

# Compressible Flow - TME085

## Lecture 14

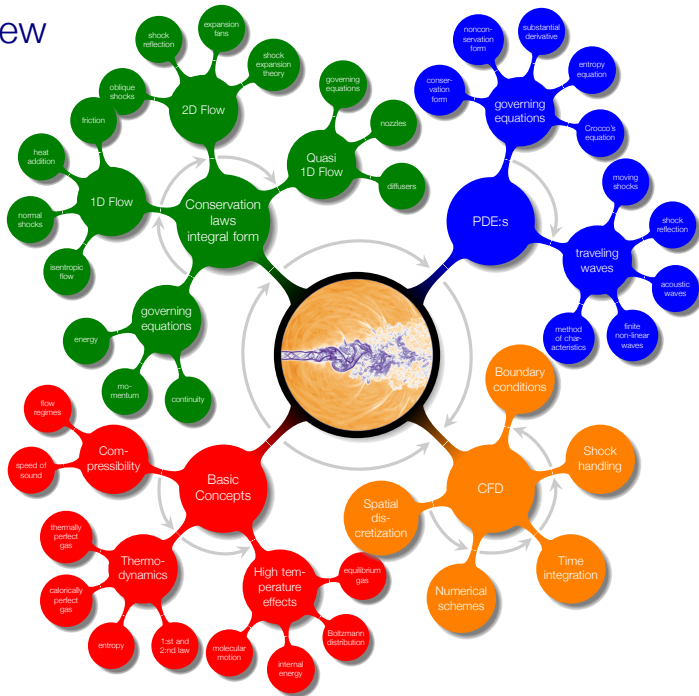
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# Overview



# Chapter 16

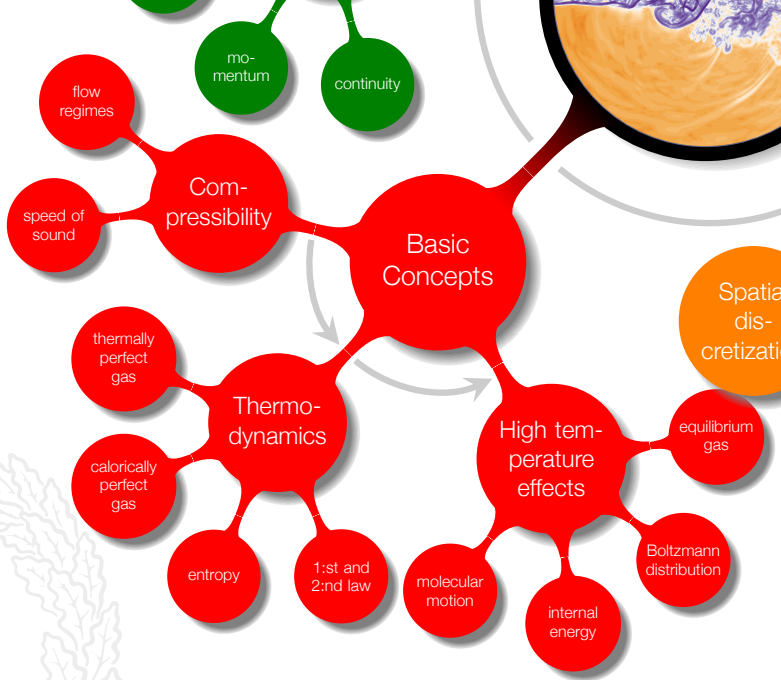
## Properties of High-Temperature Gases

# Chapter 17

## High-Temperature Flows: Basic Examples



# Overview



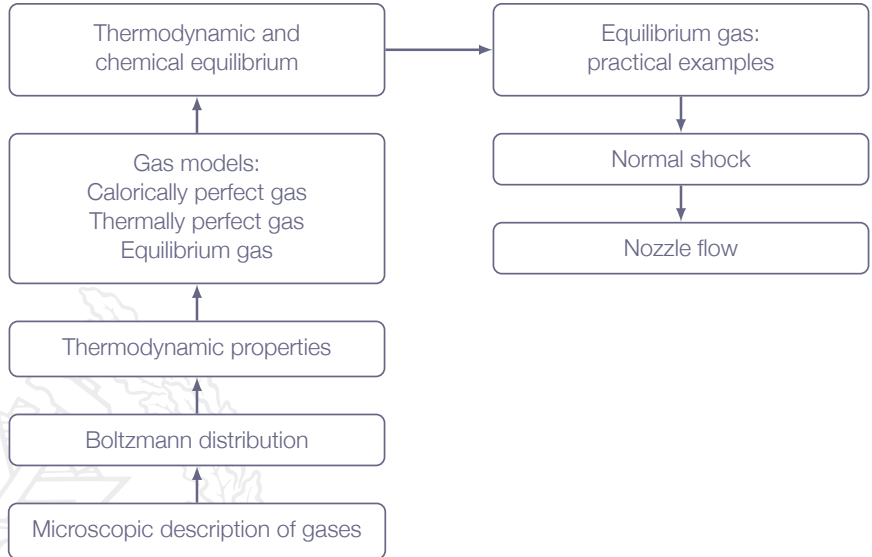
# Addressed Learning Outcomes

- 6 **Define** the special cases of calorically perfect gas, thermally perfect gas and real gas and **explain** the implication of each of these special cases

*A deep dive into the theory behind the definitions of calorically perfect gas, thermally perfect gas, and other models*



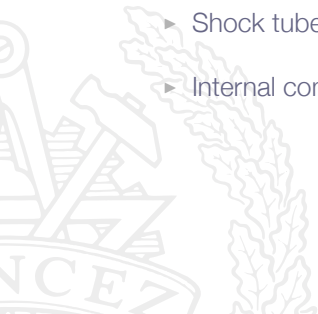
# Roadmap - High Temperature Effects



# Properties of High-Temperature Gases

## Applications:

- ▶ Rocket nozzle flows
- ▶ Reentry vehicles
- ▶ Shock tubes / Shock tunnels
- ▶ Internal combustion engines



