Rocket Propulsion

Reacting Flow Issues

Combustor Calculations

- $c^* \propto (T_o/MW)^{1/2}$
- Must include effect of product dissociation for rocket chamber calculations
  - will decrease T_o and reduce MW
- Peform **adiabatic flame temperature** calculation with full equilibrium products
  - pressure = chamber pressure
  - total enthalpy unchanged

Equivalence Ratio

- In rockets, common to present initial conditions in terms of **O/F ratio** (oxidizer to fuel) **=1/*f*** *fuel/oxidizer*
  - usually **mass** oxidizer/mass fuel
  - or **moles** fuel/moles oxidizer
- **Equivalence ratio** used by combustion engineers

$$\phi = f_{actual}/f_{stoichiometric}$$

  - ϕ = 1; **stoichiometric**
    - just enough oxidizer to **completely consume** fuel
  - ϕ < 1; **fuel lean** (excess ox.)
  - ϕ > 1; **fuel rich** (excess fuel)

H_2 Example

$$\_\_\,H_2 + \_\_\,O_2 \rightarrow \_\_\,H_2O$$

LHS ***RHS***

Stoichiometric Mixture: Hydrocarbon-O_2 Example

- Determine major products (stable, low energy)

$$C_xH_y + aO_2 \rightarrow xCO_2 + y/2\,H_2O$$

- Required (stoich.) amount of oxidizer
  - atom balances (mass conservation)

$$a = \quad x + y/4$$

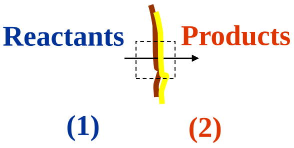
- In terms of ϕ

$$?C_xH_y + aO_2 \rightarrow$$

$$\phi = \frac{f_{actual}}{f_{stoich}} = \frac{?/a}{1/a} \Rightarrow ? = \phi \qquad \phi C_xH_y + aO_2 \rightarrow$$

Adiabatic Flame Temperature (T_{ad})

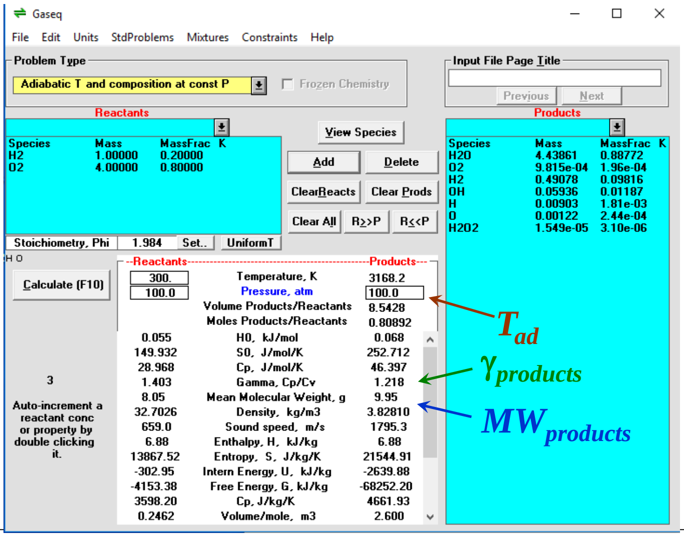
- Equilibrium temperature that would be achieved if
  - reactants converted to equilibrium products
  - without heat addition/loss or work
  - for constant pressure
  - steady



$$\dot{m}h_1 = \dot{m}h_2$$

$$h_1 = h_2$$

Example Method – Gaseq



Problem Type: Adiabatic T and composition at const P

☐ Frozen Chemistry

Input File Page Title

Reactants

Species	Mass	MassFrac	K
H2	1.00000	0.20000	
O2	4.00000	0.80000	

Stoichiometry, Phi 1.984

H O

Products

Species	Mass	MassFrac	K
H2O	4.43861	0.88772	
O2	9.815e-04	1.96e-04	
H2	0.49078	0.09816	
OH	0.05936	0.01187	
H	0.00903	1.81e-03	
O	0.00122	2.44e-04	
H2O2	1.549e-05	3.10e-06	

--Reactants--		--Products---
300.	Temperature, K	3168.2
100.0	Pressure, atm	100.0
	Volume Products/Reactants	8.5428
	Moles Products/Reactants	0.80892
0.055	H0, kJ/mol	0.068
149.932	S0, J/mol/K	252.712
28.968	Cp, J/mol/K	46.397
1.403	Gamma, Cp/Cv	1.218
8.05	Mean Molecular Weight, g	9.95
32.7026	Density, kg/m3	3.82810
659.0	Sound speed, m/s	1795.3
6.88	Enthalpy, H, kJ/kg	6.88
13867.52	Entropy, S, J/kg/K	21544.91
-302.95	Intern Energy, U, kJ/kg	-2639.88
-4153.38	Free Energy, G, kJ/kg	-68252.20
3598.20	Cp, J/kg/K	4661.93
0.2462	Volume/mole, m3	2.600

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Auto-increment a reactant conc or property by double clicking it.

