Continuous-discontinuous modelling of hygrothermal damage processes in porous media

Proefschrift

ter verkrijging van de graad van doctor
aan de Technische Universiteit Delft,
op gezag van de Rector Magnificus prof. dr. ir. J. T. Fokkema,
voorzitter van het College voor Promoties
in het openbaar te verdedigen op woensdag 10 juni 2009 om 10:00 uur

door

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geboren te Leuven, België
Results! I got a lot of results. I know several thousand things that won't work.

Thomas Alva Edison
Acknowledgement

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Peter Moonen
June 2009
This list of symbols is not exhaustive. Symbols that appear only locally in the text, and that are not important to understand the other parts of the work, are not included here.

Scalar values are denoted with italic Roman or Greek characters (e.g. $a$ or $\alpha$). Vectors and matrices are both indicated with bold characters. Lower case characters are usually assigned to vectors (e.g. $a$) and upper case characters to matrices (e.g. $A$). 4th order tensors are indicated with bold, italic, upper case characters (e.g. $C$). The individual scalar entries of a vector, matrix or tensor are referred to by making use of indices (e.g. $a_{ij}$, $A_{ij}$ or $C_{ijkl}$).

Superscripts are used to indicate to which phase or component a variable is related (e.g. $\rho^\alpha$ is the average mass density of phase $\alpha$). Several types of overbars provide additional information about a variable (e.g. $\bar{f}$ denotes that the variable $f$ has a molecular origin).

### Roman characters

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a$</td>
<td>surface of the REV</td>
<td>m²</td>
</tr>
<tr>
<td>$a$</td>
<td>acceleration vector</td>
<td>m/s²</td>
</tr>
<tr>
<td>$A$</td>
<td>surface of the body</td>
<td>m²</td>
</tr>
<tr>
<td>$A^\alpha$</td>
<td>specific Helmholtz energy of phase $\alpha$</td>
<td>J/kg</td>
</tr>
<tr>
<td>$b^\alpha$</td>
<td>Biot coefficient of phase $\alpha$</td>
<td>-</td>
</tr>
<tr>
<td>$b^\pi$</td>
<td>external supply of momentum to species $\pi$</td>
<td>m/s²</td>
</tr>
<tr>
<td>$\bar{b}^{\alpha,\pi}$</td>
<td>resulting macroscopic external supply of momentum to species $\pi$</td>
<td>m/s²</td>
</tr>
<tr>
<td>$b^\alpha$</td>
<td>mean macroscopic external supply of momentum to phase $\alpha$</td>
<td>m/s²</td>
</tr>
<tr>
<td>$b^\pi$</td>
<td>molecular supply of momentum to species $\pi$</td>
<td>m/s²</td>
</tr>
<tr>
<td>$\bar{b}^{\alpha,\pi}$</td>
<td>macroscopic supply of momentum related to molecular interaction</td>
<td>m/s²</td>
</tr>
<tr>
<td>$b^{\alpha,\pi}$</td>
<td>macroscopic supply of momentum related to phase interaction</td>
<td>m/s²</td>
</tr>
<tr>
<td>$b^{\alpha\beta}$</td>
<td>mean macroscopic supply of momentum related to phase interaction</td>
<td>m/s²</td>
</tr>
<tr>
<td>$B$</td>
<td>a body</td>
<td></td>
</tr>
</tbody>
</table>
B derivatives of shape functions -
$c^{\alpha, \pi}$ mass fraction of species $\pi$ in phase $\alpha$ -
$D$ material tangent -
$D^{\alpha, \pi}$ effective dispersion tensor of species $\pi$ in phase $\alpha$ m²/s
$E$ Young’s modulus N/m²
$f^{\pi}$ internal supply of a thermodynamic quantity $\psi^{\pi}$ */s
$f^{\alpha, \pi}$ internal supply of a macroscopic thermodynamic quantity $\bar{\psi}^{\alpha, \pi}$ */s
$f^{\pi}$ molecular supply of a thermodynamic quantity $\psi^{\pi}$ */s
$f^{\alpha}$ macroscopic effect of molecular interaction inside a phase on $\bar{\psi}^{\alpha, \pi}$ */s
$f^{\alpha}$ internal supply of a mean macroscopic thermodynamic quantity $\psi^{\alpha}$ */s
$g^{\pi}$ external supply of a thermodynamic quantity $\psi^{\pi}$ */s
$g^{\alpha, \pi}$ external supply of a macroscopic thermodynamic quantity $\bar{\psi}^{\alpha, \pi}$ */s
$g^{\alpha, \beta, \pi}$ macroscopic effect of phase interaction on $\bar{\psi}^{\alpha, \pi}$ */s
$g^{\alpha}$ external supply of a mean macroscopic thermodynamic quantity $\psi^{\alpha}$ */s
$g^{\alpha, \beta}$ mean macroscopic effect of phase interaction on $\psi^{\alpha}$ */s
$g$ gravitational acceleration vector m/s²
$h^{\pi}$ external supply of energy to species $\pi$ J/(kg s)
$h^{\alpha, \pi}$ resulting macroscopic external supply of energy to species $\pi$ J/(kg s)
$h^{\alpha}$ mean macroscopic external supply of energy to phase $\alpha$ J/(kg s)
$h^{\alpha}$ molecular supply of energy to species $\pi$ J/(kg s)
$h^{\alpha, \pi}$ macroscopic supply of energy related to molecular interaction J/(kg s)
$h^{\alpha, \beta, \pi}$ macroscopic supply of energy related to phase interaction J/(kg s)
$h^{\alpha, \beta}$ mean macroscopic supply of energy related to phase interaction J/(kg s)
$\mathcal{H}$ Heaviside function -
$H^{\alpha}$ specific enthalpy of phase $\alpha$ J/kg
$i^{\pi}$ surface flux vector of a thermodynamic quantity $\psi^{\pi}$ (* kg)/(m² s)
$i^{\alpha, \pi}$ surface flux vector of a macroscopic thermodynamic quantity $\bar{\psi}^{\alpha, \pi}$ (* kg)/(m² s)
<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$i^a$</td>
<td>Surface flux vector of a mean macroscopic thermodynamic quantity $\psi^a$</td>
<td>$(* \text{ kg})/\text{(m}^2\text{ s)}$</td>
</tr>
<tr>
<td>$I$</td>
<td>Unity matrix</td>
<td>-</td>
</tr>
<tr>
<td>$J$</td>
<td>Jacobian matrix</td>
<td>-</td>
</tr>
<tr>
<td>$J^{a,\pi}$</td>
<td>Diffusive-dispersive flux vector of species $\pi$ in phase $\alpha$</td>
<td>$\text{kg}/\text{(m}^2\text{ s)}$</td>
</tr>
<tr>
<td>$k^a$</td>
<td>Thermal conductivity of phase $\alpha$</td>
<td>$\text{W}/\text{(m K)}$</td>
</tr>
<tr>
<td>$K$</td>
<td>Bulk modulus</td>
<td>$\text{N/m}^2$</td>
</tr>
<tr>
<td>$K^a$</td>
<td>Bulk modulus of phase $\alpha$</td>
<td>$\text{N/m}^2$</td>
</tr>
<tr>
<td>$l$</td>
<td>Characteristic length of the REV</td>
<td>$\text{m}$</td>
</tr>
<tr>
<td>$\ell$</td>
<td>Characteristic size of the micro-structure</td>
<td>$\text{m}$</td>
</tr>
<tr>
<td>$L$</td>
<td>Characteristic length of the body</td>
<td>$\text{m}$</td>
</tr>
<tr>
<td>$m$</td>
<td>Mass of the REV</td>
<td>$\text{kg}$</td>
</tr>
<tr>
<td>$M$</td>
<td>Mass of the body</td>
<td>$\text{kg}$</td>
</tr>
<tr>
<td>$M^\pi$</td>
<td>Molar mass of species $\pi$</td>
<td>$\text{kg/mol}$</td>
</tr>
<tr>
<td>$n$</td>
<td>Porosity of the porous medium</td>
<td>-</td>
</tr>
<tr>
<td>$n^\pi$</td>
<td>Number of moles of species $\pi$</td>
<td>$\text{mol}$</td>
</tr>
<tr>
<td>$n$</td>
<td>Normal vector</td>
<td>-</td>
</tr>
<tr>
<td>$n^{\alpha\beta}$</td>
<td>Normal vector to the interface $\alpha\beta$</td>
<td>-</td>
</tr>
<tr>
<td>$N^a$</td>
<td>Biot modulus of phase $\alpha$</td>
<td>-</td>
</tr>
<tr>
<td>$N$</td>
<td>Shape functions</td>
<td>-</td>
</tr>
<tr>
<td>$p^a$</td>
<td>Thermodynamic pressure in phase $\alpha$</td>
<td>$\text{N/m}^2$</td>
</tr>
<tr>
<td>$q^\pi$</td>
<td>Surface flux vector of heat of species $\pi$</td>
<td>$\text{J}/(\text{m}^2\text{ s})$</td>
</tr>
<tr>
<td>$q^{a,\pi}$</td>
<td>Macroscopic surface flux vector of heat of species $\pi$ in phase $\alpha$</td>
<td>$\text{J}/(\text{m}^2\text{ s})$</td>
</tr>
<tr>
<td>$q^a$</td>
<td>Mean macroscopic surface flux vector of heat of phase $\alpha$</td>
<td>$\text{J}/(\text{m}^2\text{ s})$</td>
</tr>
<tr>
<td>$r^\pi$</td>
<td>Molecular supply of mass to species $\pi$</td>
<td>$\text{s}^{-1}$</td>
</tr>
<tr>
<td>$\bar{r}^{\alpha\pi}$</td>
<td>Macroscopic supply of mass related to molecular interaction</td>
<td>$\text{s}^{-1}$</td>
</tr>
<tr>
<td>$r^{\alpha\beta,\pi}$</td>
<td>Macroscopic supply of mass related to phase interaction</td>
<td>$\text{s}^{-1}$</td>
</tr>
<tr>
<td>$r^{\alpha\beta}$</td>
<td>Mean macroscopic supply of mass related to phase interaction</td>
<td>$\text{s}^{-1}$</td>
</tr>
<tr>
<td>$r$</td>
<td>Position vector in the reference frame of the REV</td>
<td>-</td>
</tr>
<tr>
<td>$R$</td>
<td>Universal gas constant ($8.314472$)</td>
<td>$\text{J}/(\text{K mol})$</td>
</tr>
<tr>
<td>$s^\pi$</td>
<td>External supply of entropy to species $\pi$</td>
<td>$\text{J}/(\text{kg s K})$</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
<td>Unit</td>
</tr>
<tr>
<td>---------------</td>
<td>------------------------------------------------------------------------------</td>
<td>---------------</td>
</tr>
<tr>
<td>( \bar{S}^{\alpha,\pi} )</td>
<td>resulting macroscopic external supply of entropy to species ( \pi )</td>
<td>J/(kg s K)</td>
</tr>
<tr>
<td>( s^\alpha )</td>
<td>mean macroscopic external supply of entropy to phase ( \alpha )</td>
<td>J/(kg s K)</td>
</tr>
<tr>
<td>( \bar{s}^{\pi} )</td>
<td>molecular supply of entropy to species ( \pi )</td>
<td>J/(kg s K)</td>
</tr>
<tr>
<td>( \overline{\bar{S}}^{\alpha} )</td>
<td>macroscopic supply of entropy related to molecular interaction</td>
<td>J/(kg s K)</td>
</tr>
<tr>
<td>( s^{\alpha,\beta} )</td>
<td>macroscopic supply of entropy related to phase interaction</td>
<td>J/(kg s K)</td>
</tr>
<tr>
<td>( s^{\alpha,\beta} )</td>
<td>mean macroscopic supply of entropy related to phase interaction</td>
<td>J/(kg s K)</td>
</tr>
<tr>
<td>( S^{\pi} )</td>
<td>specific entropy of species ( \pi )</td>
<td>J/(kg K)</td>
</tr>
<tr>
<td>( S^{-\alpha,\pi} )</td>
<td>macroscopic specific entropy of species ( \pi ) in phase ( \alpha )</td>
<td>J/(kg K)</td>
</tr>
<tr>
<td>( S^{\alpha} )</td>
<td>mean macroscopic specific entropy of phase ( \alpha )</td>
<td>J/(kg K)</td>
</tr>
<tr>
<td>( S^{\alpha} )</td>
<td>degree of saturation for phase ( \alpha )</td>
<td>-</td>
</tr>
<tr>
<td>( t )</td>
<td>traction vector</td>
<td>N/m²</td>
</tr>
<tr>
<td>( t )</td>
<td>time</td>
<td>s</td>
</tr>
<tr>
<td>( T )</td>
<td>absolute temperature</td>
<td>K</td>
</tr>
<tr>
<td>( u )</td>
<td>displacement vector</td>
<td>m</td>
</tr>
<tr>
<td>( v_{d}^{\alpha,\pi} )</td>
<td>diffusive-dispersive velocity vector of species ( \pi ) in phase ( \alpha )</td>
<td>m/s</td>
</tr>
<tr>
<td>( U^{\pi} )</td>
<td>specific internal energy of species ( \pi )</td>
<td>J/kg</td>
</tr>
<tr>
<td>( \overline{U}^{\alpha,\pi} )</td>
<td>macroscopic specific internal energy of species ( \pi ) in phase ( \alpha )</td>
<td>J/kg</td>
</tr>
<tr>
<td>( U^{\alpha} )</td>
<td>macroscopic specific internal energy of phase ( \alpha )</td>
<td>J/kg</td>
</tr>
<tr>
<td>( v )</td>
<td>volume of the REV</td>
<td>m³</td>
</tr>
<tr>
<td>( v^{\pi} )</td>
<td>velocity of species ( \pi )</td>
<td>m/s</td>
</tr>
<tr>
<td>( \bar{v}^{\alpha,\pi} )</td>
<td>average velocity of species ( \pi ) in phase ( \alpha )</td>
<td>m/s</td>
</tr>
<tr>
<td>( v^{\alpha} )</td>
<td>average velocity of all species in phase ( \alpha )</td>
<td>m/s</td>
</tr>
<tr>
<td>( V )</td>
<td>volume of the body</td>
<td>m³</td>
</tr>
<tr>
<td>( w^{\alpha,\beta} )</td>
<td>velocity of an interface between phases ( \alpha ) and ( \beta )</td>
<td>m/s</td>
</tr>
<tr>
<td>( x^{\alpha,\pi} )</td>
<td>mole fraction of species ( \pi ) in phase ( \alpha )</td>
<td>-</td>
</tr>
<tr>
<td>( x )</td>
<td>position vector in the reference frame of the body</td>
<td>-</td>
</tr>
</tbody>
</table>
## Greek characters

