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Theory Manual Version 4.5

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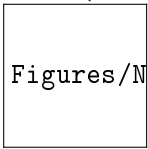Salt Lake City, Utah

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Chapter 1

Introduction

1.1   Overview of FEBio

FEBio is an implicit, nonlinear finite element solver that is specifically designed for applications in biomechanics. It offers analyses, constitutive models and boundary conditions that are relevant for this particular field. This section describes briefly the available features of FEBio. A more detailed overview of features can be found in the *FEBio User's Manual*.

FEBio supports two analysis types, namely *quasi-static* and *quasi-static poroelastic*. In a *quasi-static* analysis the (quasi-) static response of the system is sought; inertial terms are ignored. In a *quasi-static poroelastic* analysis a coupled solid-fluid problem is solved. The latter analysis type is useful for modeling tissues that have high water content and the explicit modeling of fluid movement relative to the solid phase is important.

Several nonlinear constitutive models are available to allow the user to model the often complicated biological tissue behavior. Several isotropic constitutive models are supported such as Neo-Hookean, Mooney-Rivlin, Veronda-Westmann, Arruda-Boyce and Ogden. These models have a nonlinear stress-strain response. In addition to the isotropic models, there are several anisotropic models available. These materials show anisotropic behavior in at least one preferred direction and are useful for modeling biological tissues such as tendons, muscles and other tissues that contain fibers. FEBio also contains a *rigid body* material model, which can be used to model rigid structures whose deformation is negligible compared to the deformable geometry.

Biological tissues can interact in very complicated ways. Therefore FEBio supports a wide range of boundary conditions to model these interactions. These include prescribed displacements, nodal forces, and pressure forces. Deformable models can also be connected to rigid bodies so that the user can model prescribed rotations and torques. Rigid bodies can be connected with rigid joints. Even more complicated interactions can be modeled using FEBio's contact interfaces. The user can choose between different types of contact interfaces, such as sliding interfaces, tied interfaces and rigid wall interfaces. A sliding interface is defined between two surfaces that are allowed to separate and slide across each other but are not allowed to penetrate. The rigid wall interface is also similar to the sliding interface, except that one of the contacting surfaces is a movable rigid wall. As of version 1.2, there is an implementation of a sliding interface that allows for fluid flow crossing the contact interface. The tied interface is similar to the sliding interface, but in this case, the surfaces are not allowed to slide or separate. In addition, the user may specify a body force which can be used to model the effects of gravity or base acceleration.

1.2   About this document

This document is a part of a set of three manuals that accompany FEBio: the *FEBio User's Manual*, describing how to use FEBio, the *FEBio Developer's Manual* for users who wish to modify or add features to the code, and this manual, which describes the theory behind most of the FEBio algorithms.

The purpose of this manual is to provide theoretical background on many of the algorithms that are implemented in FEBio. In this way the user can develop a better understanding of how the program works and how it can be used to create well defined biomechanical simulations. The authors have tried to be as detailed as possible to make the text coherent and comprehensible, but due to the complexity of some of the topics, some descriptions only skim the surface. Many of the theoretical ideas discussed in this manual can and have filled entire bookshelves. The explanations contained herein should be sufficient to give the reader a basic understanding of the theoretical developments. References to textbooks and the primary literature are provided for further reading.

Chapter 2 starts with a brief overview of some of the important concepts in continuum mechanics. Readers who are already familiar with this field can skip this chapter, although the material may be useful to get familiar with the notation and terminology used in this manual.

Chapter 3 describes the nonlinear finite element method. It also explains the Newton-Raphson method, which is the basis for most implementations of the nonlinear finite element method. A more specialized version of this algorithm, the BFGS method, is described as well since it is used in FEBio.

In Chapter **??** the different element types that are available in FEBio are described in detail. FEBio currently supports 3D solid elements, such as the linear hexahedral, pentahedral and tetrahedral elements, as well as quadrilateral and triangular shell elements.

Chapter 4 contains a detailed description of the material models in FEBio. Most of these models are based on hyperelasticity, which is introduced in chapter 2. Several transversely isotropic materials are described as well. This also discusses the biphasic material and its implementation in FEBio.

Chapter **??** describes the basics of the theory of contact and coupling. In FEBio the user can connect the different parts of the geometry in a variety of ways. There are rigid interfaces where a deformable model is attached to a rigid model, rigid joints where two or more rigid bodies connect, and sliding interfaces where two surfaces are allowed to separate and slide across each other but are not allowed to penetrate. The various contact and coupling algorithms are discussed as well together with their implementation in FEBio.

Chapter 2

Continuum Mechanics of Elastic Reaction-Diffusion Analyses

2.1 Elastic Reaction-Diffusion Materials

Elastic reaction-diffusion materials represent a simplification of the biphasic-solute and multiphasic materials, where there is no explicitly modeled porous media or fluid phase. Solid mechanics and chemical reaction-diffusion kinetics are formulated to be nearly independent of each other aside from additional user-defined constitutive relations where implicit feedback between stress/strain and chemical processes are defined. This approach is justified when there is a large difference in time scales between displacements associated with solid mechanics and those associated with solute transport and chemical kinetics (a common assumption of kinematic growth theory [**?**]). Additionally, this approach introduces the assumption that the entire solid mass may turn over at each new time step, resulting in a new reference configuration defined by new extensive material properties (volume, shape, etc.) but constant intensive material properties (solid density, solute concentration and diffusivity, etc.).

Elastic reaction-diffusion analyses deviate from biphasic-solute and multiphasic analyses by assuming that solute c^α concentrations, fluxes $\mathbf{j}^\alpha$, diffusivities $\mathbf{d}^\alpha$, and kinetic parameters $k_f, k_r, \hat{\zeta}$ are tracked only in an intensive sense (i.e., volumetric changes due to strain do not affect the apparent concentration or related parameters). This treatment introduces implicit sources of extensive quantities such as mass and energy which either 1) have negligible contributions when volumetric changes occur at a much longer time scale than chemical transport and kinetics, and/or 2) may be accounted for by implicit variables. Similar reasoning is used to justify the absence of porosity, hydraulic permeability, and fluid pressure (p). In the absence of fluid field variables, only isotropic diffusivity is introduced for the time being. One last distinction from biphasic and multiphasic materials is that standard thermodynamic conditions are assumed throughout the analysis. Any deviations from standard conditions may be implicitly accounted for when specifying the average material and constitutive behaviors during an analysis.

This analysis should not be used when modeling electrochemistry or short-time mechano-chemical phenomena (e.g. osmotic pressure, non-negligible solute volume fractions, convection). The user is responsible for ensuring that these assumptions are appropriate for a given problem.

2.1.1 Governing Equations

The governing equations adopted in this finite element implementation of neutral solute transport in porous media are based on the framework of mixture theory [2, 4]. The fundamental modeling assumptions adopted in this treatment are quasi-static conditions for momentum balance (negligible effects of inertia), intrinsic incompressibility of all constituents (invariant true densities), isothermal conditions, negligible volume fraction of solute relative to the solid and solvent, and negligible effects of solute viscosities (friction between similar and dissimilar solutes) relative to frictional interactions between solutes and the solid matrix. These assumptions are often made in studies of biological tissues and cells with the additional simplification that frictional interactions do not arise between the solutes and the solvent (in contrast to biphasic, biphasic-solute, triphasic, and multiphasic material formulations).

Mixture constituents are classified as components of the solid matrix (σ) or a solute ($\alpha \in \{1, 2, \ldots, s\}$). The motion of the solid matrix is described by the displacement vector $\mathbf{u}$ while solute concentrations are described by c^α (unlike prior analyses). The solid stress is described by the Cauchy stress tensor $\boldsymbol{\sigma}$. Under the established assumptions, it is common to solve the equations of motion associated with the solid mechanics and chemical kinetics separately before superimposing the chemical solution onto the mesh solved by the elastic equations of motion. The conservation of mass and linear momentum for the solid reduce to

$$\rho \frac{D\mathbf{v}}{Dt} = \operatorname{div} \boldsymbol{\sigma} \,. \tag{2.1.1}$$

Similarly, the balance of linear momentum for the solutes is given by

$$-\rho^\alpha \operatorname{grad} \tilde{\mu}^\alpha - \mathbf{f}^{\alpha\sigma} \cdot (\mathbf{v}^\alpha - \mathbf{v}^\sigma) - \mathbf{f}^{\alpha w} \cdot (\mathbf{v}^\alpha - \mathbf{v}^w) = \mathbf{0} \,, \tag{2.1.2}$$

where $\rho^\alpha = M^\alpha c^\alpha$ is the density, M^α is the (invariant) molecular weight, $\tilde{\mu}^\alpha$ is the mechano-chemical potential, $\mathbf{v}^\alpha$ is the velocity of constituent α, and $\mathbf{f}^{\alpha w}, \mathbf{f}^{\alpha w}$ are the diffusive drag tensor representing momentum exchange via frictional interactions between a given solute and the solid and implicit solvent ([**?**]).

The mechano-chemical potential is the sum of the mechanical and chemical potentials. The chemical potential μ^α of α represents the rate at which the mixture free energy changes with increasing mass of α. From classical physical chemistry, the general form of a constitutive relation for the chemical potential is $\mu^\alpha = \mu_0^\alpha(\theta) + (R\theta/M^\alpha) \ln a^\alpha$ [3], where R is the universal gas constant, θ is the absolute temperature, M^α is the molecular weight (invariant) and a^α is the activity of constituent α (a non-dimensional quantity); $\mu_0^\alpha(\theta)$ is the chemical potential at some arbitrary reference state, at a given temperature. As previously outlined in the FEBio manual (Biphasic-Solute governing equations), $a^\alpha = \gamma^\alpha c^\alpha / \kappa^\alpha c_0^\alpha = c^\alpha / \tilde{\kappa}^\alpha c_0^\alpha$ where c_0^α is the solute concentration in some standard reference state (an invariant, typically $c_0^\alpha = 1\,\text{M}$), γ^α is the non-dimensional activity coefficient (deviation from ideal physico-chemical behavior [3]), and solubility due to the fraction of the pore space which is accessible to the solute. For the elastic-solute materials, we assume both ideal physico-chemical behavior, and no exclusion of the interstitial space of the porous solid matrix throughout the analysis (i.e., $\forall t \geq 0 \; \tilde{\kappa}^\alpha = \kappa^\alpha = \gamma^\alpha = 1$).

In an elastic solute material, the mechano-electrochemical potential of each solute is simplified from to

$$\tilde{\mu}^\alpha = \mu_0^\alpha(\theta) + \frac{R\theta}{M^\alpha} \left(\ln \frac{c^\alpha}{c_0^\alpha} \right) \,. \tag{2.1.3}$$

The gradient of the mechano-chemical potential gives

$$\begin{aligned} \operatorname{grad} \tilde{\mu}^\alpha &= \frac{R\theta}{M^\alpha c^\alpha} \operatorname{grad} c^\alpha \\ &= \frac{R\theta}{\rho^\alpha} \operatorname{grad} c^\alpha \end{aligned}.$$

For elastic-solute analyses, we assume that the fluid convection over the timescale of solid deformation is negligible (i.e., $\mathbf{w} = \mathbf{v}^w - \mathbf{v}^\sigma \approx \mathbf{0}$) which implies $\mathbf{v}^\sigma = \mathbf{v}^w$. Thus, the resulting balance of linear momentum becomes

$$-R\theta \operatorname{grad} c^\alpha - (\mathbf{f}^{\alpha\sigma} + \mathbf{f}^{\alpha w}) \cdot (\mathbf{v}^\alpha - \mathbf{v}^s) = \mathbf{0}.$$

This expression can be formulated in terms of the solute molar flux ($\mathbf{j}^\alpha = c^\alpha (\mathbf{v}^\alpha - \mathbf{v}^s)$) and the effective diffusivity $\mathbf{d}^\alpha = R\theta c^\alpha (\mathbf{f}^{\alpha\sigma} + \mathbf{f}^{\alpha w})^{-1}$. Fick's first law is recovered by multiplying $c^\alpha (\mathbf{f}^{\alpha s})^{-1}$ into the above expression:

$$\mathbf{j}^\alpha = -\mathbf{d}^\alpha \operatorname{grad} c^\alpha.$$

Each constituent of the mixture must satisfy the axiom of mass balance. In the absence of chemical reactions the mass balance for constituent α is

$$\frac{\partial \rho^\alpha}{\partial t} + \operatorname{div}(\rho^\alpha \mathbf{v}^\alpha) = 0. \tag{2.1.4}$$

Using the above relations, the mass balance relation for the solute may be rewritten as

$$\frac{\partial c^\alpha}{\partial t} + \operatorname{div} \mathbf{j}^\alpha = 0. \tag{2.1.5}$$

This form of the mass balance for the solute is convenient for a finite element formulation where the mesh is defined on the solid matrix.

2.2 Chemical Reactions

Chemical reactions may be incorporated into a multiphasic mixture by adding a mass supply term to the equation of mass balance,

$$\frac{\partial c^\alpha}{\partial t} + \operatorname{div}(\mathbf{j}^\alpha) = \hat{c}^\alpha, \tag{2.2.1}$$

Where $\hat{c}^\alpha$ is the volume density of mass supply to α resulting from chemical reactions with all other mixture constituents.

