A continuum treatment of growth in biological tissue: Mass transport coupled with mechanics

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Specific goals

- Describe and simulate the processes of growth and development
- Models that are physiologically appropriate and thermodynamically valid
- Experiments on in vitro tissue in parallel
  - Descriptive model driven and validated by experiment
  - Model drives the controlled experiments

Development of biological tissue

Distinct, mathematically independent processes: [Taber - 1995]

- **Growth/Resorption:** Addition/Loss of mass
  e.g. Densification of bones

- **Remodelling:** Change in microstructure
  e.g. Alignment of trabeculae to the axis of external loading

- **Morphogenesis:** Change in macroscopic form
  e.g. Development of an embryo from a fertilized egg

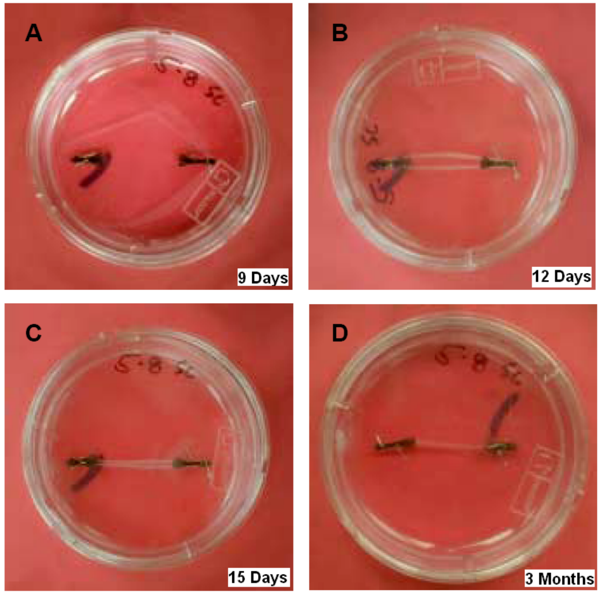
The issues that arise

- Open system *(with respect to mass)*
- Interacting and interconverting species
- Species diffusing with respect to a solid phase *(fluid, precursors, byproducts)*
- Mixture physics

Our treatment involves the introduction of sources, sinks and fluxes of mass

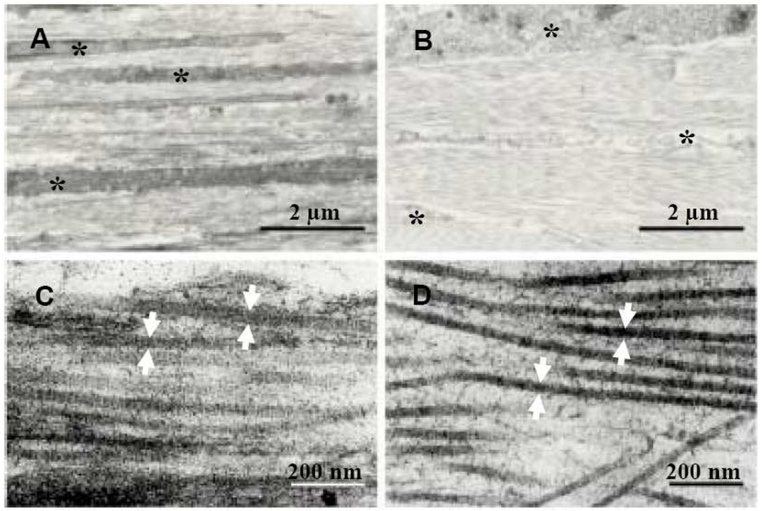
Biological model

Engineered tissue in vitro that is morphologically and functionally similar to neonatal tissue [Calve et al. - 2003]



Biological model - Morphological comparison

Morphological comparison of the engineered constructs to 2 day old neonatal rat tendon [Calve et al. - 2003]