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\alpha^\alpha)</td>
<td>thermal expansion coefficient of phase (\alpha) ((1/V)(\partial V/\partial T))</td>
<td>(K^{-1}) or (^\circ C^{-1})</td>
</tr>
<tr>
<td>(\gamma^\alpha)</td>
<td>phase distribution function of phase (\alpha)</td>
<td>-</td>
</tr>
<tr>
<td>(\gamma^{\alpha\beta})</td>
<td>surface tension at the interface between phases (\alpha) and (\beta)</td>
<td>N/m</td>
</tr>
<tr>
<td>(\delta)</td>
<td>Dirac delta distribution</td>
<td>-</td>
</tr>
<tr>
<td>(\delta_{ij})</td>
<td>Kronecker delta</td>
<td>-</td>
</tr>
<tr>
<td>(\varepsilon^\alpha)</td>
<td>volume fraction of phase (\alpha)</td>
<td>-</td>
</tr>
<tr>
<td>(\varepsilon)</td>
<td>strain tensor</td>
<td>-</td>
</tr>
<tr>
<td>(\zeta)</td>
<td>generic function</td>
<td>*</td>
</tr>
<tr>
<td>(\eta^\alpha)</td>
<td>dynamic viscosity of phase (\alpha)</td>
<td>((N \cdot s)/m^2)</td>
</tr>
<tr>
<td>(\theta, \vartheta)</td>
<td>temperature</td>
<td>(^\circ C)</td>
</tr>
<tr>
<td>(\kappa)</td>
<td>history variable (in a damage model)</td>
<td>*</td>
</tr>
<tr>
<td>(\kappa^\alpha)</td>
<td>relative permeability of phase (\alpha)</td>
<td>-</td>
</tr>
<tr>
<td>(\kappa)</td>
<td>permeability of the porous medium under single phase flow</td>
<td>m²</td>
</tr>
<tr>
<td>(\kappa^\alpha)</td>
<td>permeability</td>
<td>m²</td>
</tr>
<tr>
<td>(\lambda)</td>
<td>first Lamé parameter</td>
<td>N/m²</td>
</tr>
<tr>
<td>(\mu)</td>
<td>second Lamé parameter</td>
<td>N/m²</td>
</tr>
<tr>
<td>(\nu)</td>
<td>Poisson coefficient</td>
<td>-</td>
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<tr>
<td>(\nu^\alpha)</td>
<td>kinematic viscosity of phase (\alpha)</td>
<td>m²/s</td>
</tr>
<tr>
<td>(\xi)</td>
<td>position vector</td>
<td>-</td>
</tr>
<tr>
<td>(\sigma)</td>
<td>damage variable (Oliver)</td>
<td>l/m</td>
</tr>
<tr>
<td>(\rho^{\alpha,\pi})</td>
<td>average microscopic mass density of species (\pi) in phase (\alpha)</td>
<td>kg/m³</td>
</tr>
<tr>
<td>(\rho^\alpha)</td>
<td>average mass density of phase (\alpha)</td>
<td>kg/m³</td>
</tr>
<tr>
<td>(\rho^\pi)</td>
<td>microscopic mass density function of species (\pi)</td>
<td>kg/m³</td>
</tr>
<tr>
<td>(\sigma)</td>
<td>Stefan-Boltzmann constant ((5.67 \cdot 10^{-8}))</td>
<td>J/(m² K⁴ s)</td>
</tr>
<tr>
<td>(\sigma^\pi)</td>
<td>partial stress tensor of species (\pi)</td>
<td>N/m²</td>
</tr>
<tr>
<td>(\sigma^{\alpha,\pi})</td>
<td>macroscopic partial stress tensor of species (\pi) in phase (\alpha)</td>
<td>N/m²</td>
</tr>
<tr>
<td>(\sigma^\alpha)</td>
<td>mean macroscopic partial stress tensor of phase (\alpha)</td>
<td>N/m²</td>
</tr>
</tbody>
</table>
Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\phi^\pi$</td>
<td>surface flux vector of entropy of species $\pi$</td>
<td>J/(K m² s)</td>
</tr>
<tr>
<td>$\phi^{\alpha,\pi}$</td>
<td>macroscopic surface flux vector of entropy of species $\pi$ in phase $\alpha$</td>
<td>J/(K m² s)</td>
</tr>
<tr>
<td>$\bar{\phi}^\alpha$</td>
<td>mean macroscopic surface flux vector of entropy of phase $\alpha$</td>
<td>J/(K m² s)</td>
</tr>
<tr>
<td>$\psi^\pi$</td>
<td>typical thermodynamic property of species $\pi$</td>
<td>*</td>
</tr>
<tr>
<td>$\bar{\psi}^{\alpha,\pi}$</td>
<td>typical thermodynamic property of species $\pi$ in phase $\alpha$, macroscopic counterpart of $\psi^\pi$</td>
<td>*</td>
</tr>
<tr>
<td>$\psi^\alpha$</td>
<td>typical macroscopic thermodynamic property of phase $\alpha$</td>
<td>*</td>
</tr>
<tr>
<td>$\omega$</td>
<td>damage variable</td>
<td>-</td>
</tr>
<tr>
<td>$\Gamma$</td>
<td>boundary</td>
<td>-</td>
</tr>
<tr>
<td>$\Delta$</td>
<td>increment</td>
<td>*</td>
</tr>
<tr>
<td>$\Pi$</td>
<td>product sign</td>
<td>-</td>
</tr>
<tr>
<td>$\Sigma$</td>
<td>summation sign</td>
<td>-</td>
</tr>
<tr>
<td>$\Phi^\pi$</td>
<td>internal supply of entropy to species $\pi$</td>
<td>J/(kg K s)</td>
</tr>
<tr>
<td>$\bar{\Phi}^{\alpha,\pi}$</td>
<td>macroscopic internal supply of entropy to species $\pi$ in phase $\alpha$</td>
<td>J/(kg K s)</td>
</tr>
<tr>
<td>$\Phi^\alpha$</td>
<td>mean macroscopic internal supply of entropy to phase $\alpha$</td>
<td>J/(kg K s)</td>
</tr>
<tr>
<td>$\Omega$</td>
<td>body</td>
<td>-</td>
</tr>
</tbody>
</table>

**Roman indices**

- g: gas phase
- l: liquid phase
- s: solid phase

**Greek indices**

- $\alpha$: phase
- $\beta$: phase
- $\alpha\beta$: interface between phase $\alpha$ and phase $\beta$
- $\pi$: species
Brackets and overbars

\[ \langle \xi \rangle_\alpha \] volume average operator (with respect to phase \( \alpha \))

\[ \langle \xi \rangle^{\alpha}_\alpha \] intrinsic volume average operator (with respect to phase \( \alpha \))

\[ \bar{\xi}^{\alpha} \] mass average operator (with respect to phase \( \alpha \))

\[ \bar{\xi}^{\alpha} \] area average operator (with respect to phase \( \alpha \))

\[ \| \xi \| \] L2 norm

\[ [ \xi ] \] discontinuous jump

\[ \hat{\xi} \] regular component

\[ \tilde{\xi} \] enhanced component

\[ \bar{\xi} \] variable at molecular level

\[ \bar{\xi} \] variable collecting several other variables

\[ \xi|_b \] difference between \( \xi \) evaluated at \( b \) and evaluated at \( a \)

\[ \xi|_a \] evaluate \( \xi \) at \( a \)

Abbreviations

COD also CMOD, crack (mouth) opening displacement

DOF degree of freedom

EFG element free Galerkin

EPFM elastic-plastic fracture mechanics

FEM finite element method (variants: X-FEM, PU-FEM, GFEM, …)

LEFM linear elastic fracture mechanics

LHS left-hand side

NLFM non-linear fracture mechanics

PU partition of unity

RHS right-hand side

REV representative elementary volume

RH relative humidity

SEL size effect law

LVDT linear variable differential transformer
**Basic algebra**

Einstein summation convention is applied, meaning a summation over repeated indices.

Transpse of a matrix \( A \)

\[
A^T = A_{ji}
\]

Symmetric part of a matrix \( A \)

\[
A^s = \frac{1}{2} (A_{ij} + A_{ji})
\]

Anti-symmetric part of a matrix \( A \)

\[
A^a = \frac{1}{2} (A_{ij} - A_{ji})
\]

The dot product of two vectors \( a \) and \( b \) (scalar product)

\[
a \cdot b = a_i b_i
\]

The vector direct product of two vectors \( a \) and \( b \) (dyadic product)

\[
a \otimes b = a_j b_j
\]

The symmetric vector direct product of two vectors \( a \) and \( b \)

\[
(a \otimes b)^s = \frac{1}{2} (a_j b_j + a_i b_i)
\]

The double dot product of two matrices \( A \) and \( B \)

\[
A : B = A_{ij} B_{ji} \quad \text{or} \quad A : B = A_{ij} B_{ji}
\]

The cross product of two vectors \( a \) and \( b \) (vector product)

\[
a \times b = \begin{bmatrix}
    a_yb_z - a_zb_y, & a_zb_x - a_xb_z, & a_xb_y - a_yb_x
\end{bmatrix}^T
\]

The matrix direct product of two matrices \( A \) (m x n) and \( B \) (p x q)

\[
A \otimes B = C \quad \text{where} \quad C_{p(\cdot-1)+k,q(\cdot-1)+l} = A_{ij} B_{kl}
\]

Multiplication of a matrix \( A \) and a vector \( a \)

\[
Aa = A_j a_j
\]

Multiplication of a vector \( a \) and a matrix \( A \)

\[
aA = A_i a_i
\]

Multiplication of two matrices \( A \) and \( B \)

\[
AB = A_{ik} B_{kj}
\]
Nomenclature

Multiplication of 4th order tensor $C$ and a matrix $A$

$$CA = C_{ijkl}A_{kl}$$

Multiplication of a matrix $A$ and a 4th order tensor $C$

$$AC = A_{ij}C_{ijkl}$$

Multiplication of a 4th order tensor $C$ and a vector $a$

$$Ca = C_{ijkl}a_l$$

Multiplication of a vector $a$ and a 4th order tensor $C$

$$aC = a_lC_{ijkl}$$

The L2 norm of a vector $a$

$$\|a\| = (a_1a_2)^{\frac{1}{2}}$$

The L2 norm of a matrix $A$

$$\|A\| = (A_{ij}A_{ij})^{\frac{1}{2}}$$

Trace of a matrix $A$

$$tr(A) = A_{ii}$$

The gradient of a scalar function $f$

$$\text{grad}(f) = \nabla f = f' = \left[ \frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z} \right]$$

The gradient of a vector $a$

$$\nabla a = a_{i,j}$$

The symmetric gradient of a vector $a$

$$\nabla^s a = \frac{1}{2}(a_{i,j} + a_{j,i})$$

The divergence of a vector $F$ is defined as

$$\text{div}(F) = \nabla \cdot F = \frac{\partial F}{\partial x} + \frac{\partial F}{\partial y} + \frac{\partial F}{\partial z}$$

Material derivative

$$\frac{D^a\psi}{Dt} = \frac{\partial \psi}{\partial t} + v^a \cdot \nabla \psi$$

Gradient theorem

$$\int_a^b (\nabla f) \cdot ds = f(b) - f(a)$$
Divergence theorem (Gauss’s theorem)
\[
\int_{\Omega} (\nabla \cdot \mathbf{F}) d\Omega = \int_{\partial \Omega} \mathbf{F} \cdot \mathbf{n} dA
\]

Kronecker delta
\[
\delta_{ij} = \begin{cases} 
1 & \text{for } i = j \\
0 & \text{for } i \neq j 
\end{cases}
\]

Dirac delta distribution
\[
\int_{\Omega} \delta_{+} (x) f(x) d\Omega = \int_{\Gamma} f(x) d\Gamma
\]

Heaviside function
\[
\mathcal{H}_{\Gamma} (x) = \begin{cases} 
1 & \text{for } x \in \Omega^+ \\
0 & \text{for } x \in \Omega^-
\end{cases}
\text{ where } \Gamma \text{ is the boundary between } \Omega^+ \text{ and } \Omega^-
\]

