

Balance Equations

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Overview

Material
points

Generic
balance
equation

Particles, mass
and charge

Momentum

Energy

First main law

Entropy

Second main
law

Remarks

- Material points
- Generic balance equation
- Particles, mass and charge
- Linear and angular momentum
- Energy and First law
- Entropy and Second Law

- A material point is a piece of matter which
- is **tiny** from an engineer's point of view
- but **huge** from a physicist's point of view
- one mm^3 of an ideal gas under normal conditions
- still contains 2.7×10^{16} particles
- ideal gas: $\langle N^2 \rangle - \langle N \rangle^2 = \langle N \rangle$
- i.e. relative fluctuation is
$$\frac{\delta N}{\langle N \rangle} \approx 1 \times 10^{-8}$$
- the material point is always in thermodynamic **equilibrium**
- we usually suppress the t, \boldsymbol{x} arguments

- think of an additive and transportable quantity Y
- mass, charge, momentum, energy etc.
- the **content** of Y in a region \mathcal{V} is

$$Q(Y; t, \mathcal{V}) = \int_{\mathcal{V}} dV \varrho(Y; t, \mathbf{x})$$

- the **density** $\varrho(Y) = \varrho(Y; t, \mathbf{x})$ is a field
- the **flow** of Y through an area \mathcal{A} is

$$I(Y; t, \mathcal{A}) = \int_{\mathcal{A}} d\mathbf{A} \cdot \mathbf{j}(Y; t, \mathbf{x})$$

- the **current density** $\mathbf{j}(Y) = \mathbf{j}(Y; t, \mathbf{x})$ has a strength and a direction

- the rate of production for Y in a region \mathcal{V} is

$$\Pi(Y; t, \mathcal{V}) = \int_{\mathcal{V}} dV \pi(Y; t, \mathbf{x})$$

- the volumetric production rate $\pi(Y) = \pi(Y; t, \mathbf{x})$ describes: how much quantity Y is produced (or vanishes) per unit time and unit volume
- e.g. particles are produced in chemical reactions
- momentum is produced by external forces
- internal energy may be produced by friction
- entropy S is produced by irreversible effects
- $\pi(S) \geq 0$ is the Second main law of thermodynamics

- content of Y in \mathcal{V} changes because Y is redistributed
- i.e. flows through the surface $\partial\mathcal{V}$
- or because Y is produced inside \mathcal{V}

- as an equation

$$\frac{d}{dt}Q(Y; t, \mathcal{V}) = -I(Y; t, \partial\mathcal{V}) + \Pi(Y; t, \mathcal{V})$$

- Gauss' theorem

$$\int_{\mathcal{V}} dV \nabla \cdot \mathbf{f} = \int_{\partial\mathcal{V}} d\mathbf{A} \cdot \mathbf{f}$$

- generic balance equation

$$\dot{\rho}(Y) + \nabla \cdot \mathbf{j}(Y) = \pi(Y)$$

- must hold true for all times t and at all locations \mathbf{x}

- $Y = N^a$ denotes the number of particles of species
 $a = 1, 2, \dots$
- particle density $n^a = \varrho(N^a)$
- particle current density $\mathbf{j}^a = \mathbf{j}(N^a)$
- velocities defined by $\mathbf{j}^a = n^a \mathbf{v}^a$
- vanish or are generated in chemical reactions
- there are Γ^r chemical reactions of type r per unit time
and unit volume
- volumetric production rates are

$$\pi^a = \sum_r \Gamma^r \nu^{ra}$$

- the ν^{ra} are stoichiometric coefficients
- ν^{ra} particles of species a are produced in a reaction of
type r
- particle balance equation

$$\partial_t n^a + \partial_i n^a v_i^a = \sum_r \Gamma^r \nu^{ra}$$

- particles of species a carry a mass m^a
- mass density $\rho = \rho(M) = \sum_a m^a n^a$
- in each reaction, mass is conserved
- meaning

