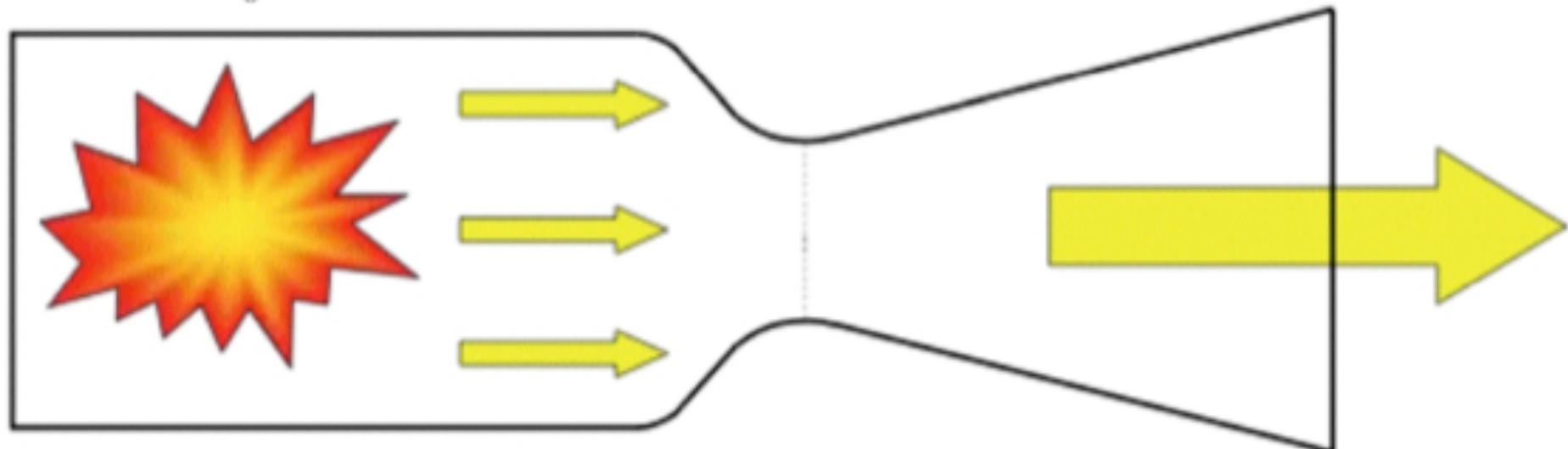


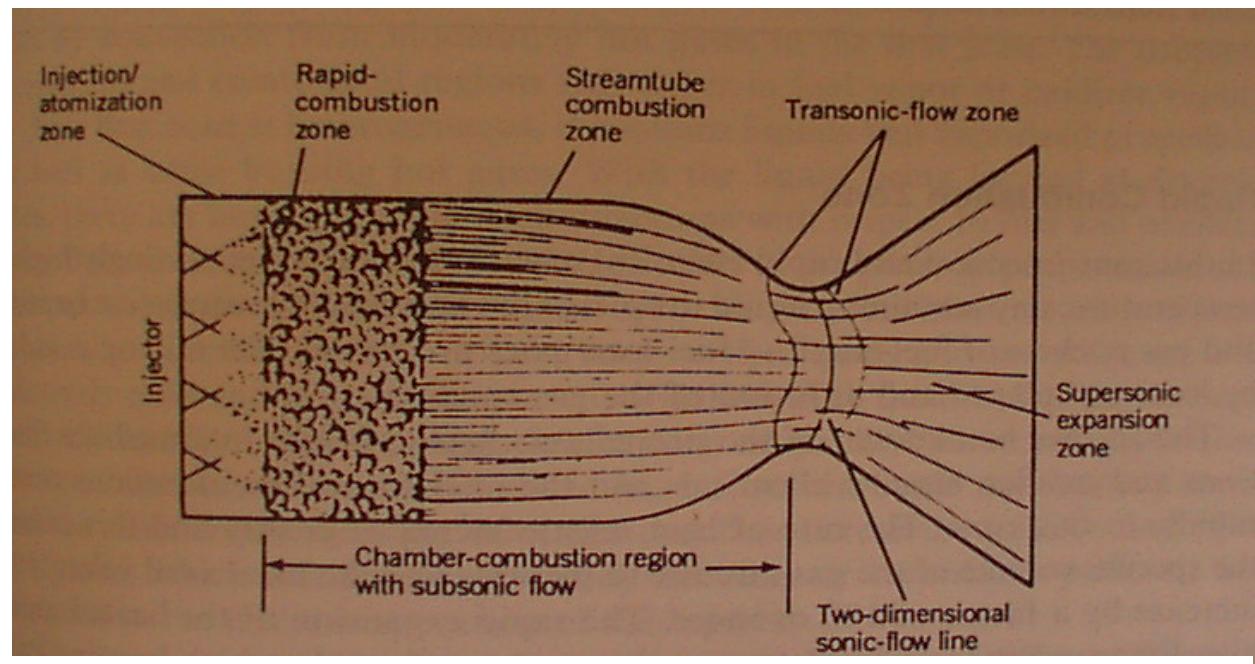
Chemical Rocket Propellant Performance Analysis

- Sutton and Biblarz: Chapter 5

$$\Delta H = \int_{T_0}^{T_c} c_p dT$$



Combustion Basics



Combustion is an exothermic chemical reaction. Often an external heat source is required (igniter) to supply the necessary energy to a threshold level where combustion is self sustaining

Propellants that combust spontaneously are referred to as *Hypergolic*

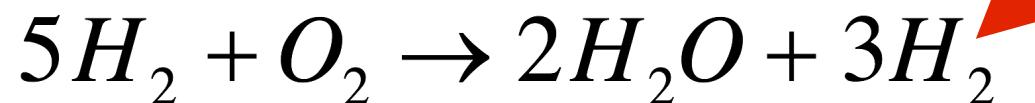
Stoichiometric Versus Non- Stoichiometric Combustion

• *Stoichiometric reaction is one in which all reactants are consumed .. Generally burns hottest*

Stoichiometric reaction:



Non- Stoichiometric reaction:



- Rockets generally burn slightly Rich (More fuel than needed for Stoich) as a balance between flame temperature and Molecular weight Of exhaust products

Desirable Propellant Properties

$$(I_{sp})_{ideal} = \frac{C^*}{g_o} \left[\gamma \sqrt{\frac{2}{\gamma - 1}} \left(\frac{2}{\gamma + 1} \right)^{\frac{\gamma + 1}{(\gamma - 1)}} \right] \Rightarrow$$

$$(I_{sp})_{ideal} = \frac{1}{g_o} \sqrt{\frac{2\gamma R_u}{\gamma - 1}} \sqrt{\frac{T_o}{M_w}}$$

- Propellants that burn Hot and have a low product Molecular weight ... have better I_{sp}

- Optimum mixture oxidizer/fuel \rightarrow high T_0
- High heat of formation, $\Delta H_f \rightarrow$ high T_0
- High hydrogen content \rightarrow low M_w

Combustion (Adiabatic Flame) Temperature

- Equilibrium properties of the reaction depends on the temperature and pressure at which the reaction occurs
- Temperature in turn depends on the heat released by the reaction and the composition of the mixture
- Pressure depends on the burn rate of the reactants
 - *..... interdependency requires iterative solution for gas composition and combustion temperature

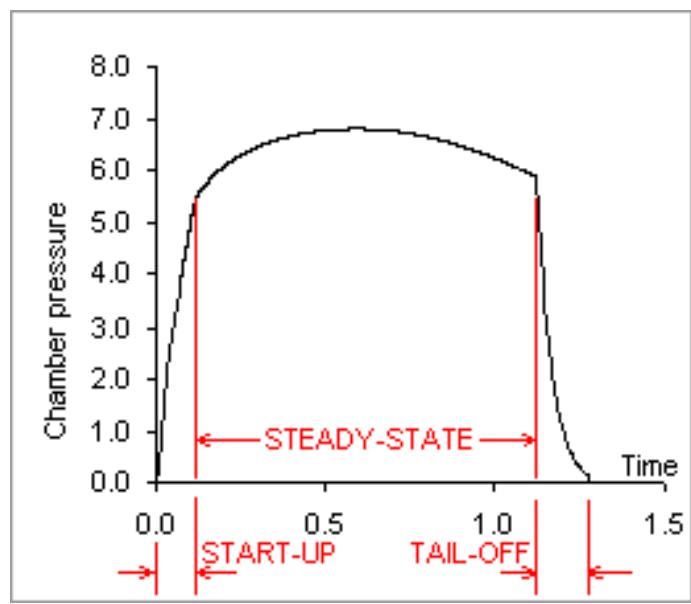
Combustion (Adiabatic Flame) Temperature

(cont'd)

- From First Law of Thermodynamics

$$i) dh = dq + vdp = dq + \frac{dp}{p}$$

- Look at “steady state” combustion in rocket $dp \approx \text{constant}$



$$ii) dh \approx dq$$

→ heat released by reaction of propellants

$$iii) dh \approx dq = h_{\text{products}} - h_{\text{reactants}}$$

→ exothermic reaction → $dh < 0$

“heat of reaction”

Heat of Formation

- Energy available in a molecule of a propellant is “Heat of formation”

ΔH_f^0 (ΔQ_f^0) \rightarrow_0 indicates standard conditions (1 atm 298 °K)

- Relative energy measure, most stable constituents like N₂ assumed to have zero heat of formation
- Knowing the standard heats of formation of the reactants and products one can estimate the heat of reaction
- Desirable to have a high positive, ΔH_f^0 , products to have a low ΔH_f^0

Example Calculation

- React 2 Molecules (moles) of gaseous diatomic hydrogen with one molecule (mole) of gaseous diatomic Oxygen



- From table 5-1 (Sutton and Biblarz)

$$\Delta H_f^0$$

$$O_2(g) = 0$$

$$H_2(g) = 0$$

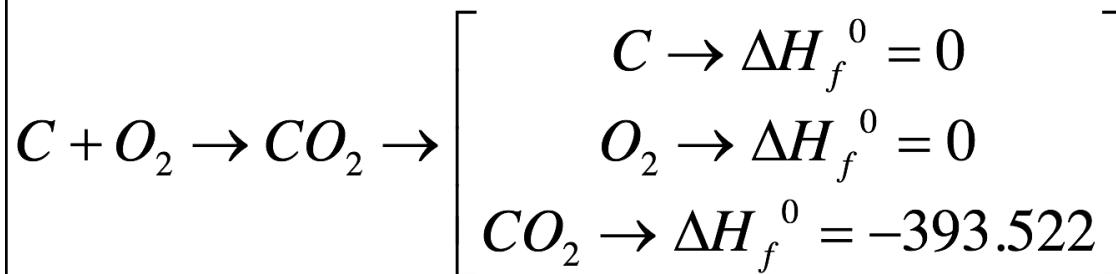
$$H_2O(g) = -241.93 \text{ KJ/mole}$$

- Heat released per mole unit reaction (standard cond't)

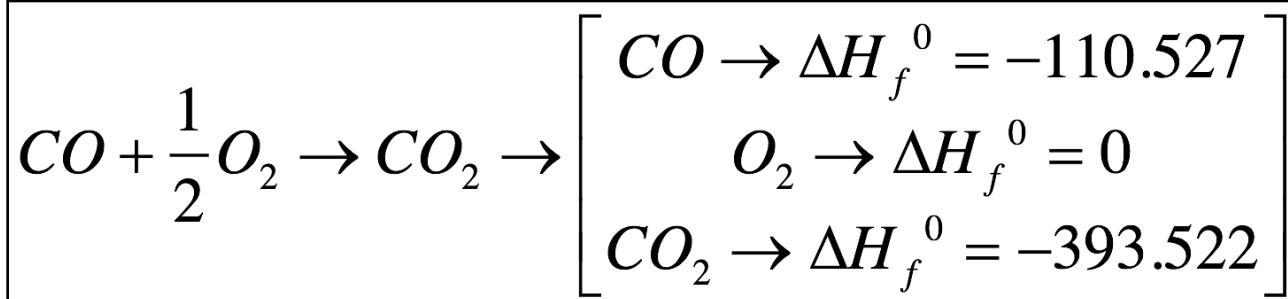
$$\Delta H_{reaction}^0 = \Delta H_{f\ products}^0 - \Delta H_{f\ reactants}^0 = -2 \cdot 241.93 \text{ KJ/mole} = -483.86 \text{ KJ/mole}$$

More Complex Example Calculation

- Hess Law ... more complex reactions can be built from simple reactions

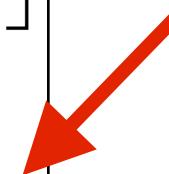


$$\Delta H_{reaction}^0 = \Delta H_{f\ products}^0 - \Delta H_{f\ reactants}^0 = \\ (-393.522 - 0)_{KJ/mole} = -393.522_{KJ/mole}$$



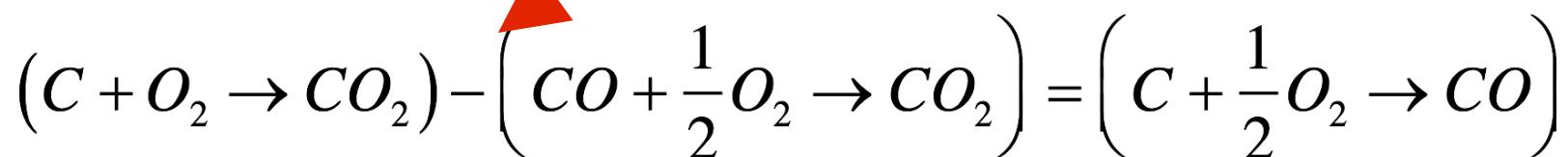
$$\Delta H_{reaction}^0 = \Delta H_{f\ products}^0 - \Delta H_{f\ reactants}^0 =$$

$$(-393.522) - (0 - 110.527)_{KJ/mole} = -282.995_{KJ/mole}$$

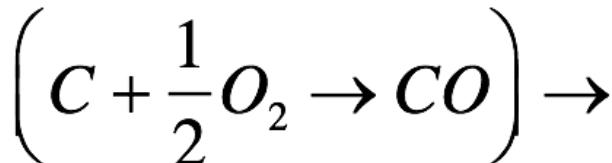


More Complex Example Calculation (cont'd)

- *Hess Law ... more complex reactions can be built from simple reactions .. Allows two reactions to be algebraically added to estimate the heat of reaction of a third reaction*
- Look at the reaction that results from the “subtraction” of the two previous reactions



- Subtract the reaction energies



$$\Delta H_{reaction}^0 1 - \Delta H_{f, reaction}^0 2 = -393.522 - (-282.995) = -110.527 \text{ kJ/mole}$$

Example Heats of Reaction (1 atm, 298 K)



Compound	KJ/mol	Compound	KJ/mol
Al(s)	0	N2(g)	0
Al2O3	-1670.53	N(g)	+472.71
C(s, graphite)	0	NH3(l)	-65.63
CO(g)	-110.59	NH3(g)	-46.21
CO2(g)	-393.68	N2H4(l)	+50.48
C(g)	+718.70	N2O4(l)	-20.13
CH4(g)	-74.90	NH4ClO4(s)	-290.58
CH3OH(l)	-238.76	HF(g)	-268.73
C2H5OH(l)	-277.77	HC(g)	-92.34
H2(g)	0	F2(l, 85k)	-12.68
H2(l, 20K)	-7.03	O2(g)	0
H(g)	+218.04	O2(l, 90K)	-9.42
H2O(g)	-241.93		
H2O(l)	-285.96		
H2O2(l)	-187.69		
HNO3(l)	-173.08		

General Reaction

- In general the heat of a particular reaction can be determined from the summation of the heats of formation of the reactants and products

$$\Delta H^0_{reaction} = \sum_j n_j (\Delta H_f^0)_{j \text{ products}} - \sum_i n_i (\Delta H_f^0)_{i \text{ reactants}}$$

$i \rightarrow$ reactants

n mole fraction of each species

$J \rightarrow$ products

General Reaction, Example

$$\Delta H^0_{reaction} = \sum_j n_j (\Delta H_f^0)_{j \text{ products}} - \sum_i n_i (\Delta H_f^0)_{i \text{ reactants}}$$



$$\{ 1(-241.93) + 1(-110.59) \} - \{ 1(0) + 1(-393.68) \} = 41.16 \text{ KJ}$$



- Oooops ... reaction is endothermic ... **wouldn't make good propellant combination!**

Reactions Occurring at Other than Standard Conditions

- At some temperature other than standard (typically higher) T_r

$$\Delta H_f^{T_r} = \Delta H_f^0 + \int_{298^\circ K}^{T_r} C_p dT$$

Cp ~
Molar
Specific Heat
J/mol-K

- And the general reaction can be written as

$$\Delta H_{reaction} = \sum_j n_j \left(\Delta H_f^0 + \int_{298^\circ K}^{T_r} C_p dT \right)_{j_{products}} - \sum_i n_i \left(\Delta H_f^0 + \int_{298^\circ K}^{T_r} C_p dT \right)_{i_{reactants}}$$

- This equation leads to an iterative process for computing the flame temperature of a reaction

“Available Heat” Flame Temperature Method

- Many different equilibrium reactions

- $\text{CO}_2 \leftrightarrow \text{CO} + \frac{1}{2} \text{O}_2$
- $\text{CO} + \text{H}_2\text{O} \leftrightarrow \text{CO}_2 + \text{H}_2$
- etc...