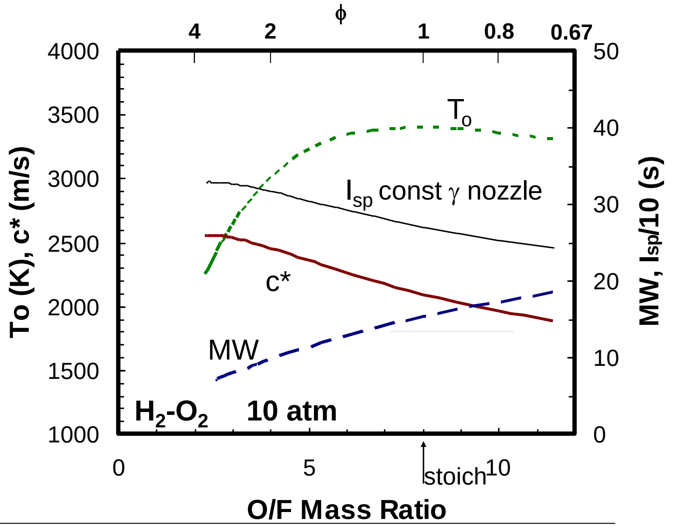
T_{ad}

$\gamma_{products}$

$MW_{products}$

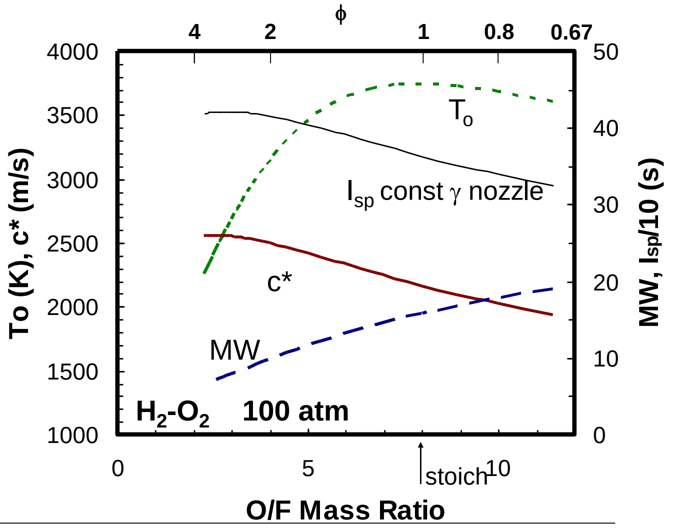
Equilibrium Combustor Chemistry

- T_{ad} peaks near stoichiometric mixture
- Peak in c^* (and I_{sp}) for rich mixture
- Why?



Pressure Effects

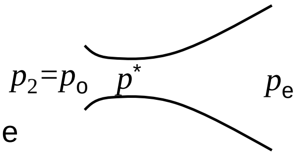
- Raise p, higher T_{ad} (less dissociation)
- Also increases MW
- Slightly higher c^*
- I_{sp} higher for same p_e

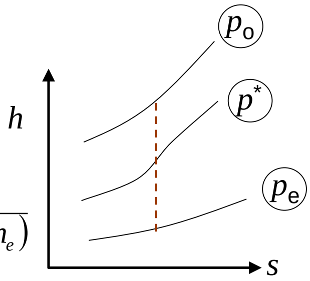


Nozzle Chemistry

- What happens to chemical composition in nozzle?
- As velocity increases
  - temperature and pressure decrease
  - will lead to change in composition