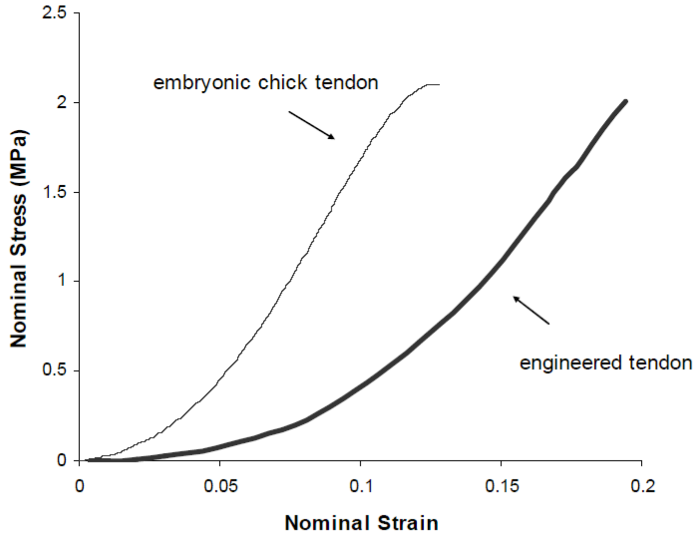


Engineered Tendon Construct

Neonatal Rat Tendon

Biological model - Mechanical comparison

Comparison of the stress-strain response of the engineered construct to embryonic chicken tendon [Calve et al. - 2003]



Tissue Engineering

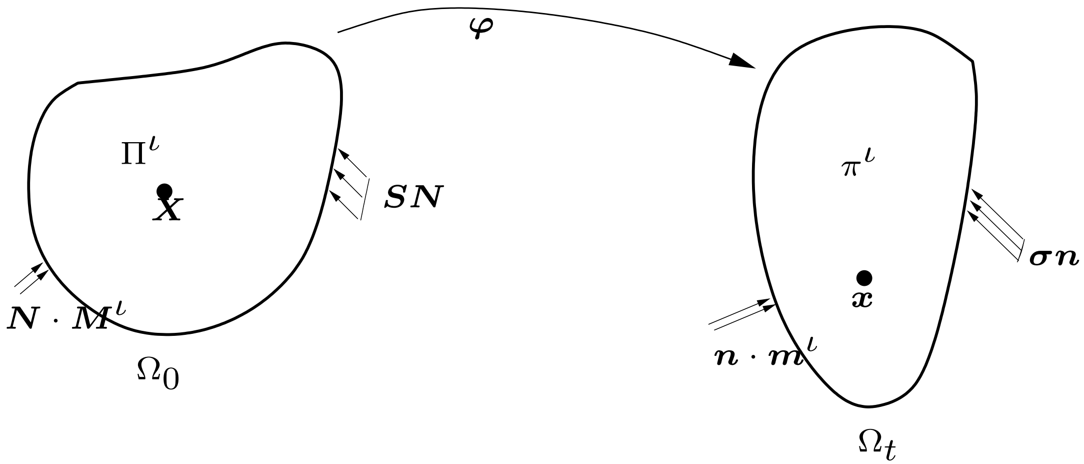
- Capability to engineer constructs which model real tissue
- Carefully control environment and apply stimuli to control growth and remodelling
  - Mechanical loading in bioreactors
  - Chemical evironment and nutrient supply

Modelling Background

Some previous work:

- Cowin and Hegedus [1976]: Solid tissue; mass source; irreversible sources of momentum and energy from perfusing fluid
- Epstein and Maugin [2000]: Mass flux; irreversible fluxes of momentum and entropy
- Kuhl and Steinmann [2002]: Configurational forces motivate mass flux

Mass Balance



- Tissue formed by reactions involving precursors and byproducts – Sources and sinks for species
- Transport of precursors, fluid and byproducts – Fluxes for species

Mass Balance - Equations

For a species ι, in local form, in Ω_0

$$\frac{\partial \rho_0^\iota}{\partial t} = \Pi^\iota - \boldsymbol{\nabla}_X \cdot \boldsymbol{M}^\iota, \; \forall\, \iota = \alpha, \ldots, \omega$$

