



AE 330/708

AEROSPACE PROPULSION

Instructor

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Importance of combustion process

Converting the chemical energy of propellants to the thermal energy

The most important performance parameters of the rocket → Specific impulse, characteristic velocity

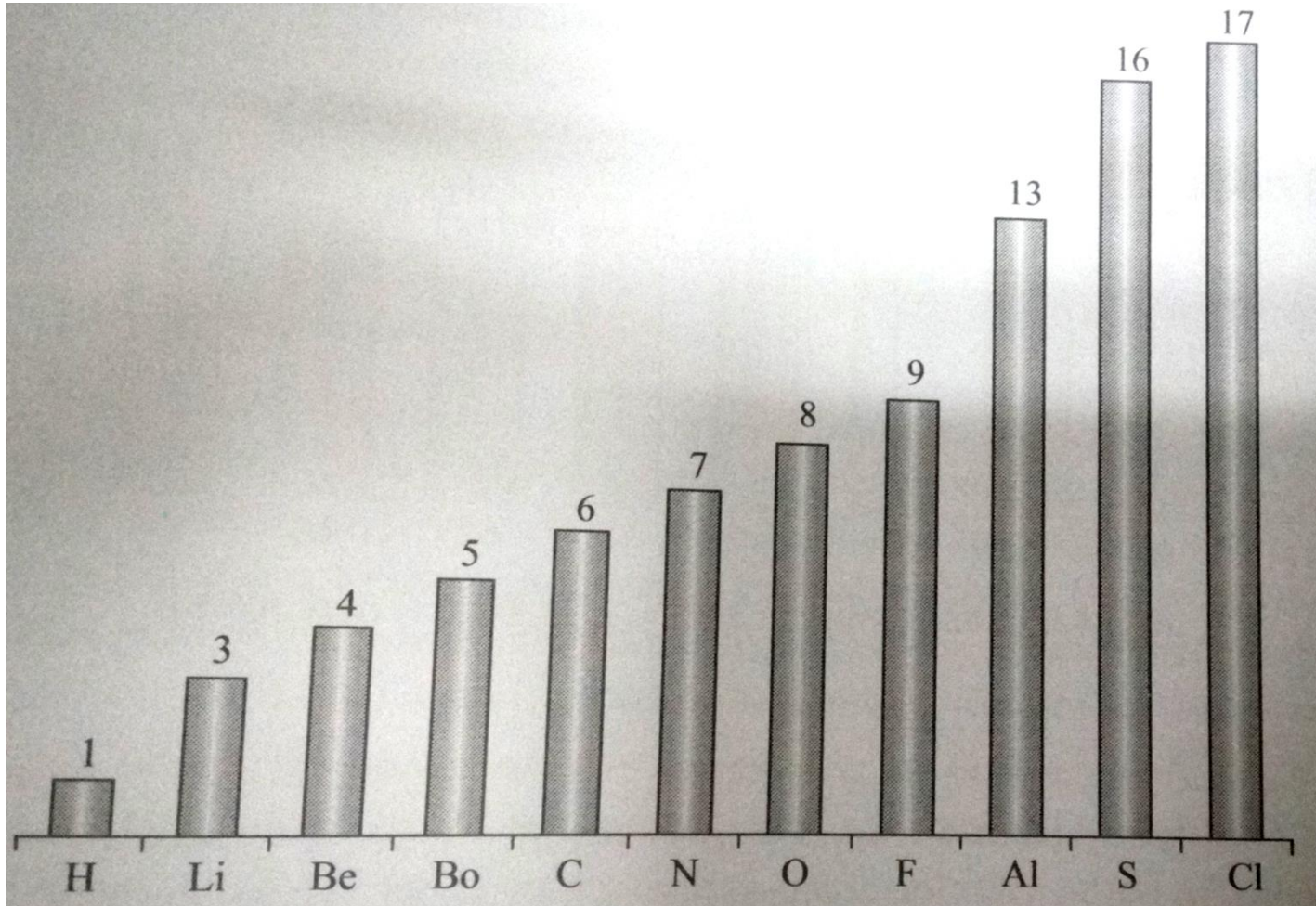
$$I_s, c^* \sim (T_1/MW)^{0.5}$$

T_1 → Combustion chamber temperature

MW → Molecular weight of the resultant gases

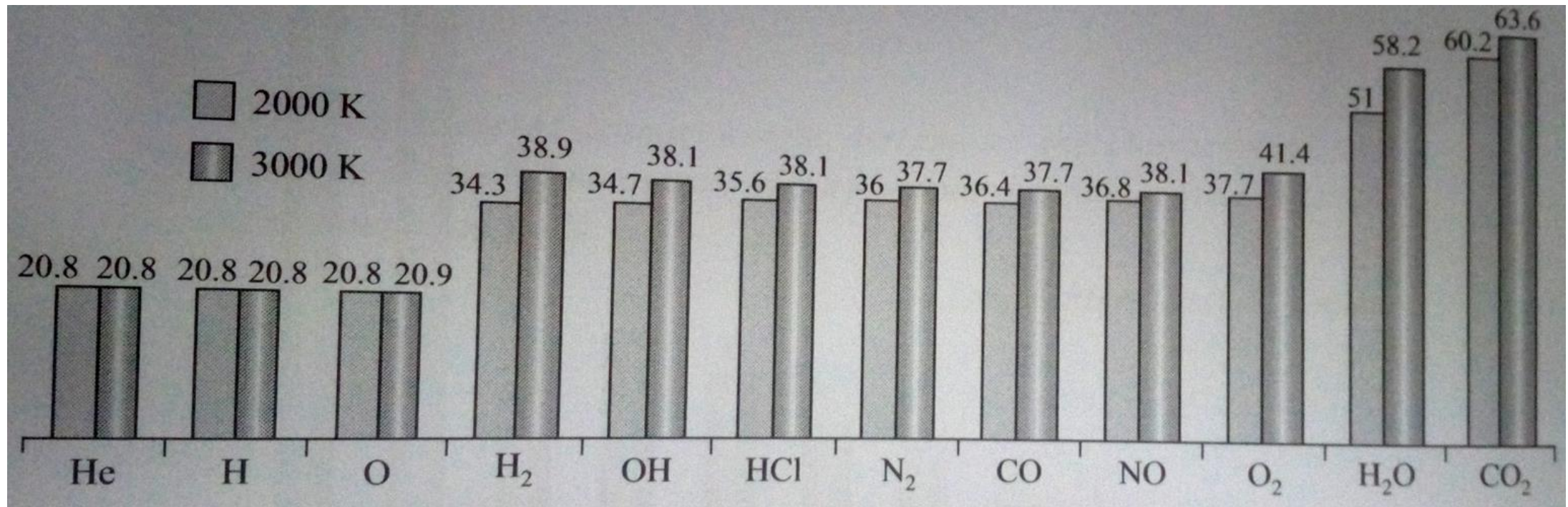
Also the other thermodynamic characteristics of gases like k , C_p also affect the nozzle performance

Elements in propellant combination



The propellant molecules should contain the elements with lower atomic number

The resulting species will then have lower molecular mass



Specific heat – function of temperature as well as the complexity of the molecule.

Lower specific heat of product species results into higher flame temperature

Simpler molecules (mono and diatomic) gases are therefore preferred as combustion products

But the molecules with complex structure have lower specific heat ratio (k)

Monoatomic : 1.66, diatomic : 1.4, tri-atomic : 1.33

