Homework 5: Thermochemistry Exploration Using CEA Code

The CEA output is very detailed and takes a total of 12 pages, so only one case (equilibrium, O/F=2.6) will be displayed here. The results are for $P_c = 70\ atm, P_e = 0.4\ atm\ \left({}^{P_c}/_{P_e} = 175\right)$, using RP-1 fuel and 02L as oxidizer.

1) For all cases run, we need the "ground jet velocity,"namely, that for $P_a = 1atm$. The code supplies only the jet velocity ("specific impulse") for ***vacuum*** and for ***matched conditions***, which we will call c_0, c_{match}, respectively. In general:

$F_0 = F_{vac} - P_a A_e$ (1)

$c = \frac{F}{\dot{m}} = \frac{F}{P_c A_t} c^*$ (2)

$c_0 = c_{vac} - \frac{P_a}{P_c}\frac{A_e}{A_t} c^*$ (3)

An alternative, more convenient formulation is:

$c = \frac{F}{\dot{m}} = \frac{F}{\rho_e u_e A_e}$ (4)

$c_0 = c_{vac} - \frac{P_a}{\rho_e u_e} = c_{vac} - \frac{P_a}{P_e}\frac{\left({}^{\mathcal{R}}/_{M_e}\right)T_e}{u_e}$ (5)

All quantities are listed as output. Here, $\frac{P_a}{P_e} = \frac{1\ atm}{0.4\ atm} = 2.5$. Notice that the exit velocity u_e is actually equal to c_{match}, and can be read directly from the output.

For the Equilibrium case we then find:

Table 1: Equilibrium Case

O/F	$c_{vac}[m/s]$	$u_e[m/s]$	$T_e[K]$	$M_e[kg/mol]$	$c_0[m/s]$
2	3205.8	3030.6	1355.5	0.02123	2767.9
2.2	3286.0	3099.1	1577.5	0.02265	2818.9
2.4	3341.4	3142.3	1810.4	0.02406	2843.7
2.6	3374.2	3161.4	2051.0	0.02545	2844.4 (opt)
2.8	3384.5	3160.6	2278.1	0.02677	2824.9

For the Frozen Flow case (nfz=2, frozen after throat), we find:

Table 2: Frozen Flow Case

O/F	$c_{vac}[m/s]$	$u_e[m/s]$	$T_e[K]$	$M_e[kg/mol]$	$c_0[m/s]$
2	3145.4	2891.7	1232.3	0.02099	2736.2
2.2	3188.0	3017.8	1364.2	0.02209	2762.7 (opt)
2.4	3196.1	3022.7	1451.9	0.02303	2762.6
2.6	3183.0	3008.5	1504.2	0.02382	2746.7
2.8	3159.1	2984.8	1531.8	0.02450	2723.2

Some observations:

a) $(c_0)_{opt}$ is 2844 m/s for equilibrium and 2763 m/s for frozen flow, a difference of 2.8%. For a rocket of large dimensions and this high pressure, the actual performance is likely to be close to equilibrium.

b) $(O/F)_{opt}$ is about 2.52 for equilibrium, but only 2.3 for frozen flow. This can be understood qualitatively: the reason an optimum exists in any case is the trade-off between higher T_c at higher O/F (closer to stoichiometric), but also higher Mat higher O/F (less extra H_2 around). There is a third effect, though: higher O/F, with its higher T_c, produces more dissociation in the chamber; if the flow is in equilibrium, most of this dissociation is reversed during the expansion, and the corresponding energy is recovered (partially) as kinetic energy. This does not happen in a frozen expansion, and so in the equilibrium case there is more of an incentive to go on to higher O/F, as observed.