The sources/sinks satisfy

$$\sum_{\iota=\alpha}^{\omega} \Pi^\iota = 0.$$

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For the solid phase

$$\frac{\partial \rho_0^s}{\partial t} = \Pi^s$$

Mass Balance - Equations

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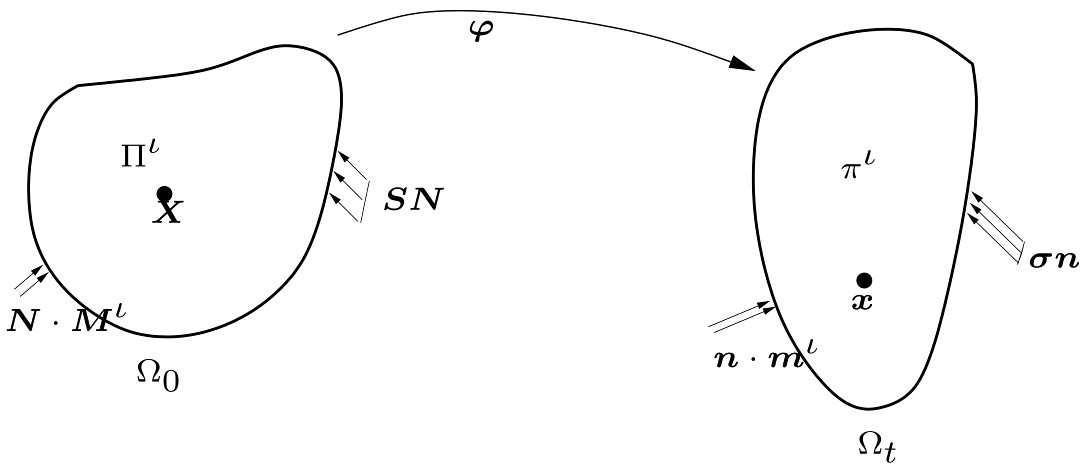
For the fluid phase

$$\frac{\partial \rho_0^f}{\partial t} = -\boldsymbol{\nabla}_X \cdot \boldsymbol{M}^f$$

Balance of Linear Momentum



- Linear momentum balance coupled with mass transport. Sources/Sinks and fluxes contribute to the momenta

- Material velocity relative to the solid $\boldsymbol{V}^\iota = (1/\rho_0^\iota)\boldsymbol{F}\boldsymbol{M}^\iota$

Balance of Linear Momentum - Equations

For a species ι, in local form, in Ω_0

$$\rho_0^\iota \frac{\partial}{\partial t}\left(\boldsymbol{V} + \boldsymbol{V}^\iota\right) = \rho_0^\iota \left(\boldsymbol{g} + \boldsymbol{q}^\iota\right) + \boldsymbol{\nabla}_X \cdot \boldsymbol{S}^\iota - \left(\boldsymbol{\nabla}_X \left(\boldsymbol{V} + \boldsymbol{V}^\iota\right)\right) \boldsymbol{M}^\iota, \; \forall\, \iota = \alpha, \ldots, \omega$$

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Relation between Π^ι's and $\boldsymbol{q}^\iota$'s,

$$\sum_{\iota=\alpha}^{\omega} \left(\rho_0^\iota \boldsymbol{q}^\iota + \Pi^\iota \boldsymbol{V}^\iota\right) = 0$$

Energy, Second Law

- Balance of energy for a species ι, in local form, in Ω_0

$$\rho_0^\iota \frac{\partial e^\iota}{\partial t} = \boldsymbol{S}^\iota : \dot{\boldsymbol{F}} + \boldsymbol{S}^\iota : \boldsymbol{\nabla}_X \boldsymbol{V}^\iota - \boldsymbol{\nabla}_X \cdot \boldsymbol{Q}^\iota + r_0^\iota + \rho_0^\iota \tilde{e}^\iota - \boldsymbol{\nabla}_X e^\iota \cdot (\boldsymbol{M}^\iota)$$

- Proceeding to
  - Write out the second law
  - Multiplying it by θ and subtracting it from the energy equation

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Constitutive relations - I

Constitutive relations:

$$\boldsymbol{S}^\iota = \rho_0^\iota \frac{\partial e^\iota}{\partial \boldsymbol{F}}, \; \forall \, \iota$$

$$\theta = \frac{\partial e^\iota}{\partial \eta^\iota}, \; \forall \, \iota$$

$$\boldsymbol{Q}^\iota = -\boldsymbol{K}^\iota \boldsymbol{\nabla}_X \theta, \; \forall \, \iota$$

$$\boldsymbol{u} \cdot \boldsymbol{K}^\iota \boldsymbol{u} \geq 0 \, \forall \boldsymbol{u} \in \mathbb{R}^3$$