Lower value of k results in better exhaust velocity and c^* - hence complex gases are preferred

Conflicting demands on the selection of propellants and their combustion!

Combustion fundamentals

* Combustion Fundamentals for Aerospace Propulsion:

Properties of mixture:

Individual gases/species

are assumed to follow ideal gas behavior.



Focus on
Gas phase combustion

Some identities:

$$n = \sum n_i$$

No. of moles of mixture

$$PV = nR_u \cdot T$$

$$P = \sum P_i$$

Dalton's law.

$$P_i V = n_i R_u \cdot T$$

Combustion fundamentals

$$\Rightarrow \frac{P_i}{P} = \frac{n_i}{n} = X_i \quad \text{Mole fraction.}$$

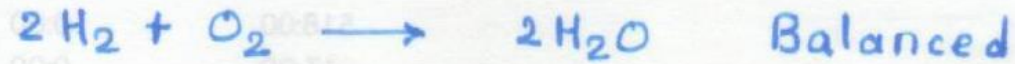
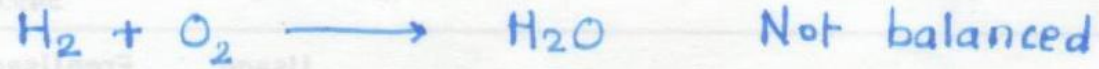
$$P = \frac{m}{V} \times \frac{R_u}{MW} \cdot T \quad \Rightarrow \quad \frac{P_i}{P} = \frac{m_i}{m} \cdot \frac{MW}{MW_i}$$

$$P_i = \frac{m_i}{V} \cdot \frac{R_u}{MW_i} \cdot T \quad \Rightarrow \quad Y_i = X_i \frac{MW_i}{MW} \quad \text{Mass fraction}$$

$$MW = \sum X_i MW_i \quad ; \quad \sum X_i = \sum Y_i = 1$$

Stoichiometry

* Stoichiometry:



Atom balance \Rightarrow Fundamental condition

Stoichiometric combustion \Rightarrow When there is no trace of reactants on the product side.



