

# 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
- Perform **adiabatic flame temperature** calculation with full equilibrium products
  - pressure = chamber pressure
  - total enthalpy unchanged

## Example Method – Gaseq

**Reactants**

Species	Mass	MassFrac	K
H2	1.00000	0.20000	
O2	4.00000	0.80000	

**Products**

Species	Mass	MassFrac	K
H2O	4.43861	0.88772	
O2	9.815e-04	1.96e-04	
H2	0.43078	0.09316	
OH	0.05336	0.01187	
H	0.00903	1.81e-03	
O	0.00122	2.44e-04	
H2O2	1.549e-05	3.10e-06	

**Thermodynamic Properties**

Property	Reactants	Products
Temperature, K	300.0	3168.2
Pressure, atm	100.0	100.0
Volume Products/Reactants		8.5428
Moles Products/Reactants		0.80892
H0, kJ/mol	0.055	0.068
S0, J/mol/K	149.932	252.712
Cp, J/mol/K	28.968	46.397
Gamma, Cp/Cv	1.403	1.218
Mean Molecular Weight, g	8.05	9.95
Density, kg/m3	32.7026	3.82810
Sound speed, m/s	659.0	1795.3
Enthalpy, H, kJ/kg	6.88	6.88
Entropy, S, J/kg/K	13867.52	21544.91
Intern Energy, U, kJ/kg	-302.95	-2639.88
Free Energy, G, kJ/kg	-4153.38	-68252.20
Cp, J/kg/K	3598.20	4661.93
Volume/mole, m3	0.2462	2.600

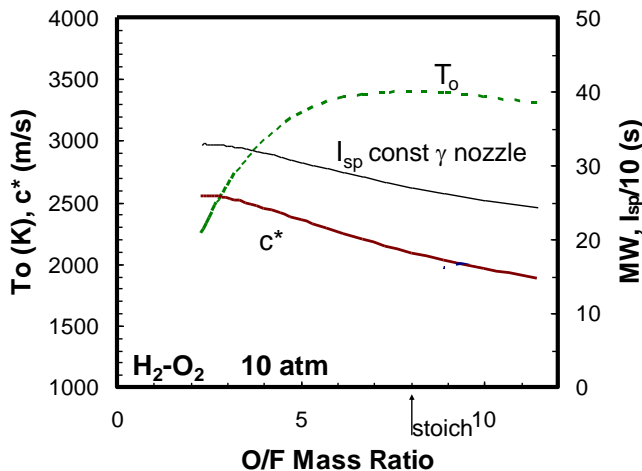
Annotations:  $T_{ad}$  (Temperature),  $\gamma_{products}$  (Gamma),  $MW_{products}$  (Mean Molecular Weight).

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## Equilibrium Combustor Chemistry

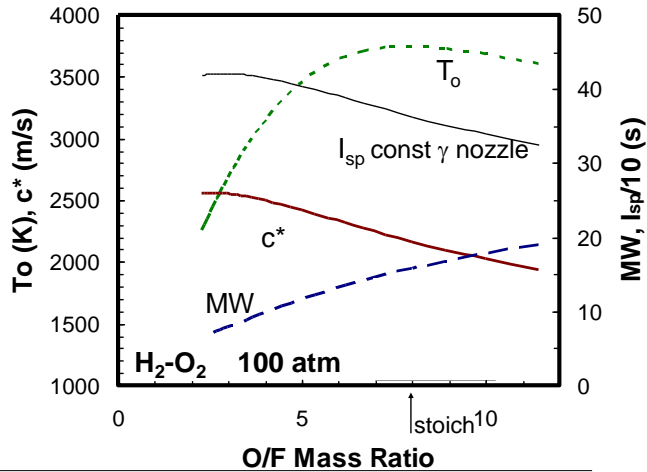
- Peak in  $T_{ad}$  near stoichiometric mixture
- Peak in  $c^*$  (&  $I_{sp} \propto c^* c_r$ ) for rich mixture?

low MW!



## Pressure Effects

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



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## Nozzle Chemistry

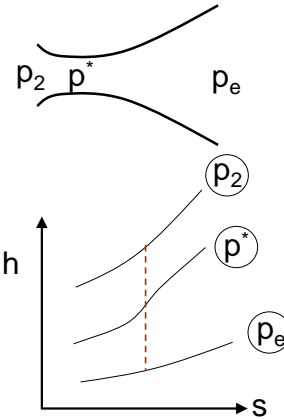
- What happens to chemical composition in nozzle?
- As velocity increases
  - temperature and pressure decrease
  - will lead to change in composition

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## Isentropic Expansion

- Constant  $\gamma$  is a very poor assumption for high temperature rocket product gases
  - can't use  $p/p_0 = (T/T_0)^{\gamma/\gamma-1}$
  - 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  $h$  (and thus  $u$ ) that matches given  $p$  and  $s$



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## Example Method – Gaseq

Species	No. Moles	Mol frac	K
O2	0.21000	0.20000	
H2	0.84000	0.80000	

Species	No. Moles	Mol frac	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	1.35e-04	
H2O2	7.144e-07	8.40e-07	

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## Example – Frozen Chemistry

Problem Type: Adiabatic compression/expansion, **Frozen Chemistry**

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	

Species	No. Moles	MolFrac	K
H2O	0.39523	0.60345	
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H2O2	5.821e-06	8.89e-06	

