

# Week 2 Hypersonics Summary of High Temperature Gass Dynamics 1

Anderson CH 9, 10, 1 → 10, 4.

The nose of a vehicle is normally not the hottest when investigating hypersonic flow. Leading edges of wings or other parts down stream from the shock interaction can be a lot hotter. This can be due to how the shockwave propagates and changing atmospheric chemistry.

Dissociation, ionization and recombination all effects thermal load.

## What High Temperatures Cause



- A lot of complex high temperature phenomena occurs in a planetary entry shock layer:

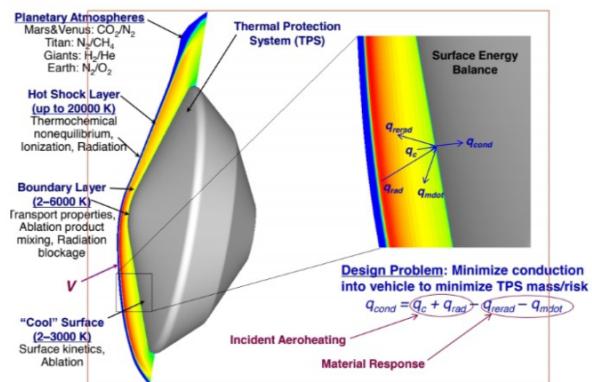
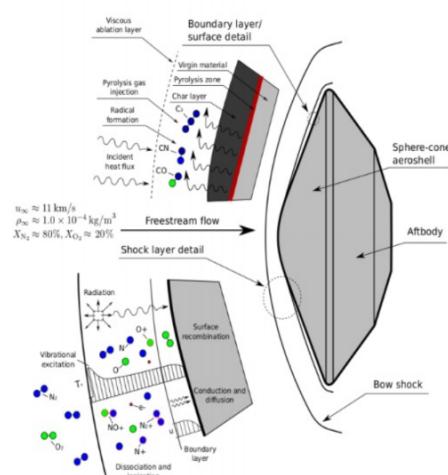


Figure: Complexities of the planetary entry shock layer from Wright and Dec [11].

## What High Temperatures Cause



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The shock stand-off is reduced for blunt bodies with also smaller oblique shock angles with reacting chemistry. (Closer to the object?)  
 ↳ High temperatures don't really effect post shock pressure. However high temperatures affect post shock temperature or density.

Non-equilibrium compression from a corner is actually curved shock waves. Any situation where a hot gas undergoes rapid expansion can result in chemical freezing → this is the sharp drop in temperature and density causes the reaction states to go to zero and is frozen in an excited state.

Flight freestream and tunnel freestream conditions are hard to keep accurate as the model moves or the gas moves. This can effect the chemistry over time or temperature changes.

And this is true for scramjets as the flight, CFD or tunnel can give different values. Either higher or lower. Non-Eq conditions.

## Perfect Gas Model



- There are many versions of the equation of state. Some examples are:

$$pv = MRT$$

$$pv = RT$$

$$p = \rho RT$$

$$pV = N R_u T$$

$$p = CR_u T$$

$$pv = \eta R_u T$$

$$pV = NkT$$

$$p = nkT$$

$$\rho = \rho \cdot R \cdot T$$

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- The useful quantities to keep in mind:

- $M$  is the total mass of the system.
- $N$  is the total number of mols
- $C$  is the concentration ( $\frac{\# \text{mols}}{\text{vol}}$ ) also  $[M]$
- $\eta$  is the mole-mass ratio ( $\frac{\# \text{mols}}{\text{mass}}$ )
- $N$  is the number of particles
- $n$  is the number density ( $\frac{\# \text{particles}}{\text{vol}}$ )

