Internal energy and The First Law

Internal energy: Energy of body not kinetic energy

1) thermal energy (heat)
2) mechanical/strain energy
3) Chemical energy
4) Magnetization

Internal energy $\mathcal{U}$ of Ω_t: $\mathcal{U}[\Omega_t] = \int_{\Omega_t} \rho(\underline{x},t)\, u(\underline{x},t)\, dV_x$

$u(\underline{x},t)$ = internal energy density/unit mass

First Law of Thermodynamics

$$\boxed{\frac{d}{dt}\mathcal{U}[\Omega_t] = Q[\Omega_t] + W[\Omega_t]} \qquad \text{for all } \Omega_t \subseteq B_t$$

Net heating: $Q[\Omega_t]$ = rate of thermal energy gain/loss

Net working: $W[\Omega_t]$ = rate of mechanical energy gain/Loss

⇒ heating first

Net heating

2 forms of heat gain / loss:

I) Body heating : $Q_b[\Omega_t] = \int_{\Omega_t} \rho(\underline{x},t)\, r(\underline{x},t)\, dV_x$

$r(\underline{x},t)$ = heat supply/loss per unit mass

Example: radiogenic heating

$$\underline{r} = H_0 e^{-\lambda t}$$

H_0 = initial power per unit mass

λ = decay constant

II) Surface heating : $Q_s[\Omega_t] = -\int_{\partial\Omega_t} \underline{q}(\underline{x},t) \cdot \underline{n}(\underline{x},t)\, dA_x$

$\underline{q}(\underline{x},t)$ = heat flux vector.

Fourier's law : $\underline{q} = -\underline{\underline{\kappa}}\, \nabla T$ (Lecture 10)

$\underline{\underline{\kappa}}$ = thermal conductivity tensor

Net heating is the rate at which heat is added or lost from Ω_t

$$\boxed{Q[\Omega_t] = Q_b[\Omega_t] + Q_s[\Omega_t] = \int_{\Omega_t} \rho(\underline{x},t)\, r(\underline{x},t)\, dV_x - \int_{\partial\Omega_t} \underline{q}(\underline{x},t) \cdot \underline{n}(\underline{x},t)\, dA_x}$$

Energy balance with net heating

First law with W = 0: $\frac{d}{dt}\mathcal{U}[\Omega_t] = Q[\Omega_t]$

where $\mathcal{U}[\Omega_t] = \int_{\Omega_t} \rho u \, dV_x$

$$Q[\Omega_t] = \int_{\Omega_t} \rho r \, dV_x - \int_{\partial\Omega_t} q \cdot \underline{n} \, dA_x$$

substituting:

$$\frac{d}{dt}\int_{\Omega_t} \rho u \, dV_x = -\int_{\partial\Omega_t} q \cdot \underline{n} \, dA_x + \int_{\Omega_t} \rho r \, dV_x$$

using derivative relative to mass and divergence Thm

$$\int_{\Omega} (\rho \dot{u} + \nabla_x \cdot q + \rho r) \, dV_x$$

by the arbitrary ness of Ω_t we have

$$\boxed{\rho \dot{u} + \nabla \cdot q = \rho r} \qquad \text{local Eulerian form}$$

Following lin. mom. balance → conservative form

$$\boxed{\frac{\partial}{\partial t}(\rho u) + \nabla \cdot [\underline{v} \rho u + \underline{q}] = \rho r} \qquad \Rightarrow \text{HW 9}$$

- still in terms of internal energy density !

Advection - Conduction Equation

Energy balance: $\frac{\partial}{\partial t}(\rho u) + \nabla \cdot [\underline{v} \rho u + \underline{q}] = \rho r$

$\underline{v} \rightarrow$ momentum balance

ρ, r parameters (given)

u, q unknown variables

1 equation with 4 unknowns

$\Rightarrow$ need to relate u and $\underline{q}$

Thermodynamics: $u = u_0 + c_p (T - T_0)$ (simplest)

Fouriers law: $q = -\kappa \nabla T$ (Lecture 10)

physical parameters:

1) c_p = specific heat capacity $\left[\frac{J}{kg\,K}\right]$

2) κ = thermal conductivity $\left[\frac{W}{m\,K} = \frac{J}{m\,s\,K}\right]$

Assume: 1) properties are constant (ρ, c_p, κ)

2) flow is incompressible $\nabla \cdot \underline{v} = 0$

substitute and simplify

$$\boxed{\rho c_p \frac{\partial T}{\partial t} - \nabla \cdot [\underline{v} \rho c_p T - \kappa \nabla T] = \rho r} \Rightarrow \text{HW9}$$

