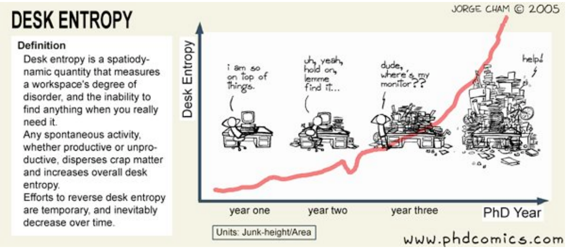
# 06 - balance equations - open systems



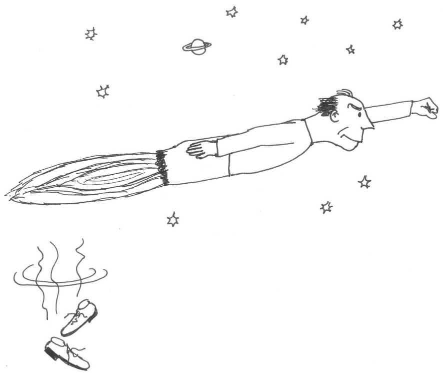



## thermodynamic systems

**open system** [ˈoʊ.pən ˈsɪs.təm] thermodynamic system which is allowed to exchange mechanical work, heat and mass, typically $\boldsymbol{P} = \boldsymbol{P}(\nabla\boldsymbol{\varphi}, ...)$ , $\boldsymbol{Q} = \boldsymbol{Q}(\nabla\theta, ...)$ and $\boldsymbol{R} = \boldsymbol{R}(\nabla\rho, ...)$ with its environment. enclosed by a deformable, diathermal, permeable membrane. characterized through its state of deformation $\boldsymbol{\varphi}$, temperature $\theta$ and density $\rho$.



## open system thermodynamics



„…thermodynamics recognizes no special role of the biological…“

Bridgman, "The nature of thermodynamics", [1941]



## open systems - balance of mass

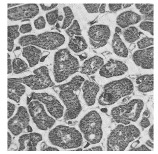
$$\mathrm{D}_t \rho_0 = \mathrm{Div}(\boldsymbol{R}) + \mathcal{R}_0$$

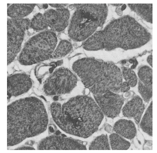
mass flux $\boldsymbol{R}$

- cell movement (migration)

mass source $\mathcal{R}_0$

- cell growth (proliferation)
- cell division (hyperplasia)
- cell enlargement (hypertrophy)

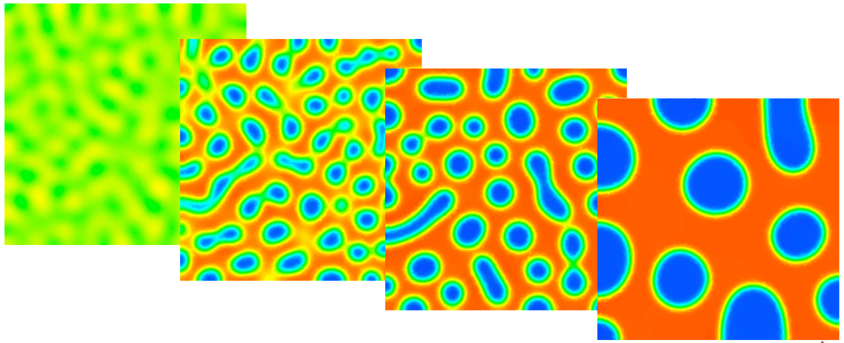




## biological equilbrium

Cowin & Hegedus [1976], Beaupré, Orr & Carter [1990], Harrigan & Hamilton [1992], Jacobs, Leveston, Beaupré, Simo & Carter [1995], Huiskes [2000]. Carter & Beaupré [2001]

## open systems - balance of mass



simulation of cell growth - cahn-hilliard equation

Kuhl & Schmid [2006], Wells, Kuhl & Garikipati [2006]



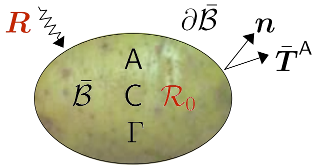
## open systems - balance of mass

the model does not take explicitly into account that the body is growing due to the absorption of some other materials. In absence of some of the vital constituents, no growth is possible. conversely, when part of the material dies, some of the bricks contained in the cellular membrane can be re-used by other cells. in this respect, an approach using mixture theory might by useful.