2.2.1 Solutes

Solutes are denoted generically by $\alpha = \iota$. In chemistry solute content is often represented in units of molar concentration (moles per fluid volume). It follows that solute molar concentration c^ι and molar supply $\hat{c}^\iota$ are related to ρ^ι and $\hat{\rho}^\iota$ via

$$c^\iota = \frac{\rho^\iota}{M^\iota}, \quad \hat{c}^\iota = \frac{\hat{\rho}^\iota}{M^\iota}. \tag{2.2.2}$$

The molar flux of constituent ι relative to the solid is given by

$$\mathbf{j}^\iota = c^\iota (\mathbf{v}^\iota - \mathbf{v}^s), \tag{2.2.3}$$

where it may be noted that $\mathbf{m}^\iota = M^\iota \mathbf{j}^\iota$.

2.2.2 Chemical Kinetics

Productions rates are described by constitutive relations which are functions of the state variables. In a biological mixture under isothermal conditions, the minimum set of state variables needed to describe reactive mixtures that include a solid matrix are: the (uniform) temperature θ, the solid matrix deformation gradient $\mathbf{F}$ (or related strain measures), and the molar content c^α of the various constituents. This set differs from the classical treatment of chemical kinetics in fluid mixtures by the inclusion of $\mathbf{F}$ and the subset of constituents bound to the solid matrix. To maintain a consistent notation in this section, solid-bound molecular species are described by their molar concentrations and molar supplies which may be related to their referential mass density and referential mass supply according to

$$c^\sigma = \frac{\rho_r^\sigma}{M^\sigma}, \quad \hat{c}^\sigma = \frac{\hat{\rho}_r^\sigma}{M^\sigma}. \tag{2.2.4}$$

Consider a general chemical reaction,

$$\sum_\alpha \nu_R^\alpha \mathcal{E}^\alpha \rightarrow \sum_\alpha \nu_P^\alpha \mathcal{E}^\alpha, \tag{2.2.5}$$

where $\mathcal{E}^\alpha$ is the chemical species representing constituent α; ν_R^α and ν_P^α represent stoichiometric coefficients of the reactants and products, respectively. Since the molar supply of reactants and products is constrained by stoichiometry, it follows that all molar supplies $\hat{c}^\alpha$ in a specific chemical reaction may be related to a production rate $\hat{\zeta}$ according to

$$\hat{c}^\alpha = \nu^\alpha \hat{\zeta}, \tag{2.2.6}$$

where ν^α represents the net stoichiometric coefficient for $\mathcal{E}^\alpha$,

$$\nu^\alpha = \nu_P^\alpha - \nu_R^\alpha. \tag{2.2.7}$$

Thus, formulating constitutive relations for $\hat{c}^\alpha$ is equivalent to providing a single relation for $\hat{\zeta}(\theta, \mathbf{F}, c^\alpha)$. When the chemical reaction is reversible,

$$\sum_\alpha \nu_R^\alpha \mathcal{E}^\alpha \rightleftharpoons \sum_\alpha \nu_P^\alpha \mathcal{E}^\alpha, \tag{2.2.8}$$

the relations of Eqs.(2.2.6)-(2.2.7) still apply but the form of $\hat{\zeta}$ would be different.

Using the relations of Eqs.(2.2.2), (2.2.4) and (2.2.6), it follows in general that $c^\alpha = \nu^\alpha \hat{\zeta}$, so that the constraint is equivalent to enforcing stoichiometry, namely,

$$\sum_\alpha \nu^\alpha = 0. \tag{2.2.9}$$

Chapter 3

The Nonlinear FE Method

This chapter discusses the basic principles of the nonlinear finite element method. The chapter begins with a short introduction to the weak formulation and the principle of virtual work. Next, the important concept of linearization is discussed and applied to the principle of virtual work. Finally the Newton-Raphson procedure and its application to the nonlinear finite element method are described.

3.1 Weak Formulation for Elastic Reaction-Diffusion Materials

The virtual work integral for a mixture of intrinsically incompressible constituents combines the balance of momentum for the mixture, the balance of mass for the mixture, and the balance of mass for each of the solutes.

For the elastic reaction-diffusion materials, it is assumed that there is a large difference in time scales between displacements and solute transport and kinetics (such as during some growth and remodeling simulations). The first consequence of this is that solute c^α concentrations, solute flux $\mathbf{j}^\alpha$, and diffusivity $\mathbf{d}^\alpha$ are unaffected by volumetric changes (i.e., J) or rotation. Thus, most of the cross linearization (i.e., interactions between solid displacements and concentration displacements) are not evaluated unless they depend on an implicitly modeled relationship ($\frac{\partial k}{\partial \mathbf{E}}, \hat{\boldsymbol{\zeta}}_\varepsilon, \boldsymbol{D}^\alpha, \frac{\delta c^\alpha}{J}, \frac{\partial \tilde{\kappa}}{J}, \mathbf{j}'_u$,etc.). The second consequence is that fluid pressure $(p, \tilde{p})$ and solute convection are assumed to be negligible (as are $\mathcal{K}, \tilde{\mathcal{K}}, \tilde{\mathbf{k}}'_c, \frac{\partial \tilde{\mathcal{K}}}{\partial c^\alpha}, \mathbf{w}'_u, \mathbf{w}'_c$). Finally, standard thermodynamic conditions are assumed throughout the analysis such that the activity coefficient, effective solubility, partition coefficient, osmotic coefficient, and diffusivities are constant (i.e., $\gamma^\alpha, \hat{\kappa}^\alpha, \tilde{\kappa}^\alpha = 1$, $\Phi = 0$, $\frac{\partial \mathbf{d}^\alpha}{\partial \tilde{c}^\gamma}, \frac{\partial \mathbf{d}^\alpha}{\partial \tilde{\kappa}^\gamma}, \mathbf{d}'_c, \frac{\partial d_0}{\partial J} = \mathbf{0}$). We leave the possibility that the stress/strain and solute concentrations may contain interaction terms (e.g., $\boldsymbol{\sigma}'_c, \frac{\partial \mathbf{S}}{\partial c}, \frac{\partial c}{\partial \boldsymbol{\sigma}}, \frac{\partial k}{\partial \mathbf{E}}, \hat{\boldsymbol{\zeta}}_\varepsilon$ may be non-zero under certain kinematic growth relations). This analysis should not be used if modeling electrochemistry or short-time mechano-chemical phenomena are desired (e.g. osmotic pressure, non-negligible solute volume fractions, convection).

The virtual work integral simplifies to:

$$
\begin{aligned}
\delta W = &\int_b \delta \mathbf{v} \cdot \operatorname{div} \boldsymbol{\sigma} \, dv \\
&+ \sum_{\alpha \neq s,w} \int_b \delta c^\alpha \left[\frac{D}{Dt} c^\alpha + \operatorname{div} \mathbf{j}^\alpha \right] dv \\
&+ \delta G,
\end{aligned}
\tag{3.1.1}
$$

where $\delta\mathbf{v}$ is the virtual velocity of the solid, δc^α is the virtual molar energy of solute α, and δG is the Gibb's free energy (due to chemical reactions). Here, b represents the mixture domain in the spatial frame and dv is an elemental volume in b. Applying the divergence theorem, δW may be split into internal and external contributions to the virtual work, $\delta W = \delta W_{\text{ext}} - \delta W_{\text{int}}$, where

$$
\begin{aligned}
\delta W_{\text{int}} = &\int_b \boldsymbol{\sigma} : \delta\mathbf{D}\,dv \\
&+ \sum_{\alpha\neq s,w}^{\alpha_s} \int_b \left[\mathbf{j}^\alpha \cdot \operatorname{grad}\delta c^\alpha - \delta c^\alpha \frac{D}{Dt} c^\alpha \right]\,dv \\
&+ \delta G,
\end{aligned}
\tag{3.1.2}
$$

d δG is given by

$$
\delta G = \sum_\alpha \sum_i \int_b \delta c^\alpha \hat{c}_i^\alpha\,dv
\tag{3.1.3}
$$

and

$$
\delta W_{\text{ext}} = \int_{\partial b} \left[\delta\mathbf{v} \cdot \mathbf{t} + \sum_{\alpha\neq s,w} \delta c^\alpha j_n^\alpha \right]\,da\,.
\tag{3.1.4}
$$

In these expressions, $\delta\mathbf{D} = \left(\operatorname{grad}\delta\mathbf{v} + \operatorname{grad}^T \delta\mathbf{v}\right)/2$, ∂b is the boundary of b, and da is an elemental area on ∂b. In this finite element formulation, $\mathbf{u}$ and c^α are used as nodal variables, and essential boundary conditions may be prescribed on these variables. Natural boundary conditions are prescribed to the mixture traction, $\mathbf{t} = \boldsymbol{\sigma} \cdot \mathbf{n}$ and normal solute flux $j_n^\alpha = \mathbf{j}^\alpha \cdot \mathbf{n}$, where $\mathbf{n}$ is the outward unit normal to ∂b.

3.1.1 Linearization along $\Delta\mathbf{u}$

The linearization of the first term in δW_{int} along $\Delta\mathbf{u}$ yields

$$
D\left(\mathbf{S} : \delta\dot{\mathbf{E}}\right)[\Delta\mathbf{u}]\,dV = \left[\delta\mathbf{d}^s : \boldsymbol{\mathcal{C}} : \Delta\boldsymbol{\varepsilon} + \boldsymbol{\sigma} : \left(\operatorname{grad}^T \Delta\mathbf{u} \cdot \operatorname{grad}\delta\mathbf{v}\right)\right]\,dv\,,
\tag{3.1.5}
$$

where $\boldsymbol{\mathcal{C}}$ is the spatial elasticity tensor of the mixture,

$$
\boldsymbol{\mathcal{C}} = J^{-1}\left[\mathbf{F} \oslash \mathbf{F}\right] : \mathbb{C} : \left[\mathbf{F}^T \oslash \mathbf{F}^T\right]\,,
\tag{3.1.6}
$$

where $\mathbb{C}$ is the material elasticity tensor of the mixture arises from $\mathbb{C}^e$ due to elastic deformation and $\mathbb{C}^g$ due to growth:

$$
\mathbb{C} = 2\frac{d\mathbf{S}(\mathbf{F}, \mathbf{F}^g)}{d\mathbf{C}} = \mathbb{C}^e + \mathbb{C}^g\,.
$$

The elastic contribution is given by

$$
\mathbb{C}^e = 2\left.\frac{\partial\mathbf{S}(\mathbf{F}, \mathbf{F}^g)}{\partial\mathbf{C}}\right|_{\mathbf{F}^g} = J^g\left[\mathbf{F}^{g-1} \oslash \mathbf{F}^{g-1}\right] : \mathbb{L}^e : \left[\mathbf{F}^{g-T} \oslash \mathbf{F}^{g-T}\right] = J^g \mathbb{L}_{ABCD}^e F_{iA}^{g-1} F_{jB}^{g-1} F_{kC}^{g-1} F_{lD}^{g-1}
$$

where $\mathbb{L}^e$ is the elasticity tensor that arises due to elastic deformation when observed from the intermediate configuration:

$$\mathbb{L}^e = 2\frac{\partial \mathbf{S}^e}{\partial \mathbf{C}^e}\bigg|_{\vartheta}.$$

The growth contribution is given by [**?**]:

$$\mathbb{C}^g = 2\left[\frac{\partial \mathbf{S}(\mathbf{C}, \vartheta)}{\partial \mathbf{F}^g}\bigg|_{\mathbf{C}} : \frac{\partial \mathbf{F}^g}{\partial \vartheta}\right] \otimes \frac{\partial \vartheta}{\partial \mathbf{C}}.$$

Currently, stress- and strain-dependent growth are not implemented in FEBio, so the first partial derivative above evaluates to the 4th order 0 tensor. Consequently there is no contribution of the growth tensor to the elasticity tensor. The spatial elasticity tensor is thus simplified as

$$\mathcal{C} = \mathcal{C}^e = J^{-1}\left(\mathbf{F} \oslash \mathbf{F}\right) : 2\frac{\partial \mathbf{S}}{\partial \mathbf{C}} : \left(\mathbf{F}^T \oslash \mathbf{F}^T\right). \tag{3.1.7}$$

The second term is given by

$$D\left(\mathbf{J}^\alpha \cdot \operatorname{Grad} \delta c^\alpha\right)[\Delta \mathbf{u}] \, dV = 0, \tag{3.1.8}$$

Since it is assumed that concentration is unaffected by deformation and molar flux is unaffected by rotation.

The last term is given by

$$D\left(\delta c^\alpha \frac{\partial c^\alpha}{\partial t}\right)[\Delta \mathbf{u}] \, dV = 0. \tag{3.1.9}$$

for cases where growth is not formulated with a dependence on stress or strain.