- The equilibrium is altered by the temperature
- What is formed depends on the temperature

- For now ignore temperature effects on reaction composition and assume that products of reaction are known (*Frozen Flow*)

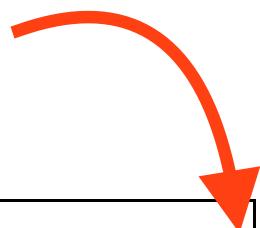
“Available Heat” Flame Temperature Method (cont’d)

- Heat released in reaction is modeled as a 3 step process
 - All reactants temperatures are cooled down or raised up to 298 K
Heat need to perform this process is modeled*
 - Standard day reaction calculations are performed, available reaction heat is calculated*
 - Once the available heat of reaction is calculated then the final reaction flame temperature is calculated ... i.e. available heat is used to raise the combustion products to the flame temperature*

$$Q_{\text{required}} = Q_{\text{available}}$$

std. day heat of reaction

$$\Delta H_{\text{reaction}}^0 = \sum_j n_j (\Delta H_f^0)_{j \text{ products}} - \sum_i n_i (\Delta H_f^0)_{i \text{ reactants}}$$



std. day react.

heat

extra heat brought in by

"hot" reactants

$$Q_{\text{available}} = \Delta H_{\text{reaction}}^0 + \sum_i \left\{ n_i \int_{298K}^{T_i} (C_p)_i \cdot dT \right\}$$

Heat capacity of products

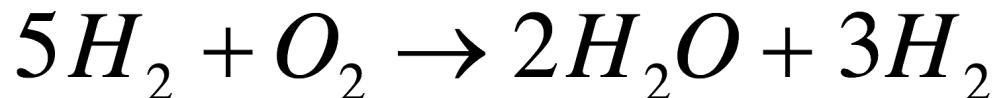
balances reaction heat

\rightarrow
 $i = \text{reactants}$
 $j = \text{products}$

$$Q_{\text{available}} = Q_{\text{required}} = \sum_j \left\{ n_j \int_{298K}^{T_{\text{reaction}}} (C_p)_j \cdot dT \right\}$$

Example “Available Heat” Calculation

- Look at fuel rich reaction at 200 atm, gases enter chamber at 500 K (T_i)



- *Standard Condition reaction heat release*

$$\Delta H^0_{reaction} = \sum_j n_j \left(\Delta H_f^0 \right)_{j \text{ products}} - \sum_i n_i \left(\Delta H_f^0 \right)_{i \text{ reactants}}$$

$$\{2(-241.93Kj / mole) + 3(O)\} - \{5(O) + 1(O)\}$$

$$-483.86KJ$$

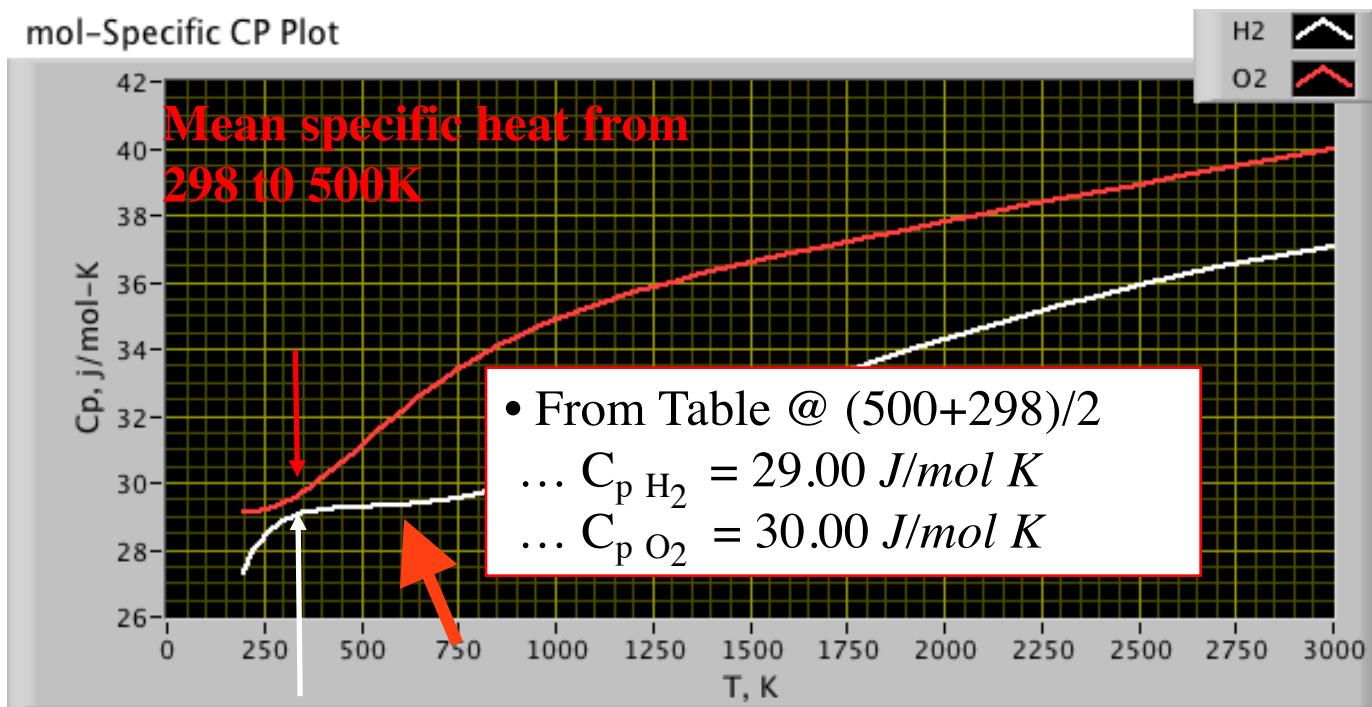


Example “Available Heat” Calculation ⁽²⁾

- Heat of Reactants at Initial conditions

Extra heat above standard conditions brought in by “hot” reactants

mol-Specific CP Plot



$$\sum_i \left\{ n_i \int_{298K}^{T_i} (C_p)_i \cdot dT \right\}$$

- Approximate Integral

$$H_2 \rightarrow \Delta Q_{500K-298K} = \int_{298^oK}^{500^oK} \bar{C}_p dT \approx 29.0 \text{ J/mol-K} (500 - 298) {}^oK = 5.86 \text{ kJ/mol}$$

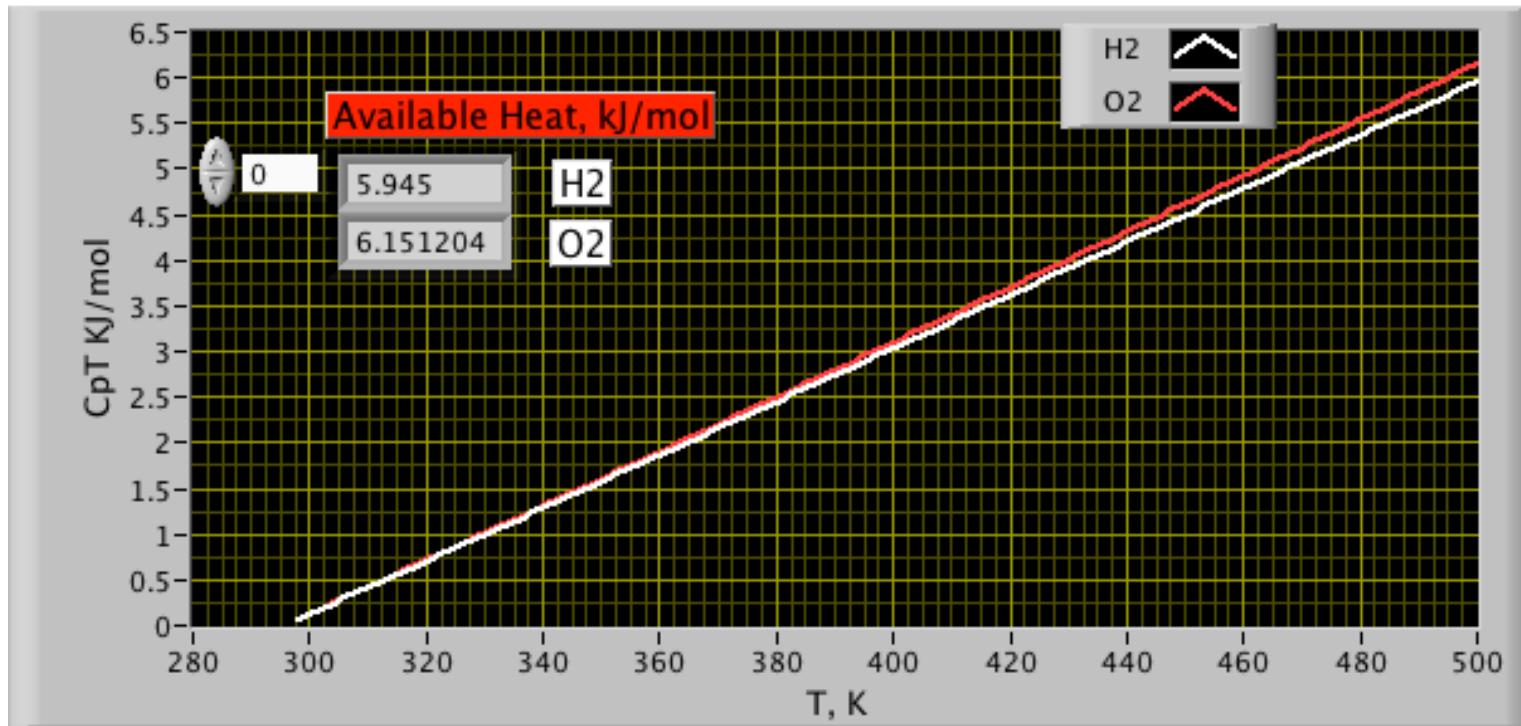
$$O_2 \rightarrow \Delta Q_{500K-298K} \int_{298^oK}^{500^oK} C_p dT \approx 30.0 \text{ J/mol-K} (500 - 298) {}^oK = 6.06 \text{ kJ / mol}$$

Example “Available Heat” Calculation ⁽²⁾

- Heat of Reactants at Initial conditions

Extra heat above standard conditions brought in by “hot” reactants

mol-Specific CpT Integral 2



$$\sum_i \left\{ n_i \int_{298K}^{T_i} (C_p)_i \cdot dT \right\}$$

- Numerical Integral

$$H_2 \rightarrow \Delta Q_{500K-298K} \int_{298^oK}^{500^oK} C_p \, dT \approx 5.945 \text{ kJ/mol}$$

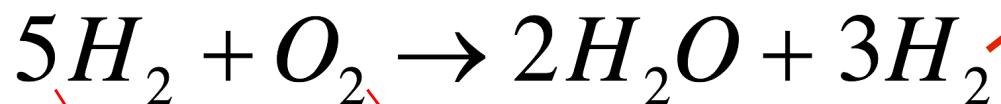
$$O_2 \rightarrow \Delta Q_{500K-298K} \int_{298^oK}^{500^oK} C_p \, dT \approx 6.151 \text{ kJ/mol}$$

Example “Available Heat”⁽³⁾

- Heat of Reactants at Initial conditions (500 K)

$$H_2 \rightarrow \Delta Q_{500K-298K} \int_{298^oK}^{500^oK} C_p dT \approx 5.945 \text{ kJ/mol}$$

$$O_2 \rightarrow \Delta Q_{500K-298K} \int_{298^oK}^{500^oK} C_p dT \approx 6.151 \text{ kJ/mol}$$



$$Q_{available} = \left(483.86 + \left(5_{n_{H_2}} \right) \cdot 5.945 + \left(1_{n_{O_2}} \right) \cdot 6.151 \right) \text{ kJ/mol} = 519.74 \text{ kJ}$$

Example Calculation ⁽⁴⁾

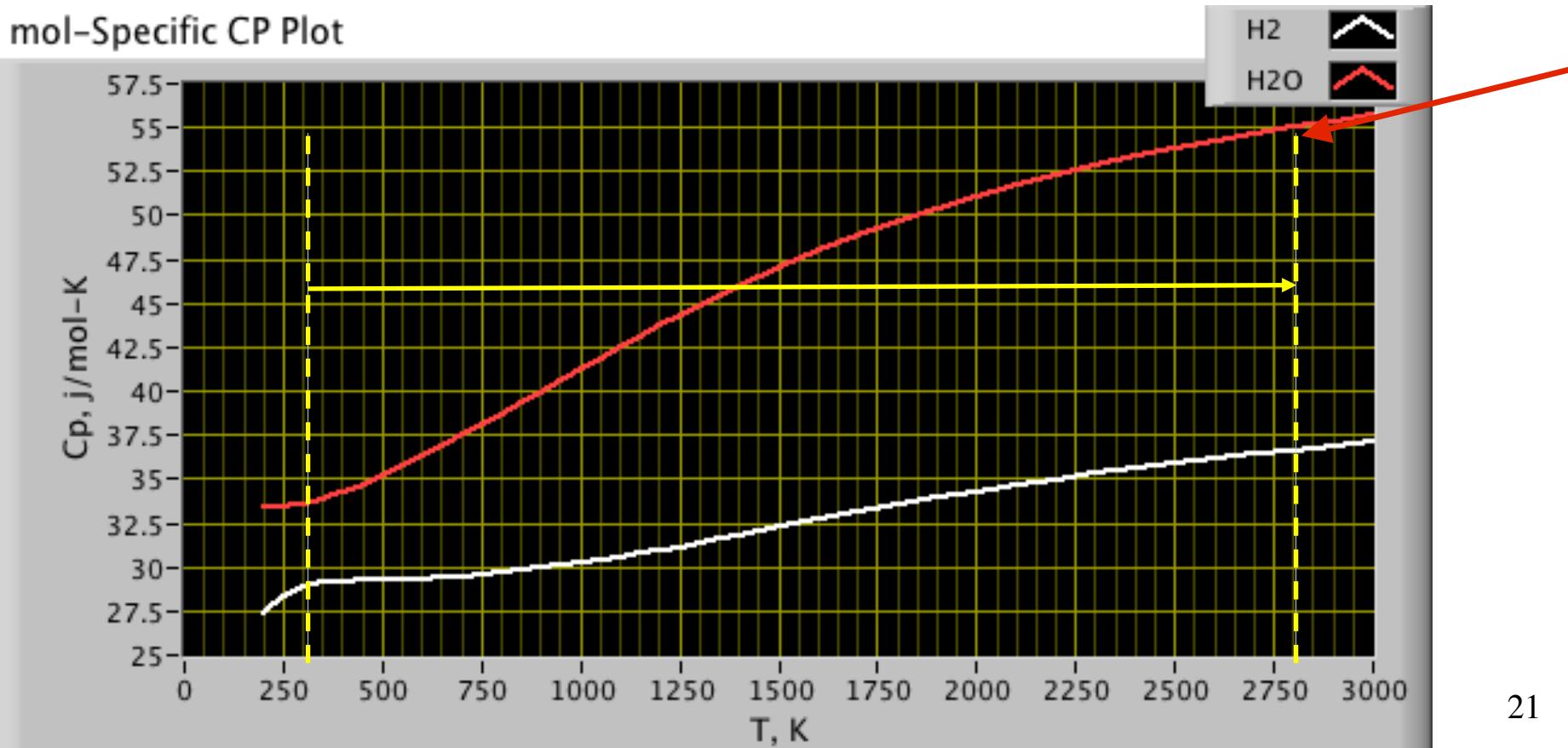
*Heat capacity of products
balances reaction heat*

$$Q_{available} = 519.74 \text{ kJ/mol}$$

$$Q_{available} = Q_{required} = \sum_j \left\{ n_j \int_{298K}^{T_{reaction}} \left(C_p \right)_j \cdot dT \right\}$$

• Guess $T_{reaction}=2800 \text{ K}$

mol-Specific CP Plot



Example Calculation (4)