# Properties of High-Temperature Gases

## Example: Reentry vehicle

Mach 32.5

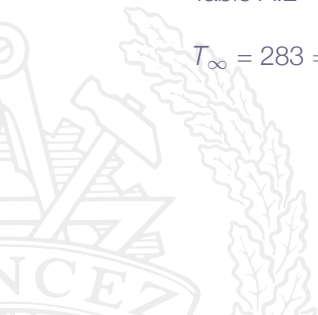
Air

Calorically perfect gas

$$T_{\infty} = 283$$

$$\text{Table A.2} \Rightarrow T_s/T_{\infty} = 206$$

$$T_{\infty} = 283 \Rightarrow T_s = 58\,300 \text{ K}$$





# Properties of High-Temperature Gases

## Example: Reentry vehicle

Mach 32.5

Air

Calorically perfect gas

$$T_{\infty} = 283$$

$$\text{Table A.2} \Rightarrow T_s/T_{\infty} = 206$$

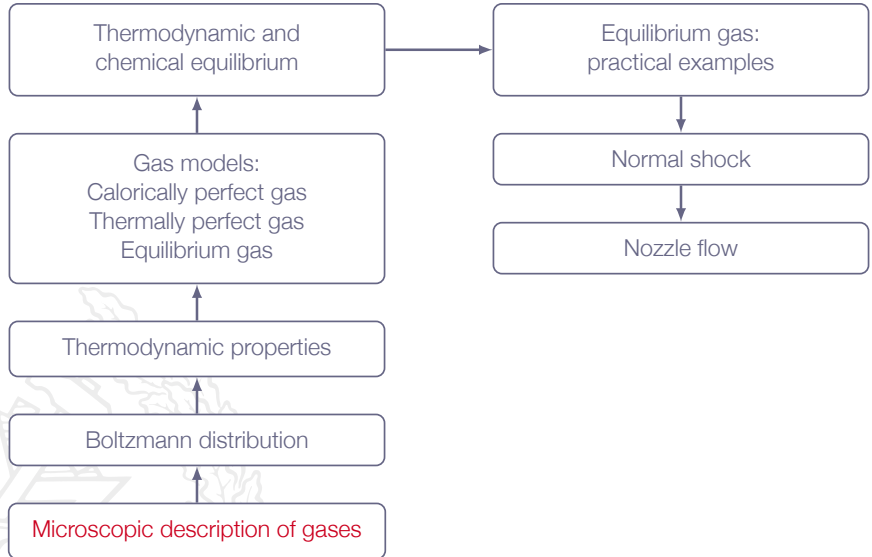
$$T_{\infty} = 283 \Rightarrow T_s = 58\,300 \text{ K}$$

A more correct value is  $T_s = 11\,600 \text{ K}$

Something is fishy here!



# Roadmap - High Temperature Effects



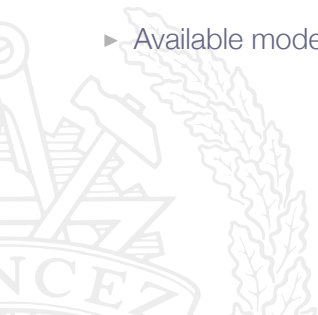
# Chapter 16.2

## Microscopic Description of Gases

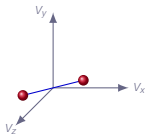


# Microscopic Description of Gases

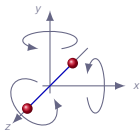
- ▶ Hard to make measurements
- ▶ Accurate, reliable theoretical models needed
- ▶ Available models do work quite well



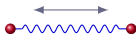
# Molecular Energy



Translational kinetic energy  
thermal degrees of freedom: 3



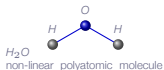
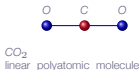
Rotational kinetic energy  
thermal degrees of freedom:  
2 for diatomic gases  
2 for linear polyatomic gases  
3 for non-linear polyatomic gases



Vibrational energy  
(kinetic energy + potential energy)  
thermal degrees of freedom: 2



Electronic energy of electrons in orbit  
(kinetic energy + potential energy)



- ▶ Translational energy
- ▶ Rotational energy  
(only for molecules - not for mono-atomic gases)
- ▶ Vibrational energy
- ▶ Electronic energy

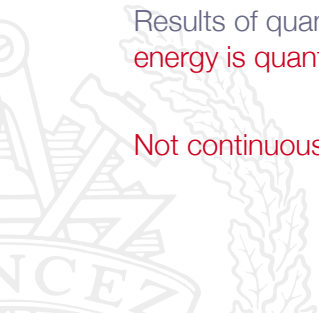
# Molecular Energy

The energy for one molecule can be described by

$$\epsilon' = \epsilon'_{trans} + \epsilon'_{rot} + \epsilon'_{vib} + \epsilon'_{el}$$

Results of quantum mechanics have shown that each energy is quantized *i.e.* they can exist only at discrete values

**Not continuous!** Might seem unintuitive



# Molecular Energy

The lowest quantum numbers defines the **zero-point energy** for each mode

- ▶ for rotational energy the zero-point energy is exactly zero
- ▶  $\epsilon'_{0trans}$  is very small but finite - *at absolute zero, molecules still moves but not much*

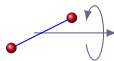
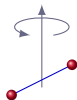
$$\epsilon_{jtrans} = \epsilon'_{jtrans} - \epsilon'_{0trans}$$

$$\epsilon_{lvib} = \epsilon'_{lvib} - \epsilon'_{0vib}$$

$$\epsilon_{krot} = \epsilon'_{krot}$$

$$\epsilon_{mel} = \epsilon'_{mel} - \epsilon'_{0el}$$

# Energy States



- ▶ three cases with the **same rotational energy**
- ▶ different direction of angular momentum
- ▶ quantum mechanics  $\Rightarrow$  different **distinguishable states**
- ▶ a finite number of possible states for each energy level



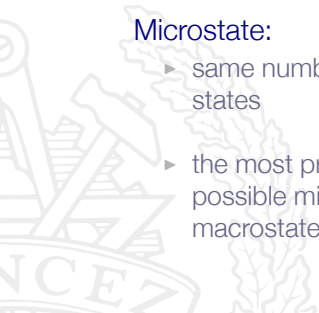
# Macrostates and Microstates

## Macrostate:

- ▶ molecules collide and exchange energy  $\Rightarrow$  the  $N_j$  distribution (the macrostate) will change over time
- ▶ some macrostates are more probable than other
- ▶ most probable macrostates (distribution)  $\Rightarrow$  **thermodynamic equilibrium**

## Microstate:

- ▶ same number of molecules in each energy level but different states
- ▶ the most probable macrostate is the one with the most possible microstates  $\Rightarrow$  possible to find the most probable macrostate by counting microstates



# Macrostates and Microstates

Macrostate I    Microstate I

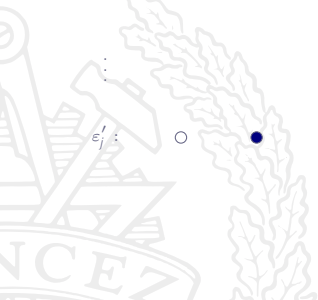
$\epsilon'_0$  :    ●    ●    ○    ○    ○     $(N_0 = 2, g_0 = 5)$

$\epsilon'_1$  :    ●    ●    ●    ○    ●    ●     $(N_1 = 5, g_1 = 6)$

$\epsilon'_2$  :    ●    ●    ●    ○    ○     $(N_2 = 3, g_2 = 5)$

⋮

$\epsilon'_j$  :    ○    ●    ●     $(N_j = 2, g_j = 3)$



# Macrostates and Microstates

Macrostate I    Microstate II

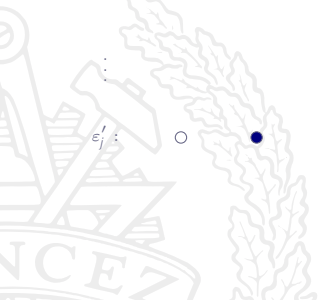
$\varepsilon'_0 :$     ○    ●    ○    ○    ●     $(N_0 = 2, g_0 = 5)$