Mixture ratio (MR) \Rightarrow Ratio of mass of oxidizer to mass of fuel [o/f ratio]. $= \frac{M_{\text{ox}}}{M_{\text{F}}}$



$\text{MR} > (\text{MR})_{\text{st}}$ oxidizer rich



$\text{MR} < (\text{MR})_{\text{st}}$ Fuel rich

Equivalence ratio (ϕ) = $\frac{(\text{MR})_{\text{st}}}{\text{MR}}$

* Heat of formation: Chemical potential associated with the species.

$\Delta h_f \Rightarrow$ available at standard state $[P=1 \text{ atm}, T=298 \text{ K}]$

Zero for naturally occurring elements in their standard states
[e.g. O_2 , H_2 , N_2 , etc]

Total enthalpy associated with species = chemical + sensible

$$\therefore h_i = \Delta h_{f,i} + \int c_{p,i} dT$$

Reactants \longrightarrow Products

} Application of the first law of thermodynamics
 \longleftarrow

Two major outcomes:

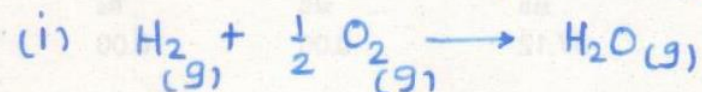
Heat of combustion $[\text{kJ/kg}]$
or (kJ/kmol)

Adiabatic flame
temperature (K)

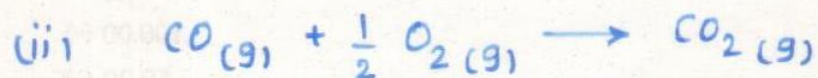
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Amount of heat liberated in a combustion reaction at standard condition. (Reactants and products both should be at standard conditions)

$$\Delta H_c = - (\Delta H_{f,p}^\circ - \Delta H_{f,R}^\circ)$$



$$\Delta H_c = - [-241 - (0 + 0)] = 241 \text{ kJ}$$



$$\Delta H_c = - [-394 - (-110 + \frac{1}{2} \times 0)] = 284 \text{ kJ}$$

At standard conditions.

* Adiabatic Flame Temperature:

Heat of combustion \rightarrow Excess amount of heat (energy) available with reactants w.r.t. products.

\rightarrow This energy is utilized for raising the sensible enthalpy ~~of~~ or temperature of the products.

If all the heat of combustion is used for raising the temperature of the products, the resulting temperature is called as the "Adiabatic Flame Temperature".

A generic chemical reaction:



We use the first law of thermodynamics to this adiabatic system.

$$[H]_{\text{product}} = [H]_{\text{reactant}}$$

$$\sum \nu_i'' [\Delta h_{f,i} + C_{p,i} (T_{\text{ad}} - T_{\text{ref}})] = \sum \nu_i' [\Delta h_{f,i} + C_{p,i} (T_R - T_{\text{ref}})]$$

T_{ad} = Adiabatic flame temp.

T_R = Reactant initial temp.

T_{ref} = Reference temp. = 298 K

For example, $2\text{H}_2 + \text{O}_2 \longrightarrow 2\text{H}_2\text{O}$

Here, $A_i = \text{H}_2, \text{O}_2, \text{H}_2\text{O}$

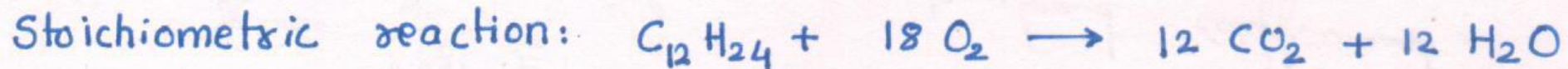
$\nu_i' = 2, 1, 0$

$\nu_i'' = 0, 0, 2$

$$\cancel{1} 2 \left[\Delta h_{f, \text{H}_2\text{O}} + C_{p, \text{H}_2\text{O}} (T_{ad} - 298\text{K}) \right] = 2 \left[\Delta h_{f, \text{H}_2} + C_{p, \text{H}_2} (T_R - 298\text{K}) \right] + 1 \left[\Delta h_{f, \text{O}_2} + C_{p, \text{O}_2} (T_R - 298) \right]$$