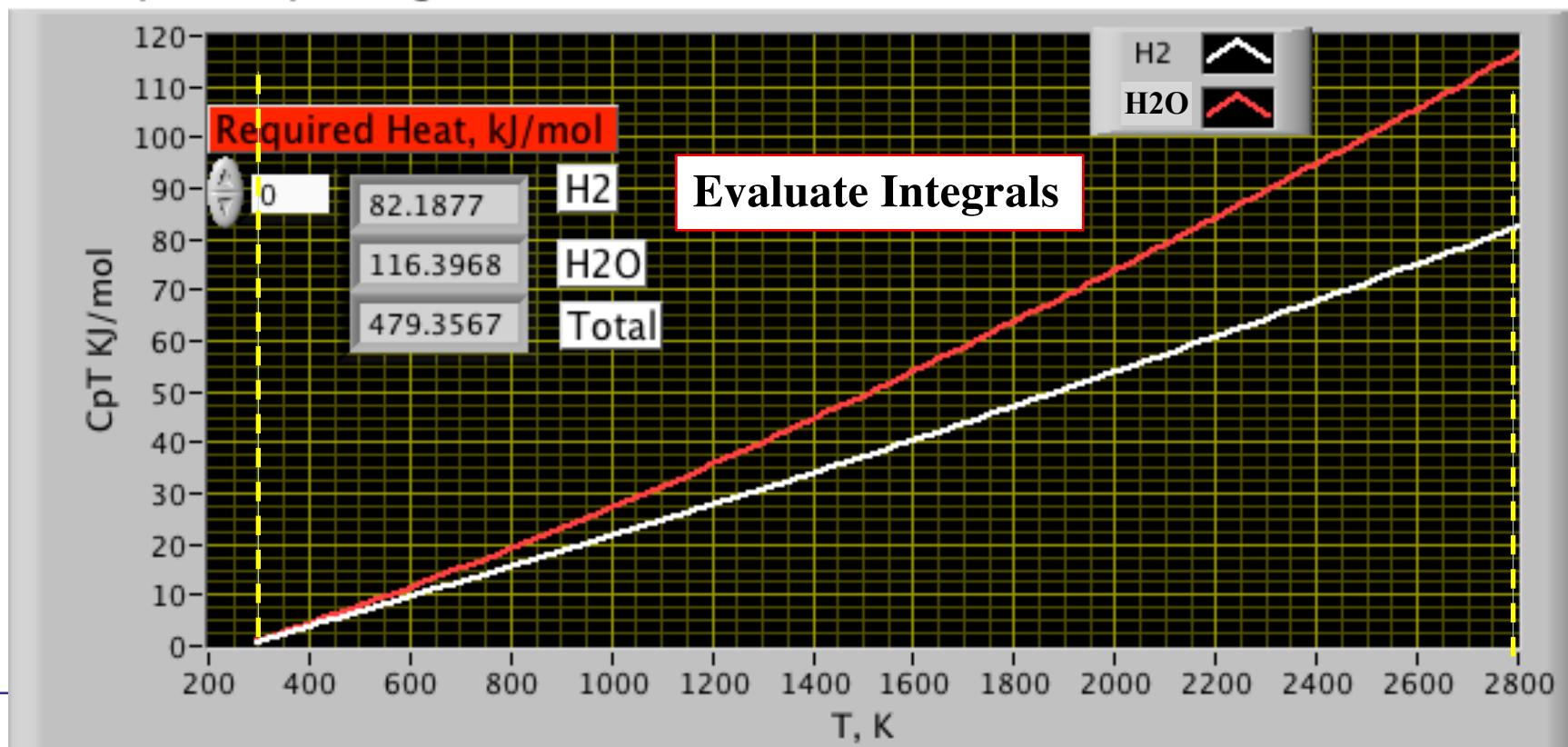
$$\int_{298K}^{T_{reaction}} \bar{C}_{P_{H_2}} \cdot dT = 82.1877 \text{ kJ/mol}$$

$$\int_{298K}^{T_{reaction}} \bar{C}_{P_{H_2O}} \cdot dT = 116.4 \text{ kJ/mol}$$

mol-Specific CpT Integral

$$Q_{available} = 2_{n_{H_2O}} \times \int_{298K}^{T_{reaction}} \bar{C}_{P_{H_2O}} \cdot dT + 3_{n_{H_2}} \times \int_{298K}^{T_{reaction}} \bar{C}_{P_{H_2}} \cdot dT$$

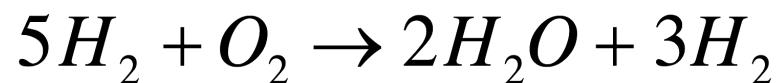
• $T_{reaction} = 2800 \text{ K}$



Example Calculation (cont'd)

*Heat capacity of products
balances reaction heat*

$$Q_{available} = Q_{required} = \sum_j \left\{ n_j \int_{298K}^{T_{reaction}} \left(C_p \right)_j \cdot dT \right\}$$



$$Q_{available} = 2_{n_{H_2O}} \times \int_{298K}^{T_{reaction}} \bar{C}_{P_{H_2}O} \cdot dT + 3_{n_{H_2}} \times \int_{298K}^{T_{reaction}} \bar{C}_{P_{H_2}} \cdot dT$$

• $T_{reaction} = 2800 \text{ K}$

$$2 \cdot 116.3968 + 3 \cdot 82.1877 = 479.357 \text{ kJ/mol}$$

$$\int_{298K}^{T_{reaction}} \bar{C}_{P_{H_2}} \cdot dT = 82.1877 \text{ kJ/mol}$$

$$\int_{298K}^{T_{reaction}} \bar{C}_{P_{H_2}O} \cdot dT = 116.4 \text{ kJ/mol}$$

Example Calculation (cont'd)

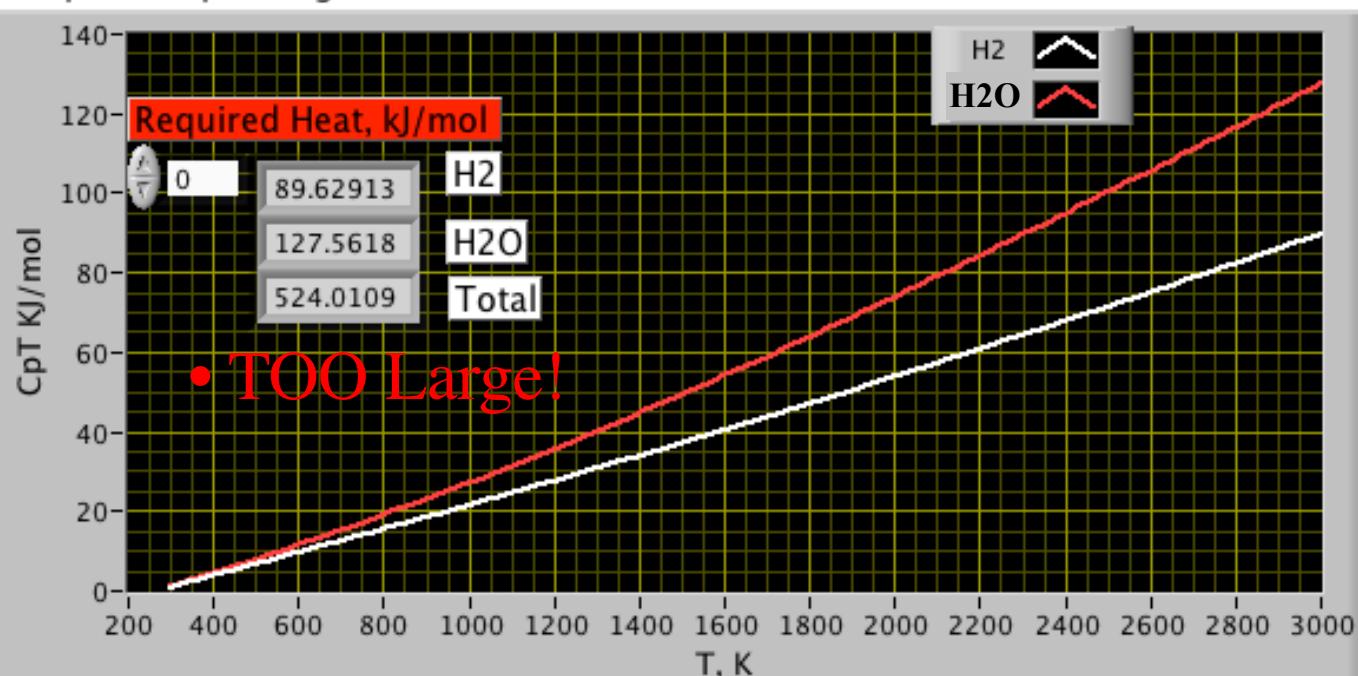
- Iterative Solution for Flame Temperature

$$Q_{available} = 519.74 \text{ kJ/mol}$$

• Guess $T_{reaction} = 3000 \text{ K}$

$$Q_{available} = 2_{n_{H_2O}} \times \int_{298K}^{T_{reaction}} \bar{C}_{P_{H_2O}} \cdot dT + 3_{n_{H_2}} \times \int_{298K}^{T_{reaction}} \bar{C}_{P_{H_2}} \cdot dT$$

mol-Specific CpT Integral



Example Calculation (cont'd)

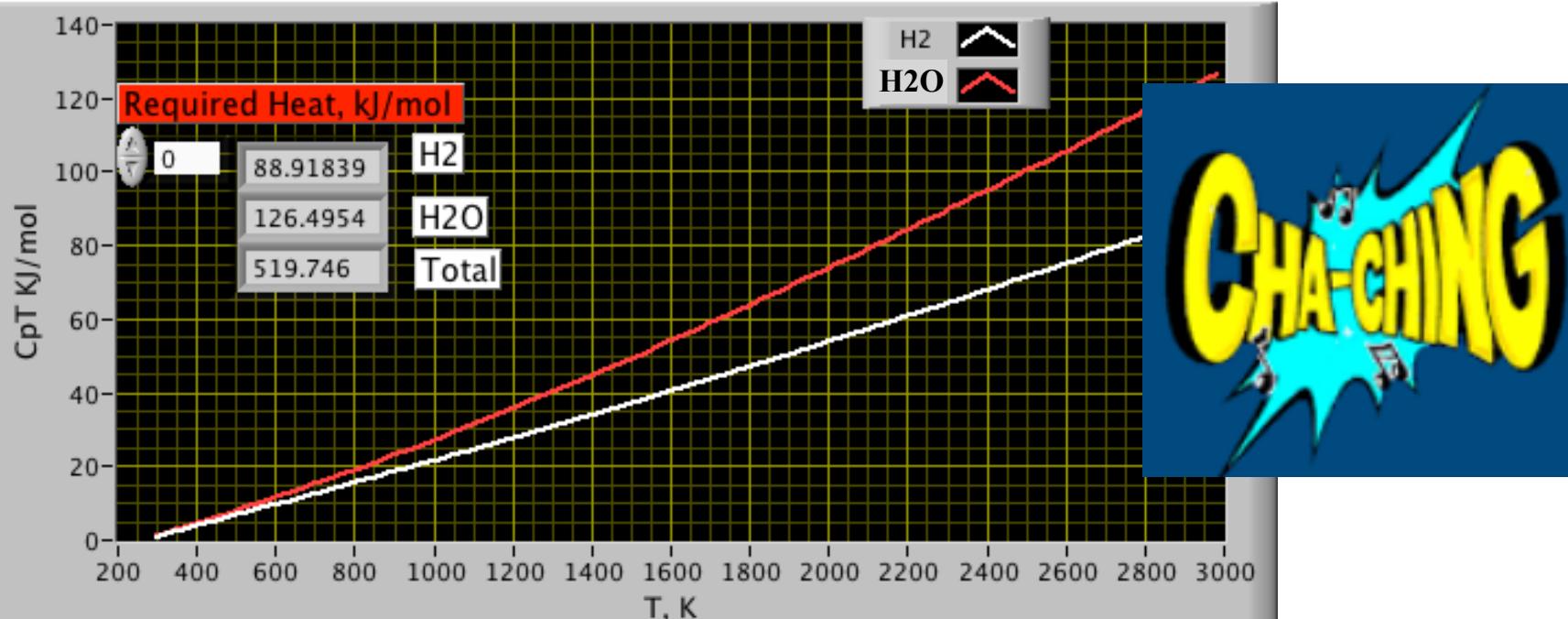
- Iterative Solution for Flame Temperature

$$Q_{available} = 519.74 \text{ kJ/mol}$$

• Guess $T_{reaction} = 2981 \text{ K}$

$$Q_{available} = 2_{n_{H_2O}} \times \int_{298K}^{T_{reaction}} \bar{C}_{P_{H_2O}} \cdot dT + 3_{n_{H_2}} \times \int_{298K}^{T_{reaction}} \bar{C}_{P_{H_2}} \cdot dT$$

mol-Specific CpT Integral



Thermo-chemical Properties of Final Reaction Mixture

$$\bar{M}_w = \frac{\sum_j n_j (M_w)_{j_{products}}}{\sum_j n_j} = \frac{2M_{w_{H_2O}} + 3M_{w_{H_2}}}{2+3} = \frac{2(18.0153 \frac{kg}{kg-mol}) + 3(2.01588 \frac{kg}{kg-mol})}{5} = 8.416 \frac{kg}{kg-mol}$$

$$R_g = \frac{\mathbb{R}_u}{\bar{M}_w} = \frac{8314.461 \frac{J/kg-kmol-K}{kg/kg-mol}}{8.416 \frac{kg}{kg-mol}} = 988.0 \frac{J/kg-K}{kg/K}$$

Molecular weights	
H ₂ , kg/kg-mol	2.01588
O ₂ , kg/kg-mol	31.9989
H ₂ O, kg/kg-mol	18.0153

Thermo-chemical Properties of Final Reaction Mixture (cont'd)

$$\bar{C}_p' = \frac{\sum_{products} n_i C_{p_i}}{\sum_{products} n_i} \quad Molar\ specific\ heat$$

$$\bar{C}_p = \frac{\bar{C}_p'}{\bar{M}_w} = \frac{1}{\bar{M}_w} \frac{\sum_{products} n_i C_{p_i}}{\sum_{products} n_i} \quad \text{Mass specific heat}$$

$$\gamma = \frac{\bar{C}_p}{\bar{C}_p - \bar{R}_g} \quad ratio\ of\ specific\ heats\ of\\ combustion\ for\ product\ mixture$$

Thermo-chemical Properties of Final Reaction Mixture (cont'd)

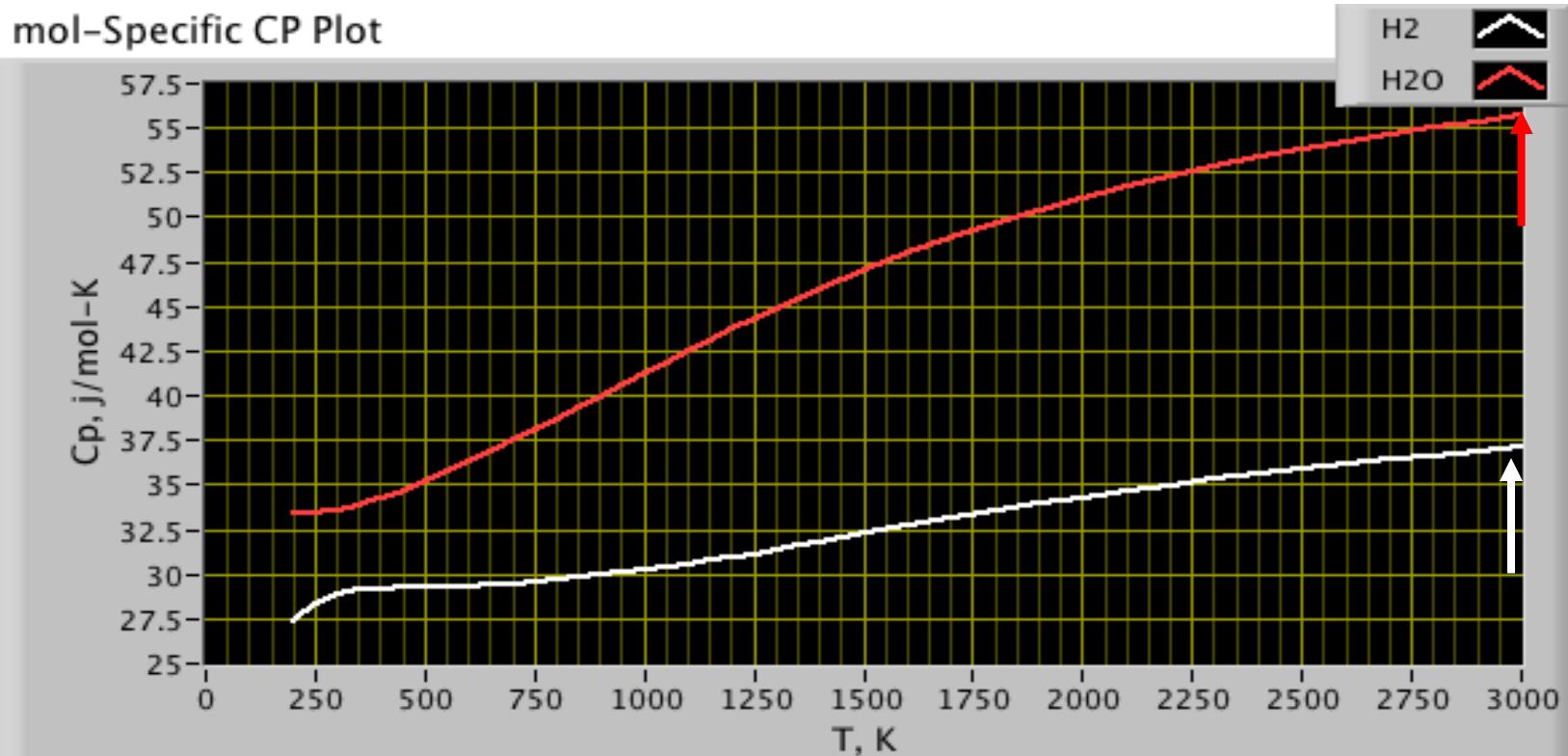
- Completing the example

$$C'_{p_{H_2O}} @ 298 \text{ K} = 55,620 \frac{\text{J}}{\text{kg-mol-K}}$$

$$C'_{p_{H_2}} @ 298 \text{ K} = 36,780 \frac{\text{J}}{\text{kg-mol-K}}$$

- Based on molar specific heat

mol-Specific CP Plot



Thermo-chemical Properties of Final Reaction Mixture (cont'd)

- Completing the example

$$C'_{p_{H_2O}} @ 298 \text{ K} = 55,620 \frac{\text{J}}{\text{kg-mol-K}}$$

$$C'_{p_{H_2}} @ 298 \text{ K} = 36,780 \frac{\text{J}}{\text{kg-mol-K}}$$

- Based on molar specific heat

$$\bar{C}_p = \frac{1}{8.416 \frac{\text{kg}}{\text{kg-mol}}} \frac{2_{\text{kg-mol}} \cdot 55,620 \frac{\text{J}}{\text{kg-mol-K}} + 3_{\text{kg-mol}} \cdot 36,780 \frac{\text{J}}{\text{kg-mol-K}}}{5_{\text{kg-mol}}} = 5265.68 \frac{\text{J}}{\text{kg-K}}$$

$$\bar{\gamma} = \frac{\bar{C}_p}{\bar{C}_p - \bar{R}_g} = \frac{5265.68 \frac{\text{J}}{\text{kg-K}}}{5265.68 \frac{\text{J}}{\text{kg-K}} - 988 \frac{\text{J}}{\text{kg-K}}} = 1.231$$

Equilibrium versus *Frozen* Combustion Flow

- Many reactants, when mixed in Stoichiometric quantities, react to form products only, in an Irreversible reaction.
- In a reversible reaction, however, the chemical process goes both ways.
- Reactants combust to form products, which then re-react to form the original reactants
- When the ratio of reactants to products becomes constant, *chemical equilibrium* has occurred

Equilibrium versus Frozen Combustion Flow

(cont'd)

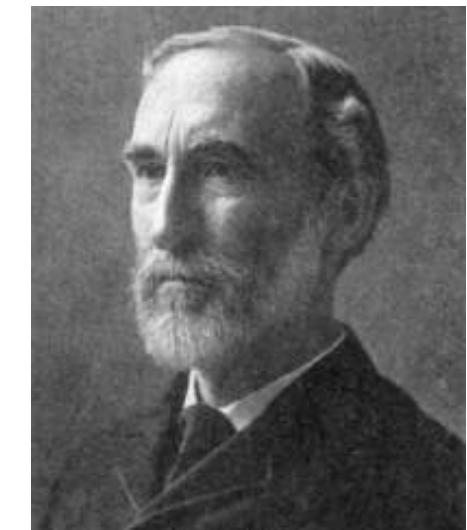
- Frozen flow assumes that the products of the reaction remain constant once the reaction occurs, no secondary reactions result
- Equilibrium flows allow combustion products to recombine and react to form other products .. Equilibrium is reached when the species combinations do not change as a function of time, as long as the external variables (Temperature and pressure)
- Changing temperature and pressure changes the equilibrium conditions

Gibbs Free Energy Analysis

(modern approach)

- Energy available to do useful work is called Gibbs free energy. It is the measure of the chemical potential of a gaseous species,
- Gibbs Free energy is given the symbol G in honor of Josiah Gibbs, a professor of chemistry at Yale University who almost single handedly developed both the concept and the quantitative equations which describe it.
- Free energy is a state function because it is formally defined only in terms of state functions, the state functions enthalpy and entropy, and the state variable temperature. The definition of free energy is:

$$G(T, P) = H - TS \rightarrow J / kg - mol$$



- H is the molar specific enthalpy, S is the entropy, and T is the absolute temperature.