3.1.2 Linearization along Δc^γ

The linearization of the first term in δW_{int} along Δc^γ yields

$$D\left(\mathbf{S} : \delta \dot{\mathbf{E}}\right)[\Delta c^\gamma] \, dV = \Delta c^\gamma \left(\boldsymbol{\sigma}'_\gamma : \delta \mathbf{d}\right) \, dv, \tag{3.1.10}$$

where $\boldsymbol{\sigma}'_\gamma$ is generally zero except for cases where chemical kinetics are mechanosensitive (dependent on the stress or strain). In this case,

$$\boldsymbol{\sigma}'_\gamma = J^{-1}\mathbf{F} \cdot \frac{\partial \mathbf{S}}{\partial c^\gamma} \cdot \mathbf{F}^T. \tag{3.1.11}$$

where symmetric growth tensors yield the expression

$$\frac{\partial \mathbf{S}}{\partial c^\gamma} = \frac{\partial \mathbf{S}}{\mathbf{F}^g} : \frac{\partial \mathbf{F}^g}{\partial \vartheta}\frac{\partial \vartheta}{\partial \dot{\vartheta}}\frac{\partial \dot{\vartheta}}{\partial \dot{c}^\gamma}\frac{\partial \dot{c}^\gamma}{\partial c^\gamma}, \tag{3.1.12}$$

where

$$\frac{\partial \mathbf{S}}{\partial \mathbf{F}^g} = \mathbf{S} \otimes \mathbf{F}^{g-T} - \left[\mathbf{F}^{g-1} \odot \mathbf{S} + \mathbf{S} \odot \mathbf{F}^{g-1}\right] - J^g\left[\mathbf{F}^{g-1} \oslash \mathbf{F}^{g-1}\right] : \mathbb{L}^e : \left[\mathbf{C}^e \oslash \mathbf{F}^{g-1} + \mathbf{F}^{g-1} \oslash \mathbf{C}^e\right], \tag{3.1.13}$$

$$\frac{\partial \mathbf{F}^g}{\partial \vartheta} = \sum_{i=1}^{N} \mathbf{n}_i \otimes \mathbf{n}_i \,,$$

$$\frac{\partial \vartheta}{\partial \dot{\vartheta}} = \Delta t \,,$$

$$\frac{\partial \dot{\vartheta}}{\partial \dot{c}^\gamma} = k(\vartheta) \frac{\partial \phi(\dot{c}^\alpha)}{\partial c^\gamma} \,,$$

$$\frac{\partial \dot{c}^\gamma}{\partial c^\gamma} = \sum \frac{\partial \hat{c}_i^\alpha}{\partial c^\gamma} \,.$$

The second term is

$$D \left(\mathbf{J}^\alpha \cdot \operatorname{Grad} \delta c^\alpha \right) [\Delta c^\gamma] \, dV = \delta_{\alpha\gamma} \operatorname{grad} \delta c^\alpha \cdot \mathbf{d}^\alpha \cdot \operatorname{grad} \Delta c^\gamma \, dv \,, \tag{3.1.14}$$

The last term is

$$D \left(\frac{\partial c^\alpha}{\partial t} \delta c^\alpha \right) [\Delta c^\gamma] \, dV = \delta c^\alpha \frac{1}{\Delta t} \frac{\partial c^\alpha}{\partial c^\gamma} \Delta c^\gamma \, dv \,, \tag{3.1.15}$$

where we similarly used a backward difference scheme to discretize the time derivative.

3.1.3 Linearization of External Virtual Work

The linearization of δW_{ext} depends on whether natural boundary conditions are prescribed as area densities or total net values over an area. Thus, in the case when $\mathbf{t} \, da$ (net force) or $j_n^\alpha da$ (net molar flow rate) are prescribed over the elemental area da, there is no variation in δW_{ext} and it follows that $D\delta W_{\text{ext}} = 0$. Alternatively, in the case when $\mathbf{t}$ or j_n^α are prescribed, the linearization may be performed by evaluating the integral in the parametric space of the boundary surface ∂b, with parametric coordinates $\left(\eta^1, \eta^2 \right)$. Accordingly, for a point $\mathbf{x} \left(\eta^1, \eta^2 \right)$ on ∂b, surface tangents (covariant basis vectors) are given by

$$\mathbf{g}_\alpha = \frac{\partial \mathbf{x}}{\partial \eta^\alpha}, \quad (\alpha = 1, 2) \tag{3.1.16}$$

and the outward unit normal is

$$\mathbf{n} = \frac{\mathbf{g}_1 \times \mathbf{g}_2}{|\mathbf{g}_1 \times \mathbf{g}_2|} \,. \tag{3.1.17}$$

The elemental area on ∂b is $da = |\mathbf{g}_1 \times \mathbf{g}_2| \, d\eta^1 d\eta^2$. Consequently, the external virtual work integral may be rewritten as

$$\delta W_{\text{ext}} = \int_{\partial b} \left(\delta \mathbf{v} \cdot \mathbf{t} + \sum_{\alpha \neq s,w}^{\alpha_s} \delta c^\alpha j_n^\alpha \right) |\mathbf{g}_1 \times \mathbf{g}_2| \, d\eta^1 d\eta^2 \,, \tag{3.1.18}$$

The directional derivative of δW_{ext} may then be applied directly to its integrand, since the parametric space is invariant [1].

If we restrict traction boundary conditions to the special case of normal tractions, then $\mathbf{t} = t_n \mathbf{n}$ where t_n is the prescribed normal traction component. Then it can be shown that the linearization of δW_{ext} along $\Delta \mathbf{u}$ produces

$$D \left(\delta W_{\text{ext}} \right) [\Delta \mathbf{u}] = \int_{\partial b} \left(t_n \delta \mathbf{v} + \sum_{\alpha \neq s,w}^{\alpha_s} \delta c^\alpha j_n^\alpha \mathbf{n} \right) \cdot \left(\frac{\partial \Delta \mathbf{u}}{\partial \eta^1} \times \mathbf{g}_2 + \mathbf{g}_1 \times \frac{\partial \Delta \mathbf{u}}{\partial \eta^2} \right) d\eta^1 d\eta^2 \,. \tag{3.1.19}$$

The linearizations along Δc^γ reduces to zero, $D\left(\delta W_{\text{ext}}\right)\left[\Delta c^\gamma\right] = 0$.

3.1.4 Discretization

To discretize the virtual work relations, let

$$
\delta \mathbf{v} = \sum_{a=1}^{m} N_a \delta \mathbf{v}_a \,, \quad \Delta \mathbf{u} = \sum_{b=1}^{m} N_b \Delta \mathbf{u}_b \,,
$$
$$
\delta c^\alpha = \sum_{a=1}^{m} N_a \delta c_a^\alpha \,, \quad \Delta c^\gamma = \sum_{b=1}^{m} N_b \Delta c_b^\gamma \,,
$$

(3.1.20)

where N_a represents the interpolation functions over an element, $\delta \mathbf{v}_a$, δc_a^α, $\Delta \mathbf{u}_a$, and Δc_a^γ respectively represent the nodal values of $\delta \mathbf{v}$, δc^α, $\Delta \mathbf{u}$, and Δc^γ; m is the number of nodes in an element.

The discretized form of δW_{int} may be written as

$$
\delta W_{\text{int}} = \sum_{e=1}^{n_e} \sum_{k=1}^{n_{\text{int}}^{(e)}} W_k J_\eta \sum_{a=1}^{m} \begin{bmatrix} \delta \mathbf{v}_a & \delta c_a^\alpha & \cdots & \delta c_a^\gamma \end{bmatrix} \cdot \begin{bmatrix} \mathbf{r}_a^u \\ r_a^\alpha \\ \vdots \\ r_a^\gamma \end{bmatrix} \,,
$$

(3.1.21)

where n_e is the number of elements in b, $n_{\text{int}}^{(e)}$ is the number of integration points in the $e-$th element, W_k is the quadrature weight associated with the $k-$th integration point, and J_η is the Jacobian of the transformation from the current spatial configuration to the parametric space of the element. In the above expression,

$$
\mathbf{r}_a^u = \boldsymbol{\sigma} \cdot \text{grad}\, N_a \,,
$$
$$
r_a^\alpha = \mathbf{j}^\alpha \cdot \text{grad}\, N_a - N_a \frac{\partial c^\alpha}{\partial t} + N_a \sum_i \hat{c}_i^\alpha \,,
$$

(3.1.22)

and it is understood that J_η, $\mathbf{r}_a^u$, and $r_a^\alpha \cdots r_a^\omega$ are evaluated at the parametric coordinates of the $k-$th integration point. Since the parametric space is invariant, time derivatives are evaluated in a material frame. For example, the time derivative $DJ\left(\mathbf{x}, t\right)/Dt$ becomes $\partial J\left(\eta_k, t\right)/\partial t$ when evaluated at the parametric coordinates $\eta_k = \left(\eta_k^1, \eta_k^2, \eta_k^3\right)$ of the $k-$th integration point. All time derivatives are discretized using a backward difference scheme.

Similarly, the discretized form of $D\delta W_{\text{int}} = D\delta W_{\text{int}}\left[\Delta \mathbf{u}\right] + \sum_\gamma D\delta W_{\text{int}}\left[\Delta c^\gamma\right]$ may be written as

$$
D\delta W_{\text{int}} = \sum_{e=1}^{n_e} \sum_{k=1}^{n_{\text{int}}^{(e)}} W_k J_\eta \sum_{a=1}^{m} \sum_{b=1}^{m} \begin{bmatrix} \delta \mathbf{v}_a & \delta c_a^\alpha & \cdots & \delta c_a^\omega \end{bmatrix} \cdot \begin{bmatrix} \mathbf{K}_{ab}^{uu} & \mathbf{k}_{ab}^{u\alpha} & \cdots & \mathbf{k}_{ab}^{u\omega} \\ \mathbf{k}_{ab}^{\alpha u} & k_{ab}^{\alpha\alpha} & \cdots & k_{ab}^{\alpha\omega} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{k}_{ab}^{\omega u} & k_{ab}^{\omega\alpha} & \cdots & k_{ab}^{\omega\omega} \end{bmatrix} \cdot \begin{bmatrix} \Delta \mathbf{u}_b \\ \Delta c_b^\alpha \\ \vdots \\ \Delta c_b^\omega \end{bmatrix} \,,
$$

where the terms in the first column are the discretized form of the linearization along $\Delta \mathbf{u}$:

$$
\mathbf{K}_{ab}^{uu} = \text{grad}\, N_a \cdot \boldsymbol{\mathcal{C}} \cdot \text{grad}\, N_b + \left(\text{grad}\, N_a \cdot \boldsymbol{\sigma} \cdot \text{grad}\, N_b\right) \mathbf{I} \,,
$$

(3.1.23)

$$
\mathbf{k}_{ab}^{\alpha u} \approx 0 \,,
$$

(3.1.24)

The terms in the remaining columns of the stiffness matrix are the discretized form of the linearization along Δc^γ:

$$\mathbf{k}_{ab}^{u\alpha} = N_b \boldsymbol{\sigma}_\alpha' \cdot \operatorname{grad} N_a \,, \tag{3.1.25}$$

$$k_{ab}^{\alpha\gamma} = -\delta_{\alpha\gamma} \operatorname{grad} N_a \cdot \mathbf{d}^\alpha \cdot \operatorname{grad} N_b - N_a N_b \frac{1}{\Delta t} + N_a N_b \sum_\alpha \sum_i \frac{\partial \hat{c}_i^\alpha}{\partial c^\gamma} \,, \tag{3.1.26}$$

The discretization of δW_{ext} has the form

$$\delta W_{\text{ext}} = \sum_{e=1}^{n_e} \sum_{k=1}^{n_{\text{int}}^{(e)}} W_k J_\eta \sum_{a=1}^{m} \left[\begin{array}{cccc} \delta\mathbf{v}_a & \delta c_a^\alpha & \cdots & \delta c_a^\gamma \end{array} \right] \cdot \left[\begin{array}{c} N_a t_n \mathbf{n} \\ N_a j_n^\alpha \\ \vdots \\ N_a j_n^\gamma \end{array} \right] , \tag{3.1.27}$$

where $J_\eta = |\mathbf{g}_1 \times \mathbf{g}_2|$. The summation is performed over all surface elements on which these boundary conditions are prescribed. The discretization of $-D\delta W_{\text{ext}}$ has the form

$$-D\delta W_{\text{ext}} = \sum_{e=1}^{n_e} \sum_{k=1}^{n_{\text{int}}^{(e)}} W_k J_\eta \sum_{a=1}^{m} \sum_{b=1}^{m} \left[\begin{array}{cccc} \delta\mathbf{v}_a & \delta c_a^\alpha & \cdots & \delta c_a^\gamma \end{array} \right] \cdot \left[\begin{array}{cccc} \mathbf{K}_{ab}^{uu} & \mathbf{k}_{ab}^{u\alpha} & \cdots & \mathbf{k}_{ab}^{u\gamma} \\ \mathbf{k}_{ab}^{\alpha u} & k_{ab}^{\alpha\alpha} & \cdots & k_{ab}^{\alpha\gamma} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{k}_{ab}^{\gamma u} & k_{ab}^{\gamma\alpha} & \cdots & k_{ab}^{\gamma\gamma} \end{array} \right] \cdot \left[\begin{array}{c} \Delta\mathbf{u}_b \\ \Delta c_b^\alpha \\ \vdots \\ \Delta c_b^\gamma \end{array} \right] , \tag{3.1.28}$$

where

$$\mathbf{K}_{ab}^{uu} = t_n N_a \boldsymbol{\mathcal{A}} \left\{ \frac{\partial N_b}{\partial \eta^1} \mathbf{g}_2 - \frac{\partial N_b}{\partial \eta^2} \mathbf{g}_1 \right\} \,, \tag{3.1.29}$$

$$\mathbf{k}_{ab}^{\alpha u} = \mathbf{0}.$$

In this expression, $\boldsymbol{\mathcal{A}}\{\mathbf{v}\}$ is the antisymmetric tensor whose dual vector is $\mathbf{v}$ (such that $\boldsymbol{\mathcal{A}}\{\mathbf{v}\} \cdot \mathbf{q} = \mathbf{v} \times \mathbf{q}$ for any vector $\mathbf{q}$).