Constitutive Relations - II

$$\boldsymbol{V}^{\iota} = -\tilde{\boldsymbol{D}}^{\iota}\left(\rho_0^{\iota}\frac{\partial \boldsymbol{V}}{\partial t} - \rho_0^{\iota}\boldsymbol{g} - \boldsymbol{\nabla}_X \cdot \boldsymbol{S}^{\iota}\right)$$

$$-\tilde{\boldsymbol{D}}^{\iota}\left(\rho_0^{\iota}\boldsymbol{F}^{-\mathrm{T}}\left(\boldsymbol{\nabla}_X e^{\iota} - \theta\boldsymbol{\nabla}_X \eta^{\iota}\right)\right),\ \forall\,\iota$$

$$\boldsymbol{u}\cdot\tilde{\boldsymbol{D}}^{\iota}\boldsymbol{u} \geq 0\,\forall \boldsymbol{u} \in \mathbb{R}^3$$

Reduced dissipation inequality

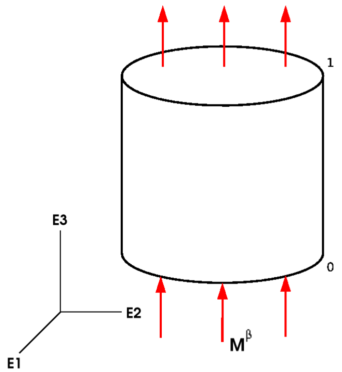
With the constitutive relations ensuring the non-positiveness of certain terms the entropy inequality is reduced to

$$\mathcal{D} = \sum_{\iota=\alpha}^{\omega} \left(\rho_0^\iota \frac{\partial e^\iota}{\partial \rho_0^\iota} \frac{\partial \rho_0^\iota}{\partial t} - \boldsymbol{S}^\iota \colon \boldsymbol{\nabla}_X \boldsymbol{V}^\iota + \rho_0^\iota \boldsymbol{V}^\iota \cdot \left(\frac{\partial \boldsymbol{V}^\iota}{\partial t} + \left(\boldsymbol{\nabla}_X \boldsymbol{V}^\iota \right) \boldsymbol{F}^{-1} \boldsymbol{V}^\iota \right) \right)$$

$$+ \sum_{\iota=\alpha}^{\omega} \Pi^\iota \left(e^\iota + \frac{1}{2} \| \boldsymbol{V} + \boldsymbol{V}^\iota \|^2 \right)$$

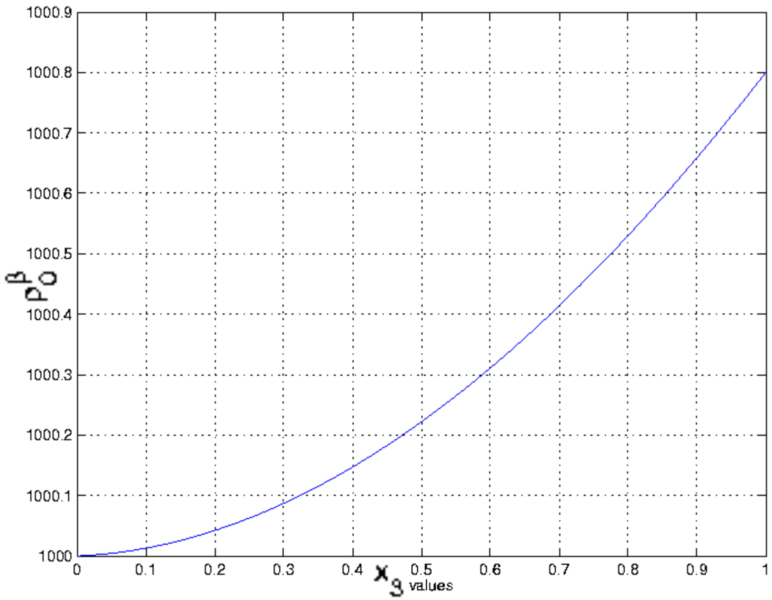
$$+ \sum_{\iota=\alpha}^{\omega} \left(\rho_0^\iota \frac{\partial}{\partial t} \left(\boldsymbol{V} + \boldsymbol{V}^\iota \right) - \rho_0^\iota \boldsymbol{g} - \boldsymbol{\nabla}_X \cdot \boldsymbol{S}^\iota + \boldsymbol{\nabla}_X \left(\boldsymbol{V} + \boldsymbol{V}^\iota \right) \left(\rho_0^\iota \boldsymbol{F}^{-1} \boldsymbol{V}^\iota \right) \right) \cdot \boldsymbol{V} \leq 0$$