## Perfect Gas Model



- By "perfect gas" we only mean that intermolecular forces are negligible.
- The categories of perfect gas we could consider are:
  - Calorically perfect gas: Constant  $C_p$ ,  $C_v$ .
  - Thermally perfect gas:  $C_p$ ,  $C_v$  functions of  $T$  only.
  - Chemically reacting mixture of perfect gases.
    - Equilibrium: composition and properties function of  $T$  and  $p$
    - Nonequilibrium: additional time and "history" dependence
- Remember that these quantities are related to internal energy and enthalpy by:

$$e = C_v dT = \int_{T_{ref}}^T C_v(T) dT \quad \text{and} \quad h = C_p dT = \int_{T_{ref}}^T C_p(T) dT$$

## Perfect Gas Mixtures



- Dalton's Law applies for perfect gas mixtures:

$$p = \sum_i p_i$$

- The mole fraction (number of moles of species  $i$  per mole of mixture) can be obtained from:

$$\frac{p_i}{p} = \frac{N_i}{N} \equiv X_i$$

- The mass fraction (mass of  $i$  per unit mass of mixture):

$$c_i = X_i \left( \frac{M_i}{\mathcal{M}} \right) = \frac{p_i}{p}$$

- Specific gas constant (J/kg K):

$$R = \sum_i c_i R_i$$

- Molar mass (kg/mol or equiv.):

$$\mathcal{M} = \frac{1}{\sum_i c_i / \mathcal{M}_i} = \sum_i X_i \mathcal{M}_i$$

- It is worth noting that  $\mathcal{M}$  is somewhat practically interchangeable with molecular weight  $m$ , which just isn't per mol.

- I strongly recommend reading carefully through Sec 10.2 of Anderson [7].

## Remember:

- ↳ Use  $R_u$  with moles universal
- ↳ Use  $R$  with mass specific
- ↳ Use Boltzmann constant  $k$  with particles

↳ Avogadro's Number  $6.022 \times 10^{23} \text{ mol}^{-1} \text{ kg}^{-1}$

## High Temperature Phenomena

### Vibrational Excitation

Air reaches such high temperatures an increase of  $C_p$  is observed due to excitation of the vibrational energy modes.

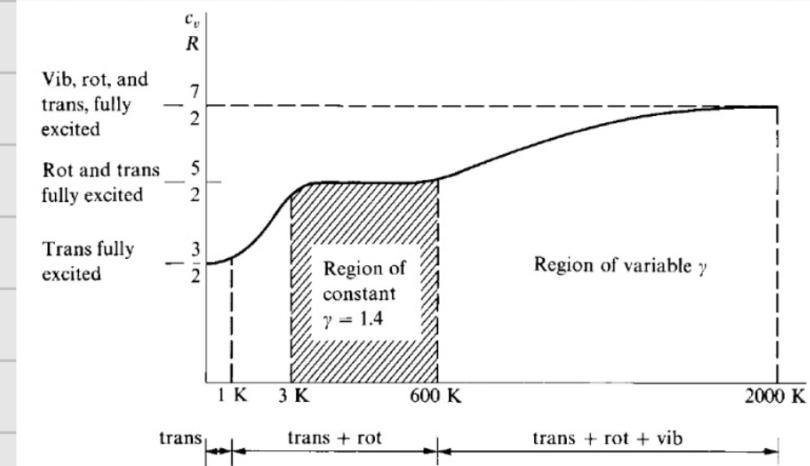


Figure: Dumbbell model from Anderson [7].

$C_p$   
Since  $\gamma = \frac{C_p}{C_V}$ , if  $C_p$  increases then  $\gamma$  will decrease.

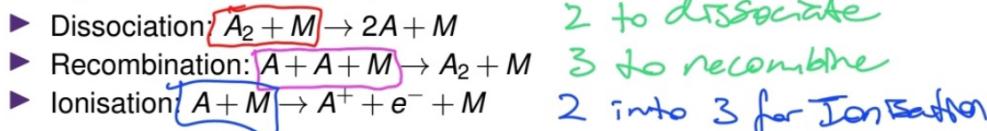
"Specific heat at constant pressure"

Chemistry occurs above 2000 K so the known relationships of  $\gamma = \frac{C_p}{C_v}$  break down.