Unit matrix \( I \)
\[
I = \delta_{ij}
\]

Volume average operator
\[
\langle \zeta \rangle_{\alpha} (x, t) = \frac{1}{dV} \int_{dV} \zeta (r, t) \gamma^\alpha (r, t) dv
\]

Intrinsic volume average operator
\[
\langle \zeta \rangle^\alpha_{\alpha} (x, t) = \frac{1}{dV^\alpha} \int_{dV^\alpha} \zeta (r, t) \gamma^\alpha (r, t) dv
\]

Mass average operator
\[
\overline{\zeta}^\alpha (x, t) = \frac{1}{\langle \rho \rangle_{\alpha} (x, t) dV} \int_{dV} \rho (r, t) \zeta (r, t) \gamma^\alpha (r, t) dv
\]

Area average operator
\[
\overline{\zeta}^\alpha (x, t) = \frac{1}{dA} \int_{dA} \zeta (r, t) \cdot \mathbf{n} \gamma^\alpha (r, t) da
\]
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1. Introduction

1.1. Context

From the moment a structure is constructed, it starts deteriorating. Especially for porous building materials, the deterioration process is strongly related to the presence of moisture. Through open pores and micro-cracks, moisture and dissolved particles (e.g. soluble salts) can penetrate into the material, rendering the structure vulnerable to various physical, chemical and biological degradation processes. Frost damage of the wetted material is only one example of a common physical degradation mechanism. In concrete, the leaching of calcium and the alkali-silica reaction are among the most widespread chemical causes of damage. Biological degradation merely affects wood and timber structures, but also concrete and stone-like materials are indirectly exposed: since e.g. vegetation retains water, drying is hindered, and therefore the wetted material becomes more susceptible to other types of moisture-related degradation. As a result of the active degradation processes, the material properties in the wetted region are altered and stresses of various origins develop. In combination with mechanical loading, initial micro-defects may grow and coalesce into macro-cracks, hereby not only reducing the structural strength and stiffness, but also creating new pathways for preferential moisture transport, both leading to an acceleration of the degradation process.

![Figure 1.1: Examples of (a) physical, (b) chemical and (c) biological degradation processes.](image)

From the above it is clear that material degradation usually does not have a single identifiable cause, but results from a complex interaction between several processes. Insight herein can be gained by conducting well-designed laboratory investigations on the one hand, and by developing theoretical models as a basis for numerical simulations on the other hand. Both methods are complementary. Laboratory experiments are performed on the real material
structure, but in general only relatively small specimens can be tested for a limited amount of
time and subjected to simplified boundary conditions. Numerical simulations can be
performed on full scale structures, for long time spans, taking into account complex boundary
conditions, but are using simplifying assumptions regarding the material structure. Including a
more detailed material structure, e.g. the composition of concrete on the meso-scale, is
possible, but implies that shorter time spans and smaller structures have to be studied - if not
the time to conduct the numerical analysis becomes prohibitively large. Therefore nowadays
much attention is directed towards the development of more efficient computational methods.
Nevertheless, the predictive capacity of a model solely depends on the ability of the
mathematical formulation to describe the observed physical phenomena correctly. In the
assessment of a proposed theory the complementary role of experimental research becomes
evident. Likewise, numerical simulations prove useful in designing experiments and
interpreting their results.
Driven by the need to understand the origin of the various degradation mechanisms and their
mutual interaction, extensive research has been carried out over the past decades, both on the
experimental and on the numerical side. For instance, standardized tests for the determination
of material properties were developed, visualization techniques became available allowing to
observe the microstructure of the material, a well-founded theoretical description of the
behaviour of continuous porous media was established, material failure under mechanical
loading was studied in detail, as well as the liquid flow in fractures, etc. Nevertheless,
material degradation is still far from being fully understood. For example, the basic
mechanism underlying corrosion in metals, which was subject of study for several decades,
has only been revealed recently by Gerhard Ertl. An achievement for which he was accredited
the 2007 Nobel Prize in Chemistry. This illustrates the fruitful interplay between basic
research and its practical application. Although the research presented in this thesis has a
much narrower scope, it also has a strong link with practice. It was motivated by some of the
challenges we are currently facing, like deciding upon the best way to conserve our historical
buildings and cultural heritage, the desire to design sustainable materials and improved
protection systems, and the determination of optimal maintenance frequencies for buildings
and civil engineering structures.
Introduction

1.2. Objectives

This research aims at developing and experimentally validating an efficient numerical model to simulate the behaviour and the degradation of porous building materials exposed to combined mechanical and hygro-thermal loading.

The following developments are envisaged:

- Incorporating the entire failure process - starting from the initial diffuse damage growth, over the subsequent formation of a failure band up to its final evolution into a macroscopic discrete crack - in a single macroscopic framework, preferably without introducing artificial parameters or parameters with a debatable physical significance.
- Taking into account the influence of the physical degradation of the material matrix on the transport processes in the pore space, and, vice versa, including the impact of the fluids inside the pore space on the mechanical behaviour.
- Designing efficient and robust algorithms to solve the resulting model equations.

To this extent, a combined experimental-numerical study has been undertaken. The cornerstone of the proposed framework is formed by a new type of cohesive zone model, ensuring a gradual transition between two states, namely the continuous state before fracture occurs, and the discontinuous state afterwards. The model essentially describes the influence of the development of a fracture on every relevant field. For example, it expresses how the fluid flow inside the material matrix is affected by the formation of a fracture. Experimental research is conducted to determine the required material properties and to assess the validity of the proposed framework.

1.3. Outline

The work consists of 9 chapters. In chapter 2, an extensive review of the state-of-the-art on the modelling of transport in and failure of porous media is given. Based on the collected literature overview on the different topics, the needs for further research are defined. The main observation is that the theory of porous media is well founded for continua, but that the influence of damage and failure is not well understood. In chapter 3, the governing equations for coupled heat and mass flow in a deformable, yet intact, porous medium are derived. Chapters 4 and 5 make up the central part of the thesis. In chapter 4, a new type of cohesive
zone model for fracture is introduced. Both the underlying concept as well as its implementation using finite elements are discussed. Selected examples show its performance to describe both material failure and interface failure. In chapter 5, the generic aspect of the new cohesive zone model is underlined, by applying the same concept to simulate heat and mass flow in fractured porous media. The aspect of imposing boundary conditions on the newly formed fracture surfaces is discussed as well. Simulations involving multiple coupled fields are time consuming. A strategy to reduce the computational cost is discussed in chapter 6. Furthermore, special attention is given to the proper treatment of discontinuous fields within the framework of the finite element method, in terms of implementation and accurate integration. In chapter 7 the model predictions are compared against experimental results. Benchmarking is performed for two reference materials, namely Meule, a layered sandstone, and masonry. The former allows analysing aspects of material failure, while the latter serves at verifying the behaviour of material interfaces. In chapter 8 the hygro-thermo-mechanical behaviour of an outside render is studied to illustrate the applicability of the proposed modelling technique in less academic cases. The conclusions of the work as well as suggestions for further research are summarised in a final chapter.
2. State of the art

The behaviour of porous building materials has been subject of study for more than a century. A concise overview of key-concepts and theories that have been developed over the years is given in this chapter. Only topics related to the present study are considered. The chapter consists of two parts. In the first part, the most relevant modelling approaches for intact porous materials are reviewed. The second part deals with the degradation of the intact material up to final failure. Attention is given to the different failure mechanisms and to the corresponding modelling techniques.

2.1. Modelling of porous continua

A porous medium or porous material is a solid (often called matrix) containing pores. These pores can form an interconnected network (known as the pore space) or can be present as isolated voids. Many building materials such as rocks, natural stones, ceramics and concrete may be considered as porous media.

As a first approximation, porous materials can be modelled by considering them as a one-component material lacking an internal structure. All defined quantities are hereby understood as averaged quantities. E.g. the material density is defined as the mass per unit volume of material, including the pore volume, and differs from the actual solid density, defined per unit volume of the matrix and hence excluding the pore volume. By using averaged quantities, the actual internal structure of the material is smeared out. The resulting homogeneous continuum can be successfully described by classical continuum mechanics.

This approach is not valid if one or more fluids (either liquid or gaseous) occupy the pore space. The different constituents or phases have their own behaviour and they mutually interact. Consider for instance a sponge saturated with water. Squeezing the sponge expels the water. Clearly, the motion of the solid matrix, the sponge, is different from that of the water initially occupying the pore space. This example illustrates that homogenizing into a one-component material is not appropriate for multi-phase porous media.

The most straightforward strategy to proceed is probably to model all individual constituents, and to apply the axioms of mechanics and thermodynamics to each of them separately. That
requires, amongst other aspects, modelling the complicated geometry of the actual pore space and the knowledge of the spatial variation of the material properties. Although it can be expected that such an approach would lead to excellent results, it is not suitable for most engineering problems. Modelling the pore space would be extremely tedious, if not unfeasible, and the actual variation of material properties is usually not known. Moreover, resolving the porous media problem with such a high level of detail is often not necessary. Returning to the example of the squeezed sponge, interest probably goes out to the amount of water that is expelled, rather than to the individual trajectories of each water molecule. Some problems can not be modelled properly using a macroscopic model, and require advanced multi-scale modelling techniques, incorporating the relevant features from lower scales. For most engineering problems however, a macroscopic approach is preferred over a description at the lower scale.

The question how to derive a macroscopic theory for multi-phase porous media has occupied scientists during the entire 20th century, although some fundamental concepts were already discovered in the preceding centuries. For an excellent overview on the historical developments in this field the interested reader is referred to de Boer (2000). Nowadays, the existing theories can broadly be classified in three groups: (i) phenomenological theories, (ii) theories originating from mixture theory, and (iii) theories relying on averaging techniques. Phenomenological theories were based on the pioneering work of Karl von Terzaghi (1883-1963). He was the first to elaborate a comprehensive theory on the mechanics of soils with his publication of *Erdbaumechanik auf bodenphysikalischer Grundlage* in 1925. Later, Maurice Biot (1905-1985) developed the phenomenological approach of von Terzaghi further (Biot 1941, Biot 1956a). In the period between 1935 and 1962 he published a number of scientific papers that laid the foundations of the theory now known as poroelasticity (Biot 1941, Biot 1956b,c), which describes the mechanical behaviour of fluid-saturated porous media. More recently, a macroscopic thermodynamic foundation of Biot’s theory was developed by Coussy (1995).

A second, often disregarded, family of phenomenological models exists. They emerged from the work of Edgar Buckingham (1867-1940) in the field of soil water physics (Buckingham 1907). Richards elaborated on the work of Buckingham, and presented a partial differential equation governing water transport in unsaturated, non-deformable soils (Richards 1931). Later, vapour transport was included as well (Philip 1954) and the theory has been extended to non-isothermal situations (Philip and De Vries 1957). Recently this transport theory
developed into a porous media theory by incorporating the effect of deformation of the soil (Jiang et al. 1994, Thomas et al. 1995).

Classical mixture theories stem from the work of Josef Stefan (1835-1893) and James Maxwell (1831-1879) on gas mixtures. In contrast to gas mixtures, the assumption of miscibility of the constituents does not hold for multi-phase porous media: each spatial point in a porous medium is either occupied by solid matrix, or by fluid. Modern mixture theory therefore makes use of the volume fraction concept, already conceived by Reinhard Woltmann in 1794, to describe at a macroscopic level the underlying microstructure (Woltmann 1794). The first mixture theory restricted by the volume fraction concept was developed by Morland (1972). However, a general one-dimensional version was already published in 1936, by a contemporary of Terzaghi, namely Paul Fillunger (1883-1937) (Fillunger 1936). Unfortunately, his contribution was nearly completely forgotten after his dead, and only rediscovered in the late 1980s. The theory of incompressible and compressible porous media was given a stronger thermodynamic background by Bowen (1980, 1982). Recent research focused on the incorporation of different material behaviour (a.o. de Boer and Kowalski 1983, de Boer and Ehlers 1986), on the study of particular phenomena, like e.g. the uplift, friction and capillarity (a.o. de Boer and Ehlers 1990) and on further improving the theoretical foundations (a.o. Li 1992).

A third approach to derive multi-phase equations employs the technique of local volume averaging. The classical balance laws of continuum mechanics, that govern the state of the system at the lower scale, are averaged over some local representative volume. The averaged, macroscopic equations are written in terms of macroscopic thermodynamic quantities. First attempts in this direction were undertaken by Whitaker (1967) and Bear (1972) for the mass transport equation. In 1977 Gray presented elegant proofs of the required averaging theorems (Gray and Lee 1977). Later Hassanizadeh and Gray developed a complete set of averaged balance equations for a multiphase porous medium (Hassanizadeh and Gray 1979a,b). In their work, the constitutive equations are obtained by systematically exploiting the entropy inequality according to the methodology proposed by Coleman and Noll (1963). An early implementation of the theory of Hassanizadeh and Gray was accomplished by Gawin and Schrefler (1996). In the early 1990s the attention shifted to the theoretical treatment of the interface between the different phases (Gray and Hassanizadeh 1989, Hassanizadeh and Gray 1990). The approach was also extended to the case where each phase consisted of a mixture of multiple components (Achanta et al. 1994).
Of the three methods discussed above, the averaging technique seems to provide the best framework to advance understanding of multi-phase flow, but the derivations can be tedious especially if the thermodynamics of the interfaces is taken into account. Nevertheless, it is obvious that, under the right assumptions, all theories should provide the same macroscopic set of equations. The equivalence between the theory based on volume averaging and the one based on mixture theory has been shown by de Boer et al. (1991). The correspondence of the latter with the phenomenological approach was proven by Coussy et al. (1998). These similarities demonstrate the essential correctness of the macroscopic equations for multiphase porous continua. However, theories for discontinuous media have not yet arrived at the same state of maturity, as will be shown in the remaining part of this chapter.