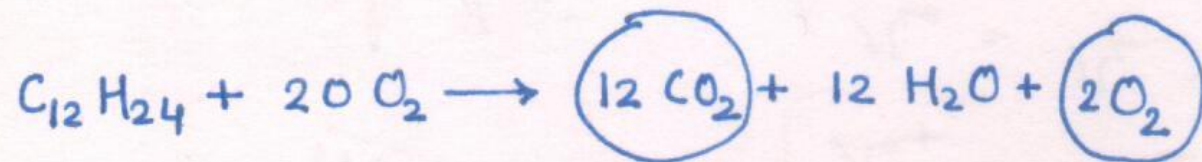
* Products of Combustion:-

Consider the reaction between Kerosene ($C_{12}H_{24}$) and O_2 .



$$(MR)_{st} = 3.43$$

Oxidizer-rich Mixture

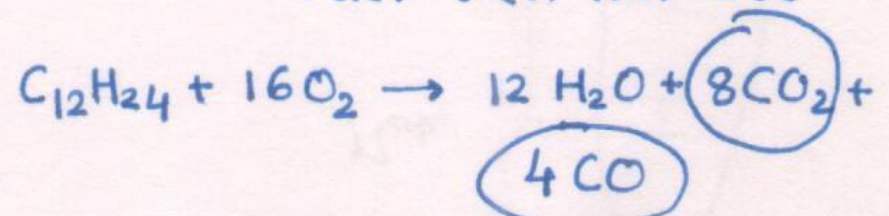


$$MR = 3.81 > (MR)_{st}$$

$$\text{Product MW} = \sum x_i MW_i$$

$$MW \approx 31.07$$

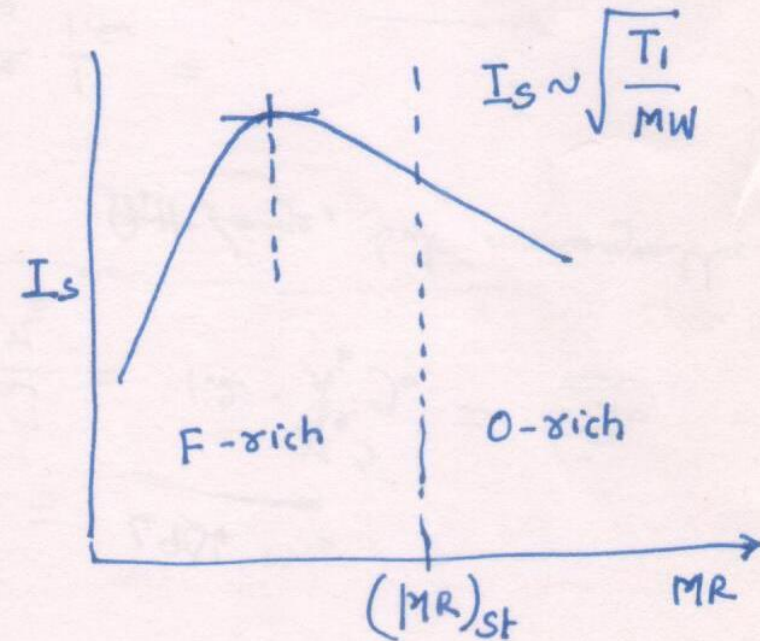
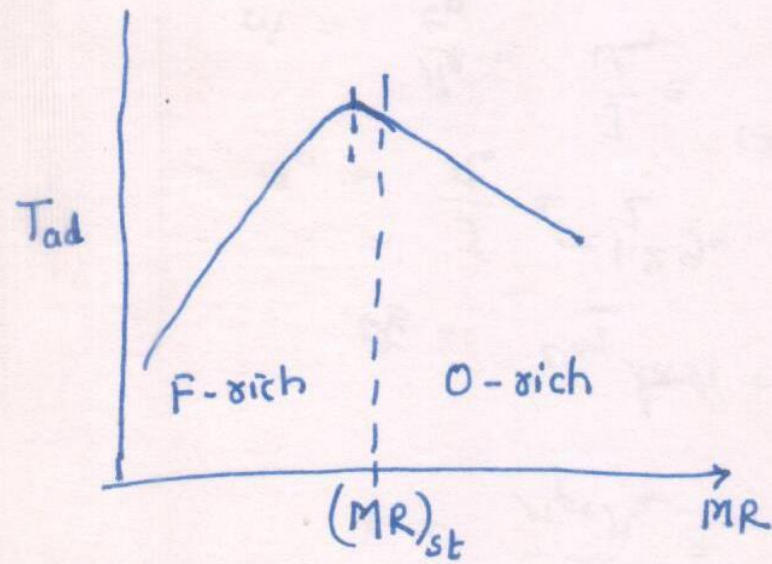
Fuel-rich mixture