Advective heat flux: $q_A = \underline{v} \rho c_p T$

Conductive heat flux: $q_c = -\kappa \nabla T$

Heat production: ρr

⇒ Advection - Diffusion - Reaction Equation

Diffusion ~ Conduction

Reaction ~ Production

In limit of $\underline{v} \rightarrow \underline{0}$

$$\boxed{\frac{\partial T}{\partial t} - D \nabla^2 T = r} \quad \underline{\text{Heat Equation}}$$

where

$\nabla^2 = \nabla \cdot \nabla$ = Laplacian (Lecture 10)

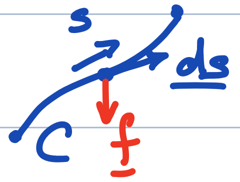
$D = \frac{\kappa}{\rho c_p}$ thermal diffusivity

Work and Power

Work is energy transferred by application of force along distance

$$W = F s$$

$$W = \int_C \underline{f} \cdot d\underline{s} = \int_{t_1}^{t_2} \underline{f} \cdot \frac{d\underline{s}}{dt}\, dt = \int_{t_1}^{t_2} \underline{f} \cdot \underline{v}\, dt$$

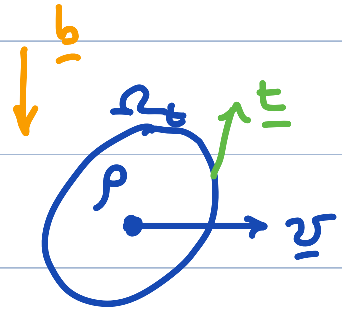


Power is the rate of work

$$\boxed{\mathcal{P} = \frac{dW}{dt} = \underline{f} \cdot \underline{v}}$$ from $$W = \int_{t_1}^{t_2} \frac{dW}{dt}\, dt = \int_{t_1}^{t_2} \underline{f} \cdot \underline{v}\, dt$$

Working is rate of work done ~ power

Exchange of mechanical energy of a body



Kinetic Energy of a continuum body is

$$\mathcal{K}[\Omega_t] = \int_{\Omega} \frac{1}{2} \rho(\underline{x},t)\, |\underline{v}(\underline{x},t)|^2\, dV_x$$

Power of **external** forces acting on Ω_t is

$$\mathcal{P}[\Omega_t] = \int_{\Omega_t} \rho(\underline{x},t)\, \underline{b}(\underline{x},t) \cdot \underline{v}(\underline{x},t)\, dV_x + \int_{\partial\Omega_t} \underline{t}(\underline{x},t) \cdot \underline{v}(\underline{x},t)\, dA_x$$

Net working $\mathcal{W}[\Omega_t]$ of external forces on Ω_t is the mechanical power not converted into motion

$$\boxed{\mathcal{W}[\Omega_t] = \mathcal{P}[\Omega_t] - \frac{d}{dt}\mathcal{K}[\Omega_t]}$$

$\mathcal{W}[\Omega_t] > 0$: mechanical energy is stored

$\mathcal{W}[\Omega_t] < 0$: stored energy is released

Net working in Eulerian form

Power: $\mathcal{P} = \underline{f} \cdot \underline{v}$

Newton's 2nd law: $\underline{f} = m\,\underline{a} \rightarrow \underline{f} = \frac{d}{dt}(m\underline{v}) = m\,\dot{\underline{v}}$

Start by taking dot product of $\underline{v}$ and lin. mom. balance

lin. mom. balance: $\rho\dot{\underline{v}} = \nabla \cdot \underline{\underline{\sigma}} + \rho\underline{b}$

$$\rho\dot{\underline{v}} \cdot \underline{v} = \rho\underline{v} \cdot \dot{\underline{v}} = (\nabla \cdot \underline{\underline{\sigma}}) \cdot \underline{v} + \rho\underline{b} \cdot \underline{v}$$