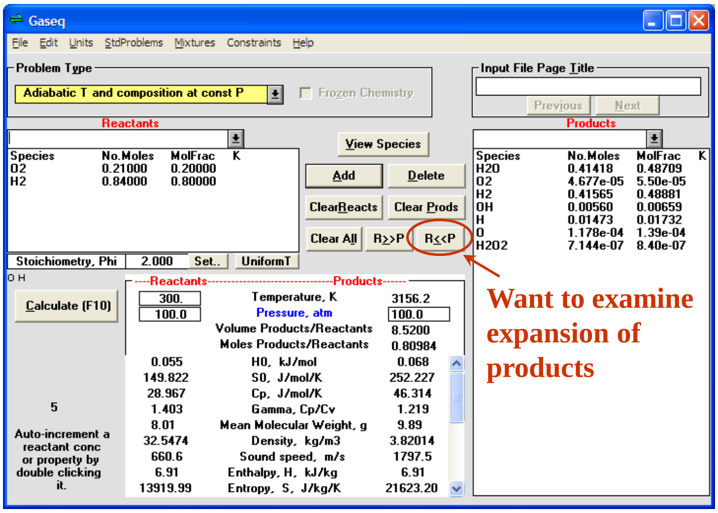
Isentropic Expansion





- Constant γ is a very poor assumption for high temperature rocket product gases
  - can't use $p/p_o = (T/T_o)^{\gamma/\gamma-1}$
  - even worse assumption if gas is reacting
- Can still calculate **isentropic** nozzle expansion for two cases
  - flow stays in **equilibrium** through nozzle (***shifting equil.***)
  - flow is **frozen** – composition can not change
  - find h that matches given p and s
  - from energy conserv. $u_e = \sqrt{2(h_o - h_e)}$

Example Method – Gaseq



Problem Type: Adiabatic T and composition at const P

☐ Frozen Chemistry

Input File Page Title

Reactants

Species	No.Moles	MolFrac	K
O2	0.21000	0.20000	
H2	0.84000	0.80000	

Stoichiometry, Phi 2.000

O H

Products

Species	No.Moles	MolFrac	K
H2O	0.41418	0.48709	
O2	4.677e-05	5.50e-05	
H2	0.41565	0.48881	
OH	0.00560	0.00659	
H	0.01473	0.01732	
O	1.178e-04	1.39e-04	
H2O2	7.144e-07	8.40e-07	

----Reactants----		----Products------
300.	Temperature, K	3156.2
100.0	Pressure, atm	100.0
	Volume Products/Reactants	8.5200
	Moles Products/Reactants	0.80984
0.055	H0, kJ/mol	0.068
149.822	S0, J/mol/K	252.227
28.967	Cp, J/mol/K	46.314
1.403	Gamma, Cp/Cv	1.219
8.01	Mean Molecular Weight, g	9.89
32.5474	Density, kg/m3	3.82014
660.6	Sound speed, m/s	1797.5
6.91	Enthalpy, H, kJ/kg	6.91
13919.99	Entropy, S, J/kg/K	21623.20

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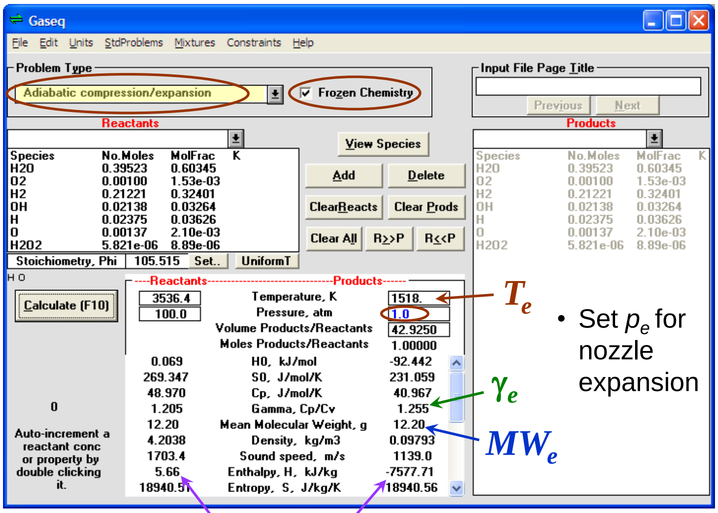
Auto-increment a reactant conc or property by double clicking it.

