Mass, Momentum and Energy Transfer in Energy Systems

-NUCL 551-

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Sept.16th, 2014

Chapter 3 Single Phase Flow Constitutive Relation

1. Closure of Equation Systems

Balance equations (Mass Momentum & Energy) not sufficient to close the math system

$$\text{Unknowns:}\quad \left.\begin{array}{ll} \text{Mass} & \rho, \vec{v} \\ \text{Momentum} & p, \tau, \vec{g} \\ \text{Energy} & u, \vec{q}, \dot{q} \end{array}\right\} \quad 8$$

Balance Equations 3

1) The balance equation should be supplemented by various constitutive relations
2) The constitutive relations should
   - Model material responses observed in experiments
   - Not to violate any physical laws
   - Have reasonably simple mathematical form
   - Fit to certain practical idealizations

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2. Second Law of Thermodynamics
   - Most Important Physical Law outside of Conservation Equations
   - Existence of Entropy s
   - Temperature T
   - 2nd Law for all materials and processes

$$\frac{d}{dt}\int_{V_m}\rho s dV+\oint_{S_m}\underbrace{\frac{\vec{q}}{T}}_{\text{Entropy flux}}\cdot n dS-\int_{V_m}\underbrace{\frac{\dot{q}}{T}}_{\text{Entropy source}}dV\geq 0$$

V_m ; fixed mass volume

Use Reynolds Transport Theorem

$$\boxed{\frac{\partial}{\partial t}\rho s+\nabla\cdot(\rho s\vec{v})+\nabla\cdot\left(\frac{\dot{q}}{T}\right)-\frac{\dot{q}}{T}\equiv\Delta\geq 0} \qquad (1)$$

Δ; entropy production

$=$; reversible system

$>$; irreversible system

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- In this form the physical meaning is not clear because the relation between *s*, *T* and other variables are not given yet. (Constitutive relations are not given yet).

- Entropy Inequality $\longrightarrow$ Restriction on Constitutive Laws

- Formulation of Constitutive Relation

  General guidelines

  - Entropy Inequality
  - Determinism — ✓ Present state can be determined from the past history
  - Frame Indifference — ✓ Material response independent of observer
  - Local Action — ✓ Material responses locally affected (no long range interactions)

- 2nd Law Restrictions (Practically)
  - Heat should not flow against the temperature gradient.
  - Frictional force acts against the motion.

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3. Type of Constitutive Relations

Equation of State	ρ, s, u, p, T
Mechanical Constitutive Equation	$\tau, \vec{g}$
Thermal Constitutive Equation	$\vec{q}, \dot{q}$

By introducing $T, s \longrightarrow$ 10 unknowns

$$\left.\begin{matrix} \rho, \vec{v} \\ p, \tau, \vec{g} \\ u, \vec{q}, \dot{q} \end{matrix}\right\} + T,\ s \quad \Longrightarrow \quad (10)$$

$$\begin{cases} \text{3 Balance Equations} \\ \text{7 Relations} \begin{cases} \tau, \vec{g} \\ \vec{q}, \dot{q} \\ s(u, \rho) \\ \text{Thermodynamic Definition of } T \text{ and } p \end{cases} \end{cases}$$

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4. Equation of State

- Fundamental Equation of State

  (for thermodynamically homogeneous material)

$$u = u(s, \rho) \qquad (2)$$

$$T \equiv \left.\frac{\partial u}{\partial s}\right|_{\rho} \quad \text{; temperature} \qquad (3)$$

$$p \equiv -\frac{\partial u}{\partial \left(1/\rho \right)} \quad \text{; thermoldynamic pressure} \qquad (4)$$

Thus $du = Tds - pd\left(1/\rho \right)$

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- Gibbs free energy $$g = u - Ts + \frac{p}{\rho} = g(T, p)$$
- Enthalpy $$i = u + \frac{p}{\rho} = i(s, p)$$
- Helmholtz free energy $$f = u - Ts = f(T, p) \text{ or } f(s, \rho)$$

- Anyone of them $\longrightarrow$ fundamental equation of state
- Legendre transformation $\longrightarrow$ Change of variable to its 1st derivative
- Practical Form of Equation of State

  Use of 1st order derivatives

  Replace 1 Fundamental Equation of State by $\left\{ \begin{array}{l} \text{Thermal Equation of State} \\ \text{Caloric Equation of State} \end{array} \right.$

  (Equivalent)

$p = p(\rho, T)$ Thermal Equation of State (5)