$\varepsilon'_1 :$     ●    ○    ●    ●    ●    ●     $(N_1 = 5, g_1 = 6)$

$\varepsilon'_2 :$     ○    ○    ●    ●    ●     $(N_2 = 3, g_2 = 5)$

⋮

$\varepsilon'_j :$     ○    ●    ●     $(N_j = 2, g_j = 3)$



# Macrostates and Microstates

Macrostate II    Microstate I

$\varepsilon'_0 :$     ○    ●    ○    ○    ○     $(N_0 = 1, g_0 = 5)$

$\varepsilon'_1 :$     ●    ○    ●    ●    ●    ●     $(N_1 = 5, g_1 = 6)$

$\varepsilon'_2 :$     ●    ○    ●    ●    ●     $(N_2 = 4, g_2 = 5)$

⋮

$\varepsilon'_j :$     ○    ○    ●     $(N_j = 1, g_j = 3)$



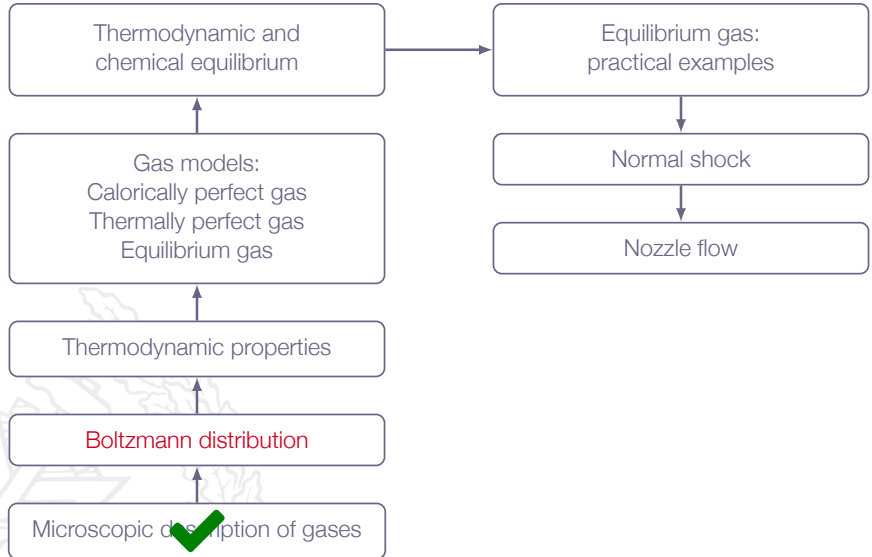
# Macrostates and Microstates

$$N = \sum_j N_j$$

$$E = \sum_j \epsilon'_j N_j$$



# Roadmap - High Temperature Effects



# Chapter 16.5

## The Limiting Case: Boltzmann Distribution



# Boltzmann Distribution

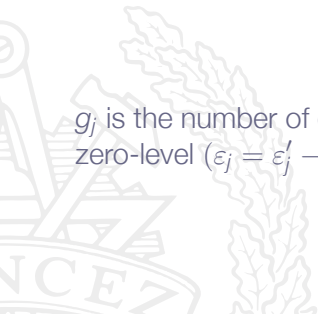
The Boltzmann distribution:

$$N_j^* = N \frac{g_j e^{-\varepsilon_j/kT}}{Q}$$

where  $Q = f(T, V)$  is the state sum defined as

$$Q \equiv \sum_j g_j e^{-\varepsilon_j/kT}$$

$g_j$  is the number of degenerate states,  $\varepsilon_j$  is the energy above zero-level ( $\varepsilon_j = \varepsilon_j' - \varepsilon_0$ ), and  $k$  is the Boltzmann constant





# Boltzmann Distribution

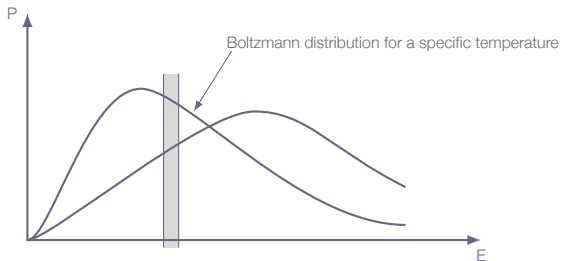
The Boltzmann distribution:

$$N_j^* = N \frac{g_j e^{-\epsilon_j/kT}}{Q}$$

*For molecules or atoms of a given species, quantum mechanics says that a set of well-defined energy levels  $\epsilon_j$  exists, over which the molecules or atoms can be distributed at any given instant, and that each energy level has a certain number of energy states,  $g_j$ .*

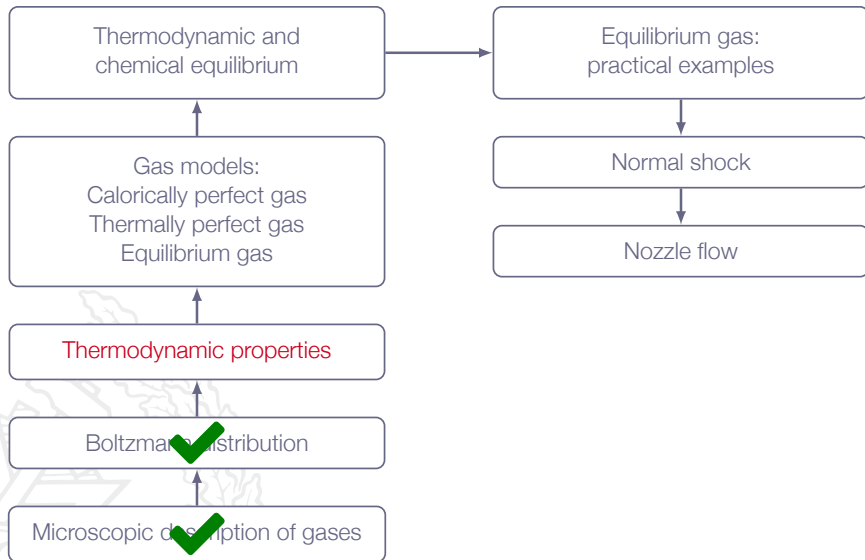
*For a system of  $N$  molecules or atoms at a given  $T$  and  $V$ ,  $N_j^*$  are the number of molecules or atoms in each energy level  $\epsilon_j$  when the system is in thermodynamic equilibrium.*

# Boltzmann Distribution



- ▶ At temperatures above  $\sim 5\text{K}$ , molecules are distributed over many energy levels, and therefore the states are generally **sparsely populated** ( $N_j \ll g_j$ )
- ▶ Higher energy levels become more populated as temperature increases

# Roadmap - High Temperature Effects



# Chapter 16.6 - 16.8

## Evaluation of Gas Thermodynamic Properties



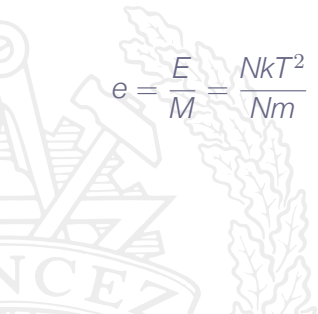
# Internal Energy

The internal energy is calculated as

$$E = NkT^2 \left( \frac{\partial \ln Q}{\partial T} \right)_V$$

The internal energy per unit mass is obtained as

$$e = \frac{E}{M} = \frac{NkT^2}{Nm} \left( \frac{\partial \ln Q}{\partial T} \right)_V = \left\{ \frac{k}{m} = R \right\} = RT^2 \left( \frac{\partial \ln Q}{\partial T} \right)_V$$



# Internal Energy - Translation

$$\epsilon'_{trans} = \frac{h^2}{8m} \left( \frac{n_1^2}{a_1^2} + \frac{n_2^2}{a_2^2} + \frac{n_3^2}{a_3^2} \right)$$

$n_1 - n_3$	quantum numbers (1,2,3,...)
$a_1 - a_3$	linear dimensions that describes the size of the system
$h$	Planck's constant
$m$	mass of the individual molecule