$$MR = 3.05 < (MR)_{st}$$

$$MW = 28.33$$

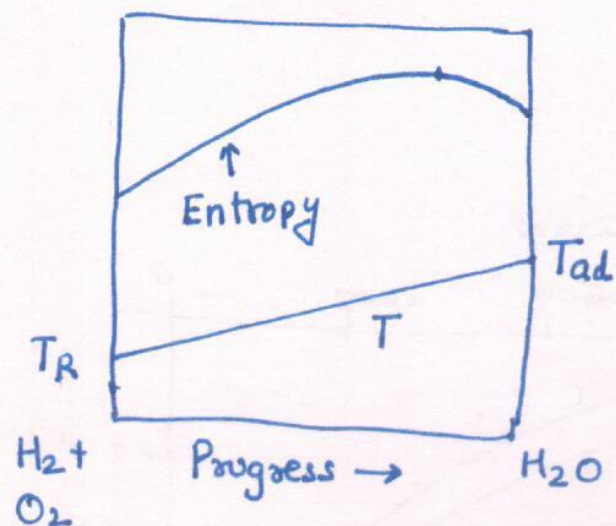
- Fuel-rich mixtures tend to give lower MW of product gases
- Lower molecular weight \Rightarrow lower specific heats \Rightarrow Higher Flame temperatures.



The effects of chemical equilibrium and dissociation have not been considered so far.

* Chemical Equilibrium:

Second Law of thermodynamics



The reaction does not actually reach a stage where only H_2O (or products) are formed.

At Higher temperatures, certain species become unstable & start to dissociate.

For instance,



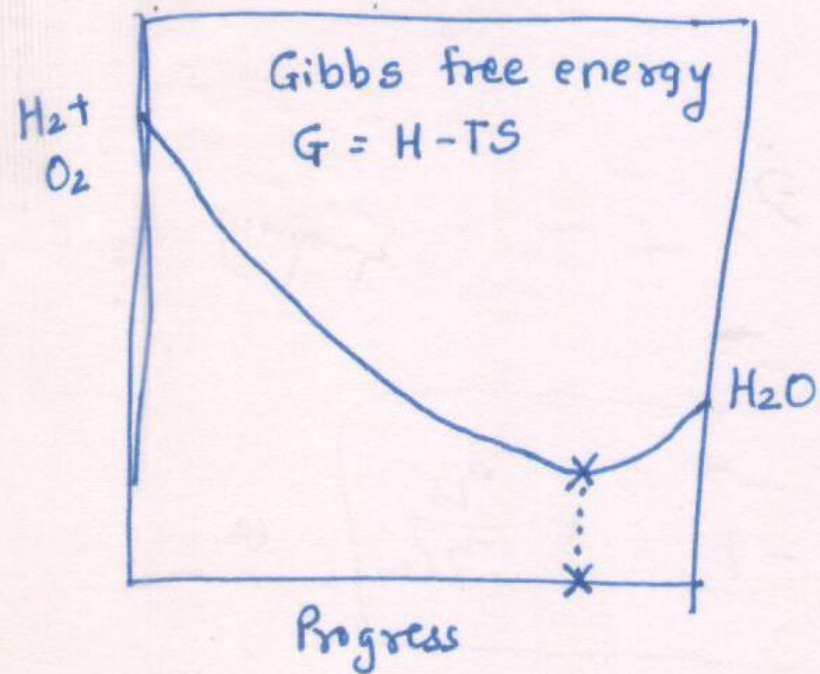
} Endothermic reactions.

Bonds break by absorbing thermal energy & complex molecules may form simpler molecules.

Result \rightarrow Temperature of the combustion products decreases

Final state of products \Rightarrow Competition betⁿ forward & backward reactions.

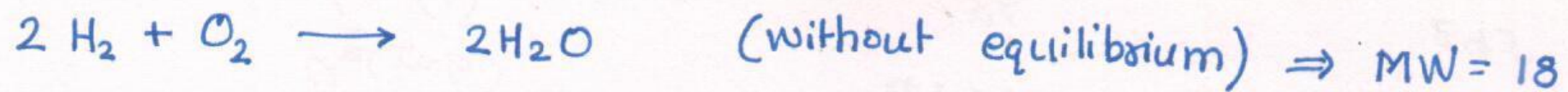
Most probable state \Rightarrow Where maximum entropy is reached or
 the point of minimum Gibbs free energy
 \Rightarrow Called as Equilibrium point.



