Lecture 1

Conservation equations for chemically reacting gas mixtures

Conservation of mass

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

\[ \frac{D\rho}{Dt} = 0 \quad \Rightarrow \quad \nabla \cdot \mathbf{v} = 0 \]

for incompressible flow

Conservation equations for a pure substance

Conservation of mass

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

\[ \frac{D\rho}{Dt} \quad \text{convective derivative} \]

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

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Conservation of momentum

\[ \rho \frac{D \mathbf{v}}{Dt} = \rho g + \nabla \cdot \sigma \]

\( \sigma = -p \mathbf{I} + \Sigma \)

stress tensor

\( \Sigma = \mu (\nabla \mathbf{v}) + (\nabla \mathbf{v})^T + (\kappa - \frac{2}{3} \mu) (\nabla \cdot \mathbf{v}) \mathbf{I} \)

viscous stress tensor (Newtonian Fluid)

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.

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

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

\( (\nabla \cdot \sigma) = \frac{\partial \sigma_{ij}}{\partial x_j} \) \( (\nabla v)_{ij} = \frac{\partial v_i}{\partial x_j} \) summation convention adopted

Conservation of energy

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

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

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)

\[ \rho \frac{D \mathbf{v}}{Dt} = \rho g + \frac{1}{2} \left( \frac{\partial v_i}{\partial x_j} \right) ^T \frac{\partial v_j}{\partial x_i} \]

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

\( \sigma : \nabla \mathbf{v} = \sigma_{ij} \frac{\partial v_i}{\partial x_j} \)
\[ \sigma = -pI + \Sigma \quad \Rightarrow \quad \frac{D\sigma}{Dt} = -p\nabla \cdot \mathbf{v} + \Phi - \nabla \cdot \mathbf{q} \]

Rate of internal energy increase by compression
\[ \Phi = \frac{1}{2} \rho \left( \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) + \left( \kappa - \frac{2}{3} \mu \right) \left( \nabla \cdot \mathbf{v} \right)^2 \]
Rate of dissipation of internal energy due to viscous forces
Dissipation function

An alternative form, in terms of the enthalpy \( h = e + p/\rho \)
\[ \frac{Dh}{Dt} = \frac{De}{Dt} + \frac{1}{\rho} \frac{D\rho}{Dt} \left( \frac{\partial\rho}{\partial p} \right) \frac{Dp}{Dt} \]
\[ = \rho \frac{Dh}{Dt} - \frac{Dp}{Dt} - p \nabla \cdot \mathbf{v} \]

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

Summary

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

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

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

Constitutive relations:
\[ \Sigma = \mu \left( \nabla \mathbf{v} + (\nabla \mathbf{v})^T \right) + \left( \kappa - \frac{2}{3} \mu \right) (\nabla \cdot \mathbf{v}) I \quad \text{Newtonian fluid} \]
\[ \nabla \cdot \mathbf{q} = -\lambda \nabla T \quad \text{Fourier Law of heat conduction} \]
(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:*

\[ p = \rho R T \quad \Rightarrow \quad p = p(\rho, T) \]

\[ e = e(T), \quad h = h(T) \quad \text{only} \]

**Specific heats at constant pressure/volume** \(c_p, c_v\)

\[
\frac{dh}{dT} = c_p \quad \Rightarrow \quad h = h^o + \int_{T^o}^T c_p dT \\
\frac{de}{dT} = c_v \quad \Rightarrow \quad e = e^o + \int_{T^o}^T c_v dT
\]

*Reference temperature

\[
\frac{dh}{dT} = \frac{de}{dT} + \frac{d}{dT} \left( \frac{p}{\rho} \right) \quad \Rightarrow \quad c_p = c_v + \frac{R}{W}
\]

**Ratio of specific heats** \(\gamma = c_p/c_v > 1\)

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**Entropy**

\[
TdS = dh - \frac{1}{\rho} dp \\
T \frac{DS}{Dt} = Dh + \frac{1}{\rho} Dp - \frac{1}{\rho} Dp
\]

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

*Reversible process: \(\Phi = 0\) \(\Delta S \sim \text{heat acquired}/T\)

*Irreversible process: \(\Phi > 0\) \(\Delta S\) larger than when \(\Phi = 0\)

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

\[
\frac{dh}{dT} = \frac{dp}{\rho} \quad \Rightarrow \quad \frac{dp}{p} = \gamma \frac{d\rho}{\rho} \quad \Rightarrow \quad p^\gamma = \text{const.}
\]

**Speed of sound**

\[
a = \sqrt{\left( \frac{\partial p}{\partial \rho} \right)_s} = \sqrt{\gamma p/\rho} = \sqrt{\gamma RT}
\]

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