## Gas Chemistry

- At sufficiently high temperatures, air will become a chemically reacting mixture. Important processes are:



- Where  $M$  is a collision partner.

2 to dissociate  
3 to recombine  
2 into 3 for Ionisation

This graph represents the approximate temperatures at 1 atm of pressure, and how each different gas dissociates or ionizes.

Note the two graphs 2000-2500 K.

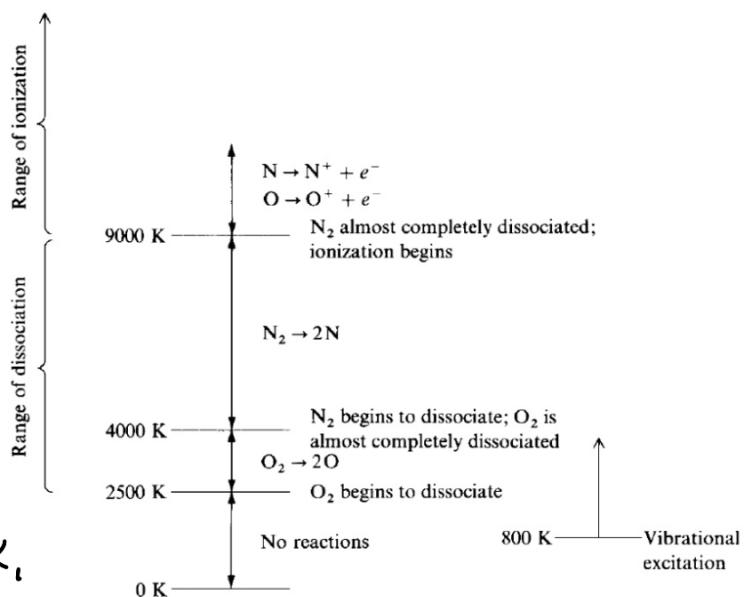
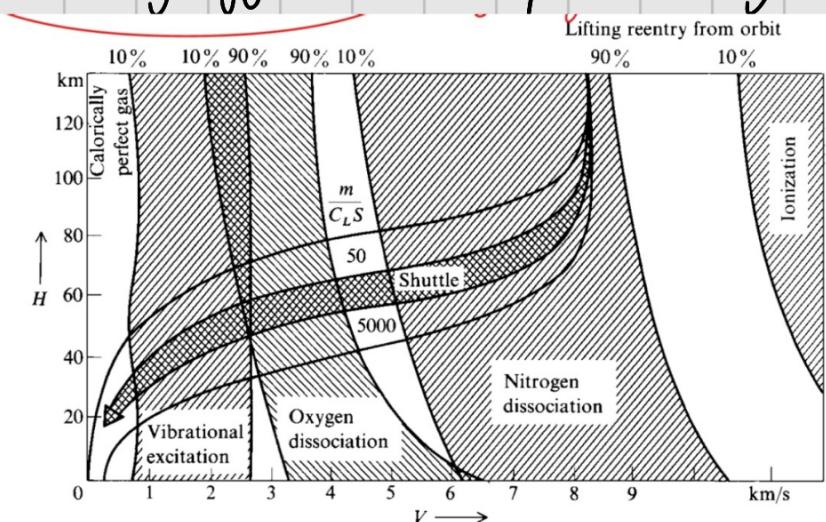


Figure: Vibrational excitation, dissociation, and ionisation for air at 1 atm [7].

Due to the large number of molecules ionizing, the electrons build up around 5000 K from coming off neutral or positive charges.

Altitude & velocity map of reentry of space shuttle into the atmosphere. With a lifting body vehicle.



# Electron Shells

Radiation is emitted when they go from high state back to low state?