Want to examine expansion of products

Rocket Thermochemistry-12

Example – Frozen Chemistry



Problem Type: Adiabatic compression/expansion

☑ Frozen Chemistry

Input File Page Title

Reactants

Species	No.Moles	MolFrac	K
H2O	0.39523	0.60345	
O2	0.00100	1.53e-03	
H2	0.21221	0.32401	
OH	0.02138	0.03264	
H	0.02375	0.03626	
O	0.00137	2.10e-03	
H2O2	5.821e-06	8.89e-06	

Stoichiometry, Phi 105.515

H O

Products

Species	No.Moles	MolFrac	K
H2O	0.39523	0.60345	
O2	0.00100	1.53e-03	
H2	0.21221	0.32401	
OH	0.02138	0.03264	
H	0.02375	0.03626	
O	0.00137	2.10e-03	
H2O2	5.821e-06	8.89e-06	

----Reactants----		----Products------
3536.4	Temperature, K	1518.
100.0	Pressure, atm	1.0
	Volume Products/Reactants	42.9250
	Moles Products/Reactants	1.00000
0.069	H0, kJ/mol	-92.442
269.347	S0, J/mol/K	231.059
48.970	Cp, J/mol/K	40.967
1.205	Gamma, Cp/Cv	1.255
12.20	Mean Molecular Weight, g	12.20
4.2038	Density, kg/m3	0.09793
1703.4	Sound speed, m/s	1139.0
5.66	Enthalpy, H, kJ/kg	-7577.71
18940.5	Entropy, S, J/kg/K	18940.56

0

Auto-increment a reactant conc or property by double clicking it.

T_e

γ_e

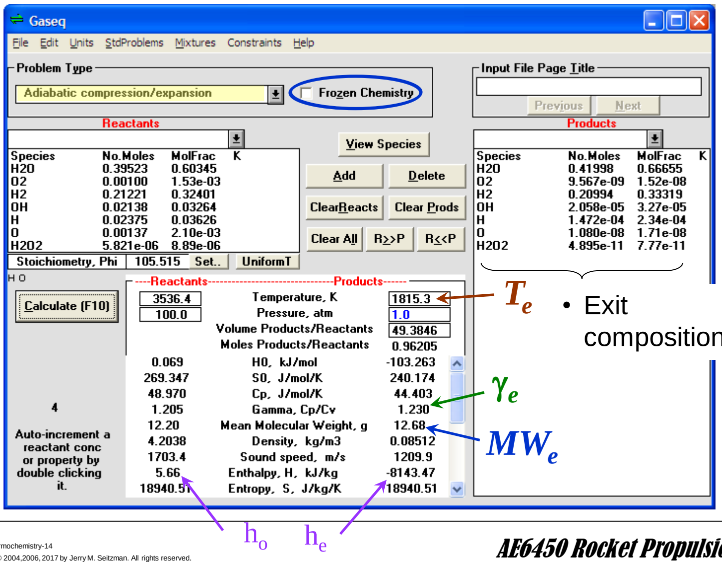
MW_e

h_o h_e

- Set p_e for nozzle expansion

Rocket Thermochemistry-13

Example – Shifting Equilibrium



Problem Type: Adiabatic compression/expansion

☐ Frozen Chemistry

Reactants

Species	No.Moles	MolFrac	K
H2O	0.39523	0.60345	
O2	0.00100	1.53e-03	
H2	0.21221	0.32401	
OH	0.02138	0.03264	
H	0.02375	0.03626	
O	0.00137	2.10e-03	
H2O2	5.821e-06	8.89e-06	

Products

Species	No.Moles	MolFrac	K
H2O	0.41998	0.66655	
O2	9.567e-09	1.52e-08	
H2	0.20994	0.33319	
OH	2.058e-05	3.27e-05	
H	1.472e-04	2.34e-04	
O	1.080e-08	1.71e-08	
H2O2	4.895e-11	7.77e-11	

Stoichiometry, Phi 105.515

H O

Reactants		Products
3536.4	Temperature, K	1815.3
100.0	Pressure, atm	1.0
	Volume Products/Reactants	49.3846
	Moles Products/Reactants	0.96205
0.069	H0, kJ/mol	-103.263
269.347	S0, J/mol/K	240.174
48.970	Cp, J/mol/K	44.403
1.205	Gamma, Cp/Cv	1.230
12.20	Mean Molecular Weight, g	12.68
4.2038	Density, kg/m3	0.08512
1703.4	Sound speed, m/s	1209.9
5.66	Enthalpy, H, kJ/kg	-8143.47
18940.51	Entropy, S, J/kg/K	18940.51