2) For $\frac{O}{F} = 2.6$, equilibrium, we read off $T_c = 3674.2K$ and, <u>*at the throat*</u>, $\gamma = 1.1340, \mathcal{M} = 0.02382\ kg/mol$. Using these as constants, we can calculate:

$$\Gamma = \sqrt{\gamma}\left(\frac{2}{\gamma+1}\right)^{\frac{\gamma+1}{2(\gamma-1)}} = 0.6354 \qquad (6)$$

$$R = \frac{8.314}{0.02382} = 349.0\ {}^{J}/_{kg * K} \qquad (7)$$

$$c^* = \frac{\sqrt{RT_c}}{\Gamma} = 1782.2 \qquad (8)$$

CEA: 1793.8 m/s

For the exit Mach number, we use $\frac{P_c}{P_e} = \left(1 + \frac{\gamma-1}{2}M_e^2\right)^{\frac{\gamma}{\gamma-1}}$, or $M_e = \sqrt{\frac{2}{\gamma-1}\left[\left(\frac{P_c}{P_e}\right)^{\frac{\gamma-1}{\gamma}} - 1\right]}$, where

$P_c = 70\ atm, P_e = 0.4\ atm.$

Therefore:

$M_e = 3.543$ (CEA: 3.536)

For exit temperature:

$$T_e = \frac{T_c}{1+\frac{\gamma-1}{2}M_e^2} = 1996K \qquad (9)$$

(CEA: 2051K)

For area ratio:

$$\frac{A_e}{A_t} = \frac{1}{M_e}\left(\frac{1+\frac{\gamma-1}{2}M_e^2}{\frac{\gamma+1}{2}}\right)^{\frac{\gamma+1}{2(\gamma-1)}} = 21.73 \qquad (10)$$

(CEA: 20.67)

For exit velocity (or matched specific impulse):

$$u_e = M_e\sqrt{\gamma R T_e} = 3149\ m/s \qquad (11)$$

(CEA: 3162 m/s)

For vacuum specific impulse:

$$c_{vac} = u_e + \frac{P_a A_e}{P_0 A_t}c^* = 3370 - \frac{1}{70} \times 21.73 \times 1782.2 = 2817\ m/s \qquad (12)$$

(CEA: 2844 m/s)

The simple model agrees to better than 5% in all the important quantities with the full equilibrium model. But you need hindsight in the choices of γ and M.

3) Atom conservation: The reactants are $CH_{1.975} + XO_2$, and imposing $O/F = 2.6$, $\frac{32x}{12+1.975} = 2.6 \rightarrow x = 1.135$. Since the *total* quantity is arbitrary, only *relative* atomic amounts matter. We have then in the reactants:

$$\frac{m_H}{m_C} = \frac{1.975}{12} = 0.165 \qquad (13)$$

$$\frac{m_O}{m_C} = \frac{1.135 \times 32}{12} = 3.027 \qquad (14)$$

For the products we read for this case the mole fractions at exit:

$y_{CO} = 0.2640$

$y_{CO_2} = 0.2419$

$y_{H_2} = 0.0918$

$y_{H_2O} = 0.4006$

$y_H = 0.0011$

$y_{OH} = 0.0006$

With very minor amounts of other molecules. Thus, the mass fractions at exit are:

$$\frac{m_H}{m_C} = \frac{y_{H_2}\times 2 + y_{H_2O}\times 2 + y_H \times 1 + y_{OH}\times 1}{y_{CO}\times 12 + y_{CO_2}\times 12} = 0.162 \qquad \text{(compare to 0.165)}$$

$$\frac{m_O}{m_C} = \frac{y_{CO}\times 16 + y_{CO_2}\times 32 + y_{H_2O}\times 16 + y_{OH}\times 16}{y_{CO}\times 12 + y_{CO_2}\times 32} = 3.028 \qquad \text{(compare to 3.027)}$$

Entropy conservation: Since $T_e = 2051K$, we need to *extrapolate* slightly from the given table of standard molar entropies; we get:

$$\tilde{s}^\circ_{CO} = 259.68\ \frac{J}{mol*K}$$

$\tilde{s}^{\circ}_{CO_2} = 310.93 \frac{J}{mol*K}$
$\tilde{s}^{\circ}_{H_2} = 189.32 \frac{J}{mol*K}$
$\tilde{s}^{\circ}_{H_2O} = 266.04 \frac{J}{mol*K}$