$\Rightarrow \dots \Rightarrow$

$$Q_{trans} = \left( \frac{2\pi mkT}{h^2} \right)^{3/2} V$$

# Internal Energy - Translation

$$Q_{trans} = \left( \frac{2\pi mkT}{h^2} \right)^{3/2} V$$

$$\ln Q_{trans} = \frac{3}{2} \ln T + \frac{3}{2} \ln \frac{2\pi mk}{h^2} + \ln V \Rightarrow$$

$$\left( \frac{\partial \ln Q_{trans}}{\partial T} \right)_V = \frac{3}{2} \frac{1}{T} \Rightarrow$$

$$e_{trans} = RT^2 \left( \frac{\partial \ln Q_{trans}}{\partial T} \right)_V = RT^2 \frac{3}{2T} = \frac{3}{2} RT$$

# Internal Energy - Rotation

$$\epsilon'_{rot} = \frac{h^2}{8\pi^2 I} J(J + 1)$$

$J$  rotational quantum number (0,1,2,...)  
 $I$  moment of inertia (tabulated for common molecules)  
 $h$  Planck's constant

$\Rightarrow \dots \Rightarrow$

$$Q_{rot} = \frac{8\pi^2 I k T}{h^2}$$





# Internal Energy - Rotation

$$Q_{rot} = \frac{8\pi^2 I k T}{h^2}$$

$$\ln Q_{rot} = \ln T + \ln \frac{8\pi^2 I k}{h^2} \Rightarrow$$

$$\left( \frac{\partial \ln Q_{rot}}{\partial T} \right)_V = \frac{1}{T} \Rightarrow$$

$$E_{rot} = RT^2 \left( \frac{\partial \ln Q_{rot}}{\partial T} \right)_V = RT^2 \frac{1}{T} = RT$$



# Internal Energy - Vibration

$$\epsilon'_{vib} = h\nu \left( n + \frac{1}{2} \right)$$

- $n$  vibrational quantum number (0,1,2,...)
- $\nu$  fundamental vibrational frequency (tabulated for common molecules)
- $h$  Planck's constant

$\Rightarrow \dots \Rightarrow$

$$Q_{vib} = \frac{1}{1 - e^{-h\nu/kT}}$$

# Internal Energy - Vibration

$$Q_{vib} = \frac{1}{1 - e^{-h\nu/kT}}$$

$$\ln Q_{vib} = -\ln(1 - e^{-h\nu/kT}) \Rightarrow$$

$$\left(\frac{\partial \ln Q_{vib}}{\partial T}\right)_V = \frac{h\nu/kT^2}{e^{h\nu/kT} - 1} \Rightarrow$$

$$e_{vib} = RT^2 \left(\frac{\partial \ln Q_{vib}}{\partial T}\right)_V = RT^2 \frac{h\nu/kT^2}{e^{h\nu/kT} - 1} = \frac{h\nu/kT}{e^{h\nu/kT} - 1} RT$$

$$\lim_{T \rightarrow \infty} \frac{h\nu/kT}{e^{h\nu/kT} - 1} = 1 \Rightarrow e_{vib} \leq RT$$

# Specific Heat

$$e = e_{trans} + e_{rot} + e_{vib} + e_{el}$$

$$e = \frac{3}{2}RT + RT + \frac{h\nu/kT}{e^{h\nu/kT}-1}RT + e_{el}$$

$$C_v \equiv \left( \frac{\partial e}{\partial T} \right)_V$$



# Specific Heat

Molecules with only translational and rotational energy

$$e = \frac{3}{2}RT + RT = \frac{5}{2}RT \Rightarrow C_v = \frac{5}{2}R$$

$$C_p = C_v + R = \frac{7}{2}R$$

$$\gamma = \frac{C_p}{C_v} = \frac{7}{5} = 1.4$$



# Specific Heat

Mono-atomic gases with only translational and rotational energy

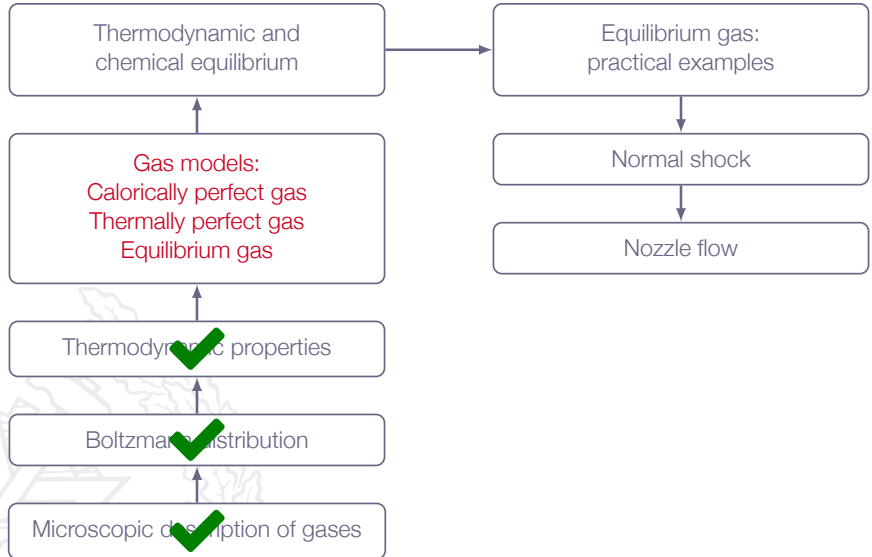
$$e = \frac{3}{2}RT \Rightarrow C_v = \frac{3}{2}R$$

$$C_p = C_v + R = \frac{5}{2}R$$

$$\gamma = \frac{C_p}{C_v} = \frac{5}{3} = 1\frac{2}{3} \simeq 1.67$$



# Roadmap - High Temperature Effects



# Calorically Perfect Gas

- ▶ In general, only **translational** and **rotational** modes of molecular excitation
- ▶ Translational and rotational energy levels are sparsely populated, according to **Boltzmann distribution** (the Boltzmann limit)
- ▶ Vibrational energy levels are practically unpopulated (except for the zero level)
- ▶ Characteristic values of  $\gamma$  for each type of molecule, e.g. mono-atomic gas, di-atomic gas, tri-atomic gas, etc
  - ▶ *He, Ar, Ne, ...* - mono-atomic gases ( $\gamma = 5/3$ )
  - ▶ *H<sub>2</sub>, O<sub>2</sub>, N<sub>2</sub>, ...* - di-atomic gases ( $\gamma = 7/5$ )
  - ▶ *H<sub>2</sub>O (gaseous), CO<sub>2</sub>, ...* - tri-atomic gases ( $\gamma < 7/5$ )



# Calorically Perfect Gas

$$\begin{aligned}p &= \rho RT & e &= C_v T \\h &= C_p T \\h &= e + p/\rho\end{aligned}$$

$$C_p - C_v = R$$

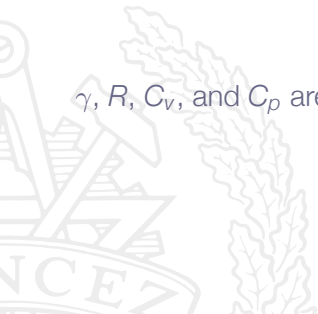
$$\gamma = C_p/C_v$$

$$C_v = \frac{R}{\gamma - 1}$$

$$C_p = \frac{\gamma R}{\gamma - 1}$$

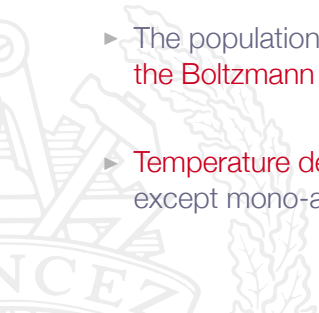
$\gamma$ ,  $R$ ,  $C_v$ , and  $C_p$  are constants

$$a = \sqrt{\frac{\gamma p}{\rho}} = \sqrt{\gamma RT}$$



# Thermally Perfect Gas

- ▶ In general, only **translational**, **rotational** and **vibrational** modes of molecular excitation
- ▶ Translational and rotational energy levels are sparsely populated, according to **Boltzmann distribution** (the Boltzmann limit)
- ▶ The population of the **vibrational energy** levels **approaches the Boltzmann limit** as temperature increases
- ▶ **Temperature dependent values of  $\gamma$**  for all types of molecules except mono-atomic (no vibrational modes possible)