3.1.5   Chemical Reactions

3.1.5.1   Virtual Work and Linearization

Due to the simplifications of the elastic-solute analysis, the following reaction terms are considered negligible: $k_f, k_r, \hat{\zeta}, \hat{\zeta}_\varepsilon, \bar{\mathcal{V}}, \hat{\varphi}^w, \hat{\boldsymbol{\varphi}}_\varepsilon^w, \frac{\partial \hat{\varphi}^w}{\partial \tilde{p}}, \frac{\partial \hat{\varphi}^w}{\partial \tilde{c}^\iota}, \frac{\partial \varphi_r^s}{\partial J}, \frac{\partial \varphi_r^s}{\partial \tilde{c}^\iota}$.

The contribution to δW due to chemical reactions is given by δG (with summation over each species ι and each reaction r

$$\delta G = \sum_\alpha \sum_i \int_b \delta c^\alpha \hat{c}_i \, dv \,. \tag{3.1.30}$$

The linearization of δG along a solid displacement increment $\Delta\mathbf{u}$ is zero unless there is either a stress- or strain- dependent relationship (as may be the case for kinematic growth models):

$$D\delta G \left[\Delta\mathbf{u} \right] = 0 \quad . \tag{3.1.31}$$

For the case of stress-dependent concentration kinetics we have

$$D\delta G \left[\Delta\mathbf{u} \right] = \sum_r \sum_\iota \nu_r^\iota \int_b \delta c^\alpha \left[\hat{c}_i^\alpha \operatorname{div} \Delta\mathbf{u} + \hat{\boldsymbol{\zeta}}_{\varepsilon,i} : \Delta\boldsymbol{\varepsilon} \right] dv \quad ,$$

where

$$\hat{\boldsymbol{\zeta}}_{\varepsilon,r} = J^{-1}\mathbf{F} \cdot \frac{\partial \hat{\zeta}_r}{\partial \mathbf{E}} \cdot \mathbf{F}^T = \frac{\partial \hat{\zeta}_r}{\partial \mathbf{e}},$$

is the tangent of the reaction rate to the strain which is dependent on the specific reaction. This tangent is zero unless there is a stress- or strain-dependent relationship. For stress-dependent kinetics the tangent becomes

$$\hat{\boldsymbol{\zeta}}_{\varepsilon,r} = \frac{\partial \hat{\zeta}_r}{\partial \boldsymbol{\sigma}} : \boldsymbol{\mathcal{C}},$$

where the specific reaction kinetics dictate $\partial \hat{\zeta}_r / \partial \boldsymbol{\sigma}$. For mass action forward reactions where the reaction rate is proportional to the trace of stress as bounded by a sigmoidal function, i.e.,

$$\hat{\zeta}_r(\boldsymbol{\sigma}) = k_F(1 + \frac{a}{1 + \exp\left(-\frac{\mathrm{tr}(\boldsymbol{\sigma})-s_0}{b}\right)},$$

the tangent is

$$\frac{\partial \hat{\zeta}_r}{\partial \boldsymbol{\sigma}} = \frac{\partial \hat{\zeta}_r}{\partial \mathrm{tr}\left(\boldsymbol{\sigma}\right)} \cdot \frac{\partial \mathrm{tr}\left(\boldsymbol{\sigma}\right)}{\partial \boldsymbol{\sigma}},$$

$$\frac{\partial \hat{\zeta}_r}{\partial \mathrm{tr}\left(\boldsymbol{\sigma}\right)} = \frac{a \exp\left(-\frac{\mathrm{tr}(\boldsymbol{\sigma})-s_0}{b}\right)}{b\left(1 + \exp\left(-\frac{\mathrm{tr}(\boldsymbol{\sigma})-s_0}{b}\right)\right)^2},$$

$$\frac{\partial \mathrm{tr}\left(\boldsymbol{\sigma}\right)}{\partial \boldsymbol{\sigma}} = \mathbf{I}.$$

The linearization along a concentration increment Δc^ι is summed over each reaction r and chemical species ι.

$$D\delta G\left[\Delta c^\iota\right] = \sum_r \sum_\gamma \nu_r^\gamma \int_b \delta c^\gamma \frac{\partial \hat{\zeta}_r}{\partial c^\iota} \Delta c^\iota \, dv \quad . \tag{3.1.32}$$

The discretized form of these expressions is given by

$$\delta G = \sum_\gamma \sum_a \delta c_a^\gamma r_a^\gamma, \tag{3.1.33}$$

where

$$r_a^\gamma = \sum_r \nu_r^\gamma \int_b N_a \hat{\zeta}_r \, dv \quad . \tag{3.1.34}$$

Similarly,

$$D\delta G\left[\Delta \mathbf{u}\right] = \sum_\gamma \sum_a \delta c_a^\gamma \sum_b \mathbf{k}_{ab}^{\gamma u} \cdot \Delta \mathbf{u}_b \quad , \tag{3.1.35}$$

where

$$\mathbf{k}_{ab}^{\gamma u} = \sum_r \nu_r^\gamma \int_a N_a \left[\hat{\zeta}_r \mathbf{I} + \hat{\boldsymbol{\zeta}}_{\varepsilon,r}\right] \cdot \mathrm{grad}\, N_b \, dv.$$

Finally,

$$D\delta G\left[\Delta \tilde{c}^{\iota}\right] = \sum_{\gamma} \sum_{a} \delta c_a^{\gamma} \sum_{b} k_{ab}^{\gamma\iota} \Delta c_b^{\iota} \quad , \tag{3.1.36}$$

where

$$k_{ab}^{\gamma\iota} = \sum_{r} \nu^{\gamma} \int_{b} N_a N_b \frac{\partial \hat{\zeta}_r}{\partial c^{\iota}} \, dv \quad . \tag{3.1.37}$$

Chapter 4

Constitutive Models

This chapter describes the theoretical background behind the constitutive models that are available in FEBio. Most materials are derived from a hyperelastic strain-energy function. Please consult Section **??** for more background information on this class of materials.

4.1 Chemical Reaction Production Rate

Production rate constitutive equations provide a relation for $\hat{\zeta}$ as a function of solid matrix strain, solute concentrations, and the concentrations of solid-bound molecular species.

4.1.1 Mass Action Forward

According to the law of mass action for forward reactions,

$$\hat{\zeta} = k\left(\theta, \mathbf{F}, \rho_r^\sigma\right) \prod_\alpha \left(c^\alpha\right)^{\nu_R^\alpha} . \tag{4.1.1}$$

A constitutive relation for the specific reaction rate $k\left(\theta, \mathbf{F}, \rho_r^\sigma\right)$ must also be provided.

4.1.2 Mass Action Reversible

According to the law of mass action for reversible reactions,

$$\hat{\zeta}_F = k_F\left(\theta, \mathbf{F}, \rho_r^\sigma\right) \prod_\alpha \left(c^\alpha\right)^{\nu_R^\alpha}$$

$$\hat{\zeta}_R = k_R\left(\theta, \mathbf{F}, \rho_r^\sigma\right) \prod_\alpha \left(c^\alpha\right)^{\nu_P^\alpha} \tag{4.1.2}$$

$$\hat{\zeta} = \hat{\zeta}_F - \hat{\zeta}_R = \hat{\zeta}_F \left[1 - K_c\left(\theta, \mathbf{F}, \rho_r^\sigma\right) \prod_\alpha \left(c^\alpha\right)^{\nu^\alpha}\right] ,$$

where $K_c = k_R/k_F$ is a function that reduces to the equilibrium constant of the reversible reaction at chemical equilibrium (when $\hat{\zeta} = 0$). Constitutive relations for the specific forward and reverse reaction rates, $k_F\left(\theta, \mathbf{F}, \rho_r^\sigma\right)$ and $k_R\left(\theta, \mathbf{F}, \rho_r^\sigma\right)$ respectively, must also be provided.

4.1.3 Michaelis-Menten

Michaelis-Menten is a model for enzyme kinetics as represented by the reactions

$$\mathcal{E}^e + \mathcal{E}^s \rightleftharpoons \mathcal{E}^{es} \to \mathcal{E}^e + \mathcal{E}^p , \tag{4.1.3}$$

where $\mathcal{E}^e$ is the enzyme, $\mathcal{E}^s$ is the substrate, $\mathcal{E}^{es}$ is the enzyme-substrate complex, and $\mathcal{E}^p$ is the product. The molar mass supply $\hat{c}^p$ producing $\mathcal{E}^p$ is related to the concentration of the substrate $\mathcal{E}^s$ via

$$\hat{c}^p = \frac{V_{max} c^s}{K_m + c^s} , \tag{4.1.4}$$

where V_{max} is the maximum rate achieved by the system, at maximum (saturating) substrate concentrations. K_m is the substrate concentration at which the reaction rate is half of V_{max}.

This relation may be derived by applying the law of mass action to the two reactions in (4.1.3). under the simplifying assumption that the reversible reaction between the enzyme and substrate reaches steady state much faster than the subsequent forward reaction forming the product. If the first and second reactions are denoted by subscripts 1 and 2, respectively, the law of mass action for the first (reversible) and second (forwar) reaction produces

$$\hat{\zeta}_1 = k_{F1} c^e c^s - k_{R1} c^{es}, \quad \hat{\zeta}_2 = k_{F2} c^{es} ,$$

$$\hat{c}^s = -\hat{\zeta}_1, \quad \hat{c}^p = \hat{\zeta}_2, \quad \hat{c}^{es} = \hat{\zeta}_1 - \hat{\zeta}_2 . \tag{4.1.5}$$

The total enzyme concentration remains constant at $c_0^e = c^e + c^{es}$, so that $\hat{\zeta}_1 = k_{F1} c_0^e c^s - (k_{F1} c^s + k_{R1}) c^{es}$. Assuming that the first reaction equilibrates much faster than the second is equivalent to letting $\hat{\zeta}_1 \approx 0$, in which case

$$c^{es} \approx \frac{c_0^e c^s}{c^s + K_m} \,, \tag{4.1.6}$$

where $K_m = k_{R1}/k_{F1}$. Then,

$$\hat{\zeta}_2 = \frac{V_{\max} c^s}{c^s + K_m} \,,$$

where $V_{\max} = k_{F2} c_0^e$ represents the maximum value of $\hat{\zeta}_2$, when $K_m \ll c^s$. In practice, choosing $k_{F1} \gg k_{F2}$ can produce the desired effect.

4.2 Specific Reaction Rate

Specific reaction rate constitutive equations provide a relation for k as a function of solid matrix strain and the concentrations of solid-bound molecular species.

4.2.1 Constant Specific Reaction Rate

For this material model, k is constant.

Appendix A

Tensor Calculus

A.1 Second-Order Tensors

A.1.1 Definition

Let $\mathbf{T}$ be a transformation, which transforms any vector into another vector, e.g.,

$$\mathbf{T} \cdot \mathbf{a} = \mathbf{b} \quad \mathbf{T} \cdot \mathbf{c} = \mathbf{d}$$

If $\mathbf{T}$ has the following properties,

$$\mathbf{T} \cdot (\mathbf{a} + \mathbf{c}) = \mathbf{T} \cdot \mathbf{a} + \mathbf{T} \cdot \mathbf{c} \tag{A.1.1}$$

$$\mathbf{T} \cdot (\alpha \mathbf{a}) = \alpha \mathbf{T} \cdot \mathbf{a} \tag{A.1.2}$$

where $\mathbf{a}$ and $\mathbf{c}$ are arbitrary vectors, and α is an arbitrary scalar, then $\mathbf{T}$ is called a *linear transformation*, a *second-order tensor*, or simply a *tensor*. Vectors are first-order tensors and scalars are zeroth-order tensors.

A.1.2 Cartesian Components of a Tensor

Let $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ form an orthonormal basis in a Cartesian coordinate system x_1, x_2, x_3. Then the Cartesian components of $\mathbf{a}$ are

$$a_1 = \mathbf{e}_1 \cdot \mathbf{a}, \quad a_2 = \mathbf{e}_2 \cdot \mathbf{a}, \quad a_3 = \mathbf{e}_3 \cdot \mathbf{a}$$

or equivalently,

$$\boxed{a_j = \mathbf{e}_j \cdot \mathbf{a}} \tag{A.1.3}$$

(Recall that $\mathbf{a} = a_i \mathbf{e}_i$, thus $\mathbf{a} \cdot \mathbf{e}_j = a_i \mathbf{e}_i \cdot \mathbf{e}_j = a_i \delta_{ij} = a_j$.)

The Cartesian components of a tensor $\mathbf{T}$ are obtained as follows. Let $\mathbf{T} \cdot \mathbf{a} = \mathbf{b}$. The components of $\mathbf{b}$ are given by $b_i = \mathbf{e}_i \cdot \mathbf{b} = \mathbf{e}_i \cdot \mathbf{T} \cdot \mathbf{a}$. But $\mathbf{a} = a_j \mathbf{e}_j$, so $b_i = a_j \mathbf{e}_i \cdot \mathbf{T} \cdot \mathbf{e}_j$. Note that $\mathbf{e}_i \cdot \mathbf{T} \cdot \mathbf{e}_j$ is the component along $\mathbf{e}_i$ of the vector $\mathbf{T} \cdot \mathbf{e}_j$. By convention, we denote this component as

$$\boxed{T_{ij} = \mathbf{e}_i \cdot \mathbf{T} \cdot \mathbf{e}_j} \quad \text{components of tensor } \mathbf{T} \tag{A.1.4}$$

components of tensor $\mathbf{T}$.