Ambrosi & Mollica [2002]



## open systems - balance equations




general format

A ... balance quantity
**B** ... flux $\quad \mathbf{B}\cdot\boldsymbol{n} = \bar{\boldsymbol{T}}^{\mathsf{A}}$
C ... source
$\Gamma$ ... production

$$\mathrm{D}_t(\rho_0 \mathsf{A}) = \mathrm{Div}(\mathbf{B} + \mathsf{A}\otimes\boldsymbol{R}) + [\mathsf{C} + \mathsf{A}\mathcal{R}_0 - \nabla_X \mathsf{A}\cdot\boldsymbol{R} + \Gamma]$$



## open systems vs. porous media

| theory of open systems [ˈoʊ.pən ˈsɪs.təms] | thoery of porous media [ˈpɔːr.əs ’miːdiː.ə] |
|---|---|
| • constituents spatially separated | • local superposition of constituents |
| • overall behavior priliminary determined by one single constituent | • consideration of mixture of multiple constituents |
| • exchange of mass, momentum, energy and entropy with environment | • exchange of mass, momentum, energy and entropy amongst constituents |

## open systems - balance of momentum

- volume specific version

$$\mathrm{D}_t(\rho_0 \boldsymbol{v}) = \mathrm{Div}(\boldsymbol{P} + \boldsymbol{v} \otimes \boldsymbol{R}) + [\boldsymbol{b}_0 + \boldsymbol{v}\mathcal{R}_0 - \nabla_X \boldsymbol{v} \cdot \boldsymbol{R}]$$

- subraction of weighted balance of mass

$$\boldsymbol{v}\,\mathrm{D}_t\rho_0 = \mathrm{Div}(\boldsymbol{v} \otimes \boldsymbol{R}) + \boldsymbol{v}\mathcal{R}_0 - \nabla_X \boldsymbol{v} \cdot \boldsymbol{R}$$

- mass specific version

$$\rho_0\,\mathrm{D}_t\boldsymbol{v} = \mathrm{Div}(\boldsymbol{P}) + \boldsymbol{b}_0$$

### mechanical equilibrium



## open systems - rocket propulsion

balance of mass

$\mathrm{D}_t\mathrm{m} = \mathcal{R}$ with $\mathcal{R} \le 0$ ejection

balance of momentum - volume specific

$$\mathrm{D}_t[\mathrm{m}\boldsymbol{v}] = \mathrm{m}\,\mathrm{D}_t\boldsymbol{v} + \mathrm{D}_t\mathrm{m}\,\boldsymbol{v} = \boldsymbol{f} + \mathcal{R}\boldsymbol{v}$$

balance of momentum - mass specific

$\mathrm{m}\,\mathrm{D}_t\boldsymbol{v} = \boldsymbol{f}$ with $\boldsymbol{f} = \boldsymbol{f}^{\text{closed}} + \boldsymbol{f}^{\text{open}}$

balance of momentum - rocket head-ejection

$$\mathrm{D}_t[\mathrm{m}\boldsymbol{v}] - \mathcal{R}\bar{\boldsymbol{v}} = \boldsymbol{f}^{\text{closed}}$$

propulsive force

$\boldsymbol{f}^{\text{open}} = [\bar{\boldsymbol{v}} - \boldsymbol{v}]\mathcal{R}$ velocity of ejection $\bar{\boldsymbol{v}}$



## open systems - rocket propulsion

a saturn v rocket like the one that took men to the moon has a mass of 2.500.000 kg on liftoff. it goes straight up vertically and burns fuel at a uniform rate of 16.000 kg/s for a duration of 2 minutes. the exhaust speed of gas from the saturn v is 3.0 km/s

what is the speed of the rocket immediately after the combustion ceases? you should include the effect of gravity near the surface of the earth, but you can neglect air resistance.

plot the burnout velocity as a function of time over the range of 0 to 120 seconds to see the increase in speed of the rocket with time.