• Chemistry gateway:

<http://www.psigate.ac.uk/newsite/reference/plambeck/chem2/p02051.htm>

Gibbs Free Energy Analysis (cont'd)

- G as a measure of the relative stability of a physical or chemical system, i.e., the tendency of the system to react or change.
- If the change in free energy, ΔG , is negative, the transformation of the system will occur spontaneously, since transitions in which the energy decreases are favored. Reactions tend to seek The minimum free energy ... *fundamental definition for chemical Equilibrium*
- Gibbs free energy for a given species is energy required to form a species from its base elements. Gibbs free energy of formation of all elements in their elemental form is zero.
- We will we will simply rely on the fact that for just about any compound we are interested in, its free energy of formation will have been measured and tabulated.

Gibbs Free Energy Analysis (cont'd)

- For a given species, G is tabulated as a function of temperature at a reference pressure of one atmosphere
- For other pressures a correction must be applied
- For a pressure other than 1atmosphere

$$\begin{aligned}G(T, P_2) - G(T, P_{1atm}) &= (H_2 - TS_2) - (H_{1atm} - TS_{1atm}) = \\(H_2 - H_{1atm}) - T(S_2 - S_{1atm})\end{aligned}$$

- But for a calorically perfect gas

$$H = C_p T$$

- And ... the expression reduces to

$$G(T, P_2) - G(T, P_{1atm}) = -T(S_2 - S_{1atm})$$

Gibbs Free Energy Analysis (cont'd)

- But as derived in *Section 5.1*

$$S_2 - S_1 = C_p \ln_2 \left[\frac{T_2}{T_1} \right] - R_g \ln \left[\frac{p_2}{p_1} \right]$$

- But since we are dealing with mol-specific and not mass-specific quantities we replace R_g with R_u , and C_p with C_p'

$$S_2 - S_1 = (C_p') \ln_2 \left[\frac{T_2}{T_1} \right] - R_u \ln \left[\frac{p_2}{p_1} \right] \rightarrow G(T, P_2) - G(T, P_{1atm}) = -T(S_2 - S_{1atm})$$

- The difference in free energy between P_2 and 1 atms at constant temperature is

$$G(T, P_2) - G(T, P_{1atm}) = TR_u \left\{ \ln \left[P_2 \right] - \ln \left[P_{1atm} \right] \right\}$$

Gibbs Free Energy Analysis (cont'd)

- Rearranging

$$G(T, P_2) = \left\{ G(T, P_{1atm}) + TR_u \ln[P_{1atm}] \right\} + TR_u \ln[P_2]$$


- From Definition (for energy of formation at 1 atms)

$$\left\{ G(T, P_{1atm}) + TR_u \ln[P_{1atm}] \right\} \equiv \Delta G_f^0(T)$$

- And the correction from 1 atms is written in general terms as

$$G(T, P) = \Delta G_f^0(T) + TR_u \ln[P]$$

Gibbs Free Energy Analysis (cont'd)

- For each species in a reaction the species free energy can be written in terms of the partial pressure of the species

$$G_i(T, P) = \Delta G_{i_f}^0(T) + TR_u \ln[P_i]$$

- And from Dalton's law ...

$$\frac{P_i}{P_T} = \frac{n_i}{n_T}$$

$$G_i(T, P) = \Delta G_{i_f}^0 + R_u T \ln \left[\frac{n_i P_T}{n_T} \right]$$

n_i = number of moles of "i" at equilibrium

Gibbs Free Energy Analysis (cont'd)

- For the mixture then ..

$$G(T, P) = \sum_i \left[n_i \Delta G_{i_f}^0(T) \right] + R_u T \sum_i \left\{ n_i \ln \left[\frac{n_i P_T}{n_T} \right] \right\}$$

- Since the reaction is equilibrium when energy state is minimized
the criterion for equilibrium is given by

$$\frac{\partial G(T, P)}{\partial n_i} = 0 \rightarrow i = 1, 2, \dots \text{number of species}$$

- Simultaneous set of non linear equations Number of moles of each species is iterated to drive G to min, constrained by the atom balance for the mixture ... i.e. products must conserve the number of atoms of the reactants

Gibbs Free Energy Analysis (cont'd)

- For a given species, G is tabulated as a function of temperature at a reference pressure of one atmosphere ... referred to as the free energy of formation ...

	ΔG_f (kJ)	ΔH_f (kJ)	S (J K ⁻¹)
NH _{3(g)}	-17	-46	193
NH _{3(aq)}	-27	-80	111
NH ₄₊ _(aq)	-79	-132	113
NO _(g)	87	90	211
NO _{2(g)}	52	34	240
N ₂ O _(g)	104	82	220
N ₂ O _{4(g)}	98	10	304
N ₂ O _{5(g)}	134	-42	178
N ₂ H _{4(l)}	149	51	121
N ₂ H ₃ CH _{3(l)}	180	54	166
HNO _{3(aq)}	-111	-207	146
HNO _{3(l)}	-81	-174	156
NH ₄ ClO _{4(s)}	-89	-295	186
NH ₄ Cl _(s)	-203	-314	96
C ₆ H ₁₂ O _{6(s)}	-911	-1275	212
CO _{2(g)}	-394	-393.5	214
H ₂ O _(l)	-237	-286	70
O _{2(g)}	0	0	205
N _{2(g)}	0	0	192
NO _{3-(aq)}	-108.7	-206.85	146.70

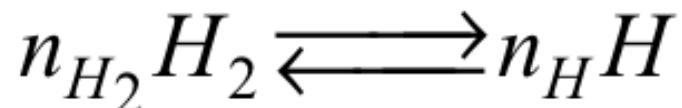
• Table shows
Thermodynamic
Properties at 1 atm
And 298 K

Per kg-mole of species

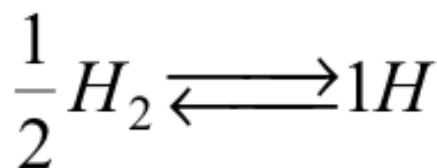
Gibbs Free Energy Analysis Example

(Credit Narayanan Komerath, Georgia Tech)

- Look at the two-way reaction where diatomic Hydrogen reacts to give mono-atomic hydrogen at 4000 K and 10 atms



- Before Combustion initiates the original mixture has a 1 half mole of H_2 and no moles of mono-atomic H
- And Stoichiometric reaction is:



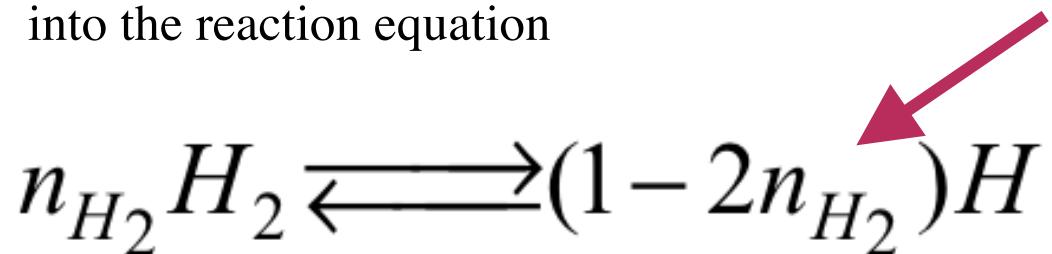
Gibbs Free Energy Analysis Example

(Credit Narayanan Komerath, Georgia Tech)

- At equilibrium temperature ... the proportions change

$$2n_{H_2} + n_H = 1 \quad \rightarrow \quad n_H = 1 - 2n_{H_2}$$

- Solving for n_{H_2} in terms of n_H and substituting into the reaction equation



- The total number of product moles is

$$n_T = n_H + n_{H_2} = (1 - 2n_{H_2}) + n_{H_2} = 1 - n_{H_2}$$

Gibbs Free Energy Analysis (cont'd)

- For the earlier example, since

$$G(T, P) = \sum_i \left[n_i \Delta G_{i_f}^0(T) \right] + R_u T \sum_i \left\{ n_i \ln \left[\frac{n_i P_T}{n_T} \right] \right\}$$

Then since

$$n_T = n_H + n_{H_2} = (1 - 2n_{H_2}) + n_{H_2} = 1 - n_{H_2}$$

$$G(T, P) = n_{H_2} \Delta G_{H_2 f(@4000^o K)}^0 + (1 - 2n_{H_2}) \Delta G_{H_f(@4000^o K)}^0 +$$

$$\left(8314.4126 \frac{J}{kg \cdot mol^o K} \right) (4000^o K) \left\{ n_{H_2} \ln \left[\frac{10_{atms} n_{H_2}}{1 - n_{H_2}} \right] + (1 - 2n_{H_2}) \ln \left[\frac{10_{atms} (1 - 2n_{H_2})}{1 - n_{H_2}} \right] \right\}$$


Gibbs Free Energy Analysis (cont'd)

- Free Energies of formation

$$\Delta G_{H_2 f}^0(T) = 0$$

$$\Delta G_{H_f}^0(T) = -15.491 \times 10^3 \frac{KJ}{kg-mol}$$

$$\frac{\partial G(4000^\circ K, P)}{\partial n_{H_2}} = (2n_{H_2} - 1)15.491 \times 10^3 \frac{KJ}{kg-mol} +$$

$$\left(4008.31 \frac{KJ}{kg-mol} \right) \left\{ n_{H_2} \ln \left[\frac{10_{atms} n_{H_2}}{1 - n_{H_2}} \right] + (1 - 2n_{H_2}) \ln \left[\frac{10_{atms} (1 - 2n_{H_2})}{1 - n_{H_2}} \right] \right\}$$

- Single parameter for minimization, n_{H_2}

$$\frac{\partial G(4000^\circ K, P)}{\partial n_{H_2}} = 0$$

Gibbs Free Energy Analysis (cont'd)

- $$\frac{\partial G(4000^\circ K, P)}{\partial n_{H_2}} =$$

$$30.982 \times 10^3 +$$

$$4008.31 \left(-2 \log \left[\frac{10 (1 - 2 n_{H_2})}{1 - n_{H_2}} \right] + \log \left[\frac{10 n_{H_2}}{1 - n_{H_2}} \right] + \frac{1}{10} \left(\frac{10 (1 - 2 n_{H_2})}{(1 - n_{H_2})^2} - \frac{20}{1 - n_{H_2}} \right) (1 - n_{H_2}) + \right.$$

$$\left. \frac{1}{10} (1 - n_{H_2}) \left(\frac{10}{1 - n_{H_2}} + \frac{10 n_{H_2}}{(1 - n_{H_2})^2} \right) \right] = 0$$

- Numerical Solution

$$n_{H_2} = 0.37782$$

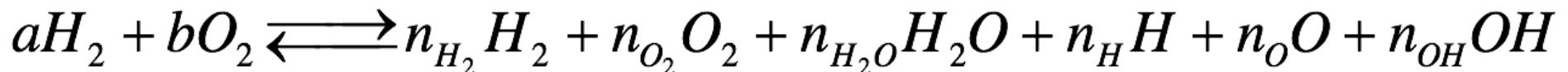
$$n_H = 1 - 2n_{H_2} = 1 - 2 \cdot 0.37782 = 0.24436$$

Ouch!

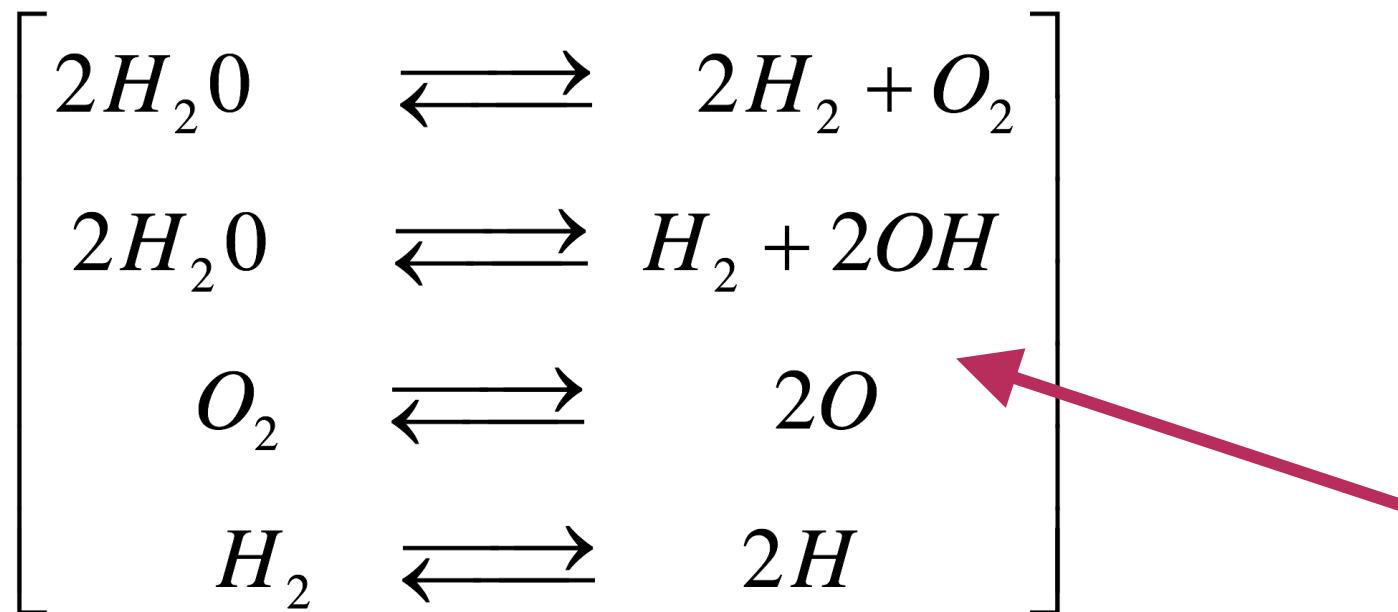
- Any more complex example than this is infeasible without a computer! ... and even this example required a computer for numerical solution

How about a more general example?

- Combustion of Oxygen and Hydrogen at 10 *atms* pressure, 298 K



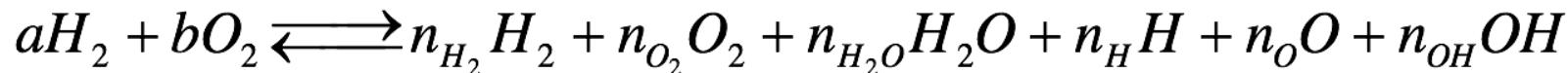
- Consider the sub-reactions that are most likely



How about a more general example?

(cont'd)

- Conservation of Atoms



... add up all “H’s”

$$2n_{H_2O} + 2n_{H_2} + n_H + n_{OH} = 2a$$

... add up all “O’s”



$$n_{H_2O} + 2n_{O_2} + n_O + n_{OH} = 2b$$

More general example?