# Thermally Perfect Gas

$$p = \rho RT$$

$$e = e(T)$$

$$C_v = de/dT$$

$$C_p - C_v = R$$

$$h = h(T)$$

$$C_p = dh/dT$$

$$\gamma = C_p/C_v$$

$$h = e + p/\rho$$

$$C_v = \frac{R}{\gamma - 1}$$

$$C_p = \frac{\gamma R}{\gamma - 1}$$

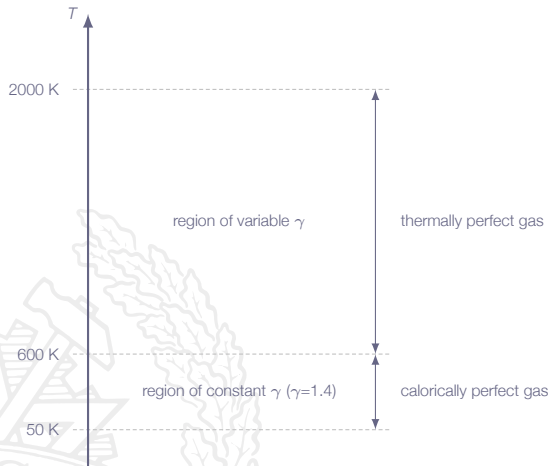
$R$  is constant

$\gamma$ ,  $C_v$ , and  $C_p$  are variable (functions of  $T$ )

$$a = \sqrt{\frac{\gamma p}{\rho}} = \sqrt{\gamma RT}$$

# High-Temperature Effects

Example: properties of air



Thermally perfect gas:  
 $e$  and  $h$  are non-linear functions of  $T$

the temperature range represents standard atmospheric pressure (lower pressure gives lower temperatures)

# High-Temperature Effects

For cases where the vibrational energy is not negligible (high temperatures)

$$\lim_{T \rightarrow \infty} e_{vib} = RT \Rightarrow C_V = \frac{7}{2}R$$

However, chemical reactions and ionization will take place long before that

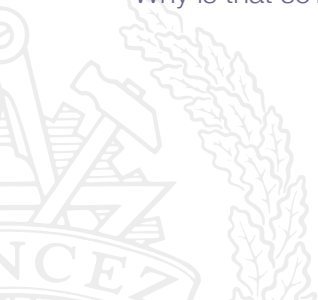
- ▶ Translational and rotational energy fully excited above  $\sim 5$  K
- ▶ Vibrational energy is non-negligible above 600 K
- ▶ Chemical reactions begin to occur above  $\sim 2000$  K



# High-Temperature Effects

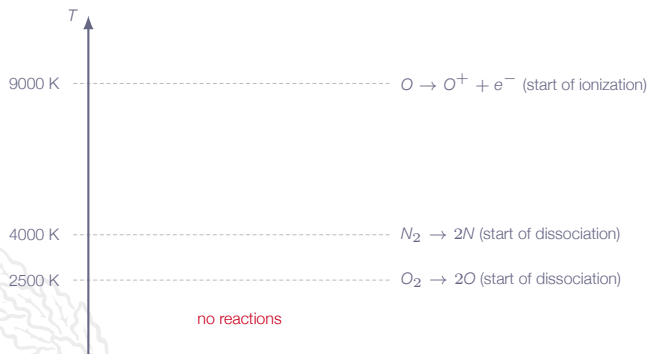
As temperature increase further vibrational energy becomes less important

Why is that so?



# High-Temperature Effects

Example: properties of air (continued)



With increasing temperature, the gas becomes more and more mono-atomic which means that vibrational modes becomes less important

# Equilibrium Gas

For temperatures  $T > \sim 2500K$

- ▶ Air may be described as being in **thermodynamic** and **chemical equilibrium** (Equilibrium Gas)
  - ▶ reaction rates (time scales) low compared to flow time scales
  - ▶ reactions in both directions (example:  $O_2 \rightleftharpoons 2O$ )
- ▶ Tables must be used (Equilibrium Air Data) or special functions which have been made to fit the tabular data





# Equilibrium Gas

How do we obtain a thermodynamic description?

$$p = p(R, T)$$

$$e = e(\nu, T)$$

$$C_v = \left( \frac{\partial e}{\partial T} \right)_\nu$$

$$h = h(p, T)$$

$$h = e + \frac{p}{\rho}$$

$$C_p = \left( \frac{\partial h}{\partial T} \right)_p$$

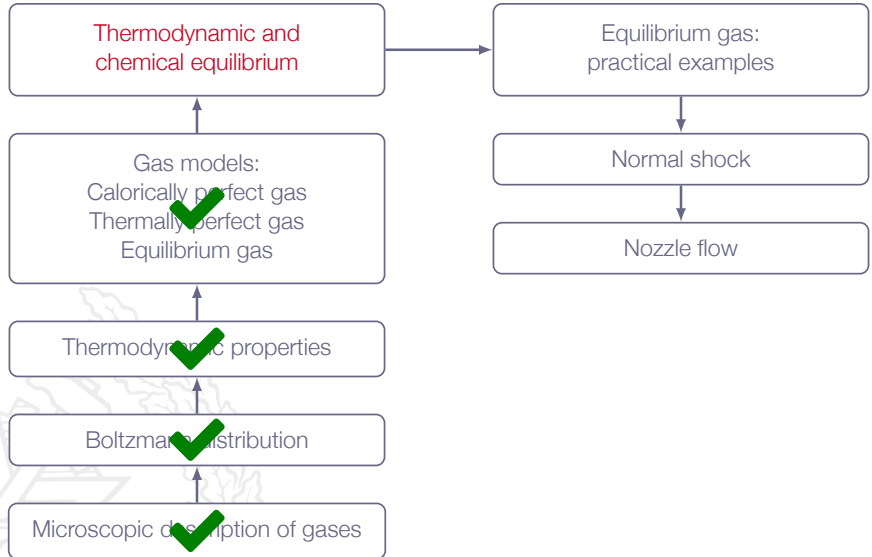
$$a_e^2 = \gamma RT \frac{1 + \frac{1}{\rho} \left( \frac{\partial e}{\partial \nu} \right)_T}{1 - \rho \left( \frac{\partial h}{\partial \rho} \right)_T}$$

$$\gamma = \frac{C_p}{C_v} = \frac{\left( \frac{\partial h}{\partial T} \right)_p}{\left( \frac{\partial e}{\partial T} \right)_\nu}$$

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

Note:  $R$  is not a constant here  
i.e. this is not the ideal gas law

# Roadmap - High Temperature Effects



# Chapter 17.1

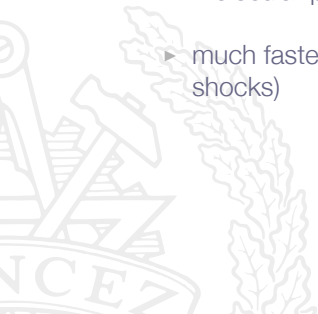
## Thermodynamic and Chemical Equilibrium