Identify $\mathcal{K}$, $\mathcal{P}$ and $\mathcal{W}$ => integrate

$$\int_{\Omega_t} \rho\underline{v} \cdot \dot{\underline{v}}\, dV_x = \int_{\Omega_t} (\nabla_x \cdot \underline{\underline{\sigma}}) \cdot \underline{v} + \rho\underline{b} \cdot \underline{v}\, dV_x$$

use identity $\nabla\cdot(\underline{\underline{A}}^T\underline{b}) = (\nabla\cdot\underline{\underline{A}})\cdot\underline{b} + \underline{\underline{A}}:\nabla\underline{b}$ (Lecture 10)

$$\int_{\Omega_t}\rho\underline{v}\cdot\dot{\underline{v}}\,dV_x = \int_{\Omega_t} -\underline{\underline{\sigma}}:\nabla_x\underline{v} + \nabla\cdot(\underline{\underline{\sigma}}^T\underline{v}) + \rho\underline{b}\cdot\underline{v}\,dV_x$$

Using $\underline{\underline{S}}:\underline{\underline{D}} = \underline{\underline{S}}:\mathrm{sym}(\underline{\underline{D}})$ if $\underline{\underline{S}} = \underline{\underline{S}}^T$

$\Rightarrow$ introduce $\underline{\underline{d}} = \mathrm{sym}(\nabla_x\underline{v}) = \frac{1}{2}(\nabla_x\underline{v} + \nabla_x\underline{v}^T)$.

$$\int_{\Omega_t}\rho\underline{v}\cdot\dot{\underline{v}}\,dV_x = \int_{\Omega_t} -\underline{\underline{\sigma}}:\underline{\underline{d}} + \rho\underline{b}\cdot\underline{v}\,dV_x + \underbrace{\int_{\partial\Omega_t}\underline{\underline{\sigma}}\underline{v}\cdot\underline{n}\,dA_x}_{\text{divergence thm.}}$$

Using $\underline{\underline{\sigma}}\underline{v}\cdot\underline{n} = \underline{v}\cdot\underline{\underline{\sigma}}^T\underline{n} = \underline{v}\cdot\underline{t}$

$$\int_{\Omega_t}\rho\underline{v}\cdot\dot{\underline{v}}\,dV_x = \int_{\Omega_t} -\underline{\underline{\sigma}}:\underline{\underline{d}}\,dV_x + \underbrace{\int_{\Omega_t}\rho\underline{b}\cdot\underline{v}\,dV_x + \int_{\partial\Omega_t}\underline{t}\cdot\underline{v}\,dA_x}_{\mathcal{P}[\Omega_t]}$$

Now we can identify the left hand side as

$$\frac{d}{dt}\mathcal{K}[\Omega_t] = \frac{d}{dt}\int_{\Omega_t}\frac{1}{2}\rho\,\underline{v}\cdot\underline{v}\,dV_x = \frac{1}{2}\int_{\Omega_t}\rho\frac{d}{dt}(\underline{v}\cdot\underline{v})\,dV_x$$

$$\frac{d}{dt}(v_i v_i) = \dot{v}_i v_i + v_i\dot{v}_i = 2(v_i\dot{v}_i)$$

$$\frac{d}{dt}\mathcal{K}[\Omega_t] = \int_{\Omega_t}\rho\,\underline{v}\cdot\dot{\underline{v}}\,dV_x$$

so that we have the result

$$\boxed{\frac{d}{dt}\mathcal{K}[\Omega_t] + \int_{\Omega_t} \underline{\underline{\sigma}} : \underline{\underline{d}} \, dV_x = \mathcal{P}[\Omega_t]}$$

by comparison with $\mathcal{W}[\Omega_t] = \mathcal{P}[\Omega_t] - \frac{d}{dt}\mathcal{K}[\Omega_t]$

$$\Rightarrow \boxed{\mathcal{W}[\Omega_t] = \int_{\Omega_t} \underline{\underline{\sigma}} : \underline{\underline{d}} \, dV_x}$$

The quantity $\underline{\underline{\sigma}} : \underline{\underline{d}}$ is called the stress power associated with a motion. It corresponds to the rate of work done by internal forces (stresses) in a continuum body.

In some cases the power of an external force can be written as $\mathcal{P}[\Omega_t] = -\frac{d}{dt} G[\Omega_t]$

where $G[\Omega_t]$ is called potential energy for ext. forces.

$$\Rightarrow \quad \frac{d}{dt}\Big(\mathcal{U}[\Omega_t] + \mathcal{K}[\Omega_t] + G[\Omega_t]\Big) = Q[\Omega_t]$$

Enrgy balance with net working

$$\frac{d}{dt}\mathcal{U}[\Omega_t] = Q[\Omega_t] + \mathcal{W}[\Omega_t]$$

where $\mathcal{U}[\Omega_t] = \int_{\Omega_t} \rho u \, dV_x$

$$Q[\Omega_t] = \int_{\Omega_t} \rho r \, dV_x - \int_{\partial\Omega_t} \underline{q}\cdot\underline{n} \, dA_x$$

$$\mathcal{W}[\Omega_t] = \int_{\Omega_t} \underline{\underline{\sigma}} : \underline{\underline{d}} \, dV_x$$