(cont'd)

- For the mixture of species

$$\begin{aligned}
 G(T, P) = & \sum_i \left[n_i \Delta G_{i_f}^0(T) \right] + R_u T \sum_i \left\{ n_i \ln \left[\frac{n_i P_T}{n_T} \right] \right\} = \\
 & n_{H_2} \Delta G_{H_2 f}^0(T) + R_u T \sum_i \left\{ n_{H_2} \ln \left[\frac{n_{H_2} P_T}{n_{H_2} + n_{O_2} + n_{H_2 O} + n_H + n_O + n_{OH}} \right] \right\} + \\
 & n_{O_2} \Delta G_{O_2 f}^0(T) + R_u T \sum_i \left\{ n_{O_2} \ln \left[\frac{n_{O_2} P_T}{n_{H_2} + n_{O_2} + n_{H_2 O} + n_H + n_O + n_{OH}} \right] \right\} + \\
 & n_{H_2 O} \Delta G_{H_2 O_f}^0(T) + R_u T \sum_i \left\{ n_{H_2 O} \ln \left[\frac{n_{H_2 O} P_T}{n_{H_2} + n_{O_2} + n_{H_2 O} + n_H + n_O + n_{OH}} \right] \right\} + \\
 & n_{OH} \Delta G_{OH_f}^0(T) + R_u T \sum_i \left\{ n_{OH} \ln \left[\frac{n_{OH} P_T}{n_{H_2} + n_{O_2} + n_{H_2 O} + n_H + n_O + n_{OH}} \right] \right\} + \\
 & n_H \Delta G_{H_f}^0(T) + R_u T \sum_i \left\{ n_H \ln \left[\frac{n_H P_T}{n_{H_2} + n_{O_2} + n_{H_2 O} + n_H + n_O + n_{OH}} \right] \right\} + \\
 & n_O \Delta G_{O_f}^0(T) + R_u T \sum_i \left\{ n_O \ln \left[\frac{n_O P_T}{n_{H_2} + n_{O_2} + n_{H_2 O} + n_H + n_O + n_{OH}} \right] \right\}
 \end{aligned}$$

n_{O_2}

More general example?

(cont'd)

- Conditions for equilibrium ... minimization of free energy

$$\frac{\partial G}{\partial n_{H_2}} = 0 \rightarrow \frac{\partial G}{\partial n_{O_2}} = 0 \rightarrow \frac{\partial G}{\partial n_{H_2O}} = 0 \rightarrow$$

$$\frac{\partial G}{\partial n_H} = 0 \rightarrow \frac{\partial G}{\partial n_O} = 0 \rightarrow \frac{\partial G}{\partial nOH} = 0$$

6 equations, 6 unknowns

More general example?

(cont'd)

- Solve for equilibrium product species concentration

$$\frac{\partial G}{\partial n_{H_2}} = 0 \rightarrow \frac{\partial G}{\partial n_{O_2}} = 0 \rightarrow \frac{\partial G}{\partial n_{H_2O}} = 0 \rightarrow$$

$$\frac{\partial G}{\partial n_H} = 0 \rightarrow \frac{\partial G}{\partial n_O} = 0 \rightarrow \frac{\partial G}{\partial nOH} = 0$$

6 equations, 6 unknowns

Species	Mole Fraction
H ₂	0.1944
O ₂	0.05521
H ₂ O	0.2498
OH	0.1695
O	0.1099
H	0.2213

More general example?

(cont'd)

- Solve for reactant mole fractions

$$2n_{H_2O} + 2n_{H_2} + n_H + n_{OH} = 2a$$

$$\frac{2 \cdot 0.2498 + 2 \cdot 0.1944 + 0.2213 + 0.1695}{2} \\ = 0.6396$$

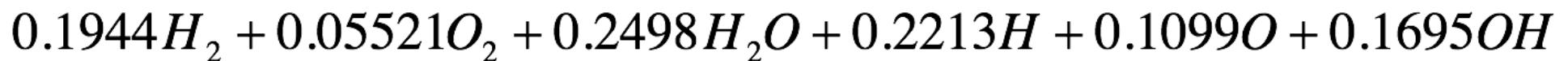
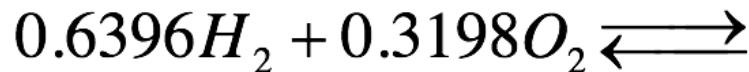
$$n_{H_2O} + 2n_{O_2} + n_O + n_{OH} = 2b$$

$$\frac{0.2498 + 2 \cdot 0.05521 + 0.1099 + 0.1695}{2} \\ = 0.3198$$

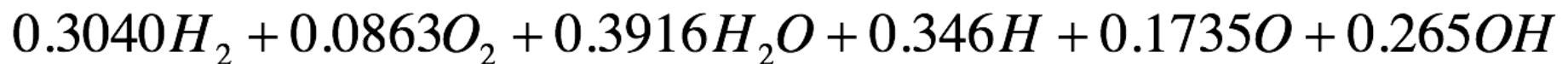
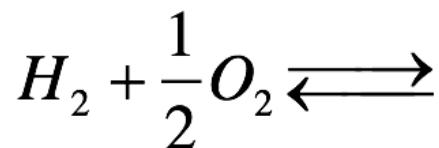
Species	Mole Fraction
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H	0.2213

More general example?

(cont'd)



→ or in terms of reactant oxidizer moles



More general example?

(cont'd)

- Flame temperature

$$\sum_j n_j \left(\int_{298^\circ K}^{T_{flame}} C_p dT \right)_{j_{products}} = -\Delta H^0_{reaction} = - \left[\sum_j n_j (\Delta H_f^0)_{j_{products}} - \sum_i n_i (\Delta H_f^0)_{i_{reactants}} \right]$$

.... Must iterate to get consistent match for data

Codes for Solving Gibbs analysis for Equilibrium Chemistry

Examples:

- “free energy” is preferred and most accurate method for computer implementation of equilibrium analysis

i) CEA Industry Standard NASA Code

<http://www.grc.nasa.gov/WWW/CEAWeb/>



ii) StanJan ... archiac DOS-based solver

<http://ww2.mne.ksu.edu/~chapman/thermo2/download.html>

iii) GasEq ... British code with MS windows interface

<http://www.gaseq.co.uk/>

iv) GUIPEP ...Decent Amateur Rocket Code mostly used for solid motors

<http://lekstutis.com/Artie/PEP/Index.html>

Chemical Equilibrium with Applications

- NASA code in development for over 45 years
- CEA is a program which calculates chemical equilibrium product Concentrations from any set of reactants and determines thermodynamic and transport properties for the product mixture.
- CEAgui is a Windows-Based Java Graphical Users Interface Application for the CEA2 Fortran program.
- Design features specifically tailored to rocket analysis are included
- Options for Both Equilibrium and Frozen Flow
- Free Download at:
<http://www.grc.nasa.gov/WWW/CEAWeb/ceaRequestForm.htm>

Chemical Equilibrium with Applications

(cont'd)

- Theoretical Documentation

NASA RP-1131

<http://www.grc.nasa.gov/WWW/CEAWeb/RP-1311.htm>

- Program Documentation

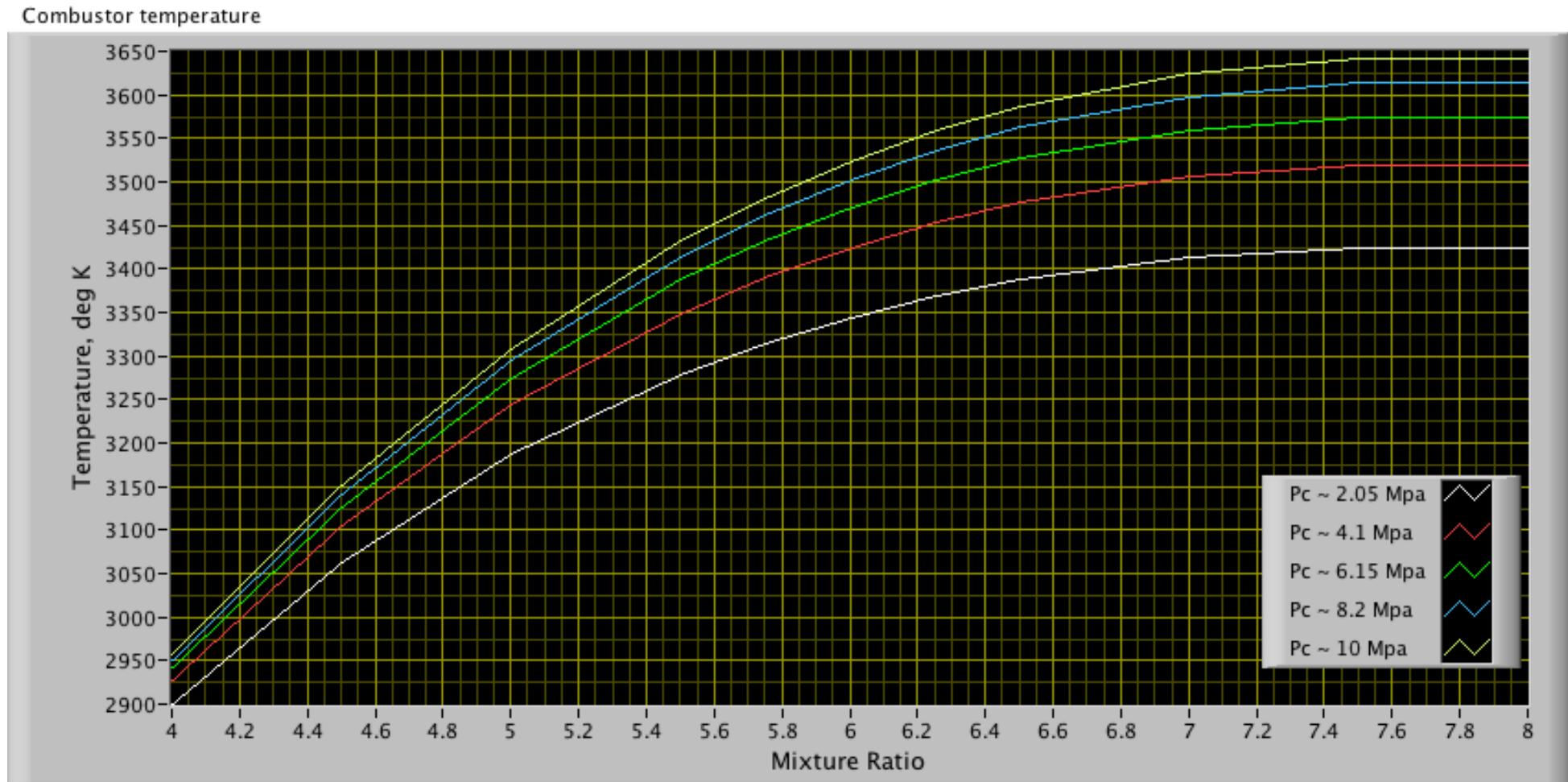
NASA RP-1131-P2

<http://www.grc.nasa.gov/WWW/CEAWeb/RP-1311P2.htm>



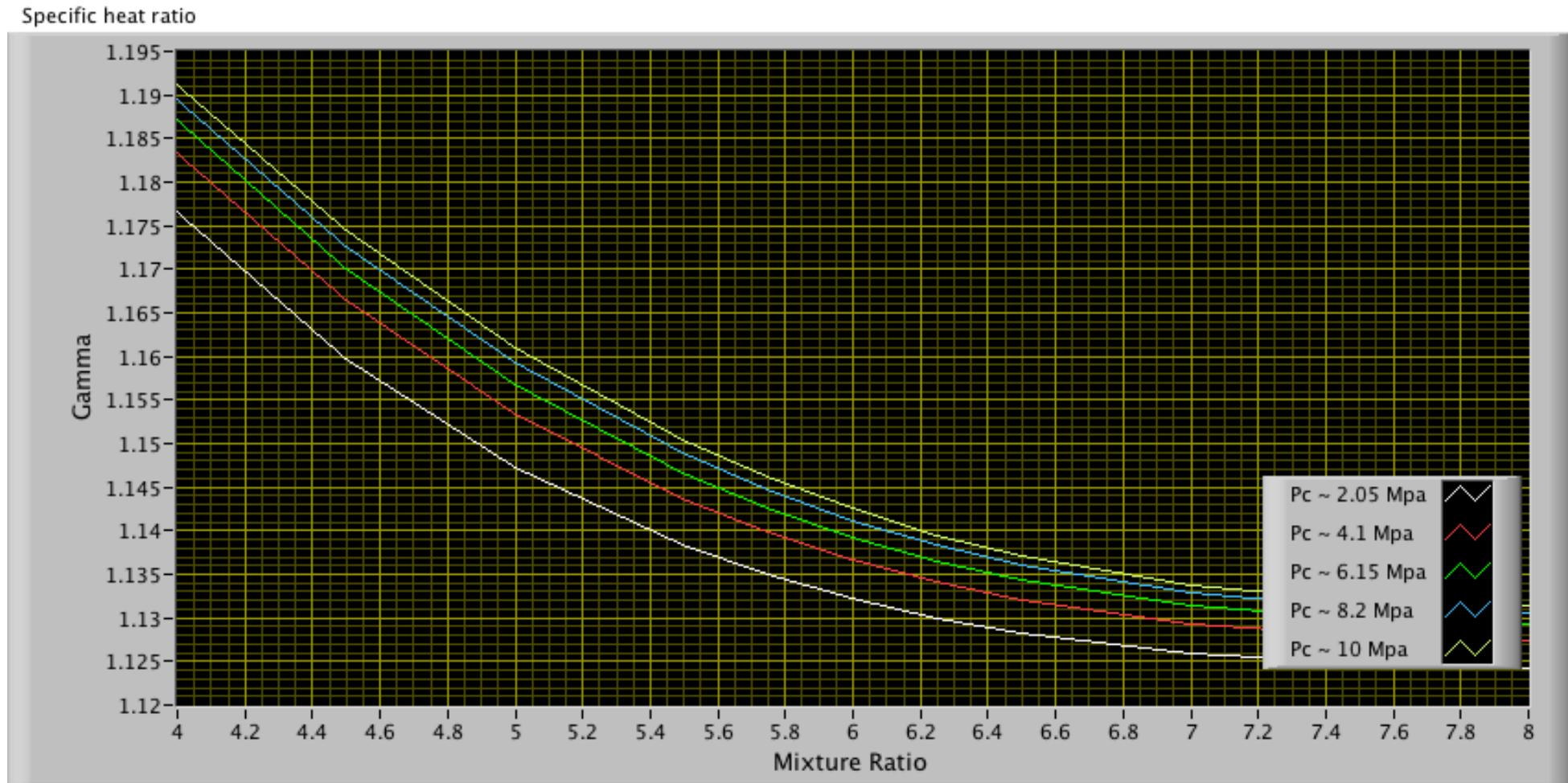
LOX/LH₂ combustion revisited

- CEA equilibrium calculations



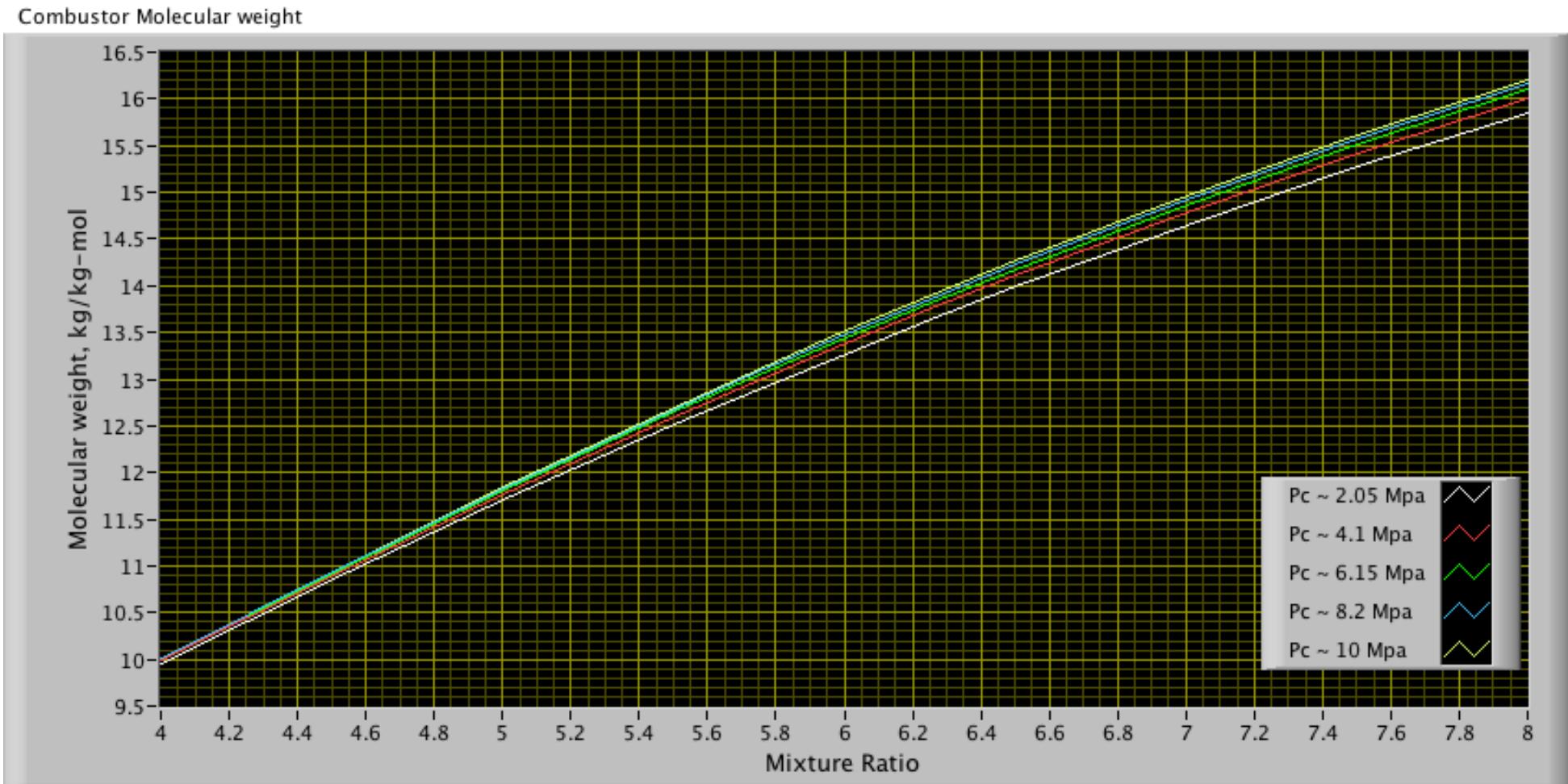
LOX/LH₂ combustion revisited (cont'd)