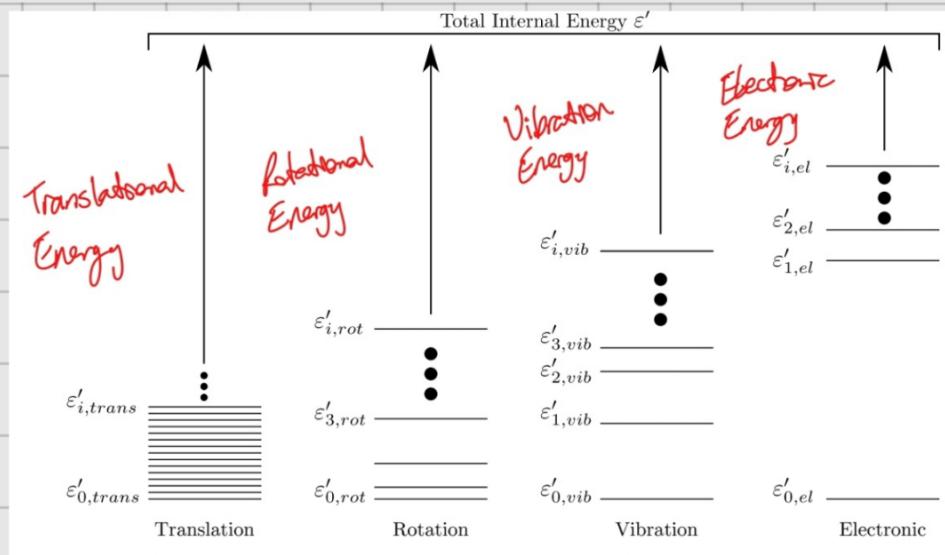


Figure: Molecular energy modes and discretisation (adapted from Anderson [7]).

Taking off electron = ionisation.

Molecules can store energy in all four modes

- ↳ Translational
- ↳ Rotational
- ↳ Vibrational
- ↳ Electrical

Atoms can only have translational & electrical modes.

A-Symmetric = no rotational etc,

Abrupt changes like a shock wave or rapid expansion can induce thermal non-equilibrium.

## Radiation

Radiative heating becomes important to address around  $10^4$  K/s or when the air is above 10,000 K. (4800  $\rightarrow$  convective & radiative heat flux)  
→ Becomes dominant source of heating as  $\varepsilon \propto T^4$

→ this modelling goes into the sublimation of heat shield design.

END THIS lecture,

rest is on next lecture L3



## AERO4470 2024 Week 2 Tutorial Problems:

1. Air is at 40 kPa and 3500 K. The composition, by mass fraction, is:  $c_{N_2} = 0.74$ ,  $c_{O_2} = 0.08$ ,  $c_{NO} = 0.05$ , and  $c_O = 0.12$ . For the mixture, find:
- The effective molar mass  $\mathcal{M}$ .
  - The specific gas constant  $R$ .
  - The mole fractions for each species.
  - The partial pressures of each species.
  - The number density of the mixture  $n$ .

Note that ignoring decimal places  $\underline{\mathcal{M}_{N_2}} = 28 \text{ kg/kmol}$ ,  $\underline{\mathcal{M}_N} = 14 \text{ kg/kmol}$ ,  $\underline{\mathcal{M}_{O_2}} = 32 \text{ kg/kmol}$ ,  $\underline{\mathcal{M}_O} = 16 \text{ kg/kmol}$ ,  $\underline{\mathcal{M}_{H_2}} = 2 \text{ kg/kmol}$ ,  $\underline{\mathcal{M}_H} = 1 \text{ kg/kmol}$ ,  $\underline{\mathcal{M}_{He}} = 4 \text{ kg/kmol}$ ,  $\underline{R_u} = 8314 \text{ J/kmol K}$ ,  $\underline{N_A} = 6.022 \times 10^{26} \text{ kmol}^{-1}$ .