Imp formulation:

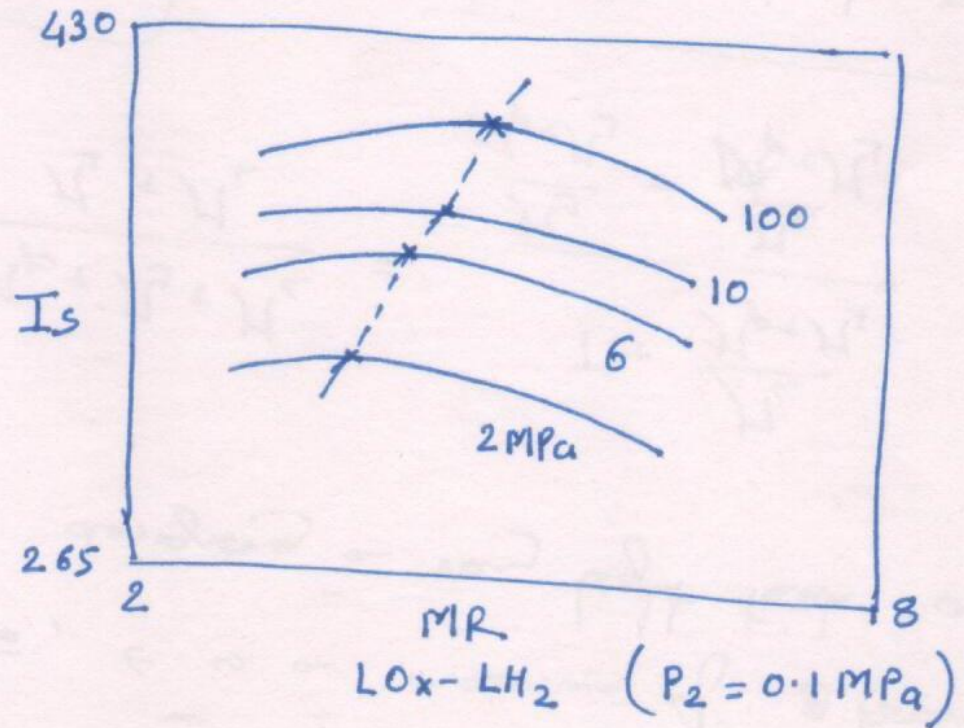
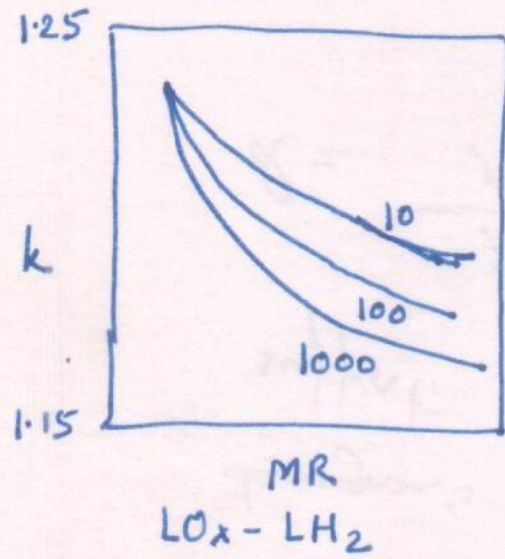
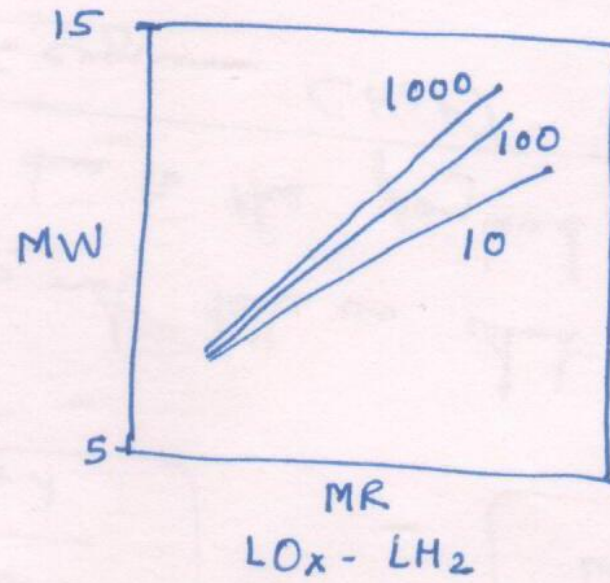
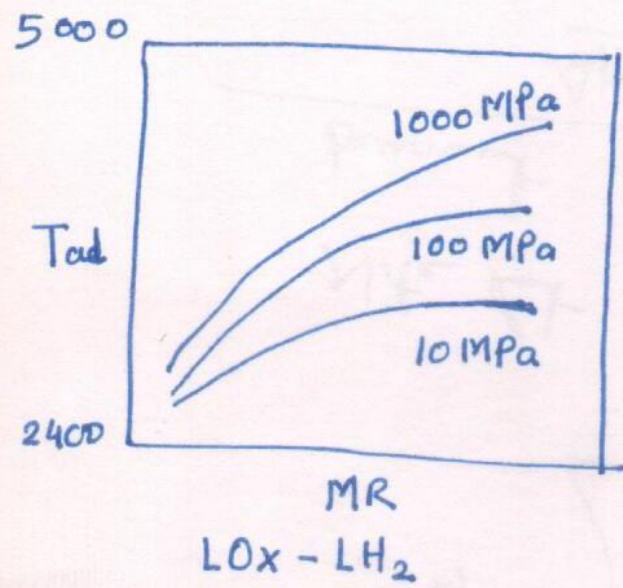
$$\exp\left(\frac{-\Delta G_T^\circ}{R_u \cdot T}\right) = \prod (P_i)^{\nu_i' - \nu_i''}$$