- CEA equilibrium calculations



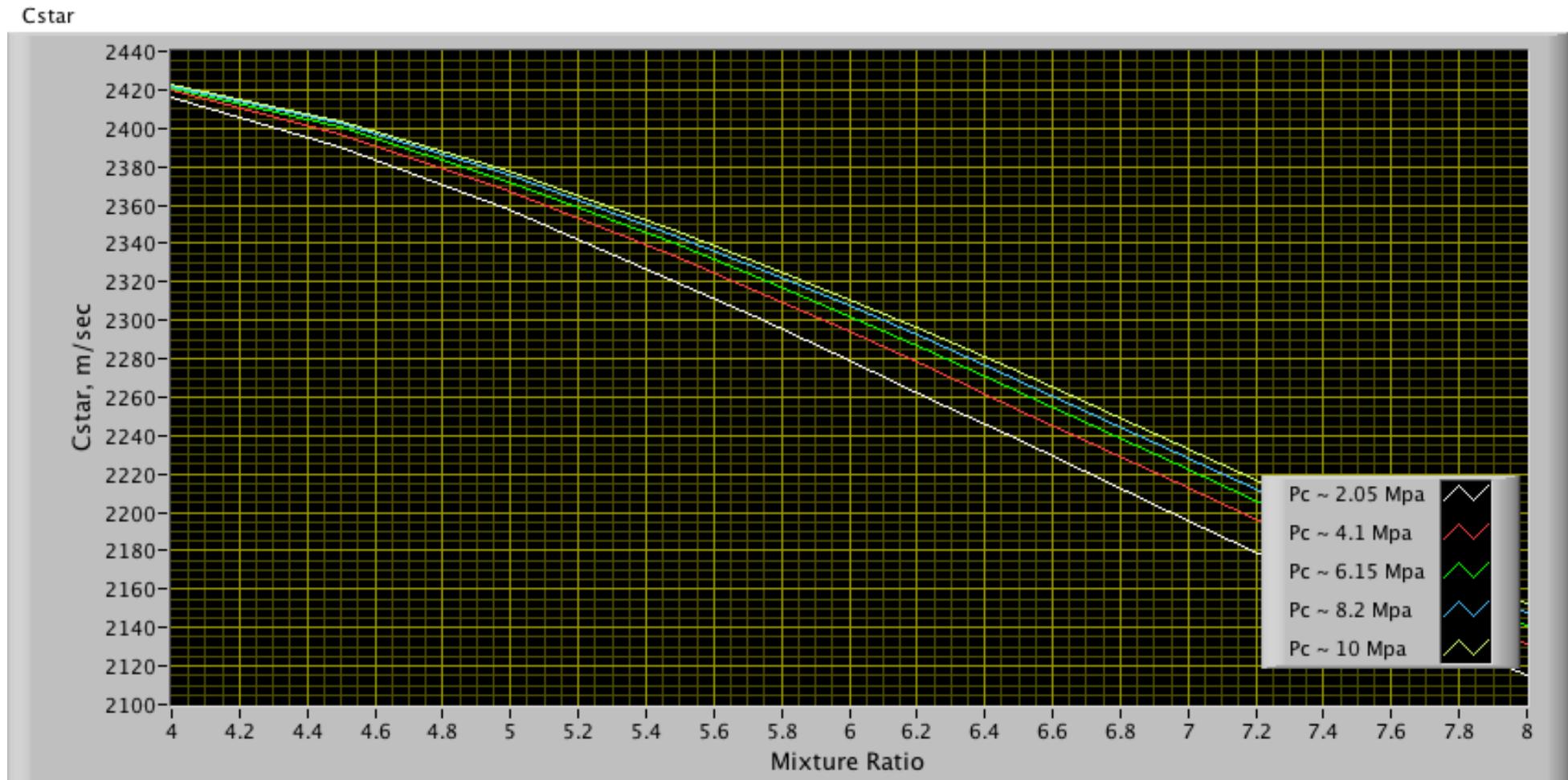
LOX/LH₂ combustion revisited (cont'd)

- CEA equilibrium calculations



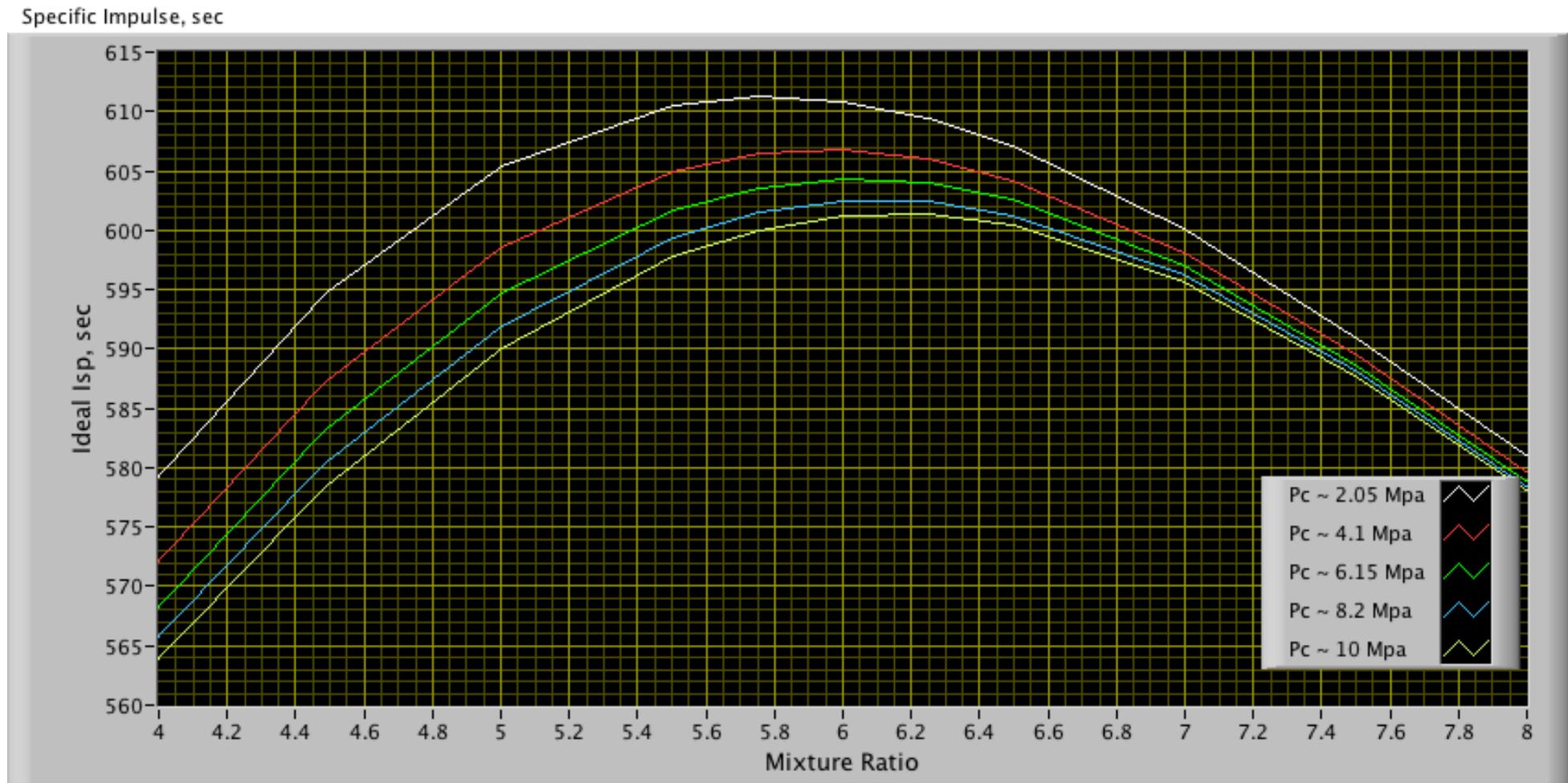
LOX/LH₂ combustion revisited (cont'd)

- CEA equilibrium calculations



LOX/LH₂ combustion revisited (cont'd)

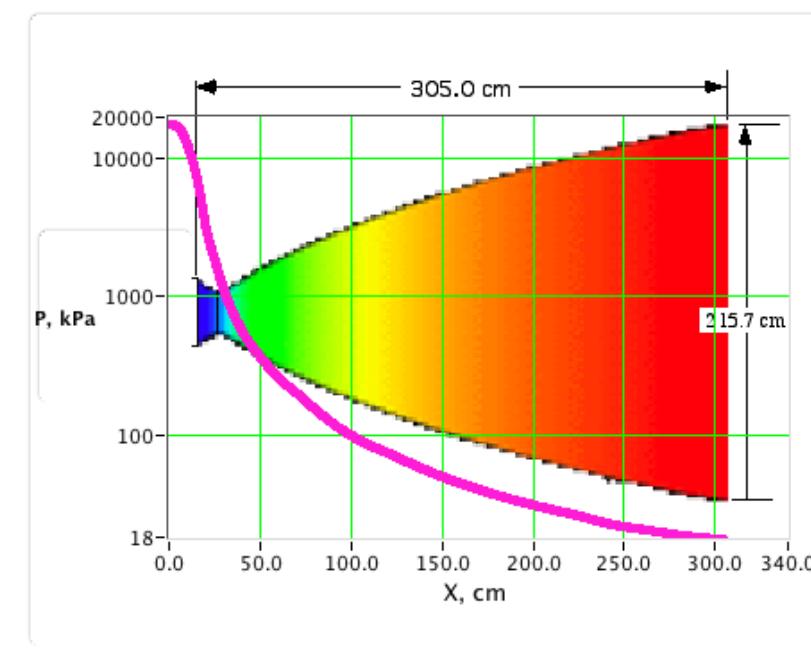
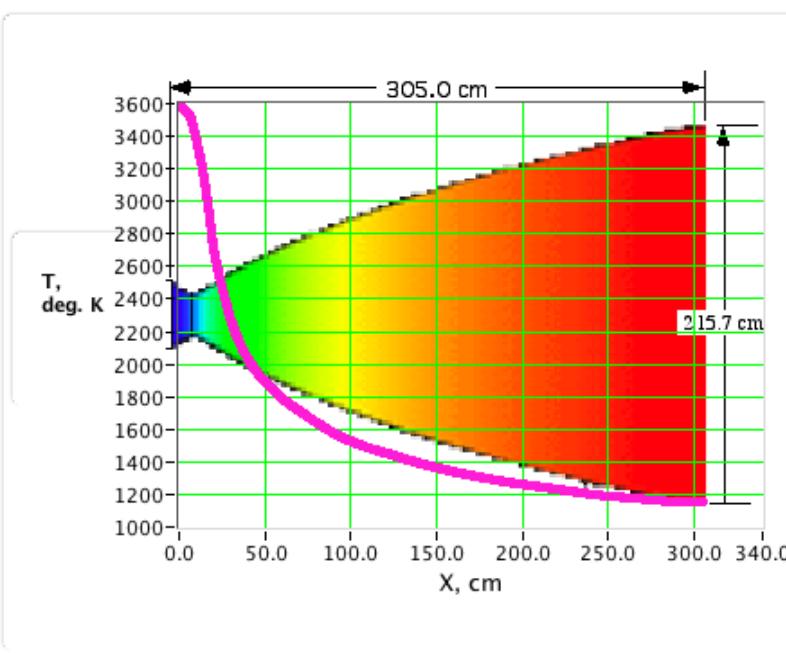
- CEA equilibrium calculations



Equilibrium versus Frozen Combustion Flow

(revisited)

- A technique that is often used for rocket analysis is “*shifting equilibrium*” ... that is the equilibrium reaction is constantly re-calculated throughout the rocket motor as the temperature and pressure drops via expansion throughout the nozzle ... basically the properties for γ , M_w , T , P ... are re-evaluated ... At each station ... by performing Gibbs analysis



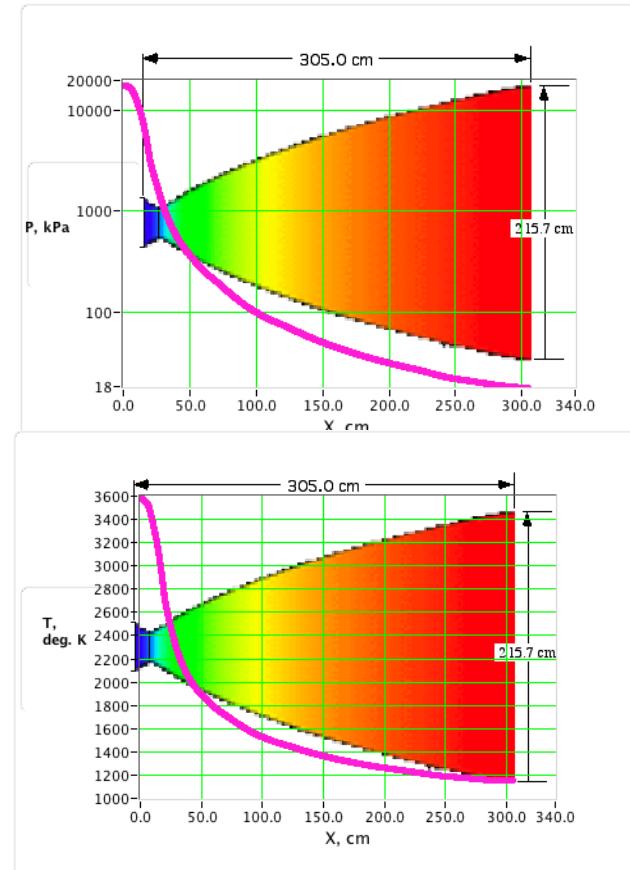
Equilibrium versus Frozen Combustion Flow

(cont'd)

- Because of the very short time the reacting flow actually spends in the Nozzle, there is much debate as to whether or not there is sufficient time for chemical reactions to actually occur as predicted by the shifting equilibrium model.
- Nozzle Geometry also plays a role, as longer nozzles provide more residence time for chemical reactions to occur.
- A common technique is to use equilibrium calculations up to the throat, and then “freeze” the mixture down stream of the throat and throughout the Nozzle
- CEA performs equilibrium analysis for combustor and throat, and also allows for frozen flow computations
- Small rockets tend to favor the frozen nozzle flow solutions; large rockets tend to be better analyzed using shifting equilibrium in the Nozzle

Shifting Equilibrium

Stagnation properties at burner



$$\gamma, M_w, T_0, P_0$$

Station A/A* downstream
In nozzle (station x)

Compute $p(x), T(x)$ based on
Current, $\gamma, M_w, \text{Combustor}$
 T_0, P_0

Given $p(x), T(x)$ compute
Gibbs free energy analysis
For species determination

Re compute γ, M_w based on
Equilibrium species concentration

Modified Ballistic Equation for Shifting Equilibrium

When “shifting equilibrium” from chamber to throat and then frozen flow at throat ... is used ... the chamber pressure equation for solid motor must be modified as ...

$$\frac{\partial P_0}{\partial t} = \frac{A_{burn} a P_o^n}{V_c} \left[\rho_p R_g T_0 - P_0 \right] - P_0 \left[\frac{A^*}{V_c} \sqrt{\gamma^* R_g^* T_0^* \left(\frac{2}{\gamma^* + 1} \right)^{\frac{\gamma^* + 1}{(\gamma^* - 1)}}} \right]$$

()* → condition at nozzle throat ... $\left\{ \gamma^*, R_g^*, T_0^*, M_w^* \right\}$

$$R_g^* = \frac{R_u}{M_w^*} \quad \gamma^* = \frac{C_p^*}{C_v^*} \quad T_0^* = T^* \cdot \left(\frac{\gamma^* + 1}{2} \right)$$

Sample CEA Calculation

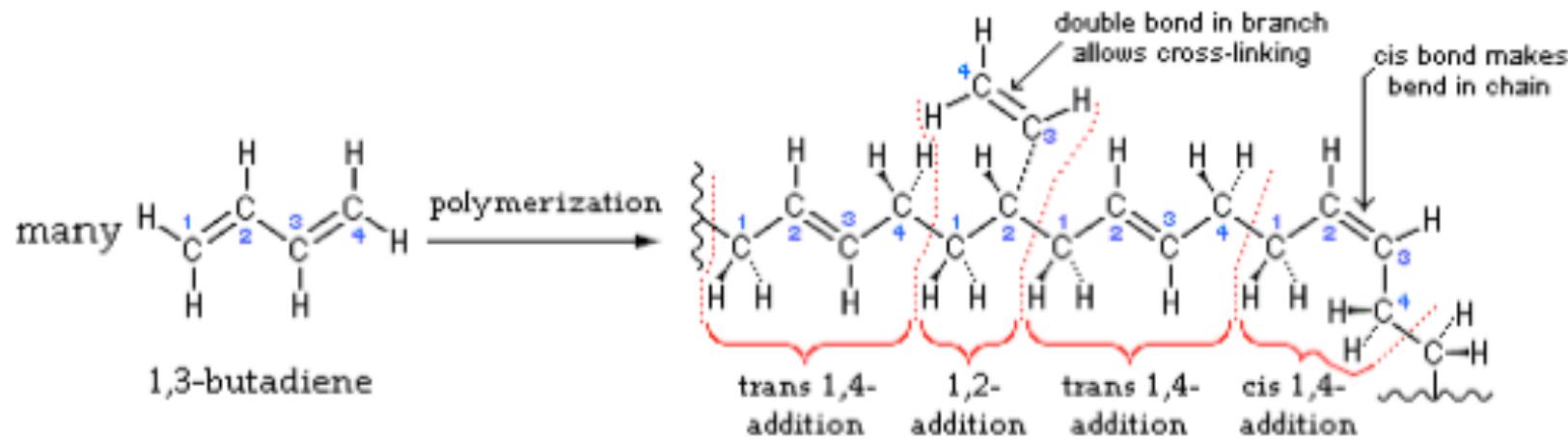
- Example for 8:5 to one Mixture ratio, Nitrous Oxide + HTPB

HTPB ... solid form $(C_4H_6)_n(OH)_2$

... A hydrocarbon butadiene molecule has two C=C double bonds

... Polybutadiene is a synthetic rubber that has a high resistance to wear and is used especially in the manufacture of tires.