Thus, $\mathbf{b} = \mathbf{T} \cdot \mathbf{a} = a_j \mathbf{T} \cdot \mathbf{e}_j = b_k \mathbf{e}_k$. Taking the dot product on both sides with $\mathbf{e}_i$ yields $a_j \mathbf{e}_i \cdot \mathbf{T} \cdot \mathbf{e}_j = a_j T_{ij} = b_k \mathbf{e}_i \cdot \mathbf{e}_k = b_k \delta_{ik} = b_i$, or

$$\boxed{b_i = T_{ij} a_j}$$

in indicial form. In matrix form,

$$\begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} = \begin{bmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix}$$

The matrix of tensor $\mathbf{T}$ with respect to $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ can also be denoted by $[\mathbf{T}]$ or $[T_{ij}]$. The columns of $[\mathbf{T}]$ are given by $\mathbf{T} \cdot \mathbf{e}_i$, e.g.,

$$[\mathbf{T} \cdot \mathbf{e}_2] = [T_{j2}\mathbf{e}_2] = \begin{bmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} T_{12} \\ T_{22} \\ T_{32} \end{bmatrix}$$

This result, when generalized, leads to the useful identity

$$\boxed{\mathbf{T} \cdot \mathbf{e}_i = T_{ji}\mathbf{e}_j} = T_{1i}\mathbf{e}_1 + T_{2i}\mathbf{e}_2 + T_{3i}\mathbf{e}_3 \qquad (A.1.5)$$

Example 1. Scaling transformation

A scaling transformation $\mathbf{T}$ with different scale factors along x_1, x_2, x_3 should satisfy the following relations by definition:

$$\mathbf{T} \cdot \mathbf{a} = s_1 (\mathbf{a} \cdot \mathbf{e}_1) \mathbf{e}_1 + s_2 (\mathbf{a} \cdot \mathbf{e}_2) \mathbf{e}_2 + s_3 (\mathbf{a} \cdot \mathbf{e}_3) \mathbf{e}_3$$

Verify that $\mathbf{T}$ is a tensor. Also find the matrix of $\mathbf{T}$ in $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$.

Solution. Is $\mathbf{T}$ a tensor? Let any $\mathbf{a} = a_i \mathbf{e}_i$ and $\mathbf{b} = b_i \mathbf{e}_i$, then

$$\begin{aligned} \mathbf{T} \cdot (\alpha \mathbf{a}) &= s_1 (\alpha \mathbf{a} \cdot \mathbf{e}_1) \mathbf{e}_1 + s_2 (\alpha \mathbf{a} \cdot \mathbf{e}_2) \mathbf{e}_2 + s_3 (\alpha \mathbf{a} \cdot \mathbf{e}_3) \mathbf{e}_3 \\ &= \alpha (s_1 (\mathbf{a} \cdot \mathbf{e}_1) \mathbf{e}_1 + s_2 (\mathbf{a} \cdot \mathbf{e}_2) \mathbf{e}_2 + s_3 (\mathbf{a} \cdot \mathbf{e}_3) \mathbf{e}_3) \\ &= \alpha \mathbf{T} \cdot \mathbf{a} \end{aligned}$$

and

$$\begin{aligned} \mathbf{T} \cdot (\mathbf{a} + \mathbf{b}) &= s_1 ((\mathbf{a} + \mathbf{b}) \cdot \mathbf{e}_1) \mathbf{e}_1 + s_2 ((\mathbf{a} + \mathbf{b}) \cdot \mathbf{e}_2) \mathbf{e}_2 + s_3 ((\mathbf{a} + \mathbf{b}) \cdot \mathbf{e}_3) \mathbf{e}_3 \\ &= s_1 (\mathbf{a} \cdot \mathbf{e}_1) \mathbf{e}_1 + s_2 (\mathbf{a} \cdot \mathbf{e}_2) \mathbf{e}_2 + s_3 (\mathbf{a} \cdot \mathbf{e}_3) \mathbf{e}_3 \\ &\quad + s_1 (\mathbf{b} \cdot \mathbf{e}_1) \mathbf{e}_1 + s_2 (\mathbf{b} \cdot \mathbf{e}_2) \mathbf{e}_2 + s_3 (\mathbf{b} \cdot \mathbf{e}_3) \mathbf{e}_3 \\ &= \mathbf{T} \cdot \mathbf{a} + \mathbf{T} \cdot \mathbf{b} \end{aligned}$$

Now that we have demonstrated that $\mathbf{T}$ is a tensor, its components are given by $T_{ij} = \mathbf{e}_i \cdot \mathbf{T} \cdot \mathbf{e}_j$, thus

$$[T_{i1}] = [\mathbf{e}_i \cdot \mathbf{T} \cdot \mathbf{e}_1] = [\mathbf{e}_i \cdot s_1 \mathbf{e}_1] = [s_1 \delta_{i1}] = \begin{bmatrix} s_1 \\ 0 \\ 0 \end{bmatrix}$$

$$[T_{i2}] = [\mathbf{e}_i \cdot \mathbf{T} \cdot \mathbf{e}_2] = [\mathbf{e}_i \cdot s_2 \mathbf{e}_2] = [s_2 \delta_{i2}] = \begin{bmatrix} 0 \\ s_2 \\ 0 \end{bmatrix}$$

$$[T_{i3}] = [\mathbf{e}_i \cdot \mathbf{T} \cdot \mathbf{e}_3] = [\mathbf{e}_i \cdot s_3 \mathbf{e}_3] = [s_3 \delta_{i3}] = \begin{bmatrix} 0 \\ 0 \\ s_3 \end{bmatrix}$$

Then, the matrix of $\mathbf{T}$ is given by

$$[\mathbf{T}] = \begin{bmatrix} s_1 & 0 & 0 \\ 0 & s_2 & 0 \\ 0 & 0 & s_3 \end{bmatrix}$$

A.1.3 Sum of Tensors

The sum of two tensors $\mathbf{T}$ and $\mathbf{S}$ is denoted by $\mathbf{T} + \mathbf{S}$ and defined by

$$\boxed{(\mathbf{T} + \mathbf{S}) \cdot \mathbf{a} = \mathbf{T} \cdot \mathbf{a} + \mathbf{S} \cdot \mathbf{a}} \tag{A.1.6}$$

for any vector $\mathbf{a}$. Thus $\mathbf{T} + \mathbf{S}$ is also a tensor, whose components are

$$(\mathbf{T} + \mathbf{S})_{ij} = \mathbf{e}_i \cdot (\mathbf{T} + \mathbf{S}) \cdot \mathbf{e}_j = \mathbf{e}_i \cdot \mathbf{T} \cdot \mathbf{e}_j + \mathbf{e}_i \cdot \mathbf{S} \cdot \mathbf{e}_j = T_{ij} + S_{ij}$$

In matrix notation, $[\mathbf{T} + \mathbf{S}] = [\mathbf{T}] + [\mathbf{S}]$.

A.1.4 Dyadic Product of Vectors

The dyadic product of two vectors $\mathbf{a}$ and $\mathbf{b}$ is denoted by $\mathbf{a} \otimes \mathbf{b}$ (or $\mathbf{ab}$) and defined as the transformation which satisfies

$$\boxed{(\mathbf{a} \otimes \mathbf{b}) \cdot \mathbf{c} = (\mathbf{b} \cdot \mathbf{c}) \mathbf{a}} \tag{A.1.7}$$

For any $\mathbf{c}$, $\mathbf{d}$, α and β, we have

$$(\mathbf{a} \otimes \mathbf{b}) \cdot (\alpha \mathbf{c} + \beta \mathbf{d}) = (\mathbf{b} \cdot (\alpha \mathbf{c} + \beta \mathbf{d})) \mathbf{a} = (\mathbf{b} \cdot \alpha \mathbf{c}) \mathbf{a} + (\mathbf{b} \cdot \beta \mathbf{d}) \mathbf{a}$$
$$= \alpha (\mathbf{b} \cdot \mathbf{c}) \mathbf{a} + \beta (\mathbf{b} \cdot \mathbf{d}) \mathbf{a} = \alpha (\mathbf{a} \otimes \mathbf{b}) \cdot \mathbf{c} + \beta (\mathbf{a} \otimes \mathbf{b}) \cdot \mathbf{d}$$

thus $\mathbf{a} \otimes \mathbf{b}$ is a tensor. Its Cartesian components with respect to $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ are

$$(\mathbf{a} \otimes \mathbf{b})_{ij} = \mathbf{e}_i \cdot (\mathbf{a} \otimes \mathbf{b}) \cdot \mathbf{e}_j = \mathbf{e}_i \cdot (\mathbf{b} \cdot \mathbf{e}_j) \mathbf{a} = b_j \mathbf{e}_i \cdot \mathbf{a} = a_i b_j$$

In matrix form,

$$[\mathbf{a} \otimes \mathbf{b}] = \begin{bmatrix} a_1 b_1 & a_1 b_2 & a_1 b_3 \\ a_2 b_1 & a_2 b_2 & a_2 b_3 \\ a_3 b_1 & a_3 b_2 & a_3 b_3 \end{bmatrix} = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} \begin{bmatrix} b_1 & b_2 & b_3 \end{bmatrix} = [\mathbf{a}] [\mathbf{b}]^T$$

Note that in general, $\mathbf{a} \otimes \mathbf{b} \neq \mathbf{b} \otimes \mathbf{a}$, i.e., the dyadic product is *not commutative*. Also note that

$$[\mathbf{e}_1 \otimes \mathbf{e}_1] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad [\mathbf{e}_1 \otimes \mathbf{e}_2] = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad [\mathbf{e}_1 \otimes \mathbf{e}_3] = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad \text{etc.}$$

thus it is possible to represent a second-order tensor in terms of its Cartesian components in $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ as $\mathbf{T} = T_{11}\mathbf{e}_1 \otimes \mathbf{e}_1 + T_{12}\mathbf{e}_1 \otimes \mathbf{e}_2 + T_{13}\mathbf{e}_1 \otimes \mathbf{e}_3 + \ldots + T_{33}\mathbf{e}_3 \otimes \mathbf{e}_3$, or

$$\boxed{\mathbf{T} = T_{ij}\mathbf{e}_i \otimes \mathbf{e}_j} \tag{A.1.8}$$

This turns out to be an important result that can be generalized to higher order tensors, e.g., third-order tensors can be represented in terms of their Cartesian components as $\mathbb{T} = T_{ijk}\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k$, and similarly for higher orders.

Example 2. The scaling transformation derived in a previous example can be represented as

$$\mathbf{T} = s_1\mathbf{e}_1 \otimes \mathbf{e}_1 + s_2\mathbf{e}_2 \otimes \mathbf{e}_2 + s_3\mathbf{e}_3 \otimes \mathbf{e}_3$$

A.1.5   Trace of a Second-Order Tensor

The trace of any dyad $\mathbf{a} \otimes \mathbf{b}$ is defined by

$$\boxed{\operatorname{tr}(\mathbf{a} \otimes \mathbf{b}) = \mathbf{a} \cdot \mathbf{b}}$$

and

$$\boxed{\operatorname{tr}(\alpha\mathbf{a} \otimes \mathbf{b} + \beta\mathbf{c} \otimes \mathbf{d}) = \alpha\operatorname{tr}(\mathbf{a} \otimes \mathbf{b}) + \beta\operatorname{tr}(\mathbf{c} \otimes \mathbf{d})}$$

The trace operator yields a scalar function. In component form,

$$\operatorname{tr}(a_i b_j) = a_i b_i$$

For any tensor $\mathbf{T}$, we can write $\mathbf{T} = T_{ij}\mathbf{e}_i \otimes \mathbf{e}_j$, thus

$$\operatorname{tr}\mathbf{T} = T_{ij}\operatorname{tr}(\mathbf{e}_i \otimes \mathbf{e}_j) = T_{ij}\mathbf{e}_i \cdot \mathbf{e}_j = T_{ij}\delta_{ij} = T_{ii} = T_{11} + T_{22} + T_{33}$$

The trace of a tensor is the sum of its diagonal components.

A.1.6   Product of Two Tensors

The products of two tensors $\mathbf{T}$ and $\mathbf{S}$ are denoted by $\mathbf{T} \cdot \mathbf{S}$ and $\mathbf{S} \cdot \mathbf{T}$ and defined respectively by

$$\boxed{(\mathbf{T} \cdot \mathbf{S}) \cdot \mathbf{a} = \mathbf{T} \cdot (\mathbf{S} \cdot \mathbf{a})} \tag{A.1.9}$$

and

$$\boxed{(\mathbf{S} \cdot \mathbf{T}) \cdot \mathbf{a} = \mathbf{S} \cdot (\mathbf{T} \cdot \mathbf{a})} \tag{A.1.10}$$

Clearly, $\mathbf{T} \cdot \mathbf{S}$ and $\mathbf{S} \cdot \mathbf{T}$ are tensors as well. Their components in $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ are given by

$$(\mathbf{T} \cdot \mathbf{S})_{ij} = \mathbf{e}_i \cdot (\mathbf{T} \cdot \mathbf{S}) \cdot \mathbf{e}_j = \mathbf{e}_i \cdot \mathbf{T} \cdot (\mathbf{S} \cdot \mathbf{e}_j) = \mathbf{e}_i \cdot \mathbf{T} \cdot (S_{kj}\mathbf{e}_k) = S_{kj}\mathbf{e}_i \cdot \mathbf{T} \cdot \mathbf{e}_k = T_{ik}S_{kj}$$

In matrix form, $[\mathbf{T} \cdot \mathbf{S}] = [\mathbf{T}][\mathbf{S}]$. Similarly,

$$(\mathbf{S} \cdot \mathbf{T})_{ij} = S_{ik}T_{kj} \quad \text{and} \quad [\mathbf{S} \cdot \mathbf{T}] = [\mathbf{S}][\mathbf{T}]$$

In general, $\mathbf{T} \cdot \mathbf{S} \neq \mathbf{S} \cdot \mathbf{T}$, however $(\mathbf{T} \cdot \mathbf{S}) \cdot \mathbf{V} = \mathbf{T} \cdot (\mathbf{S} \cdot \mathbf{V})$, i.e., the tensor product is *associative* but *not commutative*.