$$\sum_a \Gamma^{ra} m^a = 0$$

- consequently

$$\pi(M) = \sum_a \sum_r \Gamma^{ra} m^a = 0$$

- mass current density can be written as

$$\mathbf{j}(M) = \rho(M) \mathbf{v}$$

- mass continuity equation reads

$$\partial_t \rho + \partial_i \rho v_i = 0$$

- particles of species a carry a charge q^a
- charge is conserved in each chemical reaction
- consequently $\pi(Q^e) = 0$
- charge density

$$\rho^e = \sum_a q^a n^a$$

- current is split into **convection** and **conduction** part

$$\mathbf{j}(Q^e) = \mathbf{j}^e = \rho^e \mathbf{v} + \mathbf{J}^e$$

- charge **continuity equation** reads

$$\partial_t \rho^e + \partial_i \{ \rho^e v_i + J_i^e \} = 0$$

- without proof: only conduction contributions \mathbf{J} are proper vector fields
- e.g. Ohm's law refers to \mathbf{J}^e
- however, \mathbf{j}^e appears in Maxwell's equations

- Momentum P_k is an additive transportable quantity
- its density has three components

$$\rho(P_k) = \rho v_k$$

- mass times velocity per unit volume
- current densities for each component

$$j_i(P_k) = \rho v_k v_i - T_{ki}$$

- conduction part T_{ki} is stress tensor
- minus sign is a convention
- volumetric momentum production rate is force f_k per unit volume

- $f_k = \rho g_k + \rho^e E_k$

- momentum balance equation

$$\partial_t \rho v_k + \partial_i \{ \rho v_k v_i - T_{ki} \} = f_k$$

- time change as noted by a co-moving observer

$$(D_t f)(t, \mathbf{x}) = \frac{f(t + dt, \mathbf{x} + dt \mathbf{v}) - f(t, \mathbf{x})}{dt}$$

- i.e.

$$D_t f = \partial_t f + \mathbf{v} \cdot \nabla f$$

- specific quantities $\sigma(Y)$ defined by

$$\varrho(Y) = \varrho \sigma(Y)$$

- balance equations may also be written as

$$\varrho D_t \sigma(Y) = -\partial_i J_i(Y) + \pi(Y)$$

- in particular momentum balance equation

$$\varrho D_t v_k = \partial_i T_{ki} + f_k$$

- angular momentum balance requires

$$T_{ki} = T_{ik}$$

- at each location \boldsymbol{x} there is a coordinate system such that the stress tensor is orthogonal:

$$T_{ki} = T_{ik} = \begin{pmatrix} T^1 & 0 & 0 \\ 0 & T^2 & 0 \\ 0 & 0 & T^3 \end{pmatrix}$$

- a particular material can support only stress (positive T) and pressure (negative T) within certain limits
- the field of structural mechanics :
- work out the stress tensor, diagonalize it locally, and check whether its eigenvalues are within the allowed limits
- *before building the bridge*

