

Lecture 1

Conservation equations for chemically reacting gas mixtures

Conservation equations for a pure substance

Conservation of mass

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{v} = 0$$

$$\frac{\partial \rho}{\partial t} + \mathbf{v} \cdot \nabla \rho + \rho \nabla \cdot \mathbf{v} = 0$$

$$\frac{D\rho}{Dt}$$

convective
derivative

time rate of change ...
following a fluid particle

$$\Rightarrow \frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{v} = 0$$

$$\nabla \cdot \mathbf{v} = -\frac{1}{\rho} \frac{D\rho}{Dt}$$

$$\frac{D\rho}{Dt} = 0 \Rightarrow \nabla \cdot \mathbf{v} = 0$$

incompressible flow

Conservation of momentum

$$\rho \frac{D\mathbf{v}}{Dt} = \rho \mathbf{g} + \nabla \cdot \boldsymbol{\sigma}$$

$$\boldsymbol{\sigma} = \underbrace{-p\mathbf{I}}_{\text{pressure}} + \underbrace{\boldsymbol{\Sigma}}_{\text{viscous stress tensor (Newtonian Fluid)}}$$

$$\boldsymbol{\Sigma} = \mu [(\nabla \mathbf{v}) + (\nabla \mathbf{v})^T] + \left(\kappa - \frac{2}{3}\mu \right) (\nabla \cdot \mathbf{v}) \mathbf{I}$$

bulk viscosity
shear viscosity

The first term is a measure of the deformation of the fluid element and the second term is the rate of change of its volume

$$\rho \frac{D\mathbf{v}}{Dt} = -\nabla p + \nabla \cdot \boldsymbol{\Sigma} + \rho \mathbf{g}$$

$\boldsymbol{\sigma}$ is a symmetric tensor, i.e. $\sigma_{ij} = \sigma_{ji}$.

$$(\nabla \cdot \boldsymbol{\sigma})_i = \frac{\partial \sigma_{ij}}{\partial x_j} \quad (\nabla \mathbf{v})_{ij} = \frac{\partial v_i}{\partial x_j} \quad \text{summation convention adopted}$$

Conservation of energy

$$e_T = e + \frac{1}{2} \mathbf{v}^2 = \text{total energy}$$

$$\rho \frac{De_T}{Dt} = \rho \mathbf{g} \cdot \mathbf{v} + \nabla \cdot (\boldsymbol{\sigma} \cdot \mathbf{v}) - \nabla \cdot \mathbf{q}$$

rate of work done on the fluid by gravitational & viscous forces

rate of heat transferred to the fluid

\mathbf{q} - heat flux vector
(positive for outward heat transport)

$$\rho \frac{D\mathbf{v}}{Dt} = \rho \mathbf{g} + \nabla \cdot \boldsymbol{\sigma} \quad / \cdot \mathbf{v} \quad \Rightarrow \quad \rho \frac{D}{Dt} \left(\frac{1}{2} \mathbf{v}^2 \right) = \rho \mathbf{g} \cdot \mathbf{v} + (\nabla \cdot \boldsymbol{\sigma}) \cdot \mathbf{v}$$

$$\rho \frac{De}{Dt} = [\nabla \cdot (\boldsymbol{\sigma} \cdot \mathbf{v}) - (\nabla \cdot \boldsymbol{\sigma}) \cdot \mathbf{v}] - \nabla \cdot \mathbf{q}$$

$$\boldsymbol{\sigma} : \nabla \mathbf{v} = \sigma_{ij} \frac{\partial v_i}{\partial x_j}$$

$$\sigma = -p\mathbf{I} + \Sigma \quad \Rightarrow$$

$$\rho \frac{De}{Dt} = -p \nabla \cdot \mathbf{v} + \Phi - \nabla \cdot \mathbf{q}$$