# Thermodynamic Equilibrium

Molecules are distributed among their possible energy states according to the **Boltzmann distribution** (which is a **statistical equilibrium**) for the given temperature of the gas

- ▶ extremely fast process (time and length scales of the molecular processes)
- ▶ much faster than flow time scales in general (not true inside shocks)



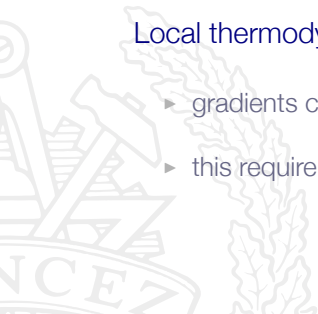
# Thermodynamic Equilibrium

## Global thermodynamic equilibrium:

- ▶ there are no gradients of  $p$ ,  $T$ ,  $\rho$ ,  $\mathbf{v}$ , species concentrations
- ▶ "true thermodynamic equilibrium"

## Local thermodynamic equilibrium:

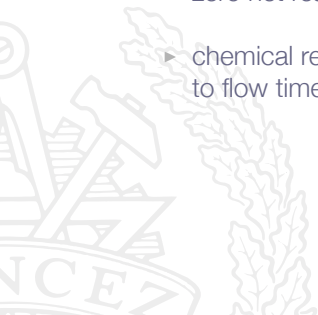
- ▶ gradients can be neglected locally
- ▶ this requirement is fulfilled in most cases (hard not to get)



# Chemical Equilibrium

**Composition** of gas (species concentrations) is **fixed in time**

- ▶ forward and backward rates of all chemical reactions are equal
- ▶ zero net reaction rates
- ▶ chemical reactions may be either slow or fast in comparison to flow time scale depending on the case studied



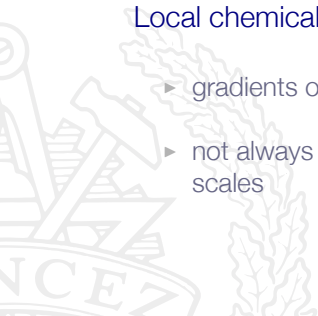
# Chemical Equilibrium

## Global chemical equilibrium:

- ▶ there are no gradients of species concentrations
- ▶ together with **global thermodynamic equilibrium**  $\Rightarrow$  all gradients are zero

## Local chemical equilibrium

- ▶ gradients of species concentrations can be neglected locally
- ▶ not always true - depends on reaction rates and flow time scales



# Thermodynamic and Chemical Equilibrium

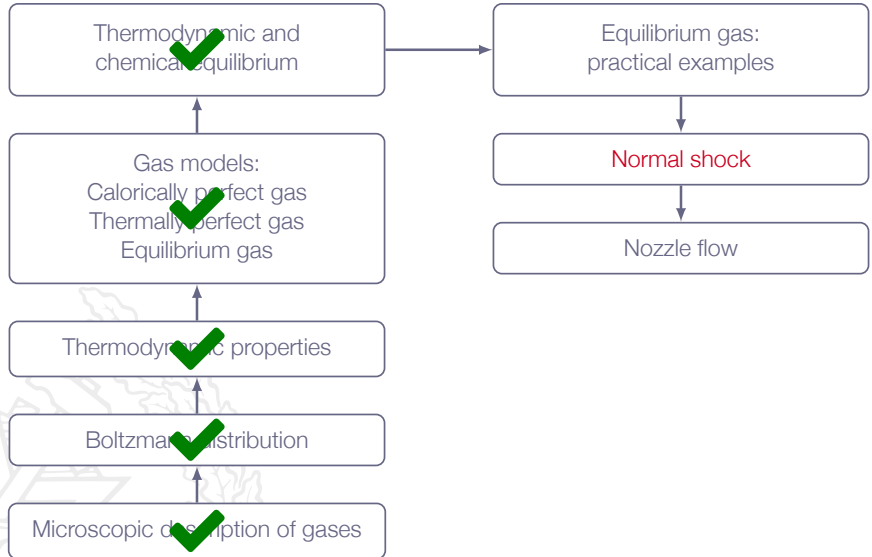
Most common cases:

	Thermodynamic Equilibrium	Chemical Equilibrium	Gas Model
1	local thermodynamic equilibrium	local chemical equilibrium	equilibrium gas
2	local thermodynamic equilibrium	chemical non-equilibrium	finite rate chemistry
3	local thermodynamic equilibrium	frozen composition	frozen flow
4	thermodynamic non-equilibrium	frozen composition	vibrationally frozen flow

- ▶ length and time scales of flow decreases from 1 to 4
- ▶ Frozen composition  $\Rightarrow$  no (or slow) reactions
- ▶ **vibrationally frozen** flow gives the same gas relations as **calorically perfect gas!**
  - ▶ no chemical reactions and unchanged vibrational energy
  - ▶ example: small nozzles with high-speed flow



# Roadmap - High Temperature Effects



# Chapter 17.2

## Equilibrium Normal Shock Wave Flows

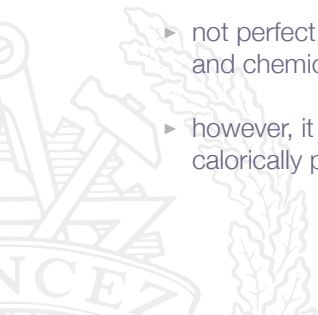


# Equilibrium Normal Shock Wave Flows

Question: Is the equilibrium gas assumption OK?

Answer:

- ▶ for hypersonic flows with very little ionization in the shock region, it is a fair approximation
- ▶ not perfect, since the assumption of local thermodynamic and chemical equilibrium is not really true around the shock
- ▶ however, it gives a significant improvement compared to the calorically perfect gas assumption



# Equilibrium Normal Shock Wave Flows

Basic relations (for all gases), stationary normal shock:

$$\left\{ \begin{array}{l} \rho_1 U_1 = \rho_2 U_2 \\ \rho_1 U_1^2 + p_1 = \rho_2 U_2^2 + p_2 \\ h_1 \frac{1}{2} U_1^2 = h_2 + \frac{1}{2} U_2^2 \end{array} \right.$$

For equilibrium gas we have:

$$\left\{ \begin{array}{l} \rho = \rho(p, h) \\ T = T(\rho, h) \end{array} \right.$$

(we are free to choose any two states as independent variables)

# Equilibrium Normal Shock Wave Flows

Assume that  $\rho_1$ ,  $u_1$ ,  $p_1$ ,  $T_1$ , and  $h_1$  are known

$$u_2 = \frac{\rho_1 u_1}{\rho_2} \Rightarrow \rho_1 u_1^2 + p_1 = \rho_2 \left( \frac{\rho_1}{\rho_2} u_1 \right)^2 + p_2 \Rightarrow$$

$$p_2 = p_1 + \rho_1 u_1^2 \left( 1 - \frac{\rho_1}{\rho_2} \right)$$

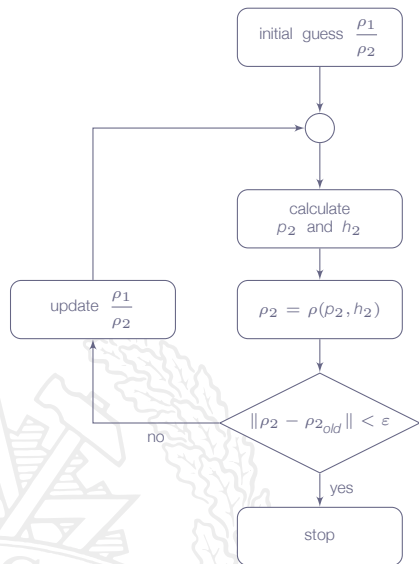
Also

$$h_1 + \frac{1}{2} u_1^2 = h_2 + \frac{1}{2} \left( \frac{\rho_1}{\rho_2} u_1 \right)^2 \Rightarrow$$

$$h_2 = h_1 + \frac{1}{2} u_1^2 \left( 1 - \left( \frac{\rho_1}{\rho_2} \right)^2 \right)$$