## open systems - rocket propulsion

## open systems - rocket propulsion

$$\mathrm{m}\mathrm{D}_t v = f^{\text{closed}} + f^{\text{open}}$$

with $f^{\text{closed}} = -\mathrm{m}\, g$ gravity

$$f^{\text{open}} = [\bar{v} - v]\mathcal{R} = w\,\mathrm{D}_t \mathrm{m}$$

$$\mathrm{m}\mathrm{D}_t v = -\mathrm{m}\, g - \mathrm{D}_t m\, w \qquad ||\ :\mathrm{m}$$

$$\mathrm{D}_t v = -g - \tfrac{1}{\mathrm{m}}\mathrm{D}_t \mathrm{m}\, w$$

integration

$$v(t) = -g\, t - w \int_{\mathrm{m}(0)}^{\mathrm{m}(t)} \tfrac{1}{\mathrm{m}} \mathrm{dm}$$

$$\mathrm{m}(t) = \mathrm{m}(0) + \mathcal{R}\, t$$

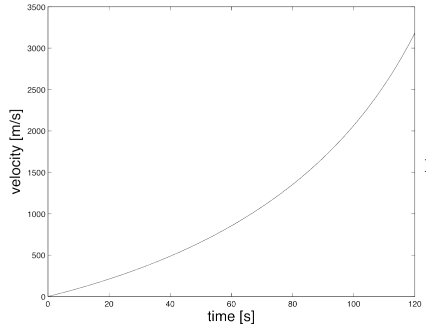
velocity

$$v(t) = -g\, t - w\, \ln \frac{\mathrm{m}(0) + \mathcal{R}\, t}{\mathrm{m}(0)}$$



## open systems - rocket propulsion

velocity $v(t) = -g\, t - w\, \ln \frac{\mathrm{m}(0) + \mathcal{R}\, t}{\mathrm{m}(0)}$

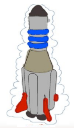



$$g = 9.8\ \mathrm{m/s}^2$$

$$w = 3000\mathrm{m/s}$$

$$\mathrm{m}(0) = 2.5 \cdot 10^6\ \mathrm{kg}$$

$$\mathcal{R}_0 = -16000\mathrm{kg/s}$$



velocity $v(t = 120\mathrm{s}) = 3207.1\ \mathrm{m/s}$



## open systems - balance of internal energy

- volume specific version

$$\mathrm{D}_t(\rho_0\, I) = \mathrm{Div}(-\boldsymbol{Q} + I\boldsymbol{R}) + [\mathcal{Q}_0 + I\,\mathcal{R}_0 - \nabla_X I \cdot \boldsymbol{R}]$$

- subraction of weighted balance of mass

$$I\,\mathrm{D}_t \rho_0 = \mathrm{Div}(I\,\boldsymbol{R}) + I\,\mathcal{R}_0 - \nabla_X I \cdot \boldsymbol{R}$$

- mass specific version

$$\rho_0 \mathrm{D}_t I = \mathrm{Div}(-\boldsymbol{Q}) + \mathcal{Q}_0$$

energy equilibrium



## open systems - balance of entropy

- volume specific version $\mathrm{H}_0^{\text{int}} \geq 0$

$$\mathrm{D}_t(\rho_0 S) = \mathrm{Div}(-\boldsymbol{H} + S\,\boldsymbol{R}) + [\mathcal{H}_0 + S\,\mathcal{R}_0 - \nabla_X S \cdot \boldsymbol{R}] + \mathrm{H}_0^{\text{int}}$$

- subraction of weighted balance of mass

$$S\,\mathrm{D}_t \rho_0 = \mathrm{Div}(S\,\boldsymbol{R}) + S\,\mathcal{R}_0 - \nabla_X S \cdot \boldsymbol{R}$$

