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Readers' Forum

Brief discussion of previous investigations in the aerospace sciences and technical comments on papers published in the AIAA Journal *are presented in this special department. Entries must be restricted to a maximum of 1000 words, or the equivalent of one* Journal *page including formulas and figures. A discussion will be published as quickly as possible after receipt of the manuscript. Neither the AIAA nor its editors are responsible for the opinions expressed by the correspondents. Authors will be invited to reply promptly.*

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

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IN Ref. 1, Westmoreland and Cinnella investigate the accuracy and overall validity of the Rogers and Chinitz[2] reduced-chemistry model, a reduced model involving five gaseous species and two reactions. They investigate this through comparison with the more detailed chemistry model of Evans and Schexnayder,[3] which has seven species and 28 chemical reactions. For the test problem of supersonic flow in a diverging nozzle section, they showed that the reduced-chemistry model predicts an overshoot of temperature and pressure near the inlet as compared to the more detailed chemistry model. Overall, it was found that the detailed chemistry model seems to indicate hydrogen combustion different from that of the reduced model, although if only flow properties (such as pressure or velocity) are of interest, the reduced models should be sufficient.

The purpose of this comment is to point out the existence of newer two-step reduced chemistry descriptions.[4–6] These two-step mechanisms are based on systematic reduction through chemical–kinetic steady-state and partial-equilibrium approximations, rather than being empirically based.[2] There are also newer and better detailed-chemistry rate parameters,[7,8] an example of these rates being the reaction set detailed in Table 1. Various review papers, such as that by Williams,[9] describe this more recent work. In particular, the two-step description

$$3H_2 + O_2 \rightleftharpoons 2H + 2H_2O \tag{1}$$

$$2H \rightleftharpoons H_2 \tag{2}$$

that involves four gaseous species and two reactions with the global rates (expressed in terms of the rates of elementary reactions)[9]

$$\omega_1 = k_1[H][O_2] - k_2[OH][O] + (k_{12} + k_{14})[HO_2][H] \tag{3}$$

$$\omega_2 = [M](k_9[H]^2 + k_{10}[H][OH] + k_{11}[H][O_2]) \tag{4}$$

utilizing the units of Table 1, can be used. In deriving this scheme, the species OH, HO_2, and O were assumed to be in steady state; steady-state expressions for these species in terms of the temperature and major species (H_2, O_2, H, and H_2O) need to be expressed. For OH, the full steady state is

$$\begin{aligned} &2k_7[OH]^2 + (k_2[O] + k_4[H] + k_5[H_2] + k_{10}[H][M] \\ &\quad + k_{16}[HO_2])[OH] - k_1[H][O_2] - k_3[H_2][O] - k_6[H][H_2O] \\ &\quad - 2k_8[H_2O][O] - 2k_{12}[HO_2][H] - k_{15}[HO_2][O] = 0 \end{aligned} \tag{5}$$

which, when combined with the other steady-state expressions, is not conducive to an analytical solution. However, because the partial equilibrium of steps 5 and 6 is quite good, it rather than the full steady-state expression should suffice to provide a value for the concentration of OH:

$$[OH] = \frac{k_6[H][H_2O]}{k_5[H_2]} \tag{6}$$

Table 1 Alternative hydrogen–oxygen mechanism

Number	Reactions	B^a	m	E, cal/mol
		Hydrogen–oxygen chain		
1	$H + O_2 \rightarrow OH + O$	3.52×10^{16}	−0.7	17,070
2	$OH + O \rightarrow H + O_2$	1.15×10^{14}	−0.324	−175
3	$H_2 + O \rightarrow OH + H$	5.06×10^{4}	2.67	6,290
4	$OH + H \rightarrow H_2 + O$	2.22×10^{4}	2.67	4,398
5	$H_2 + OH \rightarrow H_2O + H$	1.17×10^{9}	1.30	3,626
6	$H_2O + H \rightarrow H_2 + OH$	6.72×10^{9}	1.30	20,210
7	$OH + OH \rightarrow H_2O + O$	$k = 5.46 \times 10^{11} \exp(0.00149T)$		
8	$H_2O + O \rightarrow OH + OH$	7.60×10^{0}	3.84	12,780
		Direct recombination		
9[b]	$H + H + M \rightarrow H_2 + M$	7.20×10^{17}	−1.0	0
10[c]	$H + OH + M \rightarrow H_2O + M$	2.20×10^{22}	−2.0	0
		HO_2 formation and consumption		
11[c]	$H + O_2 + M \rightarrow HO_2 + M$	6.76×10^{19}	−1.4	0
12	$HO_2 + H \rightarrow OH + OH$	1.70×10^{14}	0.0	874
13	$HO_2 + H \rightarrow H_2 + O_2$	4.28×10^{13}	0.0	1,411
14	$HO_2 + H \rightarrow H_2O + O$	3.10×10^{13}	0.0	1,720
15	$HO_2 + O \rightarrow OH + O_2$	2.00×10^{13}	0.0	0
16	$HO_2 + OH \rightarrow H_2O + O_2$	2.89×10^{13}	0.0	−497

[a]Units: s^{-1} $(mol/cm^3)^{(-n+1)}$, where n is reaction order.
[b]Chaperon efficiencies: N_2, O_2: 1.0; CO: 1.9; CO_2: 3.8; H_2: 2.5; H_2O: 16.3.
[c]Chaperon efficiencies: same as listed in footnote b except H_2O: 12.0.

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This is an explicit expression in the major species and temperature. For HO_2, the full steady state is utilized and can be written as

$$[HO_2] = \frac{k_{11}[H][O_2][M]}{(k_{12} + k_{13} + k_{14})[H] + k_{15}[O] + k_{16}[OH]} = \frac{C_1}{C_2 + k_{15}[O]} \tag{7}$$

the last equality of which defines C_1 and C_2 for algebraic simplicity in later expressions. Because this expression contains the species O, it is not an explicit expression. If, however, one can express O explicitly, then an explicit expression for HO_2 is possible.

For O, we also use the full steady-state expression, which is

$$[O] = \frac{k_1[H][O_2] + k_4[OH][H] + k_7[OH]^2 + k_{14}[HO_2][H]}{k_2[OH] + k_3[H_2] + k_8[H_2O] + k_{15}[HO_2]} = \frac{C_3 + k_{14}[HO_2][H]}{C_4 + k_{15}[HO_2]} \tag{8}$$

and again the last equality defines C_3 and C_4 for later simplicity. The explicit expression for OH can then be introduced (but is not written out here, as it is wholly contained within the constants), as is the preceding expression for HO_2, and a quadratic equation for O is obtained:

$$k_{15}C_4[O]^2 + (C_2C_4 + (C_1 - C_3)k_{15})[O] - (C_2C_3 + C_1k_{14}[H]) = 0 \tag{9}$$

that can be solved using the quadratic formula to determine [O], and that value can then be used to determine the value of $[HO_2]$.

Although the resulting expressions are somewhat complicated, this scheme is explicit, should be as inexpensive to use as that of Rogers and Chinitz,[2] and should provide greater accuracy in profiles of temperature and species concentrations. It would be worthwhile to perform evaluations, similar to those reported,[1] with the improved detailed chemistry and the recent systematically reduced chemistry.

References

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Reply by the Authors to M. L. Rightley

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WE appreciate M. L. Rightley's comment that points out additional reduced mechanisms for hydrogen/air combustion. It would probably be useful to implement the newest mechanism and test it for geometries of interest to the combustion and/or fluid dynamics communities.

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Errata

Screech Tone Noise and Mode Switching in Supersonic Swirling Jets

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[AIAA Journal, 36(11), pp. 1968–1974 (1998)]

TO be consistent with the text, the captions of Figs. 6a and 6b should be exchanged. All other results remain unchanged.