A.1.7   Identity Tensor and Tensor Inverse

The identity tensor, denoted by $\mathbf{I}$, is defined by

$$\boxed{\mathbf{I} \cdot \mathbf{a} = \mathbf{a}} \tag{A.1.11}$$

for any vector $\mathbf{a}$. The Cartesian components o f $\mathbf{I}$ in $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ are given by

$$I_{ij} = \mathbf{e}_i \cdot \mathbf{I} \cdot \mathbf{e}_j = \mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij}$$

or

$$[\mathbf{I}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Given $\mathbf{T}$, if $\mathbf{S}$ exists such that $\mathbf{S} \cdot \mathbf{T} = \mathbf{I}$, we call $\mathbf{S}$ the *inverse* of $\mathbf{T}$, and $\mathbf{S} = \mathbf{T}^{-1}$. The inverse exists as long as $\det\mathbf{T} \neq 0$. Also note that $(\mathbf{T}^{-1})^{-1} = \mathbf{T}$ and $\mathbf{T}^{-1} \cdot \mathbf{T} = \mathbf{T} \cdot \mathbf{T}^{-1} = \mathbf{I}$. Also note that

$$\boxed{(\mathbf{U} \cdot \mathbf{V})^{-1} = \mathbf{V}^{-1} \cdot \mathbf{U}^{-1}}.$$

A.1.8   Transpose of a Tensor

Given a tensor $\mathbf{T}$, its transpose is denoted by $\mathbf{T}^T$ which is defined by

$$\boxed{\mathbf{a} \cdot (\mathbf{T} \cdot \mathbf{b}) = \mathbf{b} \cdot (\mathbf{T}^T \cdot \mathbf{a})} \tag{A.1.12}$$

In component form,

$$T_{ij}^T = \mathbf{e}_i \cdot \mathbf{T}^T \cdot \mathbf{e}_j = \mathbf{e}_j \cdot \mathbf{T} \cdot \mathbf{e}_i = T_{ji}$$

Also note that

$$\boxed{(\mathbf{S} \cdot \mathbf{T})^T = \mathbf{T}^T \cdot \mathbf{S}^T} \tag{A.1.13}$$

and $\left(\mathbf{S}^T\right)^T = \mathbf{S}$ and $(\mathbf{S} + \mathbf{T})^T = \mathbf{S}^T + \mathbf{T}^T$.

A.1.9   Double Product of Tensors

The double product of tensors is analogous to the dot product of vectors. Given two tensors $\mathbf{S}$ and $\mathbf{T}$, the double product (or *double contraction*) is defined as

$$\boxed{\mathbf{S} : \mathbf{T} = \operatorname{tr}\left(\mathbf{S}^T \cdot \mathbf{T}\right)} \tag{A.1.14}$$

Thus, for any tensor $\mathbf{T}$, $\operatorname{tr}\mathbf{T} = \mathbf{I} : \mathbf{T}$. In component form,

$$\mathbf{S} : \mathbf{T} = S_{ij}T_{ij}$$

The double product of second order tensors is commutative.

Example 3. Show that $\mathbf{a} \cdot \mathbf{T} \cdot \mathbf{b} = \mathbf{T} : (\mathbf{a} \otimes \mathbf{b})$ and $(\mathbf{a} \otimes \mathbf{b}) : (\mathbf{c} \otimes \mathbf{d}) = (\mathbf{a} \cdot \mathbf{c})(\mathbf{b} \cdot \mathbf{d})$.
  Using indicial notation,

$$\mathbf{a} \cdot \mathbf{T} \cdot \mathbf{b} = a_i T_{ij} b_j = T_{ij} a_i b_j = \mathbf{T} : (\mathbf{a} \otimes \mathbf{b}) \ ,$$

and

$$(\mathbf{a} \otimes \mathbf{b}) : (\mathbf{c} \otimes \mathbf{d}) = a_i b_j c_i d_j = (a_i c_i)(b_j d_j) = (\mathbf{a} \cdot \mathbf{c})(\mathbf{b} \cdot \mathbf{d}) \ .$$

A.1.10   Determinant of a Tensor

The determinant of a tensor is equal to the determinant of its components in $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$,

$$\det \mathbf{T} = \det [\mathbf{T}]_{\mathbf{e}_i} = \begin{vmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{vmatrix} = (\mathbf{T} \cdot \mathbf{e}_1 \times \mathbf{T} \cdot \mathbf{e}_2) \cdot \mathbf{T} \cdot \mathbf{e}_3 = \varepsilon_{ijk} T_{i1} T_{j2} T_{k3} \tag{A.1.15}$$

In particular, the determinant of a diagonal matrix is the product of the diagonal components,

$$\det [\mathbf{T}]_{\mathbf{e}_i} = \begin{vmatrix} T_{11} & 0 & 0 \\ 0 & T_{22} & 0 \\ 0 & 0 & T_{33} \end{vmatrix} = \varepsilon_{123} T_{11} T_{22} T_{33} = T_{11} T_{22} T_{33} \tag{A.1.16}$$

The determinant satisfies the following relations,

$$\det \mathbf{T}^{-1} = \frac{1}{\det \mathbf{T}} \tag{A.1.17}$$

$$\det (\mathbf{S} \cdot \mathbf{T}) = (\det \mathbf{S})(\det \mathbf{T}) \tag{A.1.18}$$

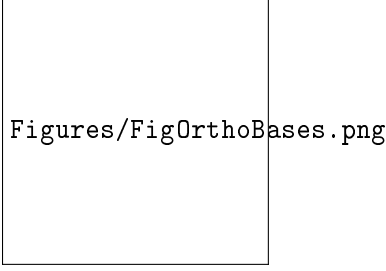Figure A.1.1: Orthonormal bases $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ and $\{\mathbf{e}'_1, \mathbf{e}'_2, \mathbf{e}'_3\}$.

A.1.11   Orthogonal Tensor

An orthogonal tensor $\mathbf{Q}$ is a linear transformation which preserves the length of a vector and the angle between vectors. Thus, by definition,

$$|\mathbf{Q} \cdot \mathbf{a}| = |\mathbf{a}| \quad \text{and} \quad \cos\left(\mathbf{Q} \cdot \mathbf{a}, \mathbf{Q} \cdot \mathbf{b}\right) = \cos\left(\mathbf{a}, \mathbf{b}\right)$$

for any vectors $\mathbf{a}$ and $\mathbf{b}$. It follows from this definition and the definition of the dot product of vectors $(\mathbf{a} \cdot \mathbf{b} = |\mathbf{a}|\,|\mathbf{b}|\cos\left(\mathbf{a}, \mathbf{b}\right))$, that

$$(\mathbf{Q} \cdot \mathbf{a}) \cdot (\mathbf{Q} \cdot \mathbf{b}) = \mathbf{a} \cdot \mathbf{b}$$

But $(\mathbf{Q} \cdot \mathbf{a}) \cdot (\mathbf{Q} \cdot \mathbf{b}) = \mathbf{b} \cdot \left(\mathbf{Q}^T \cdot \mathbf{Q}\right)\mathbf{a} = \mathbf{a} \cdot \mathbf{b} = \mathbf{b} \cdot \mathbf{I} \cdot \mathbf{a}$, which implies that $\mathbf{b} \cdot \left(\mathbf{Q}^T \cdot \mathbf{Q} - \mathbf{I}\right) \cdot \mathbf{a} = 0$. Since $\mathbf{a}$ and $\mathbf{b}$ are arbitrary, an orthogonal tensor must satisfy $\mathbf{Q}^T \cdot \mathbf{Q} = \mathbf{I}$. In indicial form, $Q^T_{im}Q_{mj} = Q_{mi}Q_{mj} = \delta_{ij}$, and in matrix form, $[\mathbf{Q}]^T [\mathbf{Q}] = [\mathbf{I}]$.

Note that $\mathbf{Q}^T \cdot \mathbf{Q} = \mathbf{I}$ implies that $\mathbf{Q}^T = \mathbf{Q}^{-1}$, i.e., the transpose of an orthogonal tensor is equal to its inverse, since $\mathbf{Q}^{-1} \cdot \mathbf{Q} = \mathbf{Q} \cdot \mathbf{Q}^{-1} = \mathbf{I}$. It follows that

$$\boxed{\mathbf{Q}^T \cdot \mathbf{Q} = \mathbf{Q} \cdot \mathbf{Q}^T = \mathbf{I}} \tag{A.1.19}$$

The determinant of an orthogonal tensor is given by

$$\det \mathbf{Q} = (\mathbf{Q} \cdot \mathbf{e}_1 \times \mathbf{Q} \cdot \mathbf{e}_2) \cdot \mathbf{Q} \cdot \mathbf{e}_3 = \left(\mathbf{e}'_1 \times \mathbf{e}'_2\right) \cdot \mathbf{e}'_3 = \pm\mathbf{e}'_3 \cdot \mathbf{e}'_3 = \pm 1$$

Here, $\{\mathbf{e}'_1, \mathbf{e}'_2, \mathbf{e}'_3\}$ is the orthonormal basis resulting from the transformation of $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ by $\mathbf{Q}$. If $\mathbf{Q}$ maintains the handedness of $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ (e.g., if both $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ and $\{\mathbf{e}'_1, \mathbf{e}'_2, \mathbf{e}'_3\}$ form a right-handed basis), then $\det \mathbf{Q} = +1$ and $\mathbf{Q}$ is called a *proper* orthogonal transformation (also equivalent to a rigid body rotation). Otherwise, in the case of a reflection which reverses the handedness of the basis vectors, $\det \mathbf{Q} = -1$ and $\mathbf{Q}$ is called *improper* (e.g., $\mathbf{e}'_1 = \mathbf{e}_1$, $\mathbf{e}'_2 = -\mathbf{e}_2$, $\mathbf{e}'_3 = \mathbf{e}_3$).

A.1.12   Transformation Laws for Cartesian Components of Vectors and Tensors

Let $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ and $\{\mathbf{e}'_1, \mathbf{e}'_2, \mathbf{e}'_3\}$ be two orthogonal bases in a Cartesian coordinate system. $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ could be made to coincide with $\{\mathbf{e}'_1, \mathbf{e}'_2, \mathbf{e}'_3\}$ through a rigid body rotation (i.e., a transformation that preserves vector length and angles),

$$\mathbf{e}'_i = \mathbf{Q} \cdot \mathbf{e}_i = Q_{mi}\mathbf{e}_m$$

where $Q_{mi}Q_{mj} = Q_{im}Q_{jm} = \delta_{ij}$. Since $Q_{mi} = \mathbf{e}_m \cdot \mathbf{Q} \cdot \mathbf{e}_i = \mathbf{e}_m \cdot \mathbf{e}'_i = \cos\left(\mathbf{e}_m, \mathbf{e}'_i\right)$, the components of $\mathbf{Q}$ are direction cosines between $\mathbf{e}_m$ and $\mathbf{e}'_i$.
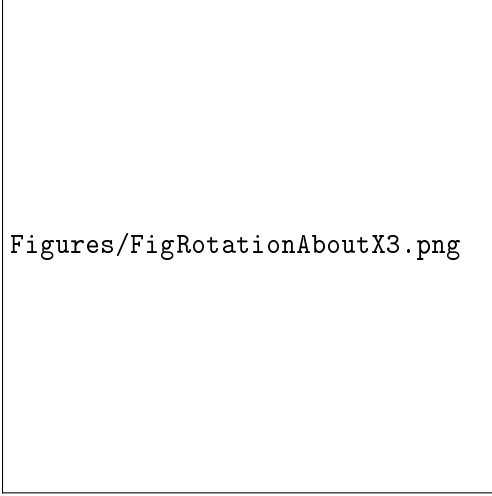
Figure A.1.2: Rotation about x_3.

Example 4. Rotation about x_3

$$[\mathbf{Q}] = \begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Reflection about $x_2 - x_3$ plane, $\mathbf{e}'_1 = \mathbf{Q} \cdot \mathbf{e}_1 = -\mathbf{e}_1$, $\mathbf{e}'_2 = \mathbf{Q} \cdot \mathbf{e}_2 = \mathbf{e}_2$, $\mathbf{e}'_3 = \mathbf{Q} \cdot \mathbf{e}_3 = \mathbf{e}_3$.

$$[\mathbf{Q}] = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

For any vector $\mathbf{a}$, its components with respect to $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ and $\{\mathbf{e}'_1, \mathbf{e}'_2, \mathbf{e}'_3\}$ are $a_i = \mathbf{e}_i \cdot \mathbf{a}$ and $a'_i = \mathbf{e}'_i \cdot \mathbf{a}$, respectively. Using the above relation,

$$a'_i = \mathbf{e}'_i \cdot \mathbf{a} = \mathbf{a} \cdot \mathbf{Q} \cdot \mathbf{e}_i = Q_{mi}\mathbf{a} \cdot \mathbf{e}_m = Q_{mi}a_m,$$

or

$$\boxed{a'_i = Q_{mi}a_m} \tag{A.1.20}$$

In matrix form,

$$\begin{bmatrix} a'_1 \\ a'_2 \\ a'_3 \end{bmatrix}_{\mathbf{e}'_i} = \begin{bmatrix} Q_{11} & Q_{21} & Q_{31} \\ Q_{12} & Q_{22} & Q_{32} \\ Q_{13} & Q_{23} & Q_{33} \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix}_{\mathbf{e}_i}$$

or

$$[\mathbf{a}]' = [\mathbf{Q}]^T[\mathbf{a}] \quad \text{or} \quad [\mathbf{a}]_{\mathbf{e}'_i} = [\mathbf{Q}]^T[\mathbf{a}]_{\mathbf{e}_i}$$

Here $[\mathbf{a}]'$ and $[\mathbf{a}]$ are matrices of the *same* vector, expressed in two different coordinate systems. This is *not the same* as $\mathbf{a}' = \mathbf{Q}^T \cdot \mathbf{a}$, where $\mathbf{a}'$ is the linear transformation of $\mathbf{a}$ by $\mathbf{Q}^T$.