# Equilibrium Normal Shock Wave Flows



when converged:

$$\left. \begin{aligned} \rho_2 &= \rho(\rho_2, h_2) \\ T_2 &= T(\rho_2, h_2) \end{aligned} \right\} \Rightarrow$$

$\rho_2, u_2, p_2, T_2, h_2$  known

# Equilibrium Air - Normal Shock

Tables of thermodynamic properties for different conditions are available

For a very strong shock case ( $M_1 = 32$ ), the table below (Table 17.1) shows some typical results for equilibrium air

	calorically perfect gas ( $\gamma = 1.4$ )	equilibrium air
$\rho_2/\rho_1$	1233	1387
$\rho_2/\rho_1$	5.97	15.19
$h_2/h_1$	206.35	212.80
$T_2/T_1$	206.35	41.64

# Equilibrium Air - Normal Shock

## Analysis:

- ▶ Pressure ratio is comparable
- ▶ Density ratio differs by factor of 2.5
- ▶ Temperature ratio differs by factor of 5

## Explanation:

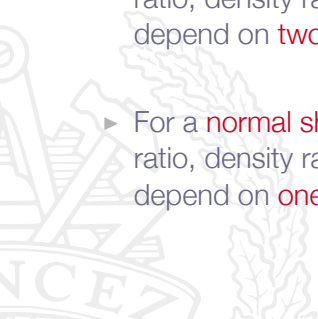
- ▶ Using equilibrium gas means that vibration, dissociation and chemical reactions are accounted for
- ▶ The chemical reactions taking place in the shock region lead to an "absorption" of energy into chemical energy
  - ▶ drastically reducing the temperature downstream of the shock
  - ▶ this also explains the difference in density after the shock



# Equilibrium Air - Normal Shock

## Additional notes:

- ▶ For a **normal shock in an equilibrium gas**, the pressure ratio, density ratio, enthalpy ratio, temperature ratio, etc all depend on **three upstream variables**, e.g.  $u_1, \rho_1, T_1$
- ▶ For a **normal shock in a thermally perfect gas**, the pressure ratio, density ratio, enthalpy ratio, temperature ratio, etc all depend on **two upstream variables**, e.g.  $M_1, T_1$
- ▶ For a **normal shock in a calorically perfect gas**, the pressure ratio, density ratio, enthalpy ratio, temperature ratio, etc all depend on **one upstream variable**, e.g.  $M_1$



# Equilibrium Gas - Detached Shock

calorically perfect gas

$M = 20$



equilibrium gas

$M = 20$



shock moves closer to body

What's the reason for the difference in predicted shock position?

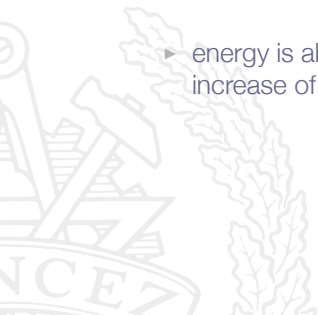
# Equilibrium Gas - Detached Shock

## Calorically perfect gas:

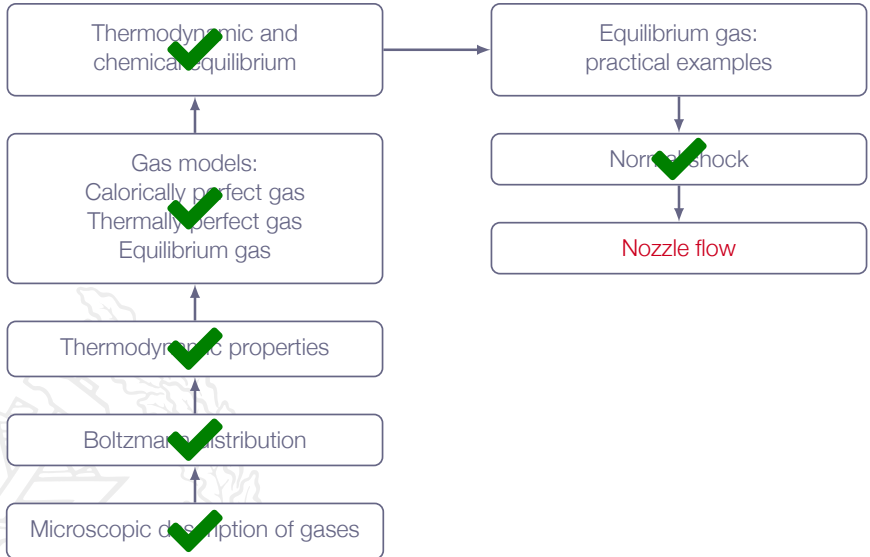
- ▶ all energy ends up in translation and rotation  $\Rightarrow$  increased temperature

## Equilibrium gas:

- ▶ energy is absorbed by reactions  $\Rightarrow$  does not contribute to the increase of gas temperature



# Roadmap - High Temperature Effects



# Chapter 17.3

## Equilibrium

### Quasi-One-Dimensional

### Nozzle Flows



# Equilibrium Quasi-1D Nozzle Flows

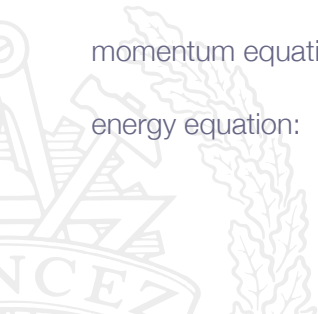
First question: Is chemically reacting gas also isentropic (for inviscid and adiabatic case)?

entropy equation:  $Tds = dh - \nu dp$

Quasi-1D equations in differential form (all gases):

momentum equation:  $dp = -\rho u du$

energy equation:  $dh + u du = 0$



# Equilibrium Quasi-1D Nozzle Flows

$$udu = -\frac{dp}{\rho} = -\nu dp$$

$$Tds = -udu - \nu dp = -udu + udu = 0 \Rightarrow$$

$$ds = 0$$

Isentropic flow!



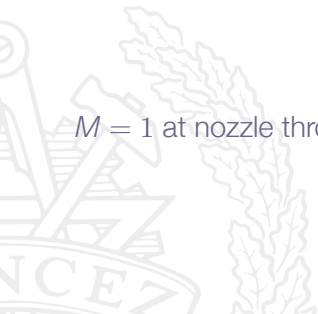
# Equilibrium Quasi-1D Nozzle Flows

Second question: Does the area-velocity relation also hold for a chemically reacting gas?