In case of $H_2 + O_2 \rightarrow H_2O$ reaction, the final products in
 real case are $\Rightarrow H_2O, H_2, O_2, H, O, OH, H_2O_2, HO_2$



Dissociation \Rightarrow Reduces MW of the product mixture.

Increase in combustion pressure \Rightarrow Reduces dissociation
 \Rightarrow increases flame temp \Rightarrow increases MW.



Shifting equilibrium in nozzles

Chemical equilibrium – a unique equilibrium composition of the chemical species at a given pressure and temperature.

Chemical equilibrium – a combine effect of forward and reverse reactions



Time scales associated with nozzle flow :

1. Flow time scale (t_f) – proportional to flow velocity
2. Reaction time scale (t_c) – proportional to rate of reaction

Flow through nozzle:

1. Pressure and temperature change along the length of the nozzle
2. Velocity of the flow increases (flow time scales decrease)
3. The species in the gaseous mixture are reactive and different reactions can take place depending on the local P and T

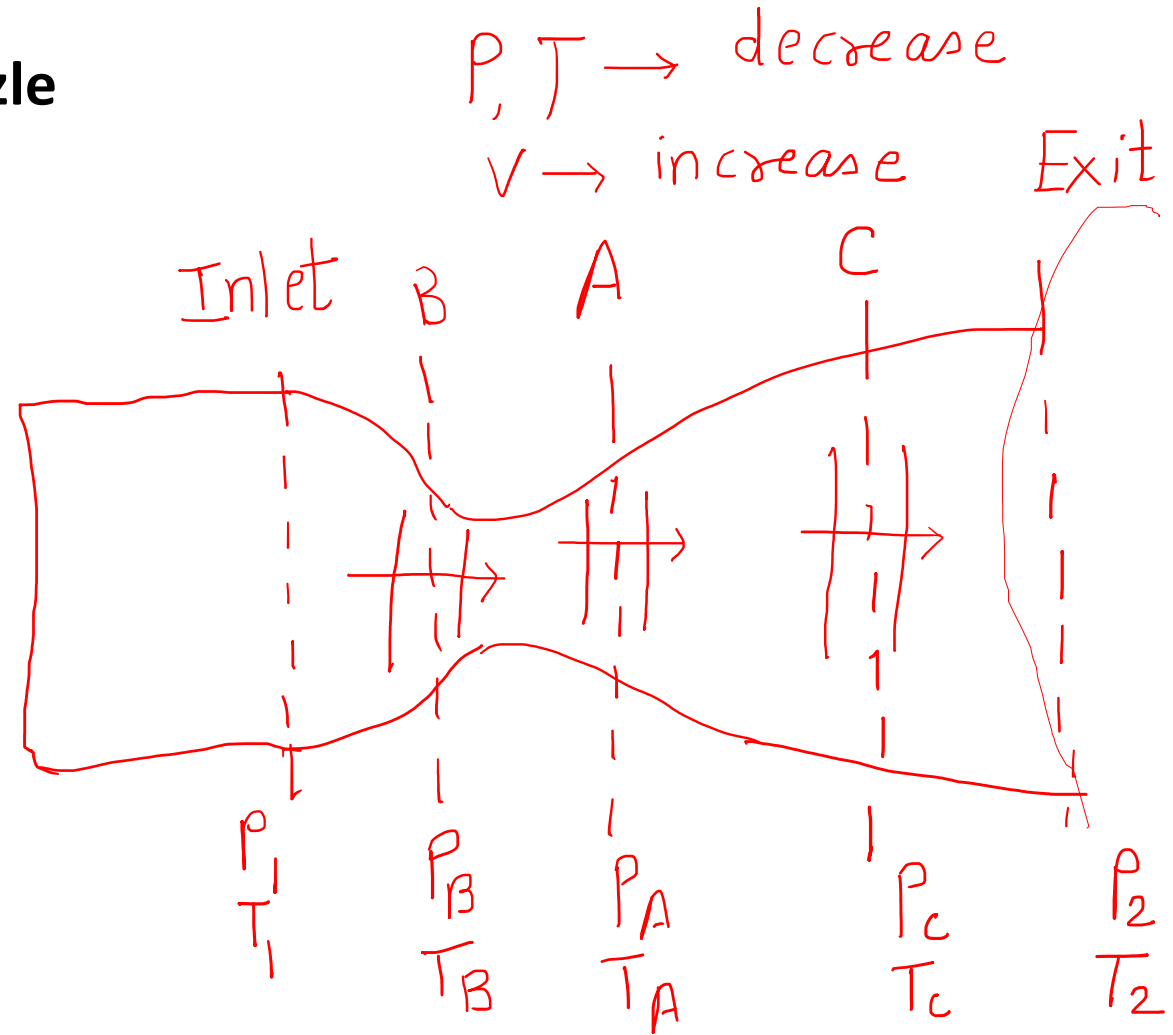
Shifting equilibrium in nozzles

Three types of flows may exist in the nozzle depending on the relative magnitudes of different time scales

Frozen flow : $t_f \ll t_c$

Equilibrium flow : $t_f \gg t_c$

Non-equilibrium flow : $t_f \sim t_c$



NTO - UDMH				LOX – LH ₂		
O/F	3.06	2.61	1.53	8.0	6.0	4.0
T _f , K	3424	3436	2779	3610	3500	2963
X _i						
CO	0.089	0.125	0.223	-	-	-
H ₂ O	0.342	0.349	0.222	0.743	0.660	0.492
H ₂	0.034	0.059	0.274	0.115	0.253	0.492