- the kinetic energy density is

$$\varrho(E^k) = \frac{\varrho}{2} \mathbf{v}^2$$

- it follows that

$$\frac{\varrho}{2} D_t \sigma(E^k) = -\partial_i J_i(E^k) + \pi(E^k)$$

- where

$$J_i(E^k) = -v_k T_{ki}$$

- and

$$\pi(E^k) = -T_{ik} G_{ik} + v_k f_k$$

- the volicity gradient is

$$G_{ik} = \frac{\partial_i v_k + \partial_k v_i}{2}$$

- quasistatic gravitational and electric potentials

$$f_k = -\varrho \partial_k \Phi^g - \varrho^e \partial_k \Phi^e$$

- density of potential energy

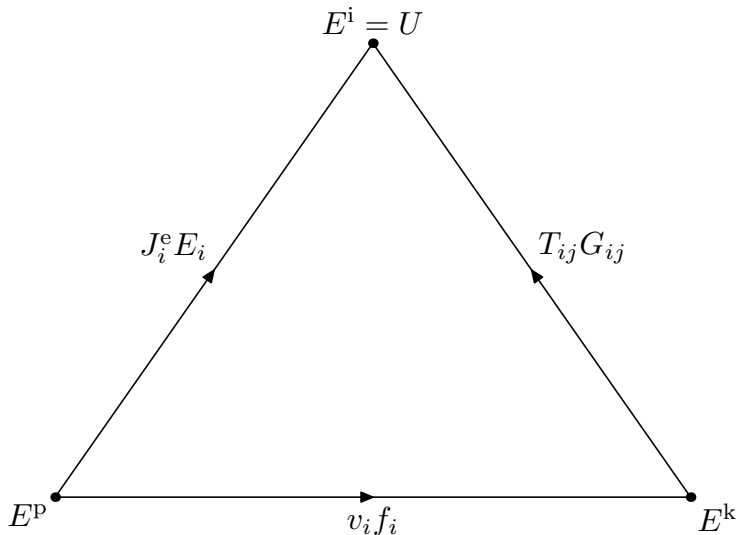
$$\varrho(E^p) = \varrho \Phi^g + \varrho^e \Phi^e$$

- it follows that

$$j_i(E^p) = \varrho j_i(M) + \varrho^e j_i(Q)$$

- with $j_i(M) = \varrho v_i$ and $j_i(Q) = \varrho^e + J_i^e$

$$\pi(E^p) = -v_i f_i - J_i^e E_i$$



Volumetric production rates for kinetic, potential and internal energy. Arrows pointing towards an energy form indicate a plus sign.

- total energy is the sum of kinetic, potential, and internal energy $E^i = U$

- total energy is conserved

$$pi(E) = \pi(E^k + E^p + U) = \pi(E^k) + \pi(E^p) + \pi(U) = 0$$

- internal energy production rate per unit volume

$$\pi(U) = T_{ik}G_{ik} + J_i^e E_i$$

- specific internal energy is denoted by u
- conduction current density for internal energy ...
- is the heat current density J_i^u
- stress tensor consists of the reversible part T'_{ik} and an irreversible part T''_{ik}
- likewise $J_i^{e'}$ and $J_i^{e''}$

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- the balance equation for internal energy is ...
- the First main law of thermodynamics

$$\rho D_t u =$$

- heat conduction

$$-\partial_i J_i^u$$

- deformation work

$$+T'_{ik} G_{ik}$$

- internal friction

$$+T''_{ik} G_{ik}$$

- polarization work

$$+J_i^{e'} E_i$$

- and Joule's heat

$$+J_i^{e''} E_i$$

- each material point is always in equilibrium
- it undergoes a reversible change
- entropy S and temperature T introduced by
$$dU = TdS + dW$$

- where dW is the work done on the system
- entropy balance equation

$$\rho D_t s = -\partial_i J_i^s + \pi(S)$$

- entropy current

$$\mathbf{j}^s = \rho s \mathbf{v} + \frac{1}{T} \mathbf{J}^u - \sum_a \frac{\mu^a}{T} \mathbf{J}^a$$

- chemical potentials μ^a
- diffusion current densities \mathbf{J}^a

- the second main law of thermodynamics says

$$0 \leq \pi(S) =$$

- heat conduction,

$$J_i^u \partial_i \frac{1}{T}$$

- diffusion

$$- \sum_a J_i^a \partial_i \frac{\mu^a}{T}$$

- friction

$$+ T_{ik}'' \frac{\partial_i v_k + \partial_k v_i}{2}$$

- Joule's heat

$$- \frac{1}{T} J_i^{e''} \partial_i \Phi^e$$

- chemical reactions

$$+ \frac{1}{T} \sum_r \Gamma^r A^r$$

- chemical affinity of reaction r is defined by

$$A^r = \sum_a \nu^{ra} \mu^a$$

- all contributions are of type 'flux times non-equilibrium indicator' which would vanish in global equilibrium.
- there are five and only five contributions to entropy production
- First and Second main law are partial differential equations
- there are much more fields than balance equations.
- therefore: additional equations required