Hence we have

$$\frac{d}{dt}\int_{\Omega_t} \rho u \, dV_x = \int_{\Omega_t} \underline{\underline{\sigma}} : \underline{\underline{d}} \, dV_x - \int_{\partial\Omega_t} \underline{q}\cdot\underline{n} \, dA_x + \int_{\Omega_t} \rho r \, dV_x$$

using derivative relative to mass and divergence Thm

$$\int_{\Omega} \left(\rho \dot{u} - \underline{\underline{\sigma}} : \underline{\underline{d}} + \nabla_x \cdot \underline{q} + \rho r\right) dV_x$$

by the arbitraryness of Ω_t we have

$$\boxed{\rho \dot{u} = \underbrace{\underline{\underline{\sigma}} : \underline{\underline{d}}}_{\text{networking}} - \nabla_x \cdot \underline{q} + \rho r}$$ local Eulerian form

$$\boxed{\frac{\partial}{\partial t}(\rho u) + \nabla_x \cdot \left[\underline{v} \rho u + \underline{q}\right] = \underline{\underline{\sigma}} : \underline{\underline{d}} + \rho r}$$ conservative local Eulerian form

Entropy and The Second Law

The Second Law expresses the fact that a body has a limit on the rate of heat uptake, but has no limit on the rate of heat release.

The second law postulates:

$$Q[\Omega_t] \leq \Xi[\Omega_t]$$

an upper bound $\Xi[\Omega_t]$ on the net heating. In the absence of net working $W[\Omega_t]=0$ we have

$$\frac{d}{dt}\mathcal{U}[\Omega_t] = Q[\Omega_t] \leq \Xi[\Omega_t]$$

$\Rightarrow$ the quantity $\Xi[\Omega_t]$ limits rate of energy storage.

The entropy of a body is defined (up to a constant)

$$\boxed{\frac{d}{dt} S[\Omega_t] = \frac{\Xi[\Omega_t]}{\Theta[\Omega_t]}}$$

where $\Theta[\Omega_t]$ is the uniform temp. of Ω_t.

Entropy is a quantity whose rate of change is equal to the upper heating bound per unit temperature.

At the atomistic level entropy is a measure of disorder, the number of atomic configurations compatible with macroscopic variables. In terms of net heating

$$\boxed{\frac{d}{dt} S[\Omega_t] \geq \frac{Q[\Omega_t]}{\Theta[\Omega_t]}}$$ Clausius-Planck Inequality

In thermo books : $dS = \frac{dQ_{rev}}{T}$ and $dS > \frac{dQ}{T}$

The irreversibility of natural processes is shown by

$$\frac{d}{dt} S[\Omega_t] \geq 0 \qquad \text{when} \qquad Q[\Omega_t] = 0$$

For a non-homogeneous body we postulate an entropy density field per unit mass, $s(\underline{x},t)$, so that

$$S[\Omega_t] = \int_{\Omega_t} \rho(\underline{x},t)\, s(\underline{x},t)\, dV_x$$

Hence the generalization of the 2nd law to inhomogeneous systems is given by the Clausius-Duhem ineq.

$$\boxed{\frac{d}{dt} S[\Omega_t] \geq \int_{\Omega_t} \frac{\rho(\underline{x},t)\, r(\underline{x},t)}{\theta(\underline{x},t)}\, dV_x - \int_{\partial\Omega_t} \frac{\underline{q}(\underline{x},t)\cdot \underline{n}(\underline{x},t)}{\theta(\underline{x},t)}\, dA_x}$$

This relation places restrictions on the constitutive relations of a body and leads to statements about energy dissipation and the flow of heat.

Note: The precise form of the 2nd law in continuum mechanics is <u>not</u> settled yet !

But all forms lead to same restrictions.