2.2. From continuous to discrete

In this section, we will first focus on the mechanical aspects of the failure process. Both the failure mechanism and the available modelling techniques will be discussed. Afterwards, attention is given to the impact of the degradation of the bulk material on the multiphase transport processes.

2.2.1. Failure characterisation

A material is said to be brittle if it is liable to fracture when subjected to stress. In e.g. glass and cast iron, discrete cracks develop almost immediately after reaching the strength of the material and brittle failure is observed. Hereby, relatively little energy is absorbed, even in materials of high strength. Most materials however do not exhibit a perfectly brittle response, but allow for some ductility, i.e. some energy dissipation prior to fracture. Plastic (or irreversible) deformations and the nucleation and growth of micro-cracks are two examples of such dissipation mechanisms. The former is of major importance in metal forming processes, whereas the latter is an important degradation mechanism of so-called quasi-brittle materials like concrete, rock and ceramics. But regardless the amount of dissipated energy, the final rupture will always be brittle to some extent.

The amount of dissipated energy during fracture depends on various factors. Both metallic and non-metallic materials exhibit a more brittle behaviour when subjected to higher loading rates and lower temperatures. For quasi-brittle porous materials, loading rate and temperature are not the only influencing factors. Also the degree of saturation influences the brittleness of the response.
The failure process of quasi-brittle materials is schematically depicted in Figure 2.1. In general it can be assumed that a material contains voids, flaws and initial defects (point A). If the material is subjected to relatively low load levels, no additional damage will occur: the material behaves elastically and the loading process is entirely reversible (stage A-B). Both linear and non-linear elastic behaviour can take place. At higher load levels (beyond point B), new defects nucleate, other defects coalesce and micro-cracks form. During the damage process, loads must be redistributed from damaged to intact parts. As long as redistribution can take place, the material can bear additional external loading (stage B-C). Eventually, the possibilities to redistribute the loading are locally exhausted. In that region strain localisation occurs, i.e. deformations (and damage growth) concentrate in that area (stage C-D, top figure). The external load applied on the structure must be decreased correspondingly in order to prevent sudden failure. The material outside the localisation region is therefore unloading.

Figure 2.1: Schematic representation of the different stages in the failure process of quasi-brittle materials, loaded in tension.

Figure 2.2: Schematic representation of the different crack propagation modes (Based on Parton 1992, Fig. 47).
and will not damage further (stage C-D, bottom figure). Finally, the micro-cracks in the localization region develop into a dominant macro-crack, and rupture occurs (point D). When referring to the global behaviour, stage A-B, B-C and C-D are usually termed the elastic, hardening and softening regime, respectively.

In the previous paragraph, macro-crack development under tensile loading was described. In general, we distinguish between three ways of applying a force to enable crack initiation and propagation:

- **Mode I (opening mode):** a tensile stress acting normal to the plane of the crack
- **Mode II (in-plane shear or sliding mode):** a shear stress acting parallel to the plane of the crack and perpendicular to the crack front
- **Mode III (out-of-plane shear or tearing mode):** a shear stress acting parallel to the plane of the crack and parallel to the crack front

Figure 2.2 schematically depicts the three pure loading modes. Real loading conditions, leading to crack propagation, can always be decomposed into a combination of pure modes. For quasi-brittle materials, mode I is the predominant failure mechanism.

### 2.2.2. Modelling failure processes

**Figure 2.3:** Schematic one dimensional representation of differences between continuous and discontinuous failure descriptions, in terms of displacement and strain field.

Modelling material behaviour and the prediction of failure have been a major research topic over the last two centuries. Traditionally, distinction is made between continuous and discontinuous descriptions of failure.
2.2.2.1. Continuum models: a continuous description of failure

Continuum models rely on the fundamental assumption that the motion of a body, as well as the fields representing properties of the material(s) composing the body, satisfy certain smoothness requirements\(^1\). The displacement field must for example be smooth and continuous throughout the entire body (Figure 2.3, first column). It is obvious that a continuum model is - by definition - not capable to describe the development of true discontinuous features like e.g. a crack.

Classical continuum models relate the stress state at a point to the strain state and the loading history at that point. In the study of failure, two major types of continuum models are distinguished, depending on the way in which strain localisation is treated. Damage formulations depart from the idea that micro-cracking is the major reason for localization. These micro-cracks are not explicitly modelled, but are represented on a higher scale by a damage variable, being a scalar in isotropic damage theories (Kachanov 1958, Janson and Hult 1977), or a tensorial quantity in anisotropic theories (Caboche 1981). With increasing damage in a region, the stiffness of the material is decreased and deformations will increase. In plastic theories, it is assumed that material rearranges in the localization region, giving rise to permanent deformations. Also here, the actual rearrangement is not modelled, but the resulting ‘flow’ is represented at a higher scale by means of a variable, namely the plastic multiplier. Like for damage formulations, both isotropic and anisotropic plastic theories have been developed (Hill 1998). The unloading stiffness is not affected by the plastic deformation.

From a conceptual point of view, damage theories apply to brittle materials (glass, rock, ceramics), whereas plastic theories describe mechanisms present in ductile materials (especially metals). In practice, both damage and plasticity models as well as combined-damage-plasticity models are used in the modelling of brittle, quasi-brittle and ductile materials.

Classical continuum models that include strain softening theoretically predict final failure in a band of zero width. Since the amount of work, performed during the fracture process, is integrated over the volume of the failure band, and since the width of this band tends towards zero, final rupture will occur without energy dissipation. At that moment, the governing equations become ill-posed. In order to maintain well-posed governing equations and in order to obtain physically meaningful results in the presence of strain softening, non-classical continuum models were introduced. The main difference with their classical counterparts is

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\(^1\) See textbooks on continuum mechanics, e.g. Chadwick 1999.
that the stress at a point is not only a function of the strain state and the loading history at that point, but also of at least one additional parameter. This parameter acts as a length scale, controlling the width of the localization zone. Depending on the choice for the additional parameter, we speak of non-local theories (Pijaudier-Cabot and Bažant 1987) or gradient theories (Peerlings et al. 1996). Well-posed equations can also be obtained by incorporating rate-dependent terms (Sluys and de Borst 1992).

2.2.2.2. Discrete models: a discontinuous description of failure

In a discontinuous approach to failure the requirements of smoothness and continuity are relaxed. The displacement field can for example exhibit a jump across a plane, rendering the theory potentially suitable to describe the behaviour of fully fractured bodies (Figure 2.3, last column).

One of the first discontinuous approaches was the use of linear elastic fracture mechanics (LEFM). In LEFM, the theory of elasticity is used to calculate the stress in a fractured, isotropic, linear elastic body. The theoretically obtained stress field is singular (i.e. infinite) at the crack tip, whereas in reality, inelastic deformations in a zone around the crack tip would limit the stresses to finite values (Figure 2.4a,b). To overcome the singularity, the stress field is decomposed into a product of a singular field, independent of the specific geometry and loading conditions, and a proportionality factor, named the stress intensity factor. Based on energy considerations, Irwin (1957) found that crack propagation would take place if the stress intensity factor would exceed a critical, material dependent value, called the fracture toughness. A fundamental assumption in Irwin's linear elastic fracture mechanics is that the size of the inelastic zone is small compared to the crack length. Non-Linear Fracture Mechanics (NLFM), also often called Elastic-Plastic Fracture Mechanics (EPFM), was developed to overcome this limitation. In NLFM, the J-integral (Rice 1968) takes the role of the stress intensity factor.

By using an energy-based criterion, LEFM and NLFM succeed in predicting crack propagation, although the stress field ahead of the crack tip is not accurately described. Dugdale (1960) and Barenblatt (1962) proposed to model the inelastic deformations ahead of the crack tip as cohesive forces (tractions) acting on a fictitious extension of the crack surface (Figure 2.4c). The magnitude of these tractions is given by a discrete model. While continuum models relate stresses to strains, discrete models express tractions in terms of the distance between the crack surfaces. Discrete models can be seen as jump conditions, imposed on surfaces. In the late seventies, Hillerborg et al. (1976) introduced the concept of fracture
energy, i.e. the energy dissipated during fracture, into the cohesive crack model and proposed a number of traction-displacement relationships for concrete.

Discrete models incorporate the localised nature of cracks. Therefore anisotropic behaviour naturally develops as cracking occurs. But more importantly, some classical problems encountered with continuum models are circumvented. For instance, the amount of work performed during the fracture process is integrated over the finite fracture area. Since the fracture surface has a non-zero area, the rupture goes hand in hand with non-zero energy dissipation, and additional regularization - like for continuum models - is unnecessary.

Several strategies have been developed to carry out numerical simulations of cohesive crack growth. The majority of them were designed within the framework of the finite element method (FEM).

The first approach consists in using zero-thickness interface elements (Goodman et al. 1968). These special elements are placed between neighbouring classical finite elements, along the expected crack path. This allows e.g. to model bond slip (Rots 1985). If the crack path is not known in advance, either remeshing is applied (Ingraffea et al. 1985), or a sufficiently fine mesh must be used containing interface elements along all inter-element boundaries (Xu and Needleman 1994, Camacho and Ortiz 1996, Tijssens et al. 2000). Since the crack path has to follow the element boundaries, some degree of mesh dependency cannot be avoided with the latter methodology. Furthermore, the high number of elements may lead to substantial calculation times. Finally, a (theoretically infinite) dummy stiffness is usually required to keep the inactive interface elements closed. The dummy stiffness might cause a poor conditioning of the system of equations and consequently inaccurate results. Other formulations use Lagrange multipliers and do not suffer from poor conditioning (Camacho and Ortiz 1996). Despite their shortcomings, interface elements are attractive because they are
straightforward in implementation and phenomena like crack branching and merging are the natural outcome of the original boundary value problem. The need for either remeshing or significant mesh refinement results from the restriction that the cohesive cracks can only propagate along element boundaries. Further research therefore aimed at developing techniques that permit arbitrary crack propagation through elements. A first step in this direction was the incorporation of a local discontinuous mode, a strain jump, in the element formulation. The strain jump captures the effect of a discontinuity in the displacement field, without actually modelling the discontinuity. These so-called enhanced assumed strain models or embedded discontinuity models were first used to model shear bands (Ortiz et al. 1987, Belytschko et al. 1988, Simo and Rifai 1990), but later also crack propagation was investigated (Oliver 1996). A comparative study regarding the performance and stability for a large number of embedded discontinuity methods has been undertaken by Jirásek (2000).

A next step consists in introducing the discontinuity directly in the displacement field. This advance relies on a seminal paper by Babuška, Caloz and Osborn (1994) dealing with the design of specific shape functions to obtain a better approximation of the solution of the investigated differential equation. Pursuing this idea, Melenk and Babuška 1996 developed the Partition of Unity Finite Element Method (PU-FEM). The method allows to incorporate a local approximation, reflecting a priori knowledge about the solution, in the finite element approximation, hereby preserving the classical displacement variational setting. One possible local approximation would be a discontinuity in the displacement field. Moes et al. (1999) and Belytschko and Black (1999) were among the first to use PU-FEM with a discontinuous approximation and termed it the extended finite element method (X-FEM). Later extensions to X-FEM include the incorporation of contact and frictional forces (Dolbow et al. 2001) and cohesive traction laws (Wells and Sluys 2001).

For completeness we mention that the finite element framework is not the only possible methodology to model cohesive crack growth. Also the Boundary Element Method (BEM) can be used (Yang and Ravi-Chandar 1998) or meshless methods, like the Element-Free Galerkin method (EFG) (Belytschko et al. 1993) and the hp-cloud method (Duarte and Oden 1996). The latter is based on the same paper of Babuška, Caloz and Osborn (1994) that lay the foundation for PU-FEM and X-FEM. The similarities between the hp-cloud method and PU-FEM inspired Duarte and Oden (2000) to publish the fundamentals for a wide class of Generalized Finite Element Methods (GFEM).
2.2.3. Modelling of fractured porous continua

In the previous section, the focus was on the mechanical aspects of failure, namely the formation of a localization zone and its development into a discrete crack. During this process, the material structure changes, and consequently its properties will do as well. Experimental research shows e.g. an increase in moisture permeability with increasing crack width (a.o. Aldea et al. 1999). Another consequence of crack formation is that the contact area between solid and liquid increases, hereby intensifying the possible interaction between both constituents.

2.2.3.1. Fluid flow in damaged regions

In literature, several models can be found that describe transport in damaged porous media. Like for the modelling of failure, distinction can be made between continuum and discrete approaches to transport.

Within the continuum family, a prominent place is taken by the dual permeability models (also called dual porosity models). Here the damaged and undamaged regions are assigned different permeabilities. The increased permeability in the damaged region is obtained from an empirical law based on an averaged crack width (a.o. Bažant et al. 1987, Gérard et al. 1996, Gérard and Marchand 2000). Despite their popularity, dual permeability models, and basically all continuum transport models, suffer from several shortcomings. The local permeability of a crack highly depends on features like the average crack width, the roughness and tortuosity of the crack surfaces, and the connectivity of the crack network. By modelling cracks as continuum features, none of these aspects are explicitly accounted for. It can be expected that the continuum approach would yield good results for a diffuse network of interconnected micro-cracks. For macro-cracks, which act as preferential flow channels, discrete models are preferred.