Isentropic process gives

$$\frac{dA}{A} = (M^2 - 1) \frac{du}{u}$$

$M = 1$  at nozzle throat still holds

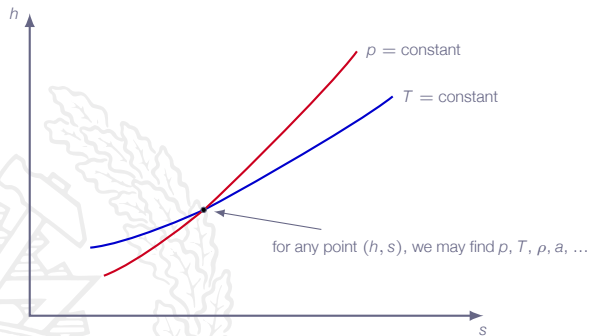




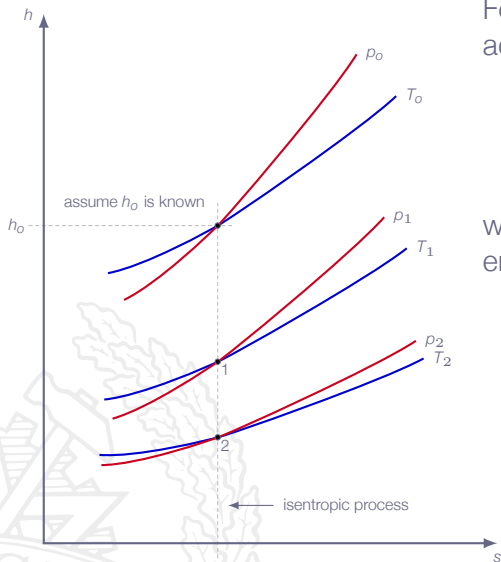
# Equilibrium Quasi-1D Nozzle Flows

For general gas mixture in thermodynamic and chemical equilibrium, we may find tables or graphs describing relations between state variables.

Example: Mollier diagram



# Equilibrium Quasi-1D Nozzle Flows



For steady-state inviscid adiabatic nozzle flow we have:

$$h_1 + \frac{1}{2}u_1^2 = h_2 + \frac{1}{2}u_2^2 = h_o$$

where  $h_o$  is the reservoir enthalpy

# Equilibrium Quasi-1D Nozzle Flows

At point 1 in Mollier diagram we have:

$$\frac{1}{2}u_1^2 = h_o - h_1 \Rightarrow u_1 = \sqrt{2(h_o - h_1)}$$

Assume that  $u_1 = a_1$  (sonic conditions) gives

$$\rho_1 u_1 A_1 = \rho^* a^* A^*$$

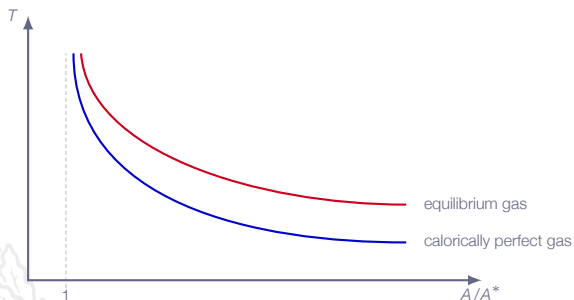
At any point along isentropic line, we have  $u = \sqrt{2(h_o - h)}$  and  $\rho$ ,  $\rho$ ,  $T$ ,  $a$  etc are all given which means that  $\rho u$  is given

$$\frac{A}{A^*} = \frac{\rho^* a^*}{\rho u}$$

may be computed for any point along isentropic line

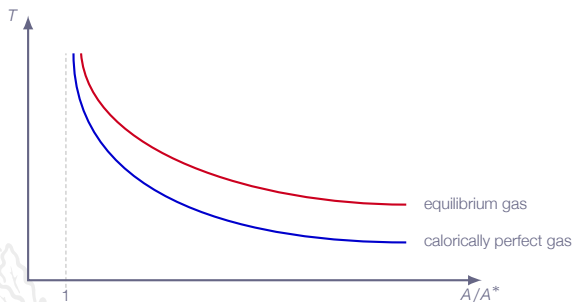
# Equilibrium Quasi-1D Nozzle Flows

- ▶ Equilibrium gas gives higher  $T$  and more thrust
- ▶ During the expansion chemical energy is released due to shifts in the equilibrium composition



# Equilibrium Quasi-1D Nozzle Flows

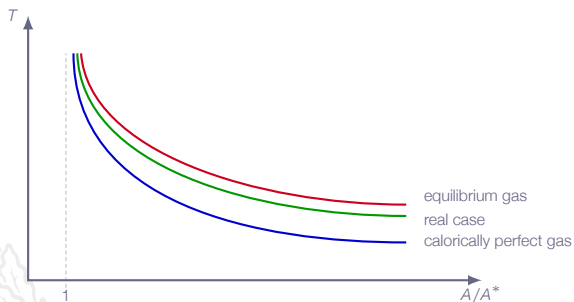
- ▶ Equilibrium gas gives higher  $T$  and more thrust
- ▶ During the expansion chemical energy is released due to shifts in the equilibrium composition



- ▶ Chemical and vibrational energy transferred to translation and rotation  $\Rightarrow$  increased temperature

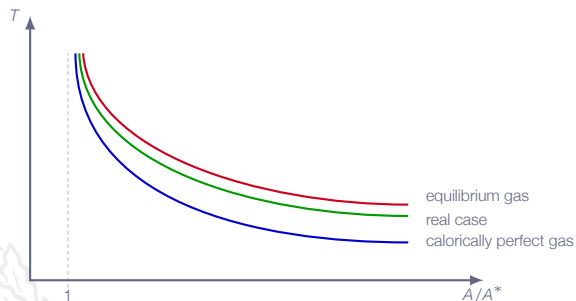
# Equilibrium Quasi-1D Nozzle Flows - Reacting Mixture

Real nozzle flow with reacting gas mixture:



# Equilibrium Quasi-1D Nozzle Flows - Reacting Mixture

Real nozzle flow with reacting gas mixture:



- ▶ Space nozzle applications:  $u_e \approx 4000$  m/s
- ▶ Required prediction accuracy 5 m/s

# Equilibrium Quasi-1D Nozzle Flows - Reacting Mixture

## Equilibrium gas:

- ▶ very **fast chemical reactions**
- ▶ local thermodynamic and chemical equilibrium

## Vibrationally frozen gas:

- ▶ very **slow chemical reactions**  
(no chemical reactions  $\Rightarrow$  frozen gas)
- ▶ **vibrational energy** of molecules have **no time to change**
- ▶ **calorically perfect gas!**





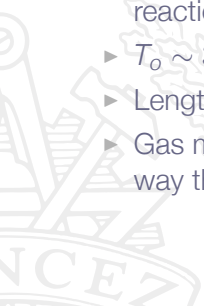
# Large Nozzles

High  $T_o$ , high  $p_o$ , high reactivity

Real case is close to **equilibrium gas** results

**Example:** Ariane 5 launcher, main engine (Vulcain 2)

- ▶  $H_2 + O_2 \rightarrow H_2O$  in principle, but many different radicals and reactions involved (at least  $\sim 10$  species,  $\sim 20$  reactions)
- ▶  $T_o \sim 3600\text{ K}$ ,  $p_o \sim 120\text{ bar}$
- ▶ Length scale  $\sim$  a few meters
- ▶ Gas mixture is quite close to equilibrium conditions all the way through the expansion



# Small Nozzles

Low  $T_o$ , low  $p_o$ , lower reactivity

Real case is close to **frozen flow** results

Example:

Small rockets on satellites (for maneuvering, orbital adjustments, etc)



# Roadmap - High Temperature Effects