**Known:** Air  $P_{AIR} = 40 \text{ kPa}$ ,  $T_{AIR} = 3500 \text{ K}$   
**Composition by MASS FRACTION**  $\Rightarrow$   $c_{N_2} = 0.74$   
 $c_{O_2} = 0.08$   
 $c_{NO} = 0.05$   
 $c_O = 0.12$   
 $R_u = 8314 \text{ J/kmol.K}$   
 $R_{AIR} = 287 \text{ J/kg.K}$   
 $\text{Total} = 0.99$

- (a) The effective molar mass  $\mathcal{M}$ . Side 38

$$\mathcal{M} = \frac{\sum_i c_i M_i}{\sum_i M_i} \Rightarrow \sum_i X_i M_i$$

► Molar mass (kg/mol or equiv.):

$$\mathcal{M} = \frac{1}{\sum_i c_i / M_i} = \sum_i X_i M_i$$

$$\mathcal{M} = \frac{c_{N_2}}{M_{N_2}} + \frac{c_{NO}}{M_{NO}} + \frac{c_{O_2}}{M_{O_2}} + \frac{c_O}{M_O}$$

$$\bar{M} = \frac{0.74}{28} + \frac{0.05}{14+16} + \frac{0.06}{16+16} + \frac{0.12}{16}$$

J / kmol · K  
 kg / kmol

$$\bar{M} = 26.25 \text{ kg/mol}$$

(b) The specific gas constant  $R$ .

62,538

► Specific gas constant (J/kg K):

$$R = \sum_i c_i R_i$$

The specific gas constant for the environment is the sum of the gas constants representing their mass fractions.

(concentration)

$$R_{\text{EARTH}} = \frac{R_u}{\bar{M}_i} (c_i)$$

$$\begin{aligned}
 c_{N_2} &= 0.74 \\
 c_{O_2} &= 0.06 \\
 c_{N_0} &= 0.05 \\
 c_O &= 0.12
 \end{aligned}$$

Note that ignoring decimal places  $M_{N_2} = 28 \text{ kg/kmol}$ ,  $M_N = 14 \text{ kg/kmol}$ ,  $M_{O_2} = 32 \text{ kg/kmol}$ ,  $M_O = 16 \text{ kg/kmol}$ ,  $M_{H_2} = 2 \text{ kg/kmol}$ ,  $M_H = 1 \text{ kg/kmol}$ ,  $M_{He} = 4 \text{ kg/kmol}$ ,  $R_u = 8314 \text{ J/kmol K}$ ,  $N_A = 6.022 \times 10^{26} \text{ kmol}^{-1}$ .

$$R_{N_2} = \frac{R_u}{\bar{M}_{N_2}} (c_{N_2}) = \frac{8314}{28} (0.74)$$

$$\rightarrow R_{N_2} = 219.73 \text{ J/kg · K}$$

$$R_{N_0} = \frac{R_u}{\bar{M}_{N_0}} (c_{N_0}) = \frac{8314}{14+16} (0.05)$$

$$\rightarrow R_{N_0} = 13.857 \text{ J/kg · K}$$

$$R_{O_2} = \frac{R_n}{M_{O_2}} (0.08) = \frac{8314}{16+16} (0.08)$$

$$\hookrightarrow R_{O_2} = \underline{\underline{20.785 \text{ J/kg.K}}}$$

$$R_O = \frac{R_n}{M_O} (0.12) = \frac{8314}{16} (0.12)$$

$$\hookrightarrow R_O = \underline{\underline{62.355 \text{ J/kg.K}}}$$

$$\sum R_{N_2, NO, O_2, O}$$

$$\sum R = R_{N_2} = 219.73$$

$$R_N = 13857$$

$$R_{O_2} = 20.785$$

$$R_O = 62.355$$

$$\sum R = \underline{\underline{316.724 \text{ J/kg.K}}} \quad \text{ANS}$$

(c) The mole fractions for each species.

Eq 10.23 HTG D Anderson 2nd.