$u = u(\rho, T)$ Caloric Equation of State (6)

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- <u>Example</u>

  a) Incompressible fluid

$$\rho = \text{constant}$$

$$u = u(T)$$

  b) Ideal gas

$$p = RT\rho$$

$$u = u(T)$$

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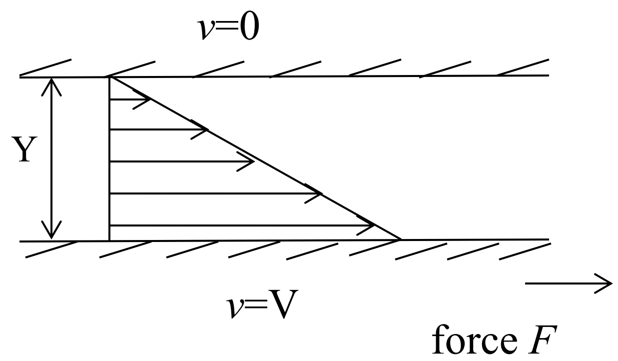
5. Mechanical Constitutive Relation (Chapter 1)
   a) Inviscid Fluid $\tau = 0$
   b) Linearly Viscous Fluid



$$\frac{F}{A} = \mu \frac{V}{Y}$$

$$\tau_{yx} = -\mu \frac{dv_x}{dy}$$

μ; viscosity

v_x; x-direction velocity

x component shear stress
acting on y direction surface

I. $\boxed{\text{Force} \sim \text{Velocity Gradient (Linear)}}$

Newton's Law of Viscosity

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II. $y \approx 0$ fluid acquires a certain amount of *x*-momentum

$y \approx \delta$ This fluid impacts some of its momentum to the adjacent layer

Hence *x*-direction momentum is transmitted through the fluid in the *y*-direction

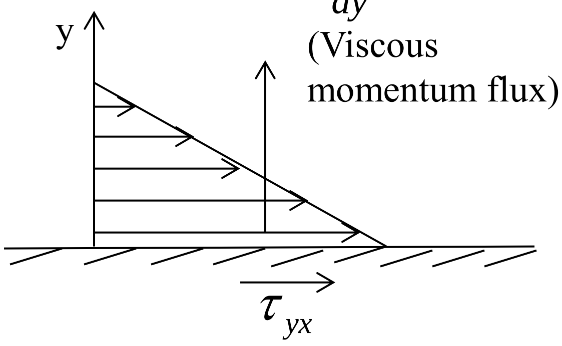
τ_{yx}; viscous flux of x-momentum in the y-direction

viscous momentum flux; in the direction of negative velocity gradient

(momentum goes from high to low velocity region)

Velocity gradient; driving force for viscous momentum transport

$$\tau_{yx} = -\mu \frac{dv_x}{dy}$$



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- Note: Similarity between
  - viscous force (Newton's Law) $\tau_{yx} = -\mu \dfrac{dv_x}{dy}$
  - heat flux (Fourier Law) $q_y = -k \dfrac{dT}{dy}$
  - diffusion mass flux (Fick's Law) $J_{ky} = -\rho D_k \dfrac{dw_k}{dy}$

v_x; velocity

μ; viscosity

T; temperature

k; thermal conductivity

w_k; mass fraction

D; diffusion coefficient

All these are linear constitutive laws

$$\Downarrow$$

Very accurately model physics in most materials

Flux	heat flux	vis. momentum flux	mass flux
Driving head	temp. grad.	vel. grad.	mass fraction grad.

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- Generalization; Linearly Viscous Fluid of Navier-Stokes

$$\tau = -\mu\left[\nabla\vec{v} + \left(\nabla\vec{v}\right)^{+}\right] + \underbrace{\left(\frac{2}{3}\mu - \mu'\right)\left(\nabla\cdot\vec{v}\right)\mathrm{I}}_{\text{Compressible effect}}$$

μ; viscosity

μ'; bulk viscosity

- However for most application, Newton's viscosity law is sufficient(in 3-D form)

$$\tau = -\mu\left[\nabla\vec{v} + \left(\nabla\vec{v}\right)^{+}\right] \qquad (7)$$

Stress Tensor is Symmetric

No need of angular momentum equation

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c) Body Force Field

$$\vec{g} = \text{constant}$$ (Newtonian gravitational field)

Electrostatic
Electromagnetic

more complicated

magneto hydrodynamics
gas dynamics

plasma physics