COMPUTATIONAL FLUID DYNAMICS

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Overview of Thermodynamics (I)

Heat capacities:

$$C_v = \left(\frac{\Delta Q}{\Delta T}\right)_V \qquad C_p = \left(\frac{\Delta Q}{\Delta T}\right)_p$$

(heat is *not* a state variable).

Internal Energy: Every equilibrium state is characterized by an internal energy *U=U(V,S)*, which is a state variable.

Given an *amount of heat* ΔQ and *work done W*, the change in internal energy is $\Delta U = \Delta Q + W$.

1st Law: For infinitesimal changes between equilibrium states:

$$dU = \bar{d}Q + dW = \bar{d}Q - pdV$$

Thermally ideal gas: $U = U(T)$ e.g. $U = \frac{3}{2} n\mathcal{R}T$ (monatomic gas)

$$pV = n\mathcal{R}T$$

$$S = S_0 + C_V \ln T + \mathcal{R} \ln V$$

where n = amount of substance (number of moles)

$\mathcal{R}$ = universal gas constant = 8.314 J mol^{-1} K^{-1}

Overview of Thermodynamics (II)

Entropy:

$$dS = \frac{\bar{d}Q}{T} \quad \Rightarrow \quad dU = TdS - pdV$$

Enthalpy:

$$H = U + pV \quad \Rightarrow \quad dH = TdS + Vdp$$

Helmholtz free energy:

$$F = U - TS \quad \Rightarrow \quad dF = -SdT - pdV$$

Overview of Thermodynamics (III)

Formulation in terms of *intensive variables*:

$$v = \frac{V}{m} = \frac{1}{\rho}$$ *specific volume*

$$e = \frac{U}{m}$$ *specific internal energy*

$$s = \frac{S}{m}$$ *specific entropy*

$$h = \frac{H}{m} = e + pv$$ *specific enthalpy*

$$f = \frac{F}{m} = e - Ts$$ *specific free energy*

$$c_v = \frac{C_V}{m}$$ *specific heat (at constant specific volume)*

$$c_p = \frac{C_p}{m}$$ *specific heat (at constant pressure)*

where *m* is the mass of the fluid or gas.

Overview of Thermodynamics (IV)

Thermodynamic relations:

$$
\begin{aligned}
de &= Tds - pdv \\
dh &= Tds + vdp \\
df &= -sdT - pdv
\end{aligned}
$$

from which one can compute, e.g.

$$
\begin{aligned}
T &= \left(\frac{\partial e}{\partial s}\right)_v \\
c_p &= \left(\frac{\partial h}{\partial T}\right)_p
\end{aligned}
$$

3 fundamental variables are needed, e.g.

$$
\begin{aligned}
&p, v, T \\
&p, v, e \\
&p, v, s \\
&e, v, s
\end{aligned}
$$

etc.

Overview of Thermodynamics (V)

Difference of specific heats:

$$c_p - c_v = R$$

where

$$R = \frac{\mathcal{R}}{w}$$

$$w = \frac{m}{n} = \quad \text{mean molecular weight}$$

<u>Thermally ideal gas EOS</u><u>:</u>

Equation of state: $pv = RT \quad \Rightarrow \quad e = e(T)$

$$c_p = c_p(T)$$

$$c_v = c_v(T)$$

Define $\gamma = \gamma(T) = \frac{c_p}{c_v}$ *(ratio of specific heats)*

Then

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

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

Overview of Thermodynamics (V)

Calorically ideal gas EOS:

For *monatomic gases*, we can assume that

$$c_v = const., \quad c_p = const.$$

$$\Rightarrow \quad \gamma = const.$$
$$e = c_v T$$

Then, the equation of state becomes:

$$p = (\gamma - 1)\rho e$$

Exercise 1

For *polyatomic gases*, c_v etc. depend on T.

Covolume EOS:

At large densities, the volume occupied by molecules is no longer negligible and there is a reduction in the volume available for molecular motion. Then:

$$p(v - b) = RT \quad \text{and} \quad p = \frac{(\gamma - 1)\rho e}{1 - b\rho}$$

where b = covolume ($m^3\ g^{-1}$).

Overview of Thermodynamics (V)

Speed of sound:

$$p = p(\rho, s) \quad \Rightarrow \quad v_s = \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_s}$$

$$p = p(\rho, e) \quad \Rightarrow \quad v_s = \sqrt{\frac{p}{\rho^2}\frac{\partial p}{\partial e} + \frac{\partial p}{\partial \rho}}$$

Examples:

$$pv = RT \quad \Rightarrow \quad v_s = \sqrt{\gamma(T)RT} = \sqrt{\frac{\gamma(T)p}{\rho}}$$

$$p = (\gamma - 1)\rho e \quad \Rightarrow \quad v_s = \sqrt{\frac{\gamma p}{\rho}}$$

$$p = \frac{(\gamma - 1)\rho e}{1 - b\rho} \quad \Rightarrow \quad v_s = \sqrt{\frac{\gamma p}{(1 - b\rho)\rho}}$$