The latter approach consists in explicitly modelling the fractures and using a discrete model to describe the flow in them (e.g. Vandersteen 2002, Vandersteen et al. 2003, Roels et al. 2003, Carmeliet et al. 2004). Discrete transport models often employ a moving front technique (a.o. Karlsen et al. 1998) to track the position of the menisci between the liquid and gaseous phases. Phenomena such as preferential flow and air entrapment can be adequately modelled.

2.2.3.2. Fluid-solid interaction in damaged regions

The pressure acting on the solid matrix depends on many factors, for instance, on the kind of fluids occupying the pore space and the resulting fluid-solid interfacial tension, on the
geometry of pore walls and menisci, and on the pressure in the fluid phases. Furthermore, if the porous material dilates, the volume of the pore space might change. The ratio between the change in pore volume and the dilatancy is expressed by the Biot coefficient. Experimental procedures for the determination of the Biot coefficient in damaged materials (Shao 1998) indicate a strong dependence of the Biot coefficient on the growth of micro-cracks. This is taken into account in recently proposed continuum models (Shao 1998, Carmeliet 1998, Lydzba and Shao 2000). In discrete cracks, the dominant fluid-solid interaction term is the fluid pressure acting on the fracture surface (e.g. pressure induced cracks in dams).

### 2.3. Need for further research

The preceding brief literature survey illustrates that multiphase porous media received much scientific interest over the past centuries. During that period, the porous media theory for continua has reached a state of maturity, meeting the principles of mechanics and thermodynamics. Various failure mechanisms have been studied, resulting in two distinct classes of models: continuum and discrete models. This duality exists for mechanical models as well as for transport models. It is clear that continuum models are conceived to describe the behaviour of continua, whereas discrete models were devised to advance our understanding of discrete phenomena.

The study of failure of porous media necessarily involves a transition from a continuum state to a discrete state. Therefore, a combined continuous-discrete approach seems necessary. The initial behaviour of the porous continuum can be described by means of the theory of porous media. During the first stages of failure inelastic strains start to localize in certain regions, and a mechanical continuum model in combination with a continuum transport model are the best candidates to model the behaviour of the porous medium. As soon as macro-cracks appear and start dominating the response, discrete mechanical and transport models adequately describe the physical reality.

Most ingredients of this continuous-discontinuous porous media theory can be found in literature. However, they generally have not been derived within a single common framework. Therefore, many open questions remain, especially related to the continuous-discontinuous transition. When do we switch from a continuum to a discrete model? How do we ensure that this transition is gradual? In this thesis a possible transition-strategy is proposed and the tools needed to perform efficient and robust numerical analyses based on this strategy are developed.
In the state of the art, three different strategies to arrive at a theory for porous continua were discussed. For specific situations, the different strategies were shown to yield the same set of governing equations, pointing out the essential correctness of the obtained theory. Out of the three approaches, the one based on local volume averaging seems to provide the best framework to reveal the implicit assumptions fundamental to the macroscopic theories currently in use. The approach starts from the fundamental axioms of continuum mechanics and thermodynamics. The majority of the assumptions are only introduced at the final stages of the analysis in order to reduce the complexity of the resulting set of macroscopic equations. Introducing simplifications a posteriori, implies that the foregoing derivation is rather general, yet tedious and laborious. A macroscopic theory, like poromechanics, provides less insight in the actual physical phenomena, but is thermodynamically sound and is more readily applicable in practice. Therefore, a hybrid approach is proposed here.

We envisage the development of a porous media theory that can be used in the study of hygro-thermo-mechanical degradation processes. Such a theory was devised by Lewis and Schrefler (1998), using the formalism of Hassanizadeh and Gray (1979a,b). However, assumptions on the number of phases, the number of constituents per phase (e.g. the gas phase is a binary mixture between dry air and water vapour) and the possible interaction between the phases (e.g. phase change) were introduced, almost at the onset of the derivation. Hassanizadeh and Gray have outlined the methodology to obtain equations (i) for a multi-phase system, including phase interaction (Gray 1983) and (ii) for a single multi-component fluid in a porous medium, including component interaction (Hassanizadeh 1986a,b). We will proceed along the same lines to obtain general equations for a multi-phase, multi-component system. The advantage of specifying the actual number of phases and constituents only at the endpoint is twofold. First of all, it paves the way to different fields of application. E.g. the study of oil recovery techniques like steam assisted gravity drainage (SAGD), where four phases play a role, namely water, steam, oil and the solid material. Another example is the study of CO₂ sequestration (i.e. storage) in subsurface aquifers, where the ion transfer is of major importance. Introducing the limitations at a later stage in the derivation has another
advantage: the formalism becomes recursive. On the micro-scale each phase is a mixture of a number of constituents. At the macro-scale, the porous medium appears as a ‘mixture’ of phases. The governing equations at each scale not only have the same format, the present variables also have the same meaning at their respective scales. The link between a variable at the macro-scale and his lower-scale counterpart is derived, and, because of the similarity between the governing equations at both scales, this relation could be applied recursively to link a series of scales. Although the practical use of this observation is limited, it adds to the theoretical understanding of the scope of the variables.

The theory is initially derived under the simplifying assumption that the interfaces between the different phases do not possess thermodynamic properties (like e.g. surface tension). This does not imply that phase interaction is not accounted for, but precludes the study of interface phenomena. In a later stage poromechanical concepts are used to include the global effect of interface phenomena. Hence, the theory presented here contains elements from mixture theory (components within a phase), volume averaging (phases within a continuum) and poromechanics (interface thermodynamics). Taking into account the interface behaviour in the averaging procedure is feasible (Hassanizadeh and Gray 1990, Achanta et al. 1994) but leads to a complex formalism. In order to meet practical requirements, a large number of simplifying assumptions need to be adopted a posteriori, hereby undoing the advantages of the cumbersome derivation to some extent. A macroscopic poromechanical approach offers a more elegant way to introduce the effect of interface thermodynamics.

The chapter starts with a short overview on the principles needed to derive the macroscopic balance equations for mass, momentum, energy and entropy of a multi-component multi-phase system. After a concise treatment of the kinematics of a porous medium in section 3.2, the actual derivation and the underlying assumptions of the governing equations are presented (section 3.3). In section 3.4, the general set of equations is transformed to a tractable set of equations by stepwise introducing several simplifications. All derivations are intentionally kept short or are given in the appendices.

This chapter should be looked upon as a concise compendium on porous media theory. Its purpose is to introduce notation, some fundamental concepts and the particular continuum theory used in the examples in the remainder of the thesis. It allows focusing more on the novel developments in the subsequent chapters.
3.1. Description of a porous medium

3.1.1. Scales of observation

In reality all quantities vary both in space and in time. Even a well-defined quantity like e.g. the mass density of a material is not at all constant. Figure 3.1 schematically depicts the mass density of a concrete sample as a function of the sample volume. For samples with a characteristic size smaller than or equal to the characteristic dimension of the material heterogeneity, a large scatter is observed. The fluctuations decrease with increasing sample size, to reach a plateau value. It is appropriate to denote this plateau value the average mass density of the material, and the smallest sample volume from which the averaged quantity can be determined is termed the representative elementary volume or REV. Since all quantities will exhibit a different spatial and temporal variation, the size of the REV is not unique, but depends on the quantity of interest.

![Figure 3.1: Schematic representation of the mass density of concrete as a function of the sample volume.](image)

The condition for a REV to exist is that its characteristic size \( l \) is sufficiently larger than the characteristic size of the lower-scale heterogeneity \( \ell \). This condition is referred to as the principle of separation of scales, and can be expressed as:

\[
\ell \ll l
\]  

(3.1)

However, the quantities obtained by homogenization (or averaging) over a REV can only be used for a continuous description of a sufficiently large material sample, i.e. the characteristic size of the sample \( L \) must be much larger than the size of the REV.

\[
l \ll L
\]  

(3.2)

Most of the time, \( L \) and \( \ell \) are separated by several orders of magnitude, hence the REV-concept can be understood as a way to bridge scales, i.e. it allows to make predictions on a higher scale, avoiding the need to know the exact lower scale structure. The mass of a concrete beam can be estimated by multiplying the average density of the heterogeneous material concrete with the volume of the beam. The average density is obtained from the volume fractions of the different phases (granulates, sand, water, cement) and the average
density of each phase. Both the volume fractions and the average density of the phases are macroscopic quantities. They are obtained from the analysis of a much smaller concrete sample, but still sufficiently large to have a representative meso-structure. However, the density within a phase (e.g. an aggregate) is not constant either. Again, the REV-concept could be used to bridge the meso-scale to the micro-scale. And one could continue to even lower scales, as long as the separation of scales principle holds. If the problem of interest does not allow defining a REV, the averaging techniques are invalid, and more precise techniques must be adopted (e.g. multi-scale modelling).

### 3.1.2. Averaging concepts

#### 3.1.2.1. Setting the scene

Consider a body $B$ occupying a volume $V$, bounded by the surface $A$ and having a characteristic dimension $L$. Each point in $B$ is the centre of a REV with volume $v$, bounded by surface $a$ and having a characteristic size $l$. Because of the separation of scales principle ($\ell \ll L$), the volume $v$ corresponds to an infinitesimal volume $dV$ of $B$. The REV contains heterogeneities with a characteristic size $\ell$ and $\ell \ll l$. Each phase $\alpha$ occupies a part $v^\alpha$ (or $dV^\alpha$) of the total volume $v$ of the REV. In general $v^\alpha$ is not a single continuous phase, but the union of a large number of isolated sub-regions. Sub-regions of different phases are separated by interfaces.

![Figure 3.2: Typical averaging volume $dV$ of a porous medium consisting of three constituents.](image)

#### 3.1.2.2. Phase distribution function

Let the position of a point of the body $B$ at time $t$ be described by position vector $x$ in the global reference frame. If a point in the REV is indicated with position vectors $r$ and $\xi$ in the global and local reference frame respectively, the following relation holds:

$$ r = x + \xi $$  \hspace{1cm} (3.3)

Define the phase distribution function $\gamma^\alpha$ for a phase $\alpha$ as (Gray and Lee 1977):
where $t$ denotes time and $N$ is the total number of phases. The function $\gamma^\alpha$ is not defined on the interfaces, but its right- and left-sided limit do exist. The phase distribution function plays an important role in the averaging theorems. It may be used to obtain the part of the volume of the REV occupied by phase $\alpha$ [m$^3$]

$$dV^\alpha(x,t) = \int_{V^\alpha} \gamma^\alpha(x + \xi, t) \, dv$$

(3.5)

Thus the integration is performed over the REV, in the local $\xi$-coordinate system. Analogously, the part of the surface of the REV in contact with phase $\alpha$ is given by [m$^2$]

$$dA^\alpha(x,t) = \int_{S^\alpha} \gamma^\alpha(x + \xi, t) \, da$$

(3.6)

The volume fraction $\varepsilon^\alpha$ of phase $\alpha$ [dimensionless] is defined as

$$\varepsilon^\alpha(x,t) = \frac{dV^\alpha}{dV} = \frac{1}{dV} \int_{V^\alpha} \gamma^\alpha(x, t) \, dv$$

(3.7)

It can be verified that $\sum_{\alpha} \varepsilon^\alpha = 1$ and $0 \leq \varepsilon^\alpha \leq 1$.

### 3.1.2.3. Averaging operators

Averaged quantities can be obtained from their microscopic counterparts by applying an appropriate averaging operator. Depending on the physical nature of the quantity, a different operator must be applied. For a volume-related quantity $\zeta$, the volume average operator and intrinsic volume average operator are defined as:

$$\langle \zeta \rangle_{av} (x,t) = \frac{1}{dV} \int_{AV} \zeta(x, t) \gamma^\alpha(x, t) \, dv$$

(3.8)

$$\langle \zeta \rangle_{av} (x,t) = \frac{1}{dV^\alpha} \int_{AV} \zeta(x, t) \gamma^\alpha(x, t) \, dv$$

(3.9)

Both operators are related via the volume fraction $\varepsilon^\alpha$ of phase $\alpha$:

$$\langle \zeta \rangle_{av} = \varepsilon^\alpha \langle \zeta \rangle_{av}$$

(3.10)

The operators (3.8) and (3.9) can e.g. be used to obtain the macroscopic density of phase $\alpha$ [kg/m$^3$] from the microscopic density $\varrho(x,t)$:

$$\langle \varrho \rangle_{av} = \varepsilon^\alpha \langle \varrho \rangle_{av}$$

(3.11)

Two other types of operators are frequently used as well: the mass averaging operator and the area averaging operator:
\[ \zeta^a(x,t) = \frac{1}{\langle \rho \rangle_a(x,t)} \int_{dV} \rho(r,t) \zeta(r,t) \gamma^a(r,t) \, dv \quad (3.12) \]

\[ \zeta^a(x,t) \equiv \frac{1}{dA} \int_{dA} \zeta(r,t) \cdot n \gamma^a(r,t) \, da \quad (3.13) \]

with \( n \) the outward normal to the boundary of the REV. If the mass and area averaging operators are applied on a partial quantity \( \zeta^x \), related to a certain component \( \pi \), shorthand notation will be used to avoid having multiple levels of superscripts:

\[ \zeta^{a,x} = \zeta^{x,a} \quad (3.14) \]

\[ \zeta^{a,x} = \zeta^{x,a} \quad (3.15) \]

### 3.2. Kinematic equations

Kinematics is the study of motion and deformation of a body or body part, without investigating their cause. A porous medium can be considered as a superposition of overlapping continua at each point, whereby each continuum represents a lower-scale component in an averaged sense. At the higher scale, the kinematics of the individual continua can be studied independently. The interaction between the different continua is guaranteed by means of the volume fraction concept (3.7), and is dealt with in the next section (section 3.3).