... Polybutadiene can be formed from many 1,3-butadiene monomers radical polymerization to make a much longer undergoing free polymer chain molecule.



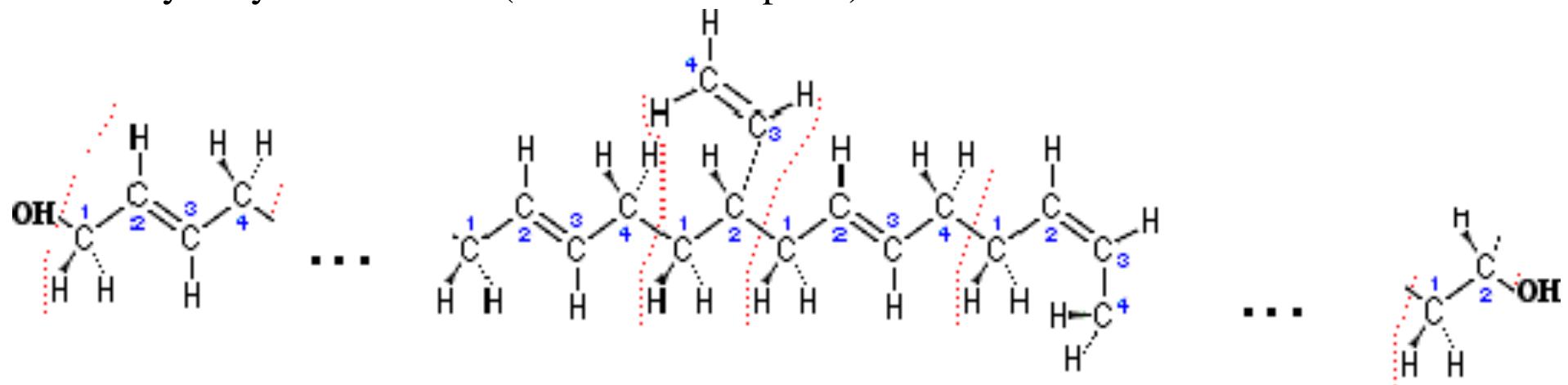
Sample CEA Calculation (cont'd)

- Example for 8:5 to one Mixture ratio, Nitrous Oxide + HTPB

HTPB ... solid form $(C_4H_6)_n(OH)_2$

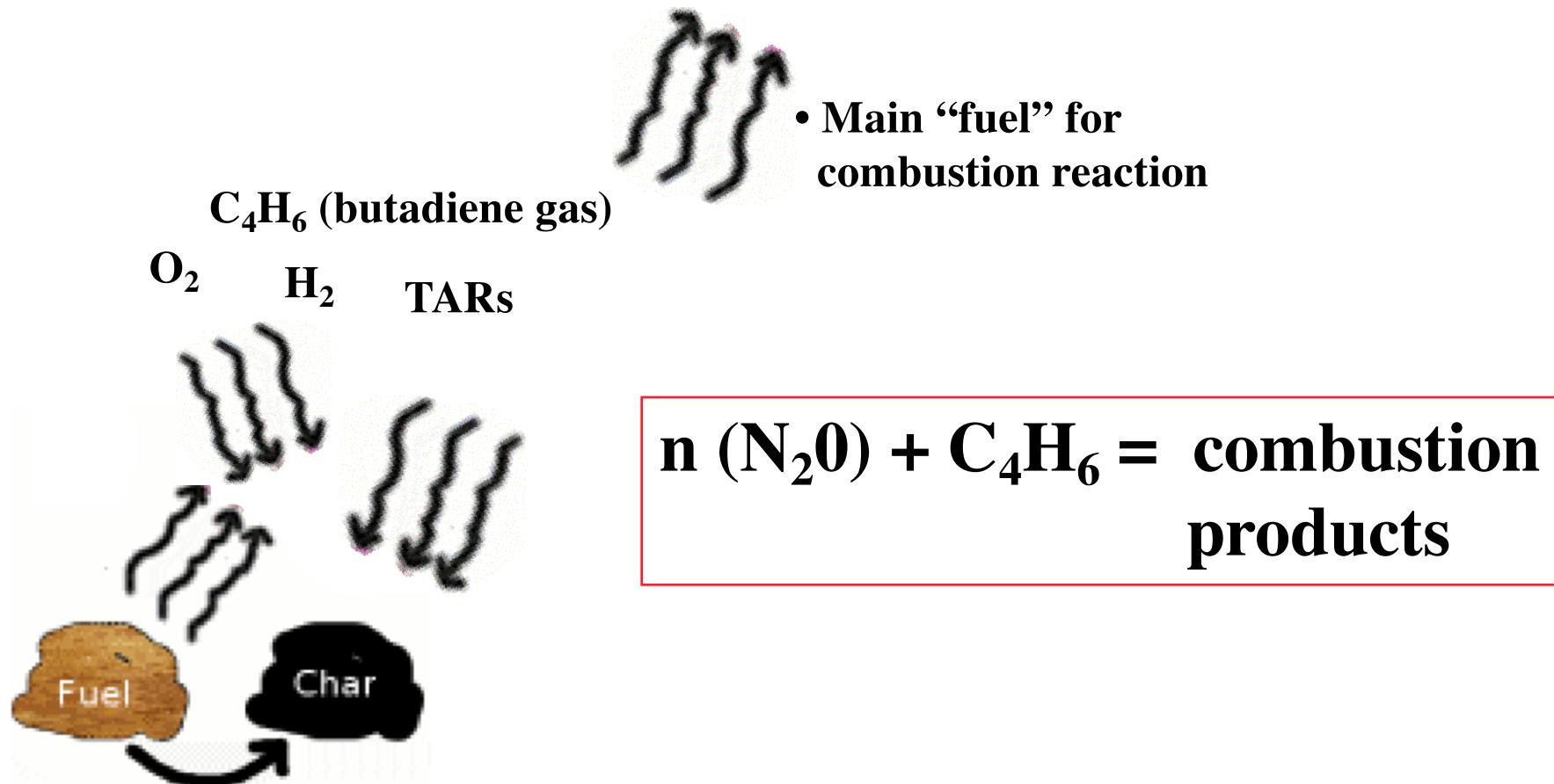
Hydroxy-terminated polybutadiene (HTPB) is a polymer of butadiene terminated at each end with a hydroxyl functional group

The effect is increased functionality of the polybutadiene on mechanical properties, thermal behavior (*lower glassification or embrittlement* temperature) and hydrolytic resistance (moisture absorption).



Sample CEA Calculation (cont'd)

- When HTPB undergoes decomposition ... that is ... it is Baked off from the solid grain core ...



Sample CEA Calculation

NASA-GLENN CHEMICAL EQUILIBRIUM PROGRAM CEA2, MAY 21, 2004

BY BONNIE MCBRIDE AND SANFORD GORDON

REFS: NASA RP-1311, PART I, 1994 AND NASA RP-1311, PART II, 1996

problem o/f=8.5, (8.5 to 1 Mixture ratio)

rocket equilibrium

p,bar=31, (reaction combustor pressure)

react

fuel=C4H6,butadiene wt=100 (fuel HTPB)

oxid=N2O wt=100 (*oxidizer, Nitrous oxide*)

end

OPTIONS: TP=F HP=F SP=F TV=F UV=F SV=F DETN=F SHOCK=F REFL=F INCD=F

RKT=T FROZ=F EQL=T IONS=F SIUNIT=T DEBUGF=F SHKDBG=F DETDBG=F TRNSPT=F

Show Input GIU Setup

Sample CEA Calculation (cont'd)

- Example for 8:5 to one Mixture ratio, Nitrous Oxide + HTPB

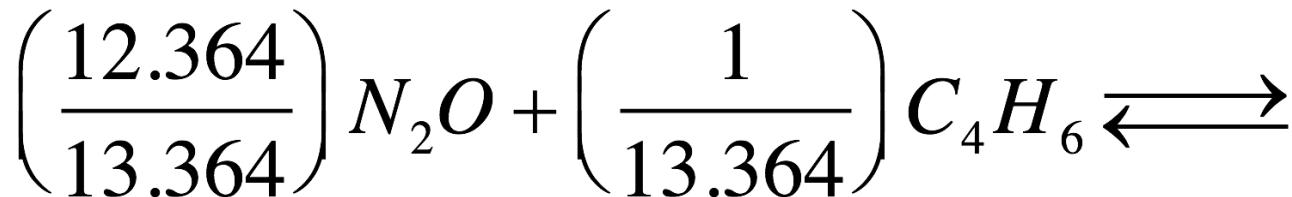
$$M_R = \frac{\dot{m}_{N_2O}}{\dot{m}_{C_4H_6}} \rightarrow \left[\begin{array}{l} \dot{moles}_{N_2O} = \frac{\dot{m}_{N_2O}}{M_{W_{N_2O}}} \\ \dot{moles}_{C_4H_6} = \frac{\dot{m}_{C_4H_6}}{M_{W_{C_4H_6}}} \end{array} \right] \rightarrow$$

$$\frac{\dot{moles}_{N_2O}}{\dot{moles}_{C_4H_6}} = \frac{\dot{m}_{N_2O}}{M_{W_{N_2O}}} \times \frac{M_{W_{C_4H_6}}}{\dot{m}_{C_4H_6}} = M_R \times \frac{\dot{m}_{C_4H_6}}{M_{W_{N_2O}}} \times \frac{M_{W_{C_4H_6}}}{\dot{m}_{C_4H_6}} =$$

$$M_R \times \frac{M_{W_{C_4H_6}}}{M_{W_{N_2O}}} \approx M_R \times \frac{4 \times 12 + 6}{2 \times 14 + 16} = 1.4545 M_R = 12.364$$

Sample CEA Calculation (cont'd)

- And the equilibrium reaction is



- Based on Gibbs free energy minimization and atomic mass balance

Species	Product Chamber	Mole fraction Throat
CO	0.06392	0.05232
CO ₂	0.15933	0.17289
H	0.00206	0.00133
HO ₂	0.00001	0.00001
H ₂	0.00840	0.00695
H ₂ O	0.15168	0.15693
NO	0.00913	0.00597
NO ₂	0.00001	0.00000
N ₂	0.57846	0.58518
O	0.00176	0.00096
OH	0.01264	0.00873
O ₂	0.01260	0.00872

Sample CEA Calculation (cont'd)

- ROCKET PERFORMANCE ASSUMING EQUILIBRIUM
- COMPOSITION DURING EXPANSION FROM INFINITE AREA COMBUSTOR

	CHAMBER	THROAT	
Pinf/P	1.0000	1.7428	Use these values for “shifting equilibrium”
P, BAR	31.000	17.787	Flow Analysis at Nozzle throat
T, K	2925.58	2744.19	
RHO, KG/CU M	3.65500	2.2555 0	
H, KJ/KG	0.00000	-454.46	
U, KJ/KG	-848.15	-1243.08	PERFORMANCE PARAMETERS (Throat)
G, KJ/KG	-26683.	9 -25484.0	
S, KJ/(KG)(K)	9.1209	9.1209	
MW, (1/n)	28.680	28.932	Ae/At
(dLV/dLP)t	-1.01044	-1.00776	1.0000
(dLV/dLT)p	1.2400	1.1912	CSTAR, M/SEC
Cp, KJ/(KG)(K)	3.1727	2.9098	1441.6
GAMMAS	1.1495	1.1526	CF
SON VEL,M/SEC	987.4	953.4	Ivac, M/SEC
MACH NUMBER	0.000	1.000	Isp, M/SEC

