>One possible iteration procedure:</u>

Guess a value of T_2 and P_2 (choose reasonable values to assist convergence).

Calculate $K_p(T_2)$ - this doesn't change for a given T_2

Calculate mole fractions of O and O_2 from T_2 and P_2 and simple dissociation equation using K_p

Calculate M_2, ρ_2, h_2

Combine continuity and momentum $u_1^2 = \dfrac{P_2 - P_1}{\rho_1 - \rho_1^2/\rho_2}$

From energy and continuity equations $u_1^2 = \dfrac{2(h_2 - h_1)}{1 - \rho_1^2/\rho_2^2}$

Iterate on P_2 at the chosen T_2 until these equations agree

Check IGL. Use as your objective function (which should be zero in the end): $P_2 - \rho_2 R_2 T_2$

Choose a new value of T_2 and guess P_2, iterate again on P_2 until the two equations agree, then recheck your objective function. Iterpolate or extrapolate to get your next guess of T_2.