Assume 1 kg mass total

$$\begin{aligned}C_{N_2} &= 0.74 \text{ kg} \\C_{O_2} &= 0.08 \text{ kg} \\C_{N_0} &= 0.05 \text{ kg} \\C_O &= 0.12 \text{ kg}\end{aligned}$$

Note that ignoring decimal places  $\mathcal{M}_{N_2} = 28 \text{ kg/kmol}$ ,  $\mathcal{M}_N = 14 \text{ kg/kmol}$ ,  $\mathcal{M}_{O_2} = 32 \text{ kg/kmol}$ ,  $\mathcal{M}_O = 16 \text{ kg/kmol}$ ,  $\mathcal{M}_{H_2} = 2 \text{ kg/kmol}$ ,  $\mathcal{M}_H = 1 \text{ kg/kmol}$ ,  $\mathcal{M}_{He} = 4 \text{ kg/kmol}$ ,  $R_u = 8314 \text{ J/kmol K}$ ,  $N_A = 6.022 \times 10^{26} \text{ kmol}^{-1}$ .

$$Total = 0.99$$

Find Funny N for each first

$$\mathcal{M}_{N_2} = \frac{C_{N_2}}{\mathcal{M}_{N_2}}$$

$$\hookrightarrow \frac{0.74 \text{ kg}}{28 \text{ kg/kmol}}$$

$$\mathcal{M}_{N_2} \hookrightarrow \underline{0.02643 \text{ kmol}}$$

$$\mathcal{M}_{N_0} = \frac{C_{N_0}}{\mathcal{M}_N + \mathcal{M}_O}$$

$$\hookrightarrow \frac{0.05 \text{ kg}}{14 + 16 \text{ kg/kmol}}$$

$$\mathcal{M}_{N_0} = \underline{0.00167 \text{ kmol}}$$

$$\mathcal{M}_{O_2} = \frac{C_{O_2}}{\mathcal{M}_{O_2}}$$

$$\hookrightarrow \frac{0.08 \text{ kg}}{16 + 16} \rightarrow \underline{0.0025 \text{ kmol}}$$

$$N_O : \frac{C_O}{M_O} = \frac{0.12 \text{ kg}}{16 \text{ kg/kmol}}$$

$$N_O = \underline{\underline{0.0075 \text{ kmol}}}$$

Now we have the funny  $N$  for each species, we can find the  $X_i$  for each species.

$$X_{N_2} = \frac{N_{N_2}}{\sum N}$$

$$X_{N_2} = \frac{0.02643 \text{ kmol}}{0.038095 \text{ kmol}}$$

Note  $\sum N =$   
 $0.038095 \text{ kmol}$

$$\underline{\underline{X_{N_2} = 0.69375}}$$

$$X_{N_0} = \frac{N_{N_0}}{\sum N}$$

$$X_{N_0} = \frac{0.00167 \text{ kmol}}{0.038095 \text{ kmol}}$$

$$\underline{\underline{X_{N_0} = 0.04375}}$$

$$X_{O_2} = \frac{N_{O_2}}{\sum N} = \frac{0.0025 \text{ kmol}}{0.038095 \text{ kmol}}$$

$$\underline{\underline{X_{O_2} = 0.065625}}$$

- The mole fraction (number of moles of species  $i$  per mole of mixture) can be obtained from:

$$\frac{p_i}{p} = \frac{N_i}{N} \equiv X_i$$

$$X_0 = \frac{N_0}{\sum N} = \frac{0.0075 \text{ kmol}}{0.038095 \text{ kmol}}$$

$$\underline{\underline{X_0 = 0.196875}}$$

$$\sum X = 0.9999999 \approx 1$$

(d) The partial pressures of each species.

► Dalton's Law applies for perfect gas mixtures:

$$p = \sum_i p_i$$

$$P_{N_2} = P \cdot X_{N_2} = \underline{\underline{27.75 \text{ kPa}}}$$

$40 \text{ kPa} \cdot 0.69375$

$$P_{N_0} = (40 \text{ kPa})(0.04375) = \underline{\underline{1.75 \text{ kPa}}}$$

$$P_{O_2} = (40 \text{ kPa})(0.065625) = \underline{\underline{2.625 \text{ kPa}}}$$

$$P_O = (40 \text{ kPa})(0.196875) = \underline{\underline{7.875 \text{ kPa}}}$$

(e) The number density of the mixture  $n$ .