The motion \( \phi \) relates the original position of every point in the continuum, denoted by \( X \), to their new position \( x \) at time \( t \), and can be mathematically expressed as:

\[ x = \phi(X,t) \quad (3.16) \]

For a fixed time \( t \), the above equation represents a mapping between the undeformed and the deformed state. For a fixed material point \( X \), equation (3.16) describes the motion of that point as a function of time. If two neighbouring points have different motions, deformation takes place. The study of deformation of a body heavily relies on the definition of the deformation gradient tensor \( F \):

\[ F = \frac{\partial \phi}{\partial X} \quad (3.17) \]

\( F \) transforms a vector \( dX \), connecting the two neighbouring points in the initial (undeformed) configuration, into a vector \( dx \), connecting the same material points in the current (deformed) configuration:

\[ dx = FdX \quad (3.18) \]
The deformation gradient tensor implicitly performs two independent operations: the vector $dX$ is both stretched and rotated. A general measure of deformation that solely relates to the stretching operation is the Lagrangian or Green strain tensor $E$:

$$E = \frac{1}{2} (F^T F - I)$$ (3.19)

Motion and deformation take place over time. It is often of interest to know the rate at which they take place. To that extent the material time derivative is introduced. For an arbitrary function $\zeta(X,t)$, expressed in initial or material coordinates $X$, it is defined as:

$$\frac{D^\alpha \zeta}{Dt} = \frac{\partial \zeta}{\partial t}|_X$$ (3.20)

The superscript $\alpha$ indicates that the material coordinates $X^\alpha$, referencing the points in phase $\alpha$, are held constant during differentiation. As a practical example, consider the velocity field $v^\alpha$ of the points in phase $\alpha$. It is obtained by taking the material time derivative of the motion (see (3.16)) of each point:

$$v^\alpha = \frac{D^\alpha \phi}{Dt} = \frac{\partial \phi}{\partial t}|_X$$ (3.21)

The material time derivative of an arbitrary function $\zeta(x,t)$, expressed in terms of the spatial position $x$ and current time $t$, is obtained by applying the chain rule of differentiation:

$$\frac{D^\alpha \zeta}{Dt} = \frac{\partial \zeta}{\partial t} + \frac{\partial \zeta}{\partial x} \frac{\partial x}{\partial t}|_X = \frac{\partial \zeta}{\partial t} + (\nabla \zeta) \cdot v^\alpha$$ (3.22)

where the definition of motion (3.16) and velocity (3.21) have been used. Note that the time derivative is actually moving together with the phase $\alpha$.

### 3.3. Conservation laws

#### 3.3.1. Methodology

In the simplest case we define two scales (Figure 3.3). At the lower scale, we consider the real, non-homogeneous, structure of the material. Each point belongs to either a phase or an interface between two phases. At the higher scale, the heterogeneous structure of the porous medium can be replaced by a model in which each phase is assumed to fill up the entire domain. Hence a phase is assumed continuous over the domain and the porous medium is considered as a superposition of overlapping continua at each point. We will apply the local volume averaging technique to obtain the higher scale description.
3.3.2. General microscopic balance equations

We consider a multiphase porous medium, where each phase is considered as a mixture of $n$ components. The balance equation for a typical thermodynamic property $\psi^\pi$ of component $\pi$ at a spatial point $r$ within phase $\alpha$, having a flux vector $i^\pi$, a molecular supply $f^\pi$, an internal supply $g^\pi$, and an external supply $g^\pi$ is given by (Hassanizadeh 1986)²:

$$\frac{\partial}{\partial t} \left( \rho^\pi \psi^\pi \right) + \nabla \cdot \left( \rho^\pi \mathbf{v}^\pi \psi^\pi \right) - \nabla \cdot \mathbf{i}^\pi = \rho^\pi \mathbf{f}^\pi + \rho^\pi \left( f^\pi + g^\pi \right)$$  \hspace{1cm} (3.23)

where $\rho^\pi$ is the mass of component $\pi$ per unit volume of phase $\alpha$ and $\mathbf{v}^\pi$ is the mass weighted mean velocity of the molecules of component $\pi$. The exchange of $\psi^\pi$ between the components $\pi$ in phase $\alpha$ can not give rise to a net production of $\psi^\pi$. Therefore the following restriction must hold:

$$\sum_{\pi} \rho^\pi \mathbf{f}^\pi = 0$$  \hspace{1cm} (3.24)

At the interface $\alpha\beta$, interaction takes place between the phases. The microscopic equations, governing these interactions, are provided by means of jump conditions, formulated for the individual components of adjacent phases:

² The notation used here deviates from the one used in Hassanizadeh (1986) but allows (i) more consistency (ii) a more straightforward formulation of the constraint equations and (iii) the formulation of a recurrence relation. An overview of the notational differences is given in Appendix C.
where \( \mathbf{w} \) is the velocity of the interface \( \alpha \beta \), \( \mathbf{n}^{\alpha \beta} \) is the unit normal vector pointing out of the \( \alpha \)-phase and into the \( \beta \)-phase at the interface \( \alpha \beta \). In the above equations the thermodynamic properties of the interfaces and contact lines have been disregarded. This assumption implies that systems in which mass accumulates at interfaces or in which interfacial tension and energy play an important role can not be modelled properly. The interested reader is referred to Achanta et al. (1994) for a discussion on multi-phase multi-component systems with interfaces, and the works of Hassanizadeh and Gray for a thorough treatment of multi-phase systems with interfaces. We will include the interface behaviour indirectly based on poromechanical concepts in section 3.4.3.1.

<table>
<thead>
<tr>
<th>Mass</th>
<th>Momentum</th>
<th>Energy</th>
<th>Entropy</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \psi^x )</td>
<td>( \mathbf{v}^x )</td>
<td>( U^x + \frac{1}{2} \mathbf{v}^x : \mathbf{v}^x )</td>
<td>( S^x )</td>
</tr>
<tr>
<td>( i^x )</td>
<td>( \mathbf{0} )</td>
<td>( \sigma^x : \mathbf{v}^x - \mathbf{q}^x )</td>
<td>( \phi^x )</td>
</tr>
<tr>
<td>( f^x )</td>
<td>( \mathbf{b}^x )</td>
<td>( \mathbf{b}^x : \mathbf{v}^x + h^x )</td>
<td>( \Phi^x )</td>
</tr>
<tr>
<td>( g^x )</td>
<td>( \mathbf{0} )</td>
<td>( \mathbf{0} )</td>
<td>( \Phi^x )</td>
</tr>
</tbody>
</table>

Table 3.1: Relation between generic and physical variables at the micro-scale.

Individual balance laws for mass, momentum, energy and entropy for a component \( \pi \) may be obtained by selecting the appropriate variables from Table 3.1. Herein, \( \tilde{r}^x \) is the molecular supply of mass to species \( \pi \) due to e.g. chemical reaction processes, \( \sigma^x \) is the microscopic partial stress tensor, \( \mathbf{b}^x \) and \( \mathbf{b}^x \) are the molecular and the external supply of momentum to species \( \pi \), \( U^x \) is the internal energy, \( \mathbf{q}^x \) is the surface flux vector of energy, \( \tilde{h}^x \) and \( h^x \) are the molecular and the external supply of energy to species \( \pi \), \( S^x \) is the internal entropy density, \( \phi^x \) is the surface flux vector of entropy, \( \tilde{s}^x \) and \( s^x \) are the molecular and the external supply of entropy to species \( \pi \) and finally, \( \Phi^x \geq 0 \) is the internal supply of entropy to species \( \pi \).

### 3.3.3. General macroscopic balance equations

The balance equations for a macroscopic property \( \tilde{\psi}^x \) are obtained by averaging the microscopic balance equations (3.23) over a representative volume \( dV \) (Hassanizadeh and
Gray 1979, Lewis and Schrefler 1998). For a component $\pi$ in phase $\alpha$ the averaged balance equation becomes:

$$
\frac{\partial}{\partial t} \left( \varepsilon^{\alpha} \rho^{\alpha,\pi} \overline{\psi}^{\alpha,\pi} \right) + \nabla \cdot \left( \varepsilon^{\alpha} \rho^{\alpha,\pi} \overline{\psi} + \overline{\psi} \right) - \nabla \cdot \mathbf{i}^{\alpha,\pi} = \varepsilon^{\alpha} \rho^{\alpha,\pi} \left( \overline{f}^{\alpha,\pi} + g^{\alpha,\pi} \right) + \varepsilon^{\alpha} \rho^{\alpha,\pi} \left( \overline{f}^{\alpha,\pi} + g^{\alpha,\pi} \right)
$$

(3.26)

Subject to restrictions on the exchange of properties among components and between phases:

$$
\sum_{\alpha} \varepsilon^{\alpha} \rho^{\alpha,\pi} \overline{f}^{\alpha,\pi} = 0 \quad \forall \alpha \quad \text{and} \quad \sum_{\alpha} \varepsilon^{\alpha} \rho^{\alpha,\pi} g^{\alpha,\pi} = 0 \quad \forall \pi
$$

(3.27)

where $\rho^{\alpha,\pi} = \left( \theta^{\alpha} \right)^{\pi}_{\alpha}$ is the macroscopic mass density function; $\mathbf{v}^{\alpha,\pi}$ is the macroscopic velocity field vector; $\mathbf{i}^{\alpha,\pi}$ is the surface flux vector of $\overline{\psi}^{\alpha,\pi}$; $\overline{f}^{\alpha,\pi}$ is the macroscopic effect of molecular exchange of $\overline{\psi}^{\alpha,\pi}$ between phases; $g^{\alpha,\pi}$ accounts for the exchange of $\overline{\psi}^{\alpha,\pi}$ with other phases through e.g. phase change or mechanical interaction; $\overline{f}^{\alpha,\pi}$ and $g^{\alpha,\pi}$ are the internal and the external supply of $\overline{\psi}^{\alpha,\pi}$.

The surface flux vector $\mathbf{i}^{\alpha,\pi}$ is related to the microscopic flux vector $\mathbf{i}^{\pi}$ by:

$$
\mathbf{N} \cdot \mathbf{i}^{\alpha,\pi} = \mathbf{i}^{\pi} - \theta^{\pi} \left( \psi^{\pi} - \overline{\psi}^{\alpha,\pi} \right) \left( \mathbf{v}^{\pi} - \overline{\mathbf{v}}^{\alpha,\pi} \right)
$$

(3.28)

where $\mathbf{N}$ is the unit normal to the area through which the flux flows.

The exchange term $g^{\alpha,\pi}$ is given by:

$$
g^{\alpha,\pi} = \frac{1}{\left( \theta^{\alpha} \right)^{\pi}_{\alpha}} \int_{\Omega} \sum_{\alpha} \left( \theta^{\pi} \psi^{\pi} \left( \mathbf{w} - \mathbf{v}^{\pi} \right) + \mathbf{i}^{\pi} \right) \cdot \mathbf{n}^{\alpha} \, da
$$

(3.29)

Specific balance laws for a component $\pi$ in phase $\alpha$ can be obtained by transforming the microscopic properties $\psi^{\pi}$, $\mathbf{i}^{\pi}$, $\overline{f}^{\pi}$, $f^{\pi}$ and $g^{\pi}$ into macroscopic properties, and inserting them into the general macroscopic balance equation. However, microscopic and macroscopic quantities with a similar physical meaning are not always directly linked by an averaging operation. As an example, consider the specific kinetic energy. At micro-scale, the specific kinetic energy is defined as the square of the particle velocity, divided by two. The averaged specific kinetic energy is then:

$$
\frac{1}{2} \mathbf{v}^{\pi} \cdot \mathbf{v}^{\pi} = \frac{1}{2} \mathbf{v}^{\alpha,\pi} \cdot \mathbf{v}^{\alpha,\pi} + \left( \mathbf{v}^{\pi} - \overline{\mathbf{v}}^{\alpha,\pi} \right) \cdot \mathbf{v}^{\pi} + \frac{1}{2} \left( \mathbf{v}^{\pi} - \overline{\mathbf{v}}^{\alpha,\pi} \right) \cdot \left( \mathbf{v}^{\pi} - \overline{\mathbf{v}}^{\alpha,\pi} \right)
$$

(3.30)

The first term on the right hand side, the square of the average phase velocity divided by two, corresponds to the macroscopic definition of specific kinetic energy. The third term will
appear as a contribution to the internal energy of the system. As a result, the macroscopic internal energy will consist of two parts, namely the average of the microscopic internal energy and the specific kinetic energy related to velocity fluctuations around the mean value:

$$\overline{U^{\alpha,\pi}} = \overline{U^{\alpha,\pi}} + \frac{1}{2} \left( \overline{v^{\pi}} - \overline{v^{\alpha,\pi}} \right) \cdot \left( \overline{v^{\pi}} - \overline{v^{\alpha,\pi}} \right)$$

(3.31)

To indicate that a macroscopic variable is not directly linked to a microscopic variable by an averaging operation, a curved overbar is used (e.g. $\overline{\zeta}$). The macroscopic quantities after averaging and subsequent recollection are listed in Table 3.2. Details on the derivations can be found in appendix A.