Property	Reactants	Products
Temperature, K	3536.4	1518
Pressure, atm	100.0	1.0
Volume Products/Reactants		42.9250
Moles Products/Reactants		1.00000
H0, kJ/mol	0.069	-92.442
S0, J/mol/K	269.347	231.059
Cp, J/mol/K	48.970	40.967
Gamma, Cp/Cv	1.205	1.255
Mean Molecular Weight, g	12.20	12.20
Density, kg/m3	4.2038	0.09793
Sound speed, m/s	1703.4	1139.0
Enthalpy, H, kJ/kg	5.66	-7577.71
Entropy, S, J/kg/K	18940.51	18940.56

Annotations:  $T_e$  (Temperature),  $Y_e$  (Mole fraction),  $MW_e$  (Mean Molecular Weight).  $h_o$  and  $h_e$  are also indicated.

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## Example – Shifting Equilibrium

Problem Type: Adiabatic compression/expansion, **Frozen Chemistry**

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	

Species	No. Moles	MolFrac	K
H2O	0.41998	0.66695	
O2	9.567e-09	1.52e-08	
H2	0.20994	0.33319	
OH	2.098e-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	

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

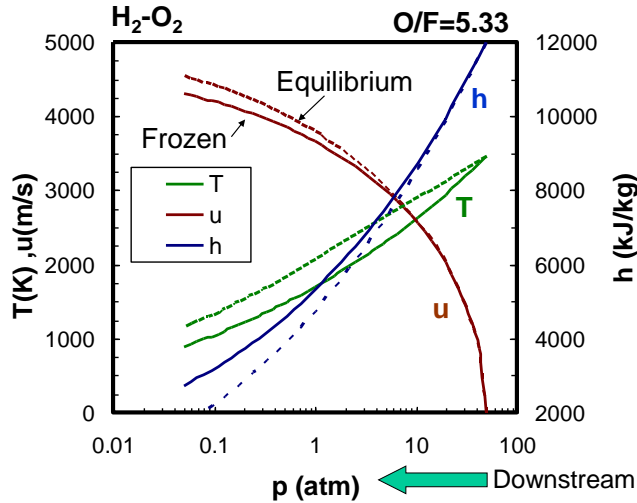
Annotations:  $T_e$  (Temperature),  $Y_e$  (Mole fraction),  $MW_e$  (Mean Molecular Weight).  $h_o$  and  $h_e$  are also indicated.

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## Frozen and Shifting Equilibrium

- Both cases have same entropy
- T drops faster for frozen flow
- $u_e$  (Isp) lower for frozen flow

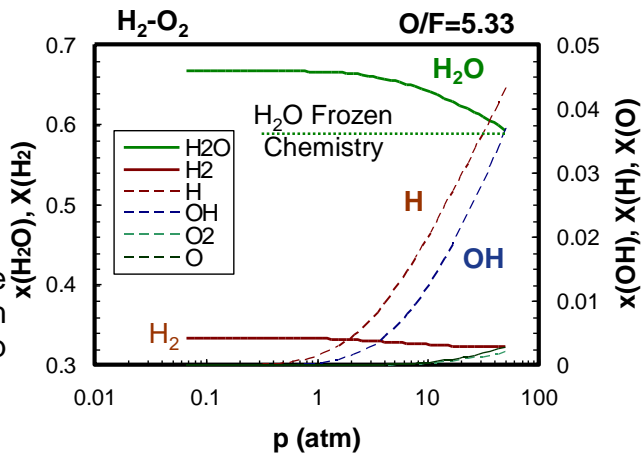


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## Shifting Equilibrium Composition

- 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)

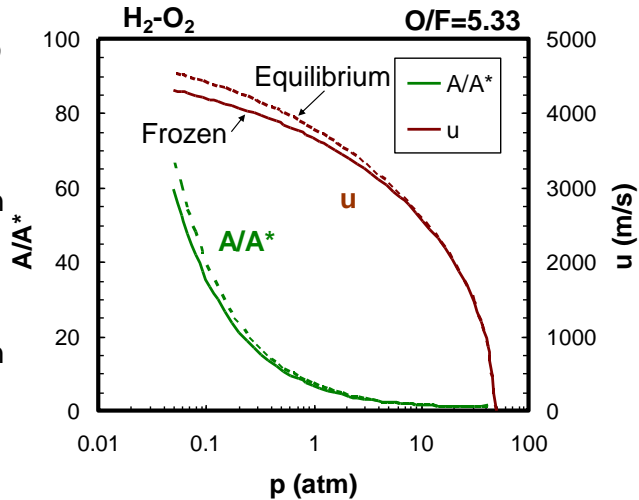


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## Area Ratio

- Compared to equil. case, frozen case requires
  - larger expansion ratio to achieve same  $u_e$
  - lower expansion ratio to achieve same  $p_e$



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## Nonequilibrium Nozzle Flow

- For adiabatic nozzles,  $I_{sp}$  will fall between the **frozen and equilibrium limits**  $\Rightarrow$  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
    - $\tau_{chem}$  VS.  $\tau_{flow}$
  - tends to get more frozen later in the nozzle colder & lower  $p \Rightarrow$  low reaction rates  $\Rightarrow \tau_{chem}$  long AND velocity high  $\Rightarrow \tau_{flow}$  short
- Can solve nonequilibrium by
  - including RATES in conservation/flow equations

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