Example

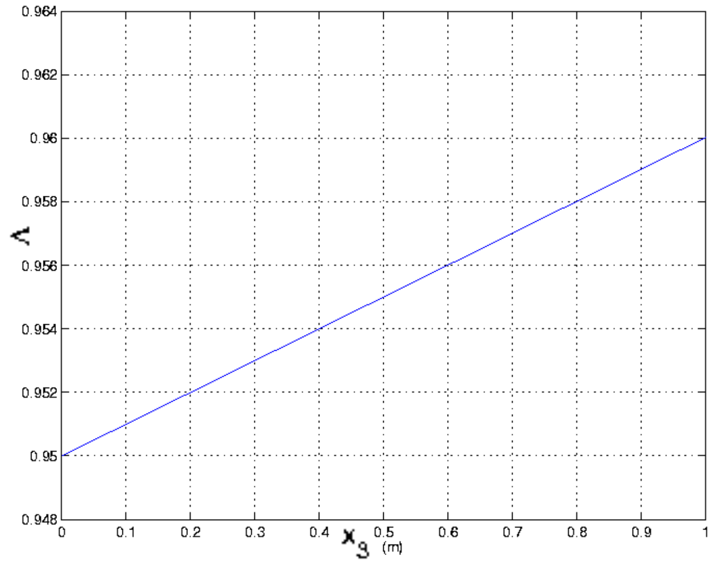


- Simplified 1D case involving two species, α, a solid and β, a fluid
- Solid is neo-hookean, fluid is compressible and ideal
- ρ_0^β and the stretch Λ vary, and calculated values are used to determine the flux $\boldsymbol{M}^\beta$

Results - Density variation along length



Results - Variation in stretch along length



Results - Observations

- Coupling of diffusion to stress
- The flux $\boldsymbol{M}^{\beta}$ ($4.5X10^{-4}kg/m^2/s$) comes out to be positive, driving the fluid against
  - Gravity
  - Concentration gradient
- Mechanics influences mass balance

Conclusions and further work

- Physiologically consistent continuum formulation describing growth in an open system
- Relevant driving forces arise from thermodynamics
- Consistent with mixture theory
- Applying present theory to 3D tissues involving multiple species diffusing and reacting
- Formulated the remodelling problem – Preliminary results

Mass Balance - Equations

For a species, in the integral form

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\Omega_0}\rho_0^\iota(\boldsymbol{X},t)\mathrm{d}V = \int\limits_{\Omega_0}\Pi^\iota(\boldsymbol{X},t)\mathrm{d}V - \int\limits_{\partial\Omega_0}\boldsymbol{M}^\iota(\boldsymbol{X},t)\cdot\boldsymbol{N}\mathrm{d}A,\ \forall\,\iota=\alpha,\ldots,\omega \quad (1)$$

ρ_0^ι being the mass concentration of species ι and $\sum\limits_{\iota=\alpha}^{\omega}\rho_0^\iota = \rho_0$

The sources/sinks satisfy

$$\sum_{\iota=\alpha}^{\omega}\Pi^\iota = 0. \quad (2)$$

Balance of Linear Momentum - Equations

For a species ι, in the integral form written in Ω_0 is

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\Omega_0} \rho_0^\iota(\boldsymbol{V} + \boldsymbol{V}^\iota)\mathrm{d}V = \int\limits_{\Omega_0} \rho_0^\iota \boldsymbol{g}\mathrm{d}V + \int\limits_{\Omega_0} \rho_0^\iota \boldsymbol{q}^\iota \mathrm{d}V + \int\limits_{\Omega_0} \Pi^\iota(\boldsymbol{V} + \boldsymbol{V}^\iota)\mathrm{d}V + \int\limits_{\partial\Omega_0} \boldsymbol{S}^\iota \boldsymbol{N}\mathrm{d}A - \int\limits_{\partial\Omega_0} (\boldsymbol{V} + \boldsymbol{V}^\iota)\boldsymbol{M}^\iota \cdot \boldsymbol{N}\mathrm{d}A \quad (3)$$

$$\boldsymbol{q}^\iota = \sum_{\vartheta=\alpha,\vartheta\neq\iota}^{\omega} \boldsymbol{q}^{\iota\vartheta} \quad (4)$$