Then, for each molecule $\boldsymbol{\tilde{s}_i} = \tilde{s}^{\circ}_i - \mathcal{R}lnP_i(atm) = \tilde{s}^{\circ}_i - \mathcal{R}ln(y_i P_e(atm))$. This gives:
$\tilde{s}_{CO} = 278.37 \frac{J}{mol*K}$
$\tilde{s}_{CO_2} = 330.35 \frac{J}{mol*K}$
$\tilde{s}_{H_2} = 216.79 \frac{J}{mol*K}$
$\tilde{s}_{H_2O} = 281.26 \frac{J}{mol*K}$

Finally, the specific entropy (per unit mass) is:

$$S_e = \frac{\sum_i y_i s_i}{\sum_i y_i M_i} = \frac{\sum_i y_i s_i}{\bar{M}} \quad (15)$$

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Using $\bar{M}_e = 0.02545 \frac{kg}{mol}$ (CEA) and the four mole fractions (CO, CO_2, H_2, H_2O), this gives:
$S_e = 11{,}230 \frac{J}{kg*K}$
Compared to $S_c = S_e = 11{,}068 \frac{J}{kg*K}$ from CEA. This is a bit high, not clear why.

THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM

COMPOSITION DURING EXPANSION FROM INFINITE AREA COMBUSTOR

Pin = 1028.7 PSIA
CASE = HWK41288

	REACTANT	WT FRACTION (SEE NOTE)	ENERGY KJ/KG-MOL	TEMP K
FUEL	RP-1	1.0000000	-24717.700	298.150
OXIDANT	O2(L)	1.0000000	-12979.000	90.170

O/F= 2.60000 %FUEL= 27.777778 R,EQ.RATIO= 1.309872 PHI,EQ.RATIO= 1.309872

	CHAMBER	THROAT	EXIT
Pinf/P	1.0000	1.7309	175.00
P, BAR	70.927	40.978	0.40530
T, K	3674.23	3489.38	2050.99
RHO, KG/CU M	5.4548 0	3.3647 0	6.0497-2
H, KJ/KG	-784.21	-1474.64	-5784.48
U, KJ/KG	-2084.48	-2692.53	-6454.44
G, KJ/KG	-42114.8	-40725.9	-28855.6
S, KJ/(KG)(K)	11.2488	11.2488	11.2488
M, (1/n)	23.494	23.822	25.454
(dLV/dLP)t	-1.04090	-1.03547	-1.00043
(dLV/dLT)p	1.7024	1.6436	1.0125
Cp, KJ/(KG)(K)	6.3458	6.1418	2.0549
GAMMAs	1.1373	1.1338	1.1941
SON VEL,M/SEC	1216.1	1175.1	894.4
MACH NUMBER	0.000	1.000	3.536

PERFORMANCE PARAMETERS

Ae/At	1.0000	20.667
CSTAR, M/SEC	1793.9	1793.9
CF	0.6551	1.7629
Ivac, M/SEC	2211.5	3374.2
Isp, M/SEC	1175.1	3162.4

MOLE FRACTIONS

*CO	3.1594-1	3.0994-1	2.6403-1
*CO2	1.5096-1	1.6349-1	2.4187-1
COOH	2.1034-5	1.2568-5	2.6919-8
*H	2.9043-2	2.5303-2	1.0883-3
HCO	2.8106-5	1.5873-5	3.6636-8
HO2	1.0280-4	6.2749-5	2.8532-9
*H2	8.0601-2	7.8728-2	9.1782-2
H2O	3.2823-1	3.4316-1	4.0063-1
H2O2	1.5347-5	9.1073-6	1.6202-9
*O	1.2293-2	9.4170-3	4.4262-6
*OH	6.3664-2	5.4067-2	5.8551-4
*O2	1.9095-2	1.5793-2	8.2751-6