<table>
<thead>
<tr>
<th>Mass</th>
<th>Momentum</th>
<th>Energy</th>
<th>Entropy</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho^{\alpha,\pi}$</td>
<td>$\rho^{\alpha,\pi}$</td>
<td>$\overline{f^{\alpha,\pi}}$</td>
<td>$\overline{g^{\alpha,\pi}}$</td>
</tr>
<tr>
<td>$i^{\alpha,\pi}$</td>
<td>$\sigma^{\alpha,\pi}$</td>
<td>$\overline{U^{\alpha,\pi}} + \frac{1}{2} \overline{v^{\alpha,\pi}} \cdot \overline{v^{\alpha,\pi}}$</td>
<td>$\overline{S^{\alpha,\pi}}$</td>
</tr>
<tr>
<td>$f^{\alpha,\pi}$</td>
<td>$\overline{f^{\alpha,\pi}}$</td>
<td>$\overline{f^{\alpha,\pi}}$</td>
<td>$\overline{f^{\alpha,\pi}}$</td>
</tr>
<tr>
<td>$g^{\alpha,\pi}$</td>
<td>$\overline{g^{\alpha,\pi}}$</td>
<td>$\overline{g^{\alpha,\pi}}$</td>
<td>$\overline{g^{\alpha,\pi}}$</td>
</tr>
</tbody>
</table>

Table 3.2: Relation between generic and physical variables at the macro-scale.

### 3.3.4. General mean macroscopic balance equations

Equation (3.26) is the general macroscopic balance law for a component $\pi$ in a phase $\alpha$. In practical problems however, it is often more interesting to describe e.g. the average motion of a phase or the diffusive motion of a component within a phase. In general, we want to describe the mean thermodynamic properties of a phase and the relative contribution of each individual component with respect to that mean value, rather than the absolute thermodynamic properties of every individual component.

Therefore, it is convenient to replace the partial density $\rho^{\alpha,\pi}$ and the average velocity $\overline{v^{\alpha,\pi}}$ of each component by the corresponding quantities averaged over the phase, and the deviation from this averaged value.

The average density $\rho^{\alpha}$ of phase $\alpha$ [kg/m³] is the sum of the partial densities of each component $\pi$:

$$\rho^{\alpha} = \sum_{\pi} \rho^{\alpha,\pi}$$

(3.32)
The mass fraction or concentration, $c^{\alpha,\pi}$ of component $\pi$ in phase $\alpha$ [dimensionless] relates the partial density, $\rho^{\alpha,\pi}$ to the average density, $\rho^\alpha$ as follows:

$$c^{\alpha,\pi} = \frac{\rho^{\alpha,\pi}}{\rho^\alpha} \quad (3.33)$$

It can easily be verified that the restrictions $\sum \pi c^{\alpha,\pi} = 1$ and $0 \leq c^{\alpha,\pi} \leq 1$ hold.

The average velocity, $v^\alpha$ of phase $\alpha$ [m/s] is given by:

$$v^\alpha = \sum_\pi c^{\alpha,\pi} \overrightarrow{v}^{\alpha,\pi} \quad (3.34)$$

with $\overrightarrow{v}^{\alpha,\pi}$ the absolute velocity of component $\pi$ in phase $\alpha$. The relative motion of a component with respect to the average phase velocity is given by the diffusive-dispersive velocity, $v_{d,\pi}^{\alpha}$ of component $\pi$ in phase $\alpha$ [m/s]:

$$v_{d,\pi}^{\alpha} = \overrightarrow{v}^{\alpha,\pi} - v^\alpha \quad (3.35)$$

The corresponding diffusive-dispersive mass flux, $J^{\alpha,\pi}$ [kg/(m²s)] is defined as:

$$J^{\alpha,\pi} = \varepsilon^\alpha \rho^{\alpha,\pi} v_{d,\pi}^{\alpha} \quad (3.36)$$

The average macroscopic balance equation for a phase $\alpha$ reads:

$$\frac{\partial \left( \varepsilon^\alpha \rho^\alpha \psi^\alpha \right)}{\partial t} + \nabla \cdot \left( \varepsilon^\alpha \rho^\alpha v^\alpha \psi^\alpha \right) - \nabla \cdot \mathbf{i}^\alpha = \varepsilon^\alpha \rho^\alpha g^{\alpha\beta} + \varepsilon^\alpha \rho^\alpha \left( f^\alpha + g^\alpha \right) \quad (3.37)$$

subjected to the restrictions:

$$\sum_\alpha \varepsilon^\alpha \rho^\alpha g^{\alpha\beta} = 0 \quad \forall \pi \quad (3.38)$$

The mean macroscopic properties are listed in Table 3.3. Details on the derivations can be found in appendix B.

<table>
<thead>
<tr>
<th></th>
<th>Mass</th>
<th>Momentum</th>
<th>Energy</th>
<th>Entropy</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\psi^\alpha$</td>
<td>1</td>
<td>$v^\alpha$</td>
<td>$U^\alpha + \frac{1}{2} v^\alpha \cdot v^\alpha$</td>
<td>$S^\alpha$</td>
</tr>
<tr>
<td>$i^\alpha$</td>
<td>0</td>
<td>$s^\alpha$</td>
<td>$\sigma^\alpha \cdot v^\alpha - q^\alpha$</td>
<td>$\phi^\alpha$</td>
</tr>
<tr>
<td>$g^{\alpha\beta}$</td>
<td>$r^{\alpha\beta}$</td>
<td>$r^{\alpha\beta} \psi^\alpha + b^{\alpha\beta}$</td>
<td>$r^{\alpha\beta} \psi^\alpha + b^{\alpha\beta} \cdot v^\alpha + h^{\alpha\beta}$</td>
<td>$r^{\alpha\beta} \psi^\alpha + s^{\alpha\beta}$</td>
</tr>
<tr>
<td>$f^\alpha$</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>$\Phi^\alpha$</td>
</tr>
<tr>
<td>$g^\alpha$</td>
<td>0</td>
<td>$b^\alpha$</td>
<td>$b^\alpha \cdot v^\alpha + h^\alpha$</td>
<td>$s^\alpha$</td>
</tr>
</tbody>
</table>

Table 3.3: Relation between generic and physical variables at the macro-scale.

The format of both the macroscopic balance equations (3.37) and the macroscopic thermodynamic properties (Table 3.3) is identical to the format of their microscopic counterparts given by equation (3.23) and in Table 3.1, respectively. The molecular
interactions have disappeared, but phase interactions are now observed to be internal to the homogenized continuum. Therefore, this averaging procedure can be seen as one step in a multi-step homogenization scheme. One could theoretically start from nano-scale, perform multiple homogenization steps and arrive at the structural scale, as long as the separation of scales principle holds in every step. The practical use of this homogenization procedure is however limited to one or two homogenization steps, for a restricted number of materials. For very small scales (e.g. nano-scale), the equations do not cover the physics accurately.

3.4. Governing equations for building physics applications

3.4.1. General assumptions

In this study, focus lies on a three-phase porous medium, consisting of a porous solid matrix, with a pore space filled with liquid and gas. We make the following assumptions:

- The solid phase consists of a single component and does not interact with the other phases, i.e. no phase change.
- The liquid phase consists of a single component, namely water. Interaction with the gas phase can take place via condensation or evaporation.
- The gas phase is a binary mixture of water vapour and dry air. Interaction with the liquid phase can take place via condensation or evaporation.
- The three phases do not chemically react.
- The studied phenomena occur slow enough to disregard inertia effects.

Furthermore we assume local thermal equilibrium (Hassanizadeh and Gray 1980, Hassanizadeh 1986a). This implies that the temperature can vary in space and time, but that all continua, coexisting at a spatial point, are at the same temperature. Therefore, only one energy balance is needed to fully describe the temperature evolution in the porous medium. This single energy balance equation is obtained as the sum of the individual energy balances (B.30) over all phases and all components. Taking into account the corresponding constraint equations (B.32), it reads:

\[
\sum_{\alpha} \left( \frac{\partial \varepsilon^\alpha \rho^\alpha (A^\alpha + S^\alpha T + \frac{1}{2} \mathbf{v}^\alpha \cdot \mathbf{v}^\alpha)}{\partial t} + \nabla \cdot \left( \varepsilon^\alpha \rho^\alpha \left( A^\alpha + S^\alpha T + \frac{1}{2} \mathbf{v}^\alpha \cdot \mathbf{v}^\alpha \right) \mathbf{v}^\alpha \right) \right)
\]

\[
= \nabla \cdot \left( \mathbf{q} + \sum_{\alpha} \boldsymbol{\sigma}^\alpha \cdot \mathbf{v}^\alpha \right)
\]  

(3.39)

where \( T \) is the absolute temperature and \( A^\alpha \) is the Helmholtz energy of phase \( \alpha \), defined by the Legendre transform:
\[ A^\alpha = U^\alpha - S^\alpha T^\alpha \] (hence \( S^\alpha = -\left( \frac{\partial A^\alpha}{\partial T^\alpha} \right)_V \))

and

\[ \mathbf{q} = \sum_{\alpha} \mathbf{q}^\alpha \]

3.4.2. Constitution

The simplified system of equations consists of 4 mass balance equations (for solid, liquid, dry air and vapour), 12 momentum balance equations (in 3D) and 1 energy balance equation. This results in 17 equations expressed in the following 57 unknowns:

\[
\begin{bmatrix}
\varepsilon^\alpha & \rho^\alpha & c_{g\text{H}_2\text{O}}^\alpha & v^\alpha & \bar{v}_{g\text{H}_2\text{O}}^\alpha & T^\alpha & r_{g\text{H}_2\text{O}}^\alpha & \sigma^\alpha & \sigma_{g\text{H}_2\text{O}}^\alpha & \mathbf{b}_{g\text{H}_2\text{O}}^\alpha & A^\alpha & S^\alpha & \mathbf{q}^\alpha
\end{bmatrix}
\]

with \( \alpha = s, l, g \)

Herein, \( \varepsilon^\alpha \) and \( \rho^\alpha \) are the volume fraction and the density of phase \( \alpha \), respectively; \( v^\alpha \) the average phase velocity, \( T \) the absolute temperature and \( \sigma^\alpha \) the mean macroscopic partial stress tensor of phase \( \alpha \); \( A^\alpha \) and \( S^\alpha \) are the specific Helmholtz energy and the specific entropy of phase \( \alpha \), respectively; \( \mathbf{q} \) is the total heat flux vector; \( c_{g\text{H}_2\text{O}}^\alpha \) is the concentration of vapour in the (binary) gas mixture; \( \bar{v}_{g\text{H}_2\text{O}}^\alpha \) the average vapour velocity and \( \sigma_{g\text{H}_2\text{O}}^\alpha \) the average partial stress tensor of the vapour within the gas phase; \( r_{g\text{H}_2\text{O}}^\alpha \) the rate of exchange of water between the gas and the liquid phase and \( \mathbf{b}_{g\text{H}_2\text{O}}^\alpha \) the corresponding exchange of momentum.

All other quantities in the balance laws are related to the above set by means of their definitions. The list of unknowns can be split into two groups, namely the primary and the secondary unknowns. The primary unknowns are basically determined by solving the system of equations. For the secondary unknowns, constitutive relations have to be postulated, describing their dependency on the primary unknowns and derived variables. We select the following 20 primary unknowns:

Set 1 = \( \{ \varepsilon^\alpha, \rho^\alpha, c_{g\text{H}_2\text{O}}^\alpha, v^\alpha, \bar{v}_{g\text{H}_2\text{O}}^\alpha, T^\alpha \} \)

In the balance equations, \( \varepsilon^\alpha \) and \( \rho^\alpha \) always appear together. If the product of both is considered as an unknown, set 1 reduces to the following set of 17 independent primary unknowns:

Set 2 = \( \{ \varepsilon^\alpha \rho^\alpha, c_{g\text{H}_2\text{O}}^\alpha, v^\alpha, \bar{v}_{g\text{H}_2\text{O}}^\alpha, T^\alpha \} \)

Set 2 can directly be computed from the 17 balance equations if the secondary unknowns are considered as given. Nevertheless, the secondary unknowns depend rather on \( \varepsilon^\alpha \) or \( \rho^\alpha \) than
on the product $\varepsilon^\alpha \rho^\alpha$, since the latter one lacks physical meaning. However, if set 1 is used, 3 additional equations are required. This is known as the classical closure problem (Bedford and Drumheller 1983, Bouré 1986). In the spirit of Hassanizadeh and Gray, we will postulate equations of state for all but one phase:

$$\rho^\alpha = f(T, \ldots) \ \text{with} \ \alpha = s, l$$ (3.42)

Furthermore we know that volume fractions are by definition related through:

$$\sum_\alpha \varepsilon^\alpha = 1$$ (3.43)

Based on relation (3.43), the three unknown volume fractions can be written in terms of the porosity $n$ of the porous medium and the fraction of the pore space filled with liquid, denoted by $S^l$:

$$\varepsilon^s = 1 - n \ ; \ \varepsilon^l = n S^l \ ; \ \varepsilon^g = n \left(1 - S^l\right)$$ (3.44)

The final set of 17 primary unknowns is:

Primary set = \{ $n$ $S^l$ $\rho^s$ $\varepsilon^{s,H,0}$ $\mathbf{v}^s$ $\mathbf{v}^{s,H,0}$ $T$ \}

The remaining 37 secondary unknowns need to be postulated. Constitutive postulates can depend on the primary unknowns and their temporal as well as their spatial derivatives. But they are subjected to the principle of admissibility. This means that they have to obey the balance laws, without violating the second law of thermodynamics, given by the entropy inequality (equation (B.40), summed over all phases $\alpha$). Furthermore, they must obey the principle of material objectivity, which states that every admissible process must remain admissible after a change of frame of the observer (Coleman and Noll 1963). In other words: the constitutive equations must remain unchanged under an orthonormal transformation of the spatial reference frame (Gray 1983).