Rate of internal energy
increase by compression

$$\Phi = \frac{1}{2}\mu \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right)^2 + \left(\kappa - \frac{2}{3}\mu \right) (\nabla \cdot \mathbf{v})^2$$

Rate of dissipation of
internal energy due to
viscous forces
Dissipation function

An alternative form, in terms of the enthalpy $h = e + p/\rho$

$$\begin{aligned} \frac{Dh}{Dt} &= \frac{De}{Dt} + \frac{1}{\rho} \frac{Dp}{Dt} - \frac{p}{\rho^2} \frac{D\rho}{Dt} \\ &= \rho \frac{De}{Dt} - \frac{Dp}{Dt} - p \nabla \cdot \mathbf{v} \end{aligned}$$

$$\rho \frac{Dh}{Dt} = \frac{Dp}{Dt} + \Phi - \nabla \cdot \mathbf{q}$$

Summary

mass $\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{v} = 0$

momentum $\rho \frac{D\mathbf{v}}{Dt} = -\nabla p + \nabla \cdot \Sigma + \rho \mathbf{g}$

energy $\rho \frac{Dh}{Dt} = \frac{Dp}{Dt} + \Phi - \nabla \cdot \mathbf{q}$

Constitutive relations:

$$\Sigma = \mu [(\nabla \mathbf{v}) + (\nabla \mathbf{v})^T] + \left(\kappa - \frac{2}{3}\mu \right) (\nabla \cdot \mathbf{v}) \mathbf{I} \quad \text{Newtonian fluid}$$

$$\nabla \cdot \mathbf{q} = -\lambda \nabla T \quad \text{Fourier Law of heat conduction (neglecting radiation, etc.)}$$

Thermodynamics

State of the gas is uniquely determined by two variables

$$p = p(\rho, T), \quad e = e(p, T), \quad \text{etc.}$$

Ideal gas:

$$p = \frac{\rho \mathcal{R} T}{W}$$

$\mathcal{R} = 8.3145 \text{ cal/mol} \cdot \text{K}$ universal gas constant

$\bar{\mathcal{R}} = \mathcal{R}/W$ specific gas constant

$e = e(T), \quad h = h(T)$ only

Specific heats at constant pressure/volume c_p, c_v

$$\frac{dh}{dT} = c_p \Rightarrow h = h^o + \int_{T^o}^T c_p dT$$

$$\frac{de}{dT} = c_v \Rightarrow e = e^o + \int_{T^o}^T c_v dT$$

* Reference temperature

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

$$\frac{dh}{dT} = \frac{de}{dT} + \frac{d}{dT} \left(\frac{p}{\rho} \right) \Rightarrow c_p = c_v + \mathcal{R}/W$$

ratio of specific heats $\gamma = c_p/c_v > 1$

entropy

$$T dS = dh - \frac{1}{\rho} dp$$

$$T \frac{DS}{Dt} = \frac{Dh}{Dt} - \frac{1}{\rho} \frac{Dp}{Dt}$$

$$\rho \frac{Dh}{Dt} = \frac{Dp}{Dt} + \Phi - \nabla \cdot \mathbf{q} \Rightarrow \rho \frac{DS}{Dt} = \frac{1}{T} (\Phi - \nabla \cdot \mathbf{q})$$

reversible process: $\Phi = 0$ $\Delta S \sim \text{heat acquired}/T$

irreversible process: $\Phi > 0$ ΔS larger than when $\Phi = 0$

In an isentropic flow (adiabatic + reversible) the entropy remain constant

$$dh = dp/\rho$$

$$dh = c_p dT$$

$$\Rightarrow \frac{dp}{p} = \gamma \frac{d\rho}{\rho}$$

$$p\rho^{-\gamma} = \text{const.}$$

speed of sound

$$a = \sqrt{\left(\frac{\partial p}{\partial \rho} \right)_s} = \sqrt{\gamma p/\rho} = \sqrt{\gamma \mathcal{R} T}$$