CO ₂	0.114	0.092	0.026	-	-	-
N ₂	0.294	0.289	0.249	-	-	-
OH	0.050	0.040	0.001	0.094	0.044	0.004
H	0.011	0.015	0.005	-	0.035	0.012
NO	0.020	0.012	-	-	-	-
O	0.009	0.006	-	0.014	0.004	-
O ₂	0.037	0.013	-	0.034	0.004	-

Effect of combustion characteristics on engine performance - Examples

LOx-LH2	O/F	Is (Equilibrium)	Is (Frozen)
	6	384	369
	4	391.6	387

	P ₁ (atm)	O/F	T _f	MW	c*	Is (Eq)
LOx-LH2	50	4.0	2951	9.95	2429	381
LOx-RP1	50	2.73	3660	24.0	1777	289.5

Performance of liquid propellant combinations at $P_1 = 70 \text{ atm}$ $I_{sp,eo}$, $I_{sp,f}$, $I_{sp,e,v}$,
are the specific impulse under equilibrium and frozen optimal expansion to 1atm
and vacuum conditions respectively

Propellants	O/F Wt.	O/F Vol	$\bar{\rho}_p$ (kg / m ³)	$I_{sp,eo}$ (N s / kg)	$I_{sp,f}$ (N s / kg)	$I_{sp,e,v}$ (N s / kg)	$\bar{\rho}_p I_{sp,eo}$ (kN s / m ³)
LOX-RP1	2.73	1.91	1023	2943	2764	3213	3010
	2.00	1.40	998	2862	2789	3085	2862
LOX-LH ₂	6.00	0.37	359	3767	3620	4086	1352
	4.00	0.25	284	3842	3800	4131	1091

Performance variation for LOX - RP1 and LOX-LH₂ at specific mixture ratios with chamber pressure with optimum expansion to 1 atm

LOX-RP1, O/F = 2.73					LOX-LH ₂ , O/F = 4			
P _c atm	T _c K	M g / mol	c* m / s	I _{sp, eo} N s / kg	T _c K	M g / mol	c* m / s	I _{sp, eo} N s / kg
30	3583	23.7	1719	2524	2931	9.95	2427	3561
50	3660	24.0	1777	2840	2951	9.95	2429	3739
70	3711	24.3	1785	2943	2963	9.97	2431	3842
100	3766	24.5	1792	3044	2974	9.97	2433	3902
200	3873	24.7	1806	3219	2992	9.98	2434	4105