Now consider a tensors $\mathbf{T}$. Its components with respect to $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ and $\{\mathbf{e}'_1, \mathbf{e}'_2, \mathbf{e}'_3\}$ are given by $T_{ij} = \mathbf{e}_i \cdot \mathbf{T} \cdot \mathbf{e}_j$ and $T'_{ij} = \mathbf{e}'_i \cdot \mathbf{T} \cdot \mathbf{e}'_j$, respectively. Thus, $T'_{ij} = (\mathbf{Q} \cdot \mathbf{e}_i) \cdot \mathbf{T} \cdot (\mathbf{Q} \cdot \mathbf{e}_j) = Q_{mi}\mathbf{e}_m \cdot \mathbf{T} \cdot Q_{nj}\mathbf{e}_n = Q_{mi}Q_{nj}\mathbf{e}_m \cdot \mathbf{T} \cdot \mathbf{e}_n = Q_{mi}Q_{nj}T_{mn}$, or

$$\boxed{T'_{ij} = Q_{mi}Q_{nj}T_{mn}} \tag{A.1.21}$$

In matrix form, $[\mathbf{T}]' = [\mathbf{Q}]^T [\mathbf{T}] [\mathbf{Q}]$, or

$$
\begin{bmatrix} T'_{11} & T'_{12} & T'_{13} \\ T'_{21} & T'_{22} & T'_{23} \\ T'_{31} & T'_{32} & T'_{33} \end{bmatrix} = \begin{bmatrix} Q_{11} & Q_{21} & Q_{31} \\ Q_{12} & Q_{22} & Q_{32} \\ Q_{13} & Q_{23} & Q_{33} \end{bmatrix} \begin{bmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{bmatrix} \begin{bmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{bmatrix}
$$

Equivalently, we can show that

$$\boxed{T_{ij} = Q_{im}Q_{jn}T'_{mn}}$$
(A.1.22)

or $[\mathbf{T}] = [\mathbf{Q}] [\mathbf{T}]' [\mathbf{Q}]^T$. As for vectors, we note that $[\mathbf{T}]$ and $[\mathbf{T}]'$ are the matrices of the *same* tensor $\mathbf{T}$, with respect to two different coordinate systems. This is *not the same* as $\mathbf{T}' = \mathbf{Q}^T \cdot \mathbf{T} \cdot \mathbf{Q}$.

A.1.13   Symmetric and Antisymmetric Tensors

A *symmetric* tensor $\mathbf{T}$ satisfies $\mathbf{T}^T = \mathbf{T}$, i.e., $T_{ji} = T_{ij}$, or in matrix form,

$$
[\mathbf{T}] = \begin{bmatrix} T_{11} & T_{12} & T_{13} \\ T_{12} & T_{22} & T_{23} \\ T_{13} & T_{23} & T_{33} \end{bmatrix}
$$

An *antisymmetric* (or *skew-symmetric*) tensor $\boldsymbol{\Omega}$ satisfies $\boldsymbol{\Omega}^T = -\boldsymbol{\Omega}$, i.e., $\Omega_{ji} = -\Omega_{ij}$ and thus $\Omega_{11} = \Omega_{22} = \Omega_{33} = 0$,

$$
[\boldsymbol{\Omega}] = \begin{bmatrix} 0 & \Omega_{12} & -\Omega_{31} \\ -\Omega_{12} & 0 & \Omega_{23} \\ \Omega_{31} & -\Omega_{23} & 0 \end{bmatrix}
$$

Any tensor can be written as the sum of a symmetric and antisymmetric tensor,

$$\mathbf{T} = \mathbf{T}^S + \mathbf{T}^A \quad \text{where} \quad \mathbf{T}^S = \frac{1}{2}\left(\mathbf{T} + \mathbf{T}^T\right) \quad \text{and} \quad \mathbf{T}^A = \frac{1}{2}\left(\mathbf{T} - \mathbf{T}^T\right)$$

This is a unique decomposition. It can be checked that $\mathbf{T}^S$ is symmetric and $\mathbf{T}^A$ is antisymmetric.

The *dual vector* $\boldsymbol{\omega}$ of an antisymmetric tensor $\boldsymbol{\Omega}$ satisfies

$$\boxed{\boldsymbol{\Omega} \cdot \mathbf{a} = \boldsymbol{\omega} \times \mathbf{a}}$$
(A.1.23)

for any vector **a**. Thus $\Omega_{ij} = \mathbf{e}_i \cdot \boldsymbol{\Omega} \cdot \mathbf{e}_j = \mathbf{e}_i \cdot (\boldsymbol{\omega} \times \mathbf{e}_j) = \omega_k \mathbf{e}_i \cdot (\mathbf{e}_k \times \mathbf{e}_j) = \omega_k \mathbf{e}_i \cdot \varepsilon_{kjl}\mathbf{e}_l = \omega_k \varepsilon_{kjl}\delta_{il}$ or

$$\boxed{\Omega_{ij} = -\varepsilon_{ijk}\omega_k}$$
(A.1.24)

In matrix form,

$$
[\boldsymbol{\Omega}] = \begin{bmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{bmatrix}
$$

Conversely, it can also be shown that

$$\boxed{\omega_i = -\frac{1}{2}\varepsilon_{ijk}\Omega_{jk}}$$
(A.1.25)

As a homework problem, it may be shown that $\varepsilon_{ijk}T_{jk} = \varepsilon_{ijk}T^A_{jk}$, since $\varepsilon_{ijk}T^S_{jk} = 0$ for any symmetric tensor $\mathbf{T}^S$.

A.1.14   Eigenvalues and Eigenvectors of Real Symmetric Tensors

A second-order tensor $\mathbf{T}$ has three pairs of eigenvalues λ and eigenvectors $\mathbf{v}$ that each satisfy

$$\mathbf{T} \cdot \mathbf{v} = \lambda \mathbf{v} \tag{A.1.26}$$

The eigenvalues λ are the roots of the characteristic equation of $\mathbf{T}$, which is the cubic polynomial produced by setting $\det(\mathbf{T} - \lambda\mathbf{I}) = 0$,

$$-\lambda^3 + I_1\lambda^2 - I_2\lambda + I_3 = 0 \tag{A.1.27}$$

where

$$\begin{aligned} I_1 &= \operatorname{tr}\mathbf{T} \\ I_2 &= \frac{1}{2}\left(I_1^2 - \operatorname{tr}\mathbf{T}^2\right) \\ I_3 &= \det\mathbf{T} \end{aligned} \tag{A.1.28}$$

are called *invariants* of $\mathbf{T}$.

According to the Cayley-Hamilton theorem, a tensor $\mathbf{T}$ satisfies its own characteristic equation,

$$-\mathbf{T}^3 + I_1\mathbf{T}^2 - I_2\mathbf{T} + I_3\mathbf{I} = \mathbf{0} \tag{A.1.29}$$

Therefore, the cubic power of $\mathbf{T}$ can be expressed in terms of its lower powers according to $\mathbf{T}^3 = I_1\mathbf{T}^2 - I_2\mathbf{T} + I_3\mathbf{I}$. Taking the trace of this equation allows us to solve for I_3 as

$$\begin{aligned} I_3 &= \frac{1}{3}\left(\operatorname{tr}\mathbf{T}^3 - I_1\operatorname{tr}\mathbf{T}^2 + I_2\operatorname{tr}\mathbf{T}\right) \\ &= \frac{1}{3}\left(\operatorname{tr}\mathbf{T}^3 - I_1^3 + 3I_1 I_2\right) \end{aligned} \tag{A.1.30}$$

Multiplying eq.(A.1.29) by $\mathbf{T}^{-1}$ also produces

$$I_3\mathbf{T}^{-1} = \mathbf{T}^2 - I_1\mathbf{T} + I_2\mathbf{I}$$

Using all these relations, we may differentiate the three invariants of $\mathbf{T}$ with respect to $\mathbf{T}$ to get

$$\begin{aligned} \frac{\partial I_1}{\partial \mathbf{T}} &= \mathbf{I} \\ \frac{\partial I_2}{\partial \mathbf{T}} &= I_1\mathbf{I} - \mathbf{T}^T \\ \frac{\partial I_3}{\partial \mathbf{T}} &= I_3\mathbf{T}^{-T} \end{aligned} \tag{A.1.31}$$

Theorem. *The eigenvalues of real symmetric tensors are real (proof not provided here).*

Theorem. *If the eigenvalues of a real symmetric tensor are all distinct, the eigenvectors are orthogonal to each other.*

Proof: Given $\mathbf{T} \cdot \mathbf{v}_1 = \lambda_1\mathbf{v}_1$, $\mathbf{T} \cdot \mathbf{v}_2 = \lambda_2\mathbf{v}_2$, $\lambda_1 \neq \lambda_2$, then $\mathbf{v}_2 \cdot \mathbf{T} \cdot \mathbf{v}_1 = \lambda_1\mathbf{v}_1 \cdot \mathbf{v}_2$ and $\mathbf{v}_1 \cdot \mathbf{T} \cdot \mathbf{v}_2 = \lambda_2\mathbf{v}_1 \cdot \mathbf{v}_2 = \mathbf{v}_2 \cdot \mathbf{T}^T \cdot \mathbf{v}_1 = \mathbf{v}_2 \cdot \mathbf{T} \cdot \mathbf{v}_1$,

$$\Rightarrow \lambda_1\mathbf{v}_1 \cdot \mathbf{v}_2 = \lambda_2\mathbf{v}_1 \cdot \mathbf{v}_2 \quad \text{or} \quad (\lambda_1 - \lambda_2)\mathbf{v}_1 \cdot \mathbf{v}_2 = 0 \quad \Rightarrow \mathbf{v}_1 \cdot \mathbf{v}_2 = 0$$

When two of the eigenvalues are repeated (a double root of the characteristic equation), the resulting eigenvectors are not necessarily orthogonal to each other; however, they remain orthogonal to the third eigenvector. This means that any vector lying in the plane normal to the third eigenvector is an eigenvector corresponding to the double root. Similarly, when all three eigenvalues are repeated (a triple root), any vector becomes an eigenvector of $\mathbf{T}$.

Example 5. In hydrostatics the stress tensor is $\mathbf{T} = -p\mathbf{I}$, where p is the hydrostatic pressure. In this case, $-p$ is a triple root of the characteristic equation of $\mathbf{T}$. Any vector $\mathbf{v}$ satisfies $\mathbf{T} \cdot \mathbf{v} = -p\mathbf{v}$, and is thus an eigenvector of $\mathbf{T}$.

In continuum mechanics the eigenvectors $\mathbf{v}$ of a tensor are generally normalized,

$$\mathbf{n} \equiv \frac{\mathbf{v}}{|\mathbf{v}|}$$

Thus, we can always find a set of three orthonormal eigenvectors $\{\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3\}$ for any real symmetric tensor $\mathbf{T}$, even when the eigenvalues are repeated. Given a tensor $\mathbf{T}$ with eigenvalues $\lambda_1, \lambda_2, \lambda_3$ and eigenvectors $\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3$, the components of $\mathbf{T}$ in the orthonormal basis $\{\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3\}$ can be obtained from

$$T_{i1} = \mathbf{v}_i \cdot \mathbf{T} \cdot \mathbf{n}_1 = \lambda_1 \mathbf{n}_i \cdot \mathbf{n}_1 = \lambda_1 \delta_{i1} \quad T_{i2} = \lambda_2 \delta_{i2} T_{i3} = \lambda_3 \delta_{i3}$$

Thus,

$$[\mathbf{T}]_{\mathbf{n}_i} = \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix} = \begin{bmatrix} T_1 & 0 & 0 \\ 0 & T_2 & 0 \\ 0 & 0 & T_3 \end{bmatrix}$$

Since $\mathbf{T} = T_{ij}\mathbf{n}_i \otimes \mathbf{n}_j = T_{i1}\mathbf{n}_i \otimes \mathbf{n}_1 + T_{i2}\mathbf{n}_i \otimes \mathbf{n}_2 + T_{i3}\mathbf{n}_i \otimes \mathbf{n}_3$, we find that

$$\mathbf{T} = \lambda_1 \mathbf{n}_1 \otimes \mathbf{n}_1 + \lambda_2 \mathbf{n}_2 \otimes \mathbf{n}_2 + \lambda_3 \mathbf{n}_3 \otimes \mathbf{n}_3 \tag{A.1.32}$$