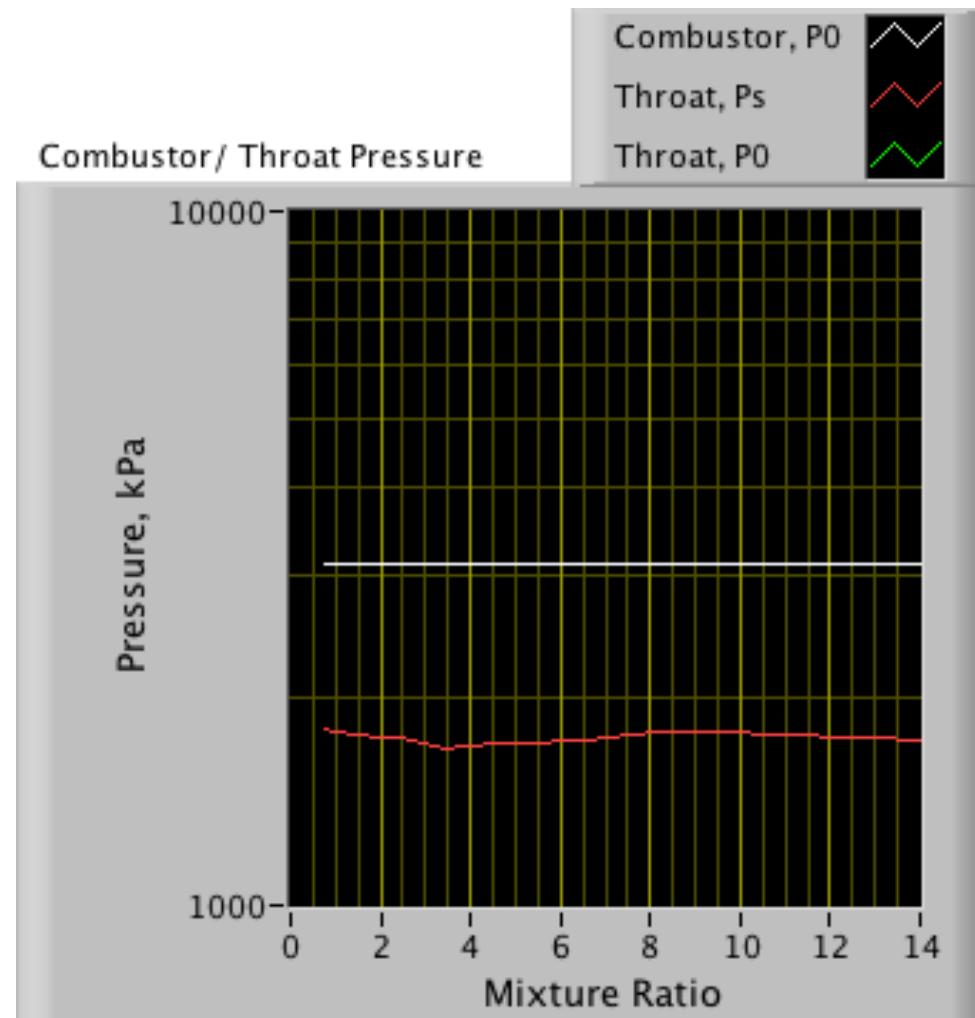
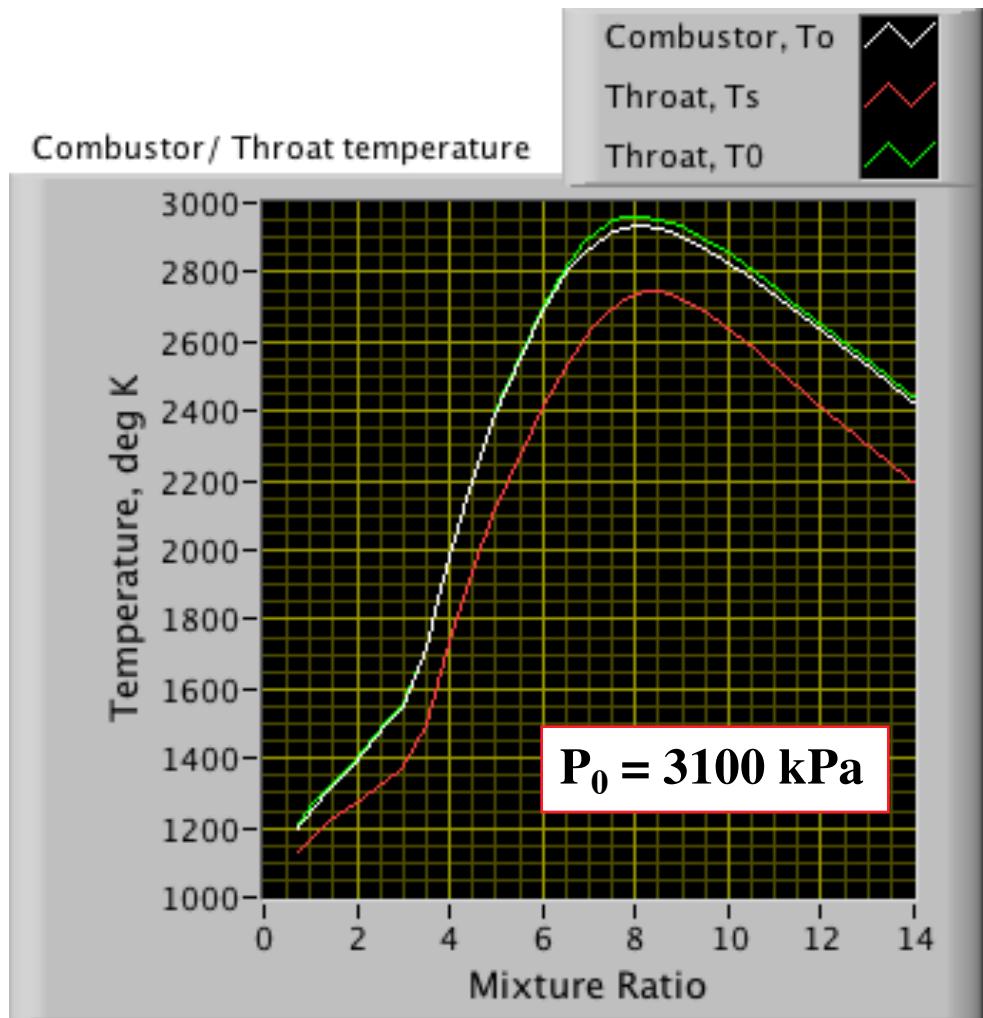
#	p	t	h	g	s	m	mw	cp	gam	mach	aeat	cf	ivac	isp
2.0500E+01	2.9000E+03	-1.2186E+03	-6.6411E+04	2.2480E+01	0.0000E+00	9.9583E+00	6.7457E+00	1.1766E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1.1612E+01	2.6710E+03	-2.5367E+03	-6.2580E+04	2.2480E+01	0.0000E+00	1.0012E+01	5.9107E+00	1.1885E+00	1.0000E+00	1.0000E+00	6.7322E-01	2.9898E+03	1.6237E+03	O/F 1
1.1612E+01	2.6710E+03	-2.5367E+03	-6.2580E+04	2.2480E+01	0.0000E+00	1.0012E+01	5.9107E+00	1.1885E+00	1.0000E+00	1.0000E+00	6.7322E-01	2.9898E+03	1.6237E+03	Pressure 1, Geometries
2.4356E+00	2.0518E+03	-5.5845E+03	-5.1709E+04	2.2480E+01	0.0000E+00	1.0074E+01	4.4844E+00	1.2296E+00	2.0477E+00	2.0000E+00	1.2252E+00	3.5281E+03	2.9550E+03	
1.2978E+00	1.8196E+03	-6.5894E+03	-4.7493E+04	2.2480E+01	0.0000E+00	1.0073E+01	4.2257E+00	1.2438E+00	2.3985E+00	3.0000E+00	1.3589E+00	3.7355E+03	3.2774E+03	
6.1260E-01	1.5650E+03	-7.6361E+03	-4.2818E+04	2.2480E+01	0.0000E+00	1.0079E+01	4.0120E+00	1.2590E+00	2.8101E+00	5.0000E+00	1.4854E+00	3.9429E+03	3.5826E+03	
3.1349E-01	1.3596E+03	-8.4433E+03	-3.9008E+04	2.2480E+01	0.0000E+00	1.0079E+01	3.8489E+00	1.2728E+00	3.1815E+00	8.0000E+00	1.5761E+00	4.0963E+03	3.8012E+03	
1.3292E-02	6.4892E+02	-1.0973E+04	-2.5560E+04	2.2480E+01	0.0000E+00	1.0079E+01	3.2900E+00	1.3346E+00	5.2256E+00	7.7500E+01	1.8314E+00	4.5381E+03	4.4169E+03	
4.1000E+01	2.9282E+03	-1.2186E+03	-6.5352E+04	2.1902E+01	0.0000E+00	9.9811E+00	6.2503E+00	1.1834E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	O/F 1
2.3173E+01	2.6859E+03	-2.5492E+03	-6.1376E+04	2.1902E+01	0.0000E+00	1.0028E+01	5.5680E+00	1.1950E+00	1.0000E+00	1.0000E+00	6.7541E-01	2.9964E+03	1.6313E+03	Pressure 2, Geometries
2.3173E+01	2.6859E+03	-2.5492E+03	-6.1376E+04	2.1902E+01	0.0000E+00	1.0028E+01	5.5680E+00	1.1950E+00	1.0000E+00	1.0000E+00	6.7541E-01	2.9964E+03	1.6313E+03	
4.8444E+00	2.0488E+03	-5.6058E+03	-5.0478E+04	2.1902E+01	0.0000E+00	1.0075E+01	4.4274E+00	1.2319E+00	2.0525E+00	2.0000E+00	1.2264E+00	3.5329E+03	2.9622E+03	
2.5810E+00	1.8154E+03	-6.6089E+03	-4.6370E+04	2.1902E+01	0.0000E+00	1.0078E+01	4.2062E+00	1.2448E+00	2.4047E+00	3.0000E+00	1.3594E+00	3.7395E+03	3.2834E+03	
1.2187E+00	1.5610E+03	-7.6525E+03	-4.1841E+04	2.1902E+01	0.0000E+00	1.0079E+01	4.0062E+00	1.2594E+00	2.8169E+00	5.0000E+00	1.4852E+00	3.9461E+03	3.5872E+03	
6.2379E-01	1.3560E+03	-8.4573E+03	-3.8156E+04	2.1902E+01	0.0000E+00	1.0079E+01	3.8456E+00	1.2731E+00	3.1885E+00	8.0000E+00	1.5754E+00	4.0989E+03	3.8049E+03	
2.6454E-02	6.4691E+02	-1.0980E+04	-2.5148E+04	2.1902E+01	0.0000E+00	1.0079E+01	3.2887E+00	1.3348E+00	5.2351E+00	7.7500E+01	1.8293E+00	4.5391E+03	4.4184E+03	
6.1500E+01	2.9424E+03	-1.2186E+03	-6.4670E+04	2.1565E+01	0.0000E+00	9.9986E+00	6.0086E+00	1.1871E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	O/F 1
3.4719E+01	2.6931E+03	-2.5554E+03	-6.0630E+04	2.1565E+01	0.0000E+00	1.0037E+01	5.4058E+00	1.1984E+00	1.0000E+00	1.0000E+00	6.7655E-01	2.9996E+03	1.6351E+03	Pressure 3, Geometries
3.4719E+01	2.6931E+03	-2.5554E+03	-6.0630E+04	2.1565E+01	0.0000E+00	1.0037E+01	5.4058E+00	1.1984E+00	1.0000E+00	1.0000E+00	6.7655E-01	2.9996E+03	1.6351E+03	
7.2474E+00	2.0472E+03	-5.6161E+03	-4.9763E+04	2.1565E+01	0.0000E+00	1.0076E+01	4.4025E+00	1.2330E+00	2.0549E+00	2.0000E+00	1.2270E+00	3.5353E+03	2.9656E+03	
3.8612E+00	1.8134E+03	-6.6181E+03	-4.5723E+04	2.1565E+01	0.0000E+00	1.0079E+01	4.1977E+00	1.2453E+00	2.4077E+00	3.0000E+00	1.3597E+00	3.7414E+03	3.2862E+03	
1.8235E+00	1.5591E+03	-7.6603E+03	-4.1281E+04	2.1565E+01	0.0000E+00	1.0079E+01	4.0037E+00	1.2596E+00	2.8201E+00	5.0000E+00	1.4851E+00	3.9477E+03	3.5894E+03	
9.3344E-01	1.3543E+03	-8.4640E+03	-3.7668E+04	2.1565E+01	0.0000E+00	1.0079E+01	3.8440E+00	1.2732E+00	3.1918E+00	8.0000E+00	1.5750E+00	4.1001E+03	3.8067E+03	
3.9591E-02	6.4596E+02	-1.0983E+04	-2.4913E+04	2.1565E+01	0.0000E+00	1.0079E+01	3.2881E+00	1.3349E+00	5.2396E+00	7.7500E+01	1.8284E+00	4.5396E+03	4.4191E+03	
8.2000E+01	2.9515E+03	-1.2186E+03	-6.4160E+04	2.1325E+01	0.0000E+00	1.0007E+01	5.8566E+00	1.1896E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	O/F 1
4.6257E+01	2.6975E+03	-2.5594E+03	-6.0085E+04	2.1325E+01	0.0000E+00	1.0042E+01	5.3057E+00	1.2006E+00	1.0000E+00	1.0000E+00	6.7729E-01	3.0015E+03	1.6376E+03	Pressure 4, Geometries
4.6257E+01	2.6975E+03	-2.5594E+03	-6.0085E+04	2.1325E+01	0.0000E+00	1.0042E+01	5.3057E+00	1.2006E+00	1.0000E+00	1.0000E+00	6.7729E-01	3.0015E+03	1.6376E+03	
9.6473E+00	2.0462E+03	-5.6224E+03	-4.9259E+04	2.1325E+01	0.0000E+00	1.0077E+01	4.3878E+00	1.2336E+00	2.0564E+00	2.0000E+00	1.2274E+00	3.5367E+03	2.9678E+03	
5.1400E+00	1.8122E+03	-6.6238E+03	-4.5269E+04	2.1325E+01	0.0000E+00	1.0079E+01	4.1927E+00	1.2455E+00	2.4095E+00	3.0000E+00	1.3598E+00	3.7426E+03	3.2879E+03	
2.4276E+00	1.5579E+03	-7.6651E+03	-4.0887E+04	2.1325E+01	0.0000E+00	1.0079E+01	4.0021E+00	1.2597E+00	2.8221E+00	5.0000E+00	1.4851E+00	3.9486E+03	3.5907E+03	
1.2428E+00	1.3532E+03	-8.4681E+03	-3.7326E+04	2.1325E+01	0.0000E+00	1.0079E+01	3.8431E+00	1.2733E+00	3.1939E+00	8.0000E+00	1.5749E+00	4.1009E+03	3.8078E+03	
5.2714E-02	6.4538E+02	-1.0985E+04	-2.4748E+04	2.1325E+01	0.0000E+00	1.0079E+01	3.2877E+00	1.3349E+00	5.2424E+00	7.7500E+01	1.8279E+00	4.5400E+03	4.4195E+03	
1.0000E+01	2.8656E+03	-1.2186E+03	-6.7356E+04	2.3080E+01	0.0000E+00	9.9258E+00	7.3793E+00	1.1691E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	
5.6795E+00	2.6514E+03	-2.5215E+03	-6.3716E+04	2.3080E+01	0.0000E+00	9.9899E+00	6.3669E+00	1.1809E+00	1.0000E+00	1.0000E+00	6.7067E-01	2.9813E+03	1.6143E+03	
5.6795E+00	2.6514E+03	-2.5215E+03	-6.3716E+04	2.3080E+01	0.0000E+00	9.9899E+00	6.3669E+00	1.1809E+00	1.0000E+00	1.0000E+00	6.7067E-01	2.9813E+03	1.6143E+03	
1.1968E+00	2.0555E+03	-5.5562E+03	-5.2997E+04	2.3080E+01	0.0000E+00	1.0071E+01	4.5698E+00	1.2262E+00	2.0418E+00	2.0000E+00	1.2237E+00	3.5215E+03	2.9454E+03	

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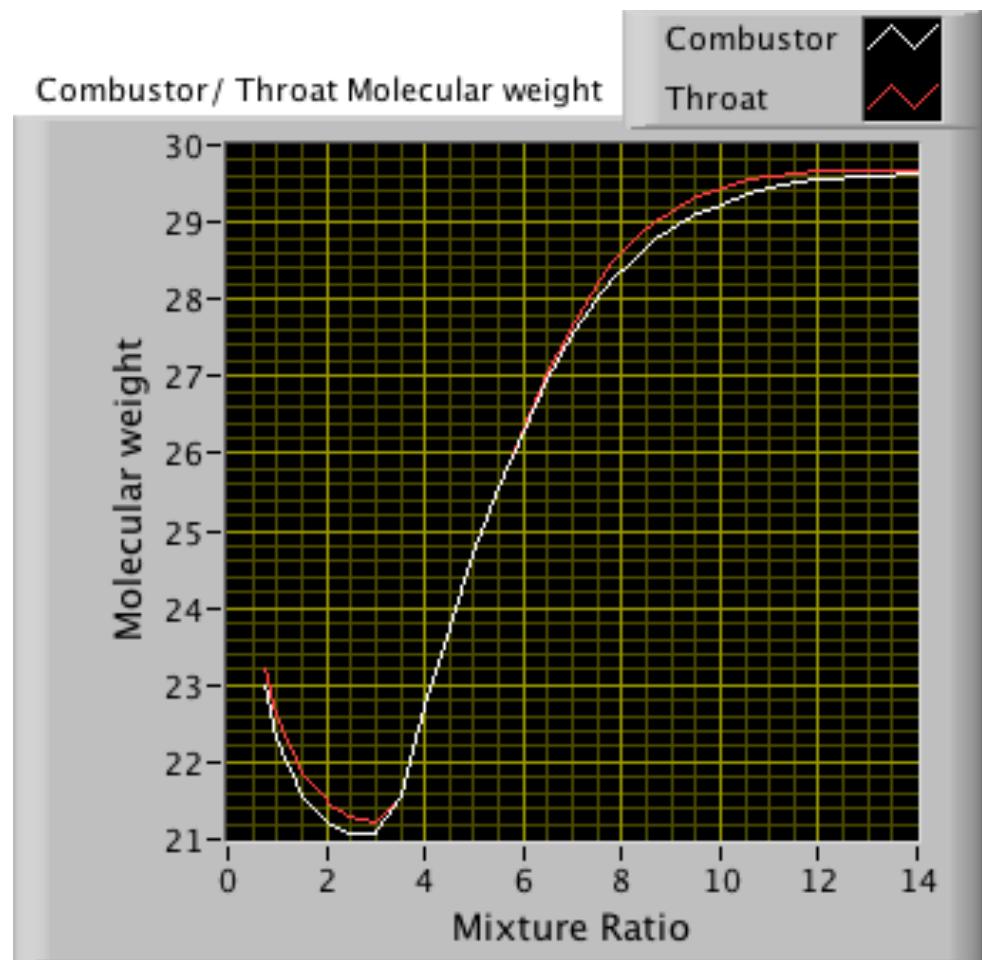
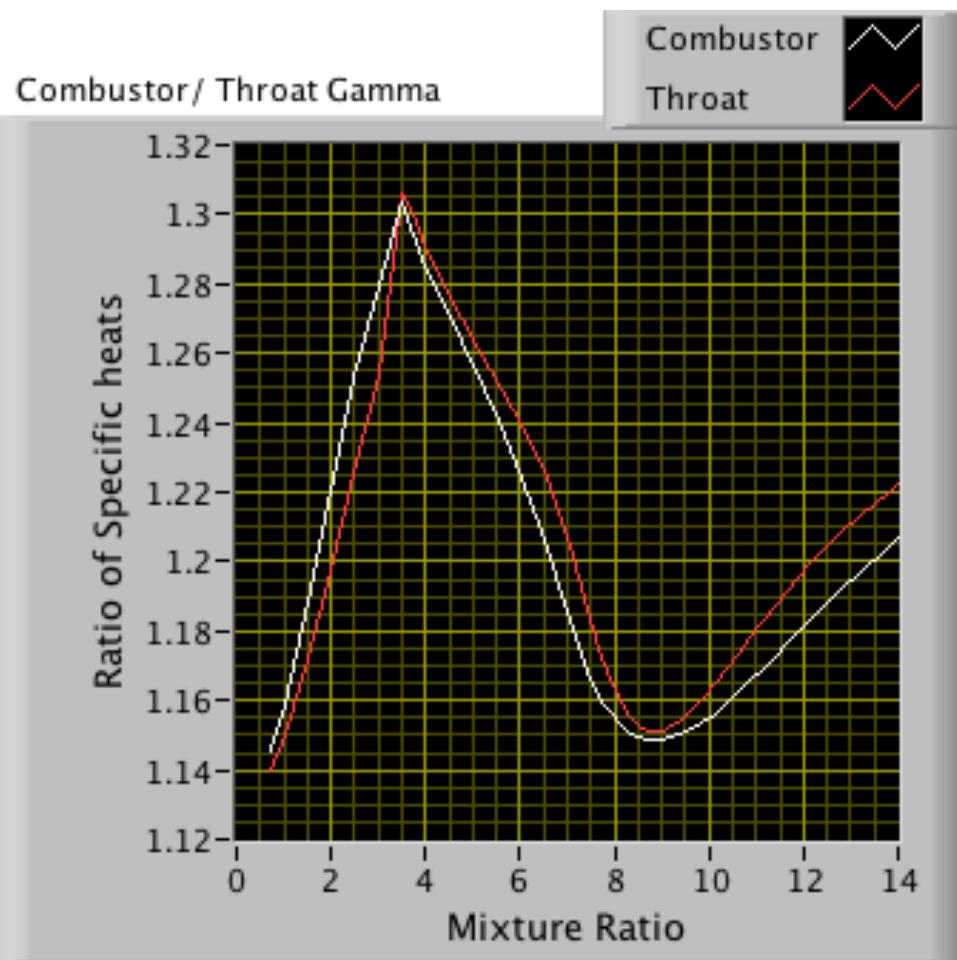
Sample CEA Calculation (cont'd)

- Combustion Properties



Sample CEA Calculation (cont'd)

- Combustion Product Properties



Sample CEA Calculation (cont'd)

- Combustion Performance Properties