Density from  $P = \rho RT$  @ 3500K  
using total R value then  $n$ .

$$P = \rho RT$$

$$\rho = \frac{P}{RT}$$

$$\rho = \frac{40000}{(316.724)(3500)}$$

$$\begin{aligned}C_{N_2} &= 0.74 \\C_{O_2} &= 0.06 \\C_{N_0} &= 0.05 \\C_O &= 0.12\end{aligned}$$

Total R

$$\rho_{\text{mix}} = 0.03608 \text{ kg/m}^3$$

$$C_{\text{mix}} = \frac{0.03608}{26.25}$$

$$C_{\text{mix}} = 0.001375 \text{ kmol/m}^3$$

$$R = Av \#$$

$$6.022 \times 10^{23} \text{ mol}$$

$$6.022 \times 10^{26} \text{ kmol}$$

$$\begin{aligned}n &= 6.022 \times 10^{26} \cdot 0.001375 \\&= 8.278 \times 10^{23}\end{aligned}$$

as per kmol

Q2.

2. Now consider a mixture of 85% H<sub>2</sub> and 15% He by mole fraction at 40 kPa and 2000 K. Assume it is fully vibrationally excited and non-reacting. Find:
- $C_v$  and  $C_p$  of the mixture.
  - The specific heat ratio  $\gamma$ .
  - The sound speed of the mixture  $a$ .
  - What would be different if the mixture was reacting?

Note that ignoring decimal places  $\mathcal{M}_{N_2} = 28 \text{ kg/kmol}$ ,  $\mathcal{M}_N = 14 \text{ kg/kmol}$ ,  $\mathcal{M}_{O_2} = 32 \text{ kg/kmol}$ ,  $\mathcal{M}_O = 16 \text{ kg/kmol}$ ,  $\mathcal{M}_{H_2} = 2 \text{ kg/kmol}$ ,  $\mathcal{M}_H = 1 \text{ kg/kmol}$ ,  $\mathcal{M}_{He} = 4 \text{ kg/kmol}$ ,  $R_u = 8314 \text{ J/kmol K}$ ,  $N_A = 6.022 \times 10^{26} \text{ kmol}^{-1}$ .

$$X_{H_2} = 0.85$$

$$X_{He} = 0.15$$

$$P = 40 \text{ kPa}$$

$$T = 2000 \text{ K}$$

Assumptions

Assume a flat earth.

mole fraction.

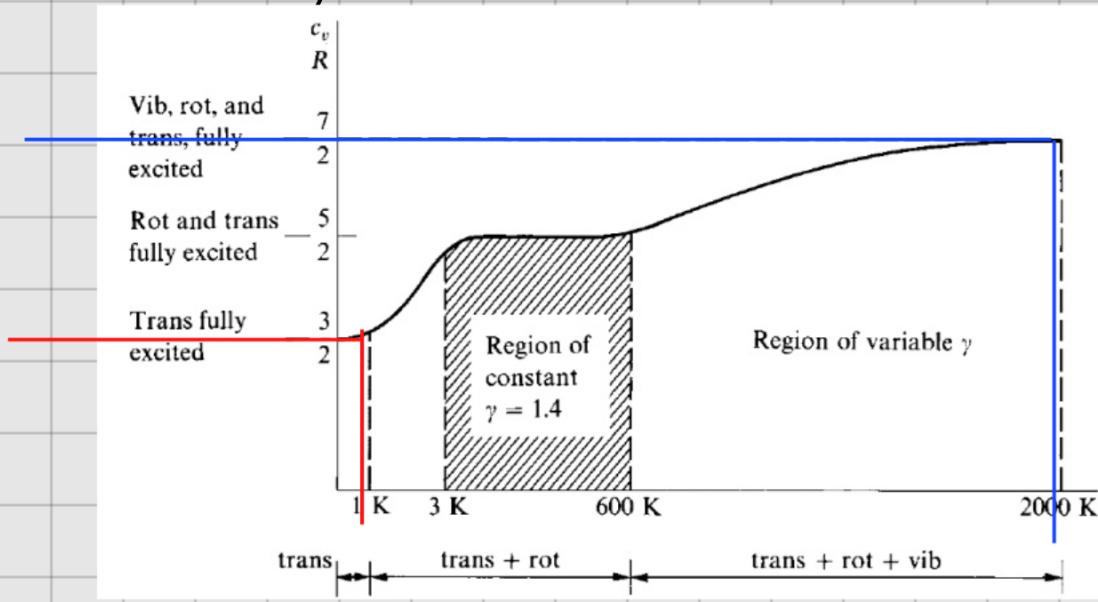
► The mole fraction (number of moles of species  $i$  per mole of mixture) can be obtained from:

$$\frac{p_i}{p} = \frac{\mathcal{N}_i}{\mathcal{N}} \equiv X_i$$

Some 4800 things  
are hard to let go of  
((w))

$$a) R_{H_2} = \frac{R_u}{2} = \frac{8314}{2} = 4157.5 \text{ J/kg.K}$$

$$R_{He} = \frac{R_u}{4} = \frac{8314}{4} = 2078.5 \text{ J/kg.K}$$



Cv

= #DOF  
2 -  $\frac{g_f}{g_o}$

$$C_V H_2 = \frac{R_u}{2} \cdot \frac{7}{2} = 4157 \cdot \frac{7}{2} = \underline{\underline{14549,5}}$$

All units  $J/kg \cdot K$

$$C_V He = \frac{R_u}{2} \cdot \frac{3}{2} = 2078,5 \cdot \frac{3}{2} = \underline{\underline{3117,5}}$$

$$C_p = R + C_V$$

$$C_p H_2 = R_{H_2} + C_V H_2 = 4157 + 14549,5 = \underline{\underline{18706,5}}$$

$$C_p He = R_{He} + C_V He = 2078,5 + 3117,5 = \underline{\underline{5196,25}}$$

$$\bar{M} = (0,85)(2) + (0,15)(4) = \underline{\underline{2,3}} \text{ kg/kmol}$$

$$C_{H_2} = \frac{x_{H_2} \cdot M_{H_2}}{\bar{M}_{\text{tot}}} = \frac{0,85 \cdot 2}{2,3} = \underline{\underline{0,73913}}$$

$$C_{He} = \frac{x_{He} \cdot M_{He}}{\bar{M}_{\text{tot}}} = \frac{0,15 \cdot 4}{2,3} = \underline{\underline{0,26087}}$$

Concentration of  $H_2$  in this env =  $\underline{\underline{0,73913}}$

Concentration of  $He$  in this env =  $\underline{\underline{0,26087}}$

$$C_V = C_{V\text{H}_2} \cdot C_{\text{H}_2} + C_{V\text{He}} \cdot C_{\text{He}}$$

$$\text{env} = 14549.5 \cdot 0.73913 + 3117.5 \cdot 0.26087$$

Gives  $11567.3 \text{ J/kg.K}$

$$C_p = C_{p\text{H}_2} \cdot C_{\text{H}_2} + C_{p\text{He}} \cdot C_{\text{He}}$$

$$18706.5 \cdot 0.73913 + 5196.25 \cdot 0.26087$$

$C_p \rightarrow 15182.08 \text{ J/kg.K}$

b)  $\gamma = \frac{C_p}{C_v} \Rightarrow \frac{15182.08}{11567.3} = 1.3125$

c)  $\alpha = \sqrt{\gamma R T}$

$$\alpha = \sqrt{1.3125 \cdot 3614.78 \cdot 2000 \text{ K}} = 3080.4 \text{ m/s}$$

When  $R = C_p - C_v$

$$R = 15182.08 - 11567.3 = 3614.78 \text{ J/kg.K}$$

d) Each property changes, since the mass fraction would change, the mixture at each stage would be different in non-eq.

The  $C_p$  &  $C_v$  would change if either  $\text{H}_2$  or He dissociate, ionisation, therefore  $R$  for each species & their ratio of excitational states