This is known as the *spectral representation* of the tensor $\mathbf{T}$. In particular, since the eigenvalues of the identity tensor are $\lambda_1 = \lambda_2 = \lambda_3 = 1$, and since any vector is an eigenvector of $\mathbf{I}$, we can select the basis vectors $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$ so that the spectral representation of $\mathbf{I}$ may be given by

$$\mathbf{I} = \mathbf{e}_i \otimes \mathbf{e}_i = \mathbf{e}_1 \otimes \mathbf{e}_1 + \mathbf{e}_2 \otimes \mathbf{e}_2 + \mathbf{e}_3 \otimes \mathbf{e}_3 \tag{A.1.33}$$

A.1.15 Orthogonal Transformation of Tensors

An orthogonal transformation $\mathbf{Q}$ transforms any vector $\mathbf{a}$ into the vector $\mathbf{Q} \cdot \mathbf{a}$, which we may denote as

$$\mathbf{a}^* = \mathbf{Q} \cdot \mathbf{a} \tag{A.1.34}$$

Recall that a tensor $\mathbf{T}$ may be expressed in its spectral representation as per eq.(A.1.32). Each of its eigenvectors $\mathbf{n}$ is transformed by $\mathbf{Q}$ into $\mathbf{n}^* = \mathbf{Q} \cdot \mathbf{n}$. Since eigenvalues of $\mathbf{T}$ are invariant to orthogonal transformations, it follows that

$$\begin{aligned} \mathbf{T}^* &= \lambda_1 \mathbf{n}_1^* \otimes \mathbf{n}_1^* + \lambda_2 \mathbf{n}_2^* \otimes \mathbf{n}_2^* + \lambda_3 \mathbf{n}_3^* \otimes \mathbf{n}_3^* \\ &= \lambda_1 (\mathbf{Q} \cdot \mathbf{n}_1) \otimes (\mathbf{Q} \cdot \mathbf{n}_1) + \lambda_2 (\mathbf{Q} \cdot \mathbf{n}_2) \otimes (\mathbf{Q} \cdot \mathbf{n}_2) + \lambda_3 (\mathbf{Q} \cdot \mathbf{n}_3) \otimes (\mathbf{Q} \cdot \mathbf{n}_3) \\ &= \mathbf{Q} \cdot (\lambda_1 \mathbf{n}_1 \otimes \mathbf{n}_1 + \lambda_2 \mathbf{n}_2 \otimes \mathbf{n}_2 + \lambda_3 \mathbf{n}_3 \otimes \mathbf{n}_3) \cdot \mathbf{Q}^T \\ &= \mathbf{Q} \cdot \mathbf{T} \cdot \mathbf{Q}^T \end{aligned}$$

Thus, the transformation of the second-order tensor $\mathbf{T}$ by $\mathbf{Q}$ is $\mathbf{T}^* = \mathbf{Q} \cdot \mathbf{T} \cdot \mathbf{Q}^T$.

A.2 Higher Order Tensors

Note that $\mathbf{a} \cdot \mathbf{T} \cdot \mathbf{b} = \mathbf{a} \otimes \mathbf{b} : \mathbf{T} = \mathbf{T} : \mathbf{a} \otimes \mathbf{b}$, and $\mathbf{a} \otimes \mathbf{b} : \mathbf{c} \otimes \mathbf{d} = (\mathbf{a} \cdot \mathbf{c})(\mathbf{b} \cdot \mathbf{d})$. Similarly, $(\mathbf{a} \otimes \mathbf{b}) \cdot (\mathbf{c} \otimes \mathbf{d}) = (\mathbf{b} \cdot \mathbf{c}) \mathbf{a} \otimes \mathbf{d}$. We will be using generalizations of these relations when examining higher order tensors.

A.2.1 Third-Order Tensors

A third-order tensor $\mathbb{T}$ is a linear transformation that transforms any vector $\mathbf{a}$ into a second-order tensor $\mathbf{S}$,

$$\boxed{\mathbb{T} \cdot \mathbf{a} = \mathbf{S}} \tag{A.2.1}$$

In general, the dyadic product of three vectors is a third-order tensor which satisfies

$$\boxed{(\mathbf{a} \otimes \mathbf{b} \otimes \mathbf{c}) \cdot (\alpha \mathbf{u} + \beta \mathbf{v}) = (\alpha \mathbf{c} \cdot \mathbf{u} + \beta \mathbf{c} \cdot \mathbf{v}) (\mathbf{a} \otimes \mathbf{b})} \quad \forall \, \mathbf{u}, \mathbf{v} \,. \tag{A.2.2}$$

Any third-order tensor $\mathbb{T}$ can be expressed in terms of its Cartesian components T_{ijk} as

$$\boxed{\mathbb{T} = T_{ijk}\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k} \tag{A.2.3}$$

and the Cartesian components of a third-order tensor may be evaluated from

$$\boxed{T_{ijk} = \mathbf{e}_i \cdot (\mathbb{T} \cdot \mathbf{e}_k) \cdot \mathbf{e}_j} \tag{A.2.4}$$

It follows from Eqs.(A.2.2) and (A.2.3) that

$$\mathbb{T} \cdot \mathbf{a} = T_{ijk} (\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k) \cdot \mathbf{a} = T_{ijk} (\mathbf{e}_k \cdot \mathbf{a}) (\mathbf{e}_i \otimes \mathbf{e}_j) = T_{ijk}a_k (\mathbf{e}_i \otimes \mathbf{e}_j) = \mathbf{S} = S_{ij} (\mathbf{e}_i \otimes \mathbf{e}_j)$$

so that the indicial form of eq.(A.2.1) is

$$T_{ijk}a_k = S_{ij} \tag{A.2.5}$$

In particular,

$$\mathbb{T} \cdot \mathbf{e}_k = T_{ijk}\mathbf{e}_i \otimes \mathbf{e}_j \tag{A.2.6}$$

The double dot product of a third-order tensor with a second-order tensor is defined by

$$\boxed{(\mathbf{a} \otimes \mathbf{b} \otimes \mathbf{c}) : (\mathbf{d} \otimes \mathbf{e}) = (\mathbf{b} \cdot \mathbf{d}) (\mathbf{c} \cdot \mathbf{e}) \mathbf{a}} \,,$$

and

$$\boxed{(\mathbf{a} \otimes \mathbf{b}) : (\mathbf{c} \otimes \mathbf{d} \otimes \mathbf{e}) = (\mathbf{a} \cdot \mathbf{c}) (\mathbf{b} \cdot \mathbf{d}) \mathbf{e}} \,.$$

Therefore, the double dot product of a third-order tensor with a second-order tensor is a vector given by

$$\mathbb{T} : (\mathbf{a} \otimes \mathbf{b}) = (\mathbb{T} \cdot \mathbf{b}) \cdot \mathbf{a} \,. \tag{A.2.7}$$

Proof: Using $\mathbb{T} \cdot \mathbf{b} = T_{ijk}b_k (\mathbf{e}_i \otimes \mathbf{e}_j)$, we find that $(\mathbb{T} \cdot \mathbf{b}) \cdot \mathbf{a} = T_{ijk}b_k (\mathbf{e}_i \otimes \mathbf{e}_j) \cdot \mathbf{a} = T_{ijk}b_k (\mathbf{a} \cdot \mathbf{e}_j) \mathbf{e}_i = T_{ijk}a_j b_k \mathbf{e}_i$. Similarly, $\mathbb{T} : (\mathbf{a} \otimes \mathbf{b}) = T_{ijk} (\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k) : (\mathbf{a} \otimes \mathbf{b}) = T_{ijk} (\mathbf{e}_j \cdot \mathbf{a}) (\mathbf{e}_k \cdot \mathbf{b}) \mathbf{e}_i = T_{ijk}a_j b_k \mathbf{e}_i$, thus completing the proof.

For any second-order tensor $\mathbf{S}$, it also follows that

$$\mathbb{T} : \mathbf{S} = T_{ijk}S_{jk}\mathbf{e}_i \,.$$

Example 6. If we introduce the notation $\mathbb{E}$ as the third-order (pseudo-)tensor of Cartesian components ε_{ijk}, the relation between an antisymmetric tensor and its dual vector can also be written as

$$\boxed{\boldsymbol{\Omega} = -\mathbb{E} \cdot \boldsymbol{\omega}} \tag{A.2.8}$$

Similarly,

$$\boxed{\boldsymbol{\omega} = -\frac{1}{2}\mathbb{E} : \boldsymbol{\Omega}} \tag{A.2.9}$$

A.2.2   Fourth-Order Tensors

The dyadic product of four vectors is a fourth-order tensor $\mathbf{a} \otimes \mathbf{b} \otimes \mathbf{c} \otimes \mathbf{d}$, defined as

$$(\mathbf{a} \otimes \mathbf{b} \otimes \mathbf{c} \otimes \mathbf{d}) \cdot \mathbf{v} = (\mathbf{d} \cdot \mathbf{v}) \, (\mathbf{a} \otimes \mathbf{b} \otimes \mathbf{c}) \tag{A.2.10}$$

The Cartesian components of a fourth-order tensor $\mathcal{T}$ are given by

$$T_{ijkl} = (\mathbf{e}_i \otimes \mathbf{e}_j) : \mathcal{T} : (\mathbf{e}_k \otimes \mathbf{e}_l) \tag{A.2.11}$$

such that

$$\mathcal{T} = T_{ijkl}\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_l \tag{A.2.12}$$

Therefore, a fourth-order tensor transforms a vector into a third-order tensor,

$$\mathcal{T} \cdot \mathbf{a} = (T_{ijkl}\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_l) \cdot \mathbf{a} = T_{ijkl}a_l\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \equiv S_{ijk}\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k = \mathbb{S} \tag{A.2.13}$$

The double dot product of a fourth-order tensor with a second-order tensor is a second-order tensor defined as

$$\boxed{\mathcal{T} : (\mathbf{a} \otimes \mathbf{b}) = (\mathcal{T} \cdot \mathbf{b}) \cdot \mathbf{a}} \tag{A.2.14}$$

from which it can be shown that

$$\mathcal{T} : \mathbf{S} = T_{ijmn}S_{mn}\mathbf{e}_i \otimes \mathbf{e}_j \tag{A.2.15}$$

or equivalently, $(\mathcal{T} : \mathbf{S})_{ij} = T_{ijkl}S_{kl}$.

A fourth-order tensor can exhibit three levels of symmetry, which can be represented using Cartesian components as

$$\begin{aligned} T_{ijkl} &= T_{jikl} && \text{left minor symmetry} \\ T_{ijkl} &= T_{ijlk} && \text{right minor symmetry} \\ T_{ijkl} &= T_{klij} && \text{major symmetry} \end{aligned} \tag{A.2.16}$$

Whereas a general fourth-order tensor may have 81 distinct components, a tensor with one minor symmetry has 54 distinct components; a tensor with both minor symmetries has 36 distinct components; and a tensor with minor and major symmetries has 21distinct components. We may represent the major symmetry of $\mathcal{T}$ as $\mathcal{T} = \mathcal{T}^T$, whose Cartesian representation is provided above. It follows from this definition that

$$\mathbf{S} : \mathcal{T} = \mathcal{T}^T : \mathbf{S}$$
$$(\mathbf{S} : \mathcal{T})_{ij} = S_{kl}T_{klij} = T_{ijkl}^T S_{kl}$$

A.2.3   Additional Tensor Products

Earlier we saw that the dyadic product of vectors can produce tensors. Similarly, we can define dyadic products of tensors which produce higher-order tensors. In particular, the following products of second-order tensors $\mathbf{A}$ and $\mathbf{B}$ produce fouth-order tensors, satisfying

$$\begin{aligned} (\mathbf{A} \otimes \mathbf{B}) : \mathbf{S} &= (\mathbf{B} : \mathbf{S}) \, \mathbf{A} \\ (\mathbf{A} \oslash \mathbf{B}) : \mathbf{S} &= \mathbf{A} \cdot \mathbf{S} \cdot \mathbf{B}^T \\ (\mathbf{A} \obslash \mathbf{B}) : \mathbf{S} &= \mathbf{A} \cdot \mathbf{S}^T \cdot \mathbf{B}^T \\ (\mathbf{A} \odot \mathbf{B}) : \mathbf{S} &= \frac{1}{2}(\mathbf{A} \oslash \mathbf{B} + \mathbf{A} \obslash \mathbf{B}) : \mathbf{S} = \frac{1}{2}\left(\mathbf{A} \cdot \mathbf{S} \cdot \mathbf{B}^T + \mathbf{A} \cdot \mathbf{S}^T \cdot \mathbf{B}^T\right) \end{aligned} \tag{A.2.17}$$

where **S** is any second-order tensor. Using Cartesian components of tensors, the indicial form of these tensor products are

$$(\mathbf{A} \otimes \mathbf{B})_{ijkl} = A_{ij} B_{kl}$$

$$(\mathbf{A} \oslash \mathbf{B})_{ijkl} = A_{ik} B_{jl}$$

$$(\mathbf{A} \oslash \mathbf{B})_{ijkl} = A_{il} B_{jk} \tag{A.2.18}$$

$$(\mathbf{A} \odot \mathbf{B})_{ijkl} = \frac{1}{2} \left(A_{ik} B_{jl} + A_{il} B_{jk} \right)$$

Bibliography

[1] Javier Bonet and Richard D. Wood. *Nonlinear continuum mechanics for finite element analysis*. Cambridge University Press, 1997.

[2] R.M. Bowen. Theory of mixtures. *Continuum physics*, 3(Pt I), 1976.

[3] I. Tinoco Jr., K. Sauer, and J. C. Wang. *Physical chemistry : principles and applications in biological sciences*. Prentice Hall, 1995.

[4] C. Truesdell and R. Toupin. *The classical field theories*, volume III/1 of *Handbuch der physik*. Springer, Heidelberg, 1960.