Local Eulerian Form of the Second Law

The integral form of the Clausius-Duhem form of the the Second Law is

$$\frac{d}{dt}\int_{\Omega_t} \rho s \, dV_x \geq \int_{\Omega_t} \frac{\rho r}{\theta} dV_x - \int_{\partial\Omega_t} \frac{q\cdot n}{\theta} dA_x$$

After applying the Divergence Thm and invoking the arbitrariness of Ω_t we have

$$\boxed{\rho \dot{s} \geq \rho r/\theta - \nabla_x \cdot (q/\theta)}$$

Clausius-Duhem inequality in local Eulerian form

After multiplying by θ and expanding the divergence

$$\theta \rho \dot{s} \geq \rho r - \nabla_x \cdot q + \theta^{-1} q \cdot \nabla_x \theta$$

Which can be written as

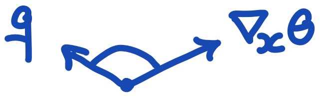
$$\boxed{\delta - \theta^{-1} q \cdot \nabla_x \theta \geq 0}$$

where $\delta = \theta \rho \dot{s} - (\rho r - \nabla_x \cdot q)$ is the internal dissipation density per unit volume. Difference between local entropy increase and the local heating.

Note:

I) Any point where $\nabla_x \theta = 0$ the dissipation is non-negative, $\delta \geq 0$. $\Rightarrow$ bodies with homogeneous θ have non-neg. dissipation.

II) If $\delta = 0$, i.e. a reversible process, then $q \cdot \nabla_x \theta \leq 0$.



Thus q is at an angle > 90 from $\nabla_x \theta$.

$\Rightarrow$ heat flows down the temperature gradient.

To study the consequences of Clausius-Duhem inequality for constitutive laws we introduce the field

$$\boxed{\psi(\underline{x},t) = \phi(\underline{x},t) - \theta(\underline{x},t)\, s(\underline{x},t)}$$

Helmholtz free energy density. This is the portion of the free energy available for performing work at const. θ.

$\Rightarrow$ Reformulate Clausius-Duhem in terms of ψ

Material derivative of free energy

$$\frac{d}{dt}(\theta s) = \frac{\partial}{\partial t}(\theta s) + \nabla_x(\theta s)\cdot\underline{v} = \theta\frac{\partial s}{\partial t} + s\frac{\partial \theta}{\partial t} + \theta\nabla_x s\cdot\underline{v} + s\nabla_x\theta\cdot\underline{v}$$

$$= \theta\left(\frac{\partial s}{\partial t} + \nabla_x s\cdot\underline{v}\right) + s\left(\frac{\partial \theta}{\partial t} + \nabla_x\theta\cdot\underline{v}\right)$$

$$= \theta\dot{s} + s\dot{\theta}$$

from definition of $\dot{\psi}$

$$\dot{\psi} = \dot{u} - \theta\dot{s} - \dot{\theta}s \quad\Rightarrow\quad \dot{u} = \dot{\psi} + \theta\dot{s} + s\dot{\theta}$$

substituting into local form of 1st law

$$\rho\dot{u} = \underline{\underline{\sigma}} : \underline{\underline{d}} - \nabla_x\cdot q + \rho r$$

$$\rho\dot{\psi} + \rho\theta\dot{s} + \rho s\dot{\theta} = \underline{\underline{\sigma}} : \underline{\underline{d}} - \nabla_x\cdot q + \rho r$$

$$\rho\theta\dot{s} = \underline{\underline{\sigma}} : \underline{\underline{d}} - \nabla_x\cdot q + \rho r - \rho\dot{\psi} - \rho s\dot{\theta}$$

substituting into 2nd law

$$\theta\rho\dot{s} \geq \rho r - \nabla_x\cdot q + \theta^{-1} q\cdot\nabla_x\theta$$

$$\underline{\underline{\sigma}} : \underline{\underline{L}} - \cancel{\nabla_x\cdot q} + \cancel{\rho r} - \rho\dot{\psi} - \rho s\dot{\theta} \geq \cancel{\rho r} - \cancel{\nabla_x\cdot q} + \theta^{-1} q\cdot\nabla_x\theta$$

solve for $\rho\dot{\psi}$

$$\boxed{\rho\dot{\psi} \leq \underline{\underline{\sigma}} : \underline{\underline{d}} - \rho s\dot{\theta} - \theta^{-1} q\cdot\nabla_x\theta}$$

This is called the reduced Clausius-Duhem inequality, because it is independent of local heat supply r and heat flux, q, if $\nabla_x \theta = 0$. ⇒ homogeneous bodies of classical thermo.

Note:

In a homogeneous body, $\nabla\theta = 0$, we have that

$$\rho\dot{\phi} \leq \underline{\underline{\sigma}} : \underline{\underline{d}}$$

for a reversible process this becomes an equality.

⇒ rate of change of free energy is equal to the stress power.