On application of balance of mass, in local form, for the entire system

$$\sum_{\iota=\alpha}^{\omega} \rho_0^\iota \frac{\partial}{\partial t} \left(\boldsymbol{V} + \boldsymbol{V}^\iota \right) = \sum_{\iota=\alpha}^{\omega} \rho_0^\iota \left(\boldsymbol{g} + \boldsymbol{q}^\iota \right) + \sum_{\iota=\alpha}^{\omega} \boldsymbol{\nabla}_X \cdot \boldsymbol{S}^\iota - \sum_{\iota=\alpha}^{\omega} \left(\boldsymbol{\nabla}_X \left(\boldsymbol{V} + \boldsymbol{V}^\iota \right) \right) \boldsymbol{M}^\iota \quad (5)$$

Relation between Π^ι's and $\boldsymbol{q}^\iota$'s,

$$\sum_{\iota=\alpha}^{\omega} \left(\rho_0^\iota \boldsymbol{q}^\iota + \Pi^\iota \boldsymbol{V}^\iota \right) = 0 \quad (6)$$

Balance of Angular Momentum - Equations

- In a purely mechanical theory, balance of angular momentum implies $\boldsymbol{\sigma} = \boldsymbol{\sigma}^{\mathrm{T}}$.

- For a single species ι, in integral form in Ω_0,

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} \int\limits_{\Omega_0} \boldsymbol{\varphi} \times \rho_0^\iota (\boldsymbol{V} + \boldsymbol{V}^\iota) \mathrm{d}V \quad &= \quad \int\limits_{\Omega_0} \boldsymbol{\varphi} \times \left[\rho_0^\iota \left(\boldsymbol{g} + \boldsymbol{q}^\iota \right) + \Pi^\iota \left(\boldsymbol{V} + \boldsymbol{V}^\iota \right) \right] \mathrm{d}V \\ &+ \int\limits_{\partial\Omega_0} \boldsymbol{\varphi} \times \left(\boldsymbol{S}^\iota - \left(\boldsymbol{V} + \boldsymbol{V}^\iota \right) \otimes \boldsymbol{M}^\iota \right) \boldsymbol{N} \mathrm{d}A \end{aligned} \tag{7}$$

On simplification,

$$\int_{\Omega_0} \boldsymbol{V} \times \rho_0^\iota \boldsymbol{V}^\iota \mathrm{d}V \quad = \quad -\int_{\Omega_0} \boldsymbol{\epsilon} \colon \left(\left(\boldsymbol{S}^\iota - (\boldsymbol{V} + \boldsymbol{V}^\iota) \otimes \underbrace{\boldsymbol{M}^\iota}_{\rho_0^\iota \boldsymbol{F}^{-1} \boldsymbol{V}^\iota} \right) \boldsymbol{F}^{\mathrm{T}} \right) \mathrm{d}V \quad (8)$$

On localizing,

$$\left(\boldsymbol{S}^\iota - \boldsymbol{V}^\iota \otimes \rho_0^\iota \boldsymbol{F}^{-1} \boldsymbol{V}^\iota \right) \boldsymbol{F}^{\mathrm{T}} = \boldsymbol{F} \left(\boldsymbol{S}^\iota - \boldsymbol{V}^\iota \otimes \rho_0^\iota \boldsymbol{F}^{-1} \boldsymbol{V}^\iota \right)^{\mathrm{T}} \quad (9)$$

But, $(\boldsymbol{V}^\iota \otimes \boldsymbol{F}^{-1} \boldsymbol{V}^\iota) \boldsymbol{F}^{\mathrm{T}} = \boldsymbol{V}^\iota \otimes \boldsymbol{V}^\iota$, which implies the symmetry: $\boldsymbol{S}^\iota \boldsymbol{F}^{\mathrm{T}} = \boldsymbol{F} (\boldsymbol{S}^\iota)^{\mathrm{T}}$

This implies the partial Cauchy stresses are symmetric: $\boldsymbol{\sigma}^\iota = (\boldsymbol{\sigma}^\iota)^{\mathrm{T}}$