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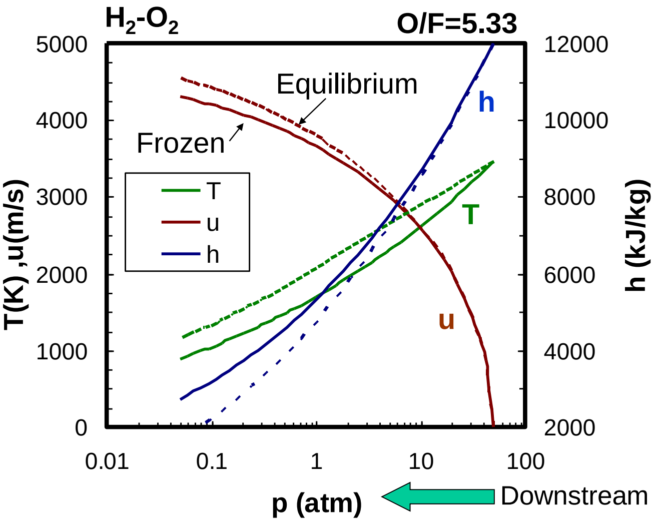
Auto-increment a reactant conc or property by double clicking it.

- Exit composition

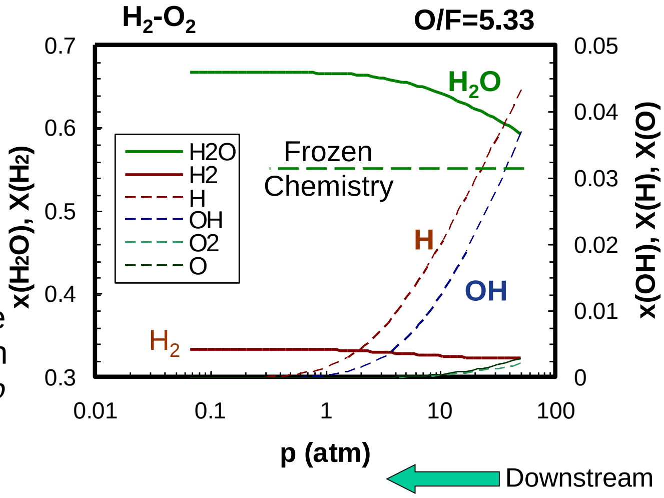
Frozen and Shifting Equilibrium

- Both cases have same entropy
- *T* drops faster for frozen flow
- u_e (I_{sp}) lower for frozen flow



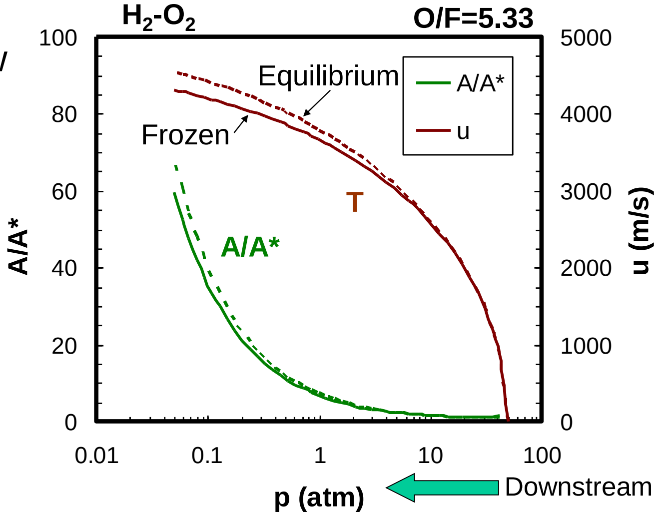
Shifting Equilibrium Chemistry

- As *T* drops, minor species recombine (H,OH)
- Chemical energy converted to thermal energy
- *T* does not have to drop as much to reach same *p* (c_p effectively higher)



Area Ratio

- Frozen flow requires larger expansion ratio to achieve same p_e



Nonequilibrium Nozzle Flow

- For adiabatic nozzles, I_{sp} will fall between the **frozen and equilibrium limits** ⇒ not isentropic! – **nonequilibrium flow**
  - – chemistry isn't so fast compared to nozzle expansion rate, so composition can't stay in equilibrium, but not so slow to be frozen
    - τ_{chem} vs. τ_{flow}
  - – tends to get more frozen later in the nozzle colder & lower p⇒ low reaction rates ⇒ τ_{chem} long AND velocity high ⇒ τ_{flow} short
- Can solve nonequilibrium by
  - – including RATES in conservation/flow equations