- mass specific version

$$\rho_0 \mathrm{D}_t S = \mathrm{Div}(-\boldsymbol{H}) + \mathcal{H}_0 + \mathrm{H}_0^{\text{int}}$$

entropy inequality

## open systems - dissipation inequality

- dissipaltion inequality
  $$\mathrm{D}_0 := \vartheta \mathrm{H}_0^{\mathrm{int}} = \rho_0 \vartheta \mathrm{D}_t S + \vartheta \mathrm{Div}(\boldsymbol{H}) - \vartheta \mathcal{H}_0 \geq 0$$
- identification $\boldsymbol{H} = \frac{1}{\vartheta}\boldsymbol{Q} + \boldsymbol{S}$ $\quad \mathcal{H}_0 = \frac{1}{\vartheta}\mathcal{Q}_0 + \mathcal{S}_0$
- free energy $\psi = \psi(\rho_0, \boldsymbol{F}, \vartheta)$
- definition of stress and entropy
  $$\boldsymbol{P} = \rho_0 \, \mathrm{D}_F \psi \qquad S = -\mathrm{D}_\vartheta \psi$$
- thermodynamic restrictions
  $$\mathcal{S}_0 \leq \rho_0 \mathrm{D}_{\rho_0} \psi \tfrac{1}{\vartheta} \mathcal{R}_0 \qquad \boldsymbol{S} \geq \rho_0 \mathrm{D}_{\rho_0} \psi \tfrac{1}{\vartheta} \boldsymbol{R} \qquad \boldsymbol{Q} \cdot \nabla_X \ln(\vartheta) \geq 0$$

„... a living organism can only keep alive by continuously drawing from its environment negative entropy. it feeds upon negative entropy to compensate the entropy increase it produces by living."

Schrödinger „What is life?" [1944]



## open systems - dissipation inequality

- dissipaltion inequality
  $$\mathrm{D}_0 := \ldots \mathrm{H}_0^{\mathrm{int}} = \rho_0 \ldots S + \ldots \mathrm{v}(\boldsymbol{H}) - \vartheta \mathcal{H}_0 \geq 0$$
- identification $\ldots = \frac{1}{\vartheta}\mathcal{Q}_0 + \mathcal{S}_0$
- free energy
- definition of s...
  $$\boldsymbol{F} \ldots \quad - \mathrm{D}_\vartheta \psi$$
- thermodynamic restric...ns
  $$\mathcal{S}_0 \leq \rho_0 \mathrm{D}_{\rho_0} \psi \tfrac{1}{\vartheta} \mathcal{R}_0 \qquad \boldsymbol{S} \ldots \rho_0 \mathrm{D}_{\rho_0} \psi \tfrac{1}{\vartheta} \boldsymbol{R} \qquad \boldsymbol{Q} \ldots$$

„... a living organism can only keep alive by continuously drawing from its en... entropy. it feeds upon negative entropy to compensate the entropy increase ..."

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## open systems - dissipation inequality

$$\mathrm{D}_0 = \boldsymbol{P} : \mathrm{D}_t \boldsymbol{F} - \rho_0 \mathrm{D}_t \psi - \rho_0 \, S \, \mathrm{D}_t \vartheta - \mathsf{s}_0 \, \vartheta + \boldsymbol{Q} \cdot \nabla_X \ln(\vartheta) \geq 0$$

with definition of arguments of free energy

$$\psi = \psi(\rho_0, \boldsymbol{F}, \vartheta) \qquad \mathrm{D}_t \psi = \mathrm{D}_\rho \psi \, \mathrm{D}_t \rho + \mathrm{D}_F \psi : \mathrm{D}_t \boldsymbol{F} + \mathrm{D}_\vartheta \psi \, \mathrm{D}_t \vartheta$$

evaluation of dissipation inequality

$$\mathrm{D}_0 = [\, \boldsymbol{P} - \rho_0 \mathrm{D}_F \psi \,] : \mathrm{D}_t \boldsymbol{F} - [\, \rho_0 \, S - \rho_0 \, \mathrm{D}_\vartheta \psi \,] \, \mathrm{D}_t \vartheta + \ldots \geq 0$$

provides guidelines for the appropriate choice of the constitutive equations $\quad \boldsymbol{P} = \rho_0 \, \mathrm{D}_F \psi \qquad S = -\mathrm{D}_\vartheta \psi$

thermodynamically conjugate pairs $\quad \boldsymbol{P} \rightleftharpoons \boldsymbol{F} \qquad S \rightleftharpoons \vartheta$