Balance of Energy - Equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\Omega_0} \rho_0^\iota \left(e^\iota + \frac{1}{2}\|\boldsymbol{V} + \boldsymbol{V}^\iota\|^2\right)\mathrm{d}V = \int\limits_{\Omega_0} \left(\rho_0^\iota \boldsymbol{g}\cdot(\boldsymbol{V} + \boldsymbol{V}^\iota) + r_0^\iota\right)\mathrm{d}V$$

$$+ \int\limits_{\Omega_0} \rho_0^\iota \boldsymbol{q}^\iota \cdot (\boldsymbol{V} + \boldsymbol{V}^\iota)\mathrm{d}V$$

$$+ \int\limits_{\Omega_0} \left(\Pi^\iota \left(e^\iota + \frac{1}{2}\|\boldsymbol{V} + \boldsymbol{V}^\iota\|^2\right) + \rho_0^\iota \tilde{e}^\iota\right)\mathrm{d}V$$

$$+ \int\limits_{\partial\Omega_0} \left((\boldsymbol{V} + \boldsymbol{V}^\iota)\cdot \boldsymbol{S}^\iota - \boldsymbol{M}^\iota \left(e^\iota + \frac{1}{2}\|\boldsymbol{V} + \boldsymbol{V}^\iota\|^2\right) - \boldsymbol{Q}^\iota\right)\cdot \boldsymbol{N}\mathrm{d}A. \qquad (10)$$

On simplification localizing, and summing over all ι,

$$\sum_{\iota=\alpha}^{\omega} \rho_0^\iota \frac{\partial e^\iota}{\partial t} = \sum_{\iota=\alpha}^{\omega} \left(\boldsymbol{S}^\iota : \dot{\boldsymbol{F}} + \boldsymbol{S}^\iota : \boldsymbol{\nabla}_X \boldsymbol{V}^\iota - \boldsymbol{\nabla}_X \cdot \boldsymbol{Q}^\iota + r_0^\iota + \rho_0^\iota \tilde{e}^\iota \right) - \sum_{\iota=\alpha}^{\omega} \boldsymbol{\nabla}_X e^\iota \cdot (\boldsymbol{M}^\iota) \quad (11)$$

Where $\tilde{e}^\iota$ satisfies the relation,

$$\sum_{\iota=\alpha}^{\omega} \left(\rho_0^\iota \boldsymbol{q}^\iota \cdot (\boldsymbol{V} + \boldsymbol{V}^\iota) + \Pi^\iota \left(e^\iota + \frac{1}{2} \|\boldsymbol{V} + \boldsymbol{V}^\iota\|^2 \right) + \rho_0^\iota \tilde{e}^\iota \right) = 0 \quad (12)$$

The different terms - Mechanics

In the reference configuration Ω_0,

Π^ι is the source/sink term for species ι
$\boldsymbol{M}^\iota$ is the mass flux term for species ι
$\boldsymbol{S}^\iota$ is the partial first Piola-Kirchhoff stress on species ι
$\boldsymbol{N}$ is the outward normal at the surface
$\boldsymbol{g}$ is the body force acting on the entire system

The different terms - Mechanics

In the current configuration Ω_t,

π^ι is the source/sink term for species ι
$\boldsymbol{m}^\iota$ is the mass flux term for species ι
$\boldsymbol{\sigma}^\iota$ is the partial Cauchy stress on species ι
$\boldsymbol{n}$ is the outward normal at the surface
$\boldsymbol{g}$ is the body force acting on the entire system

The different terms - Mechanics

$\boldsymbol{V}$ is the velocity of the solid phase

$\boldsymbol{V}^{\iota}$ is the material velocity relative to the solid phase defined as $\boldsymbol{V}^{\iota} = (1/\rho_0^{\iota})\boldsymbol{F}\boldsymbol{M}^{\iota}$

$\boldsymbol{q}^{\iota}$ is the net force exerted on species ι by all other species in the system

The different terms - Energy

e^ι is the internal energy of each species ι
$\boldsymbol{F}$ is the deformation gradient
$\boldsymbol{Q}^\iota$ is the heat flux term for species ι
r_0^ι is the heat supplied to species ι per unit reference volume
$\tilde{e}$ is the internal energy transferred to species ι from all other species