

Combustor Calculations

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

Example Method – Gaseq

Problem Type: Adiabatic T and composition at const P

Reactants

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

$$m_{O_2} / m_{H_2} = (0.2 \times 32) / (0.8 \times 2) = 4$$

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	

Stoichiometry, Phi: 2.000 Set.. UniformT

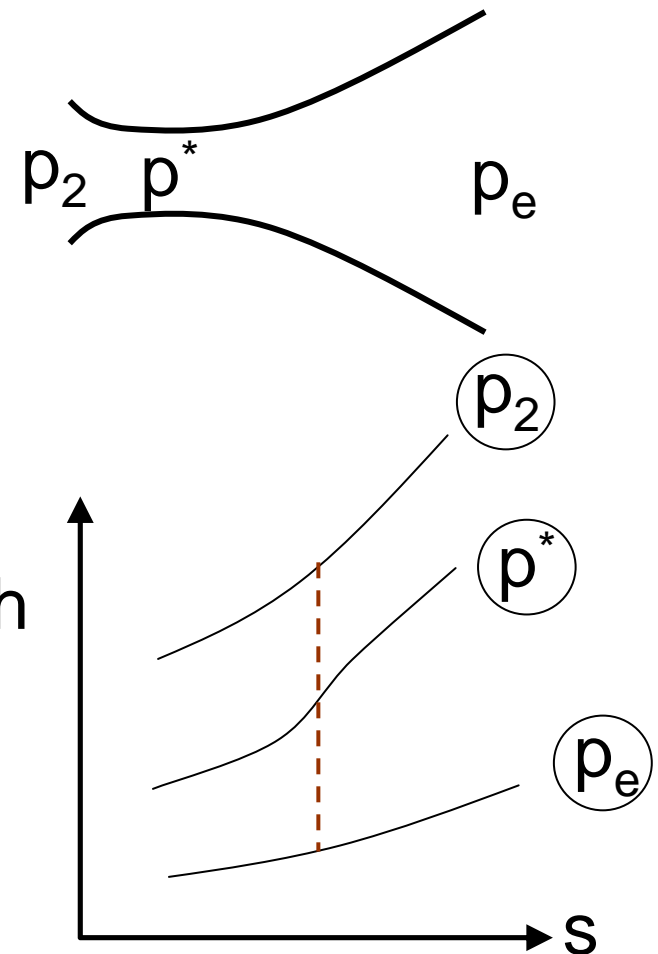
Calculate (F10)

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	HO, kJ/mol: 0.068
149.822	SO, 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

Annotations:
 - T_{ad} points to the adiabatic temperature (3156.2 K).
 - $\gamma_{products}$ points to the gamma value (1.219).
 - $MW_{products}$ points to the mean molecular weight (9.89 g).

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 (and thus u) that matches given p and s



Example Method – Gaseq

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Reactants Table:

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H2O2	7.144e-07	8.40e-07	

Control Panel: View Species, Add, Delete, Clear Reacts, Clear Prods, Clear All, R>>P, **R<<P**

Stoichiometry, Phi: 2.000 Set.. UniformT

Calculate (F10)

Property Table:

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
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Want to examine expansion of products

Example – Frozen Chemistry

The screenshot shows the Gaseq software interface. The 'Problem Type' is set to 'Adiabatic compression/expansion' and 'Frozen Chemistry' is checked. The 'Reactants' table lists species H2O, O2, H2, OH, H, O, and H2O2 with their respective moles and mol fractions. The 'Products' table shows the same species. A 'Calculate (F10)' button is visible. Below the tables, a property table compares reactant and product properties.

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

• Set p_e for nozzle expansion

h_o h_e

Example – Shifting Equilibrium

Gaseq

File Edit Units StdProblems Mixtures Constraints Help

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

Input File Page Title: _____

Previous Next

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	

View Species

Add Delete

Clear Reacts Clear Prods

Clear All R>>P R<<P

Stoichiometry, Phi 105.515 Set.. UniformT

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	

Calculate (F10)

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

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

T_e (Exit Temperature)
 γ_e (Exit Gamma)
 MW_e (Exit Mean Molecular Weight)
 h_o (Enthalpy of Reactants)
 h_e (Enthalpy of Products)

• Exit composition