Many authors (e.g. Hassanizadeh, Gray, Achanta, Schrefler) have derived constitutive relationships by systematically exploring the entropy inequality based on the approach proposed by Coleman and Noll (1963). In this way they were capable to provide a scientific foundation to well-known principles, like the effective stress principle (Bishop 1959), and to derive the conditions under which renowned empirical relationships, like Darcy’s law for fluid transport and Fick’s law for diffusion, are valid. A detailed thermodynamic analysis is beyond the scope of this thesis and would mainly duplicate work that has been undertaken by other researchers. In the next section we provide the equations of state and the missing constitutive relations for the secondary unknowns, based on results published in literature.
### 3.4.3. Constitutive relations and state equations

#### 3.4.3.1. Partial stress tensors

The systematic exploration of the entropy inequality leads to the following general expression for the partial stress tensor $\sigma^\alpha$ of a fluid phase $\alpha$, containing constituents $\pi$ (Hassanizadeh 1986):

$$
\sigma^\alpha = -\varepsilon^\alpha \left( p^\alpha I + \sum_\pi c^{\alpha,\pi} v_d^{\alpha,\pi} \cdot v_d^{\alpha,\pi} \right)
$$

(3.45)

where $p^\alpha$ is the (thermodynamic) pressure, $I$ a second order unit tensor. The last term of equation (3.45) represents the stress contribution that originates from the motion of the species $\pi$ in phase $\alpha$. For the solid phase, the general expression reads:

$$
\sigma^s = \sigma - \varepsilon^s \left( p^s I + \sum_\pi c^{s,\pi} v_d^{s,\pi} \cdot v_d^{s,\pi} \right)
$$

(3.46)

where $\sigma$ is the effective stress tensor (section 3.4.3.2) and $p^s$ the solid pressure. At thermodynamic equilibrium, the latter is given by:

$$
p^s = S^l p^l + S^g p^g = p^g - S^l (p^g - p^l)
$$

(3.47)

The total stress tensor $\sigma^{tot}$ is the sum of the partial stress tensors:

$$
\sigma^{tot} = \sigma^s + \sigma^l + \sigma^g = \sigma - p^l I - \sum_\alpha \left( \varepsilon^\alpha \sum_\pi c^{\alpha,\pi} v_d^{\alpha,\pi} \cdot v_d^{\alpha,\pi} \right)
$$

(3.48)

Equation (3.48) is a more general form of the effective stress principle, formulated by Terzaghi (1936) for saturated porous media and later by Bishop (1959) for the unsaturated case. Nevertheless, (3.48) has been derived under the assumption that the interfaces between the different phases do not possess thermodynamic properties, and consequently (3.48) is not ‘correct’ either. Derivations, including interface thermodynamics, were conducted e.g. by Gray and Schrefler (2001). Such studies are theoretically valuable to provide insight in e.g. the effect of the interface geometry on the solid pressure and the effective stress. Their practical use is however rather limited, since crucial information, like the average interface curvature, is usually unavailable in reality. But interface thermodynamics can also be taken into account indirectly, using the theory of poromechanics (Coussy 1995). This is a macroscopic thermodynamic approach, and therefore no information on the geometry of the microstructure is required. The poromechanical effective stress principle, for a single component solid material (i.e. $v_d^{s,\pi} = 0$) reads:
\( \mathbf{\sigma}' = \mathbf{\sigma} - b' p' \mathbf{I} \) \hspace{1cm} (3.49)

where \( b' \) is the Biot coefficient, introduced to account for the deformability of the grains, and \( p' \) the solid pressure, now defined as:

\[
p' = p^s - S^l \left( p^g - p^l \right) - U \quad \text{with} \quad U = \int_{S_l} \left( p^g - p^l \right) dS_l
\] \hspace{1cm} (3.50)

The term \( U \) is the macroscopic contribution of the interfaces to the solid pressure. Equations (3.49)-(3.50) will be used in the remaining part of this thesis, instead of (3.46)-(3.47).

### 3.4.3.2. Effective stress tensor

Several material models have been developed to describe the dependency of the effective stress tensor on material deformation. The simplest model assumes an isotropic linear elastic material and is given by:

\[
\mathbf{\sigma} = \mathbf{D}\varepsilon
\] \hspace{1cm} (3.51)

with \( \mathbf{D} = \lambda \mathbf{I} \otimes \mathbf{I} + 2\mu \mathbf{I} \) the elasticity tensor, \( \mathbf{I} \) and \( \mathbf{I} \) the second and fourth order unit tensors, and \( \lambda \) and \( \mu \) the Lamé constants. \( \varepsilon \) is the second order strain tensor. Linear elasticity is suitable to model the mechanical behaviour of many quasi-brittle materials under moderate loading conditions. For higher load levels, more advanced models incorporating material damage must be used, like the stress-based continuum damage model by Simo and Ju (1987). The stress-strain relation for this model reads:

\[
\mathbf{\sigma} = (1 - d) \mathbf{D}\varepsilon
\] \hspace{1cm} (3.52)

where \( d \) is a scalar damage variable which varies between zero, for the initial undamaged state, and one, corresponding to fully damaged material. The damage variable is obtained from an internal stress-like variable \( r \) and a postulated hardening or softening function \( q \), also depending on \( r \):

\[
d = 1 - \frac{q(r)}{r} \quad \text{where} \quad r \in [r_0, +\infty)
\] \hspace{1cm} (3.53)

and \( r_0 \) the threshold for damage initiation. Damage growth is (for the materials under study) an irreversible process. Mathematically, it can be considered a constrained problem of evolution, restricted by the following loading/unloading conditions:

\[
f \leq 0; \; \dot{r} \geq 0; \; \dot{r}f = 0; \; \ddot{r}f = 0
\] \hspace{1cm} (3.54)

where \( f \) is the damage criterion, for instance a Rankine criterion, given by:

\[
f(\mathbf{\sigma}, q) = \sigma_j - q
\] \hspace{1cm} (3.55)
and $\sigma$, the maximal principal stress. In literature, several examples of hardening/softening functions $q$ can be found, ranging from constant, over linear to exponential softening. Less well-know, but physically meaningful is the Weibull-based softening law (Krajcinovic 1989):

$$q = r \exp \left(-\left(\frac{r - r_c}{\lambda_r}\right)^{k_r}\right)$$

(3.56)

where $\lambda_r > 0$ is the scale parameter and $k_r > 0$ the shape parameter of a Weibull distribution of the material strength. The Weibull distribution can mimic the behaviour of other statistical distributions such as the normal ($k_w = 3.4$) and the exponential distribution ($k_w = 1$).

Thermodynamic consistency of the constitutive stress-strain relationship has only been proven for elastic and thermo-elastic materials. A proof for the stress-based continuum damage model is still missing.

3.4.3.3. Heat conduction

According to Gray (1983), the exploration of the entropy inequality leads to the following expression for the transport of heat in a phase $\alpha$:

$$q^\alpha = -k^\alpha \nabla T$$

(3.57)

with $k^\alpha$ the thermal conductivity tensor of phase $\alpha$. Equation (3.57) is known as Fourier’s law of heat conduction. In the derivation of equation (3.57) the simplifying assumption has been adopted that differences in phase velocity do not give rise to heat transfer.

The total heat flux is given by:

$$q = -k \nabla T$$

(3.58)

with $k = \sum_\alpha k^\alpha$ the total thermal conductivity of the porous medium.

3.4.3.4. Equation of state for solid material

Assume the following functional dependency for the solid density:

$$\rho^s(p^s, I_1, T)$$

(3.59)

where $p^s$ is the solid pressure, $I_1$ the first invariant of the effective stress and $T$ the absolute temperature. According to Lewis and Schrefler (1998) the material derivative of the solid density can then be expressed as:

$$\frac{1}{\rho^s} \frac{D\rho^s}{Dt} = \frac{1}{1-n} \left[ (b^s - n) \frac{1}{K^s} \frac{D^s p^s}{Dt} - \alpha^s (b^s - n) \frac{D^s T}{Dt} - (1-b^s) \nabla \cdot \mathbf{v}^s \right]$$

(3.60)
with $K^s$ the bulk modulus of the solid grain material, $\alpha^s$ the thermal expansion coefficient for the solid, $n$ the porosity and $b^s$ the Biot coefficient, defined as:

$$b^s = 1 - \frac{K}{K^s} \leq 1$$

(3.61)

with $K$ the bulk modulus of the material (solid grains and pore space). For incompressible grain material $1/K^s = 0$ and $b^s = 1$. This does however not imply that the solid skeleton is rigid, since rearrangement of the pore space can still take place. In this case, equation (3.60) reduces to:

$$\frac{1}{\rho^s} \frac{D\rho^s}{Dt} = -\alpha^s \frac{D'T}{Dt}$$

(3.62)

### 3.4.3.5. Equation of state for liquid water

As a first approximation, water is considered incompressible:

$$\rho^l = \text{cst}$$

(3.63)

More realistic equations of state, including the dependency on the liquid pressure and temperature can be found in literature (e.g. Fernandez 1972).

### 3.4.4. Manipulation of the system of equations

The constitutive relations and state equation given in the previous section allow determining the majority of the secondary unknowns. For the other unknowns constitutive postulates exist as well, however, by the appropriate manipulation of the remaining 17 governing equations these variables can be eliminated.

#### 3.4.4.1. Solid mass balance

The solid mass balance reads:

$$\frac{\partial (\varepsilon^s \rho^s)}{\partial t} + \nabla \cdot (\varepsilon^s \rho^s \mathbf{v}^s) = 0$$

(3.64)

Substituting the volume fraction by means of (3.44) and inserting the equation of state for the solid material (3.60), we obtain:

$$\frac{\partial n}{\partial t} + \mathbf{v}^s \cdot \nabla n = (b^s - n) \left[ \nabla \cdot \mathbf{v}^s + \frac{1}{K^s} \frac{D'\rho^s}{Dt} - \alpha^s \frac{D'T}{Dt} \right]$$

(3.65)

Given the material properties $b^s$, $K^s$ and $\alpha^s$, and the evolution of the variables $\mathbf{v}^s$, $T$ and $p^s$ the evolution of the porosity $n$ can be computed.
3.4.4.2. H₂O mass balance

The mass balance equations for liquid water and for water vapour can be combined in order to eliminate the mass exchange term \( \rho^{g,H₂O} \).

\[
\frac{\partial (\varepsilon \rho^l)}{\partial t} + \frac{\partial (\varepsilon^g \rho^{g,H₂O})}{\partial t} + \nabla \cdot (\varepsilon \rho^l v^l) + \nabla \cdot (\varepsilon^g \rho^{g,H₂O} v^g) + \nabla \cdot \mathbf{J}^{g,H₂O} = 0
\] (3.66)

After substituting the volume fractions by means of (3.44) and rearranging, the conservation equation for water reads:

\[
\frac{\partial (nS^l \rho^l + n(1-S^l) \rho^{g,H₂O})}{\partial t} + \nabla \cdot \left( nS^l \rho^l v^l + n(1-S^l) \rho^{g,H₂O} v^g \right) + \nabla \cdot \mathbf{J}^{g,H₂O} = 0
\] (3.67)

Or in terms of the relative velocities of the fluid and gas with respect to the solid:

\[
\frac{D^s (nS^l \rho^l + n(1-S^l) \rho^{g,H₂O})}{Dt} + \left( nS^l \rho^l + n(1-S^l) \rho^{g,H₂O} \right) \nabla \cdot \mathbf{v}^s + \nabla \cdot \left( nS^l \rho^l (\mathbf{v}^l - \mathbf{v}^s) + n(1-S^l) \rho^{g,H₂O} (\mathbf{v}^g - \mathbf{v}^s) \right) + \nabla \cdot \mathbf{J}^{g,H₂O} = 0
\] (3.68)

According to Durner (1992, 1994), the degree of liquid saturation \( S^l \) for porous materials with multimodal pore-sizes can be expressed in terms of the capillary pressure \( p_e = p^g - p^l \) using a superposition of Van Genuchten-type functions:

\[
S^l (p_e) = \sum_{i=1}^{n_{ps}} \left( 1 + (c_i p_e)^{-n_i} \right)^{-\left(1-n_i \right) / n_i}
\] (3.69)

where \( l_i \) is the weight factor of subsystem \( i \) of the multimodal function, \( c_i \) and \( n_i \) are shape parameters of subsystem \( i \) and \( n_{ps} \) is the number of pore systems for the material.

It is assumed that water vapour behaves as an ideal gas:

\[
\rho^{g,H₂O} = \frac{M^{H₂O}}{RT} p^{g,H₂O}
\] (3.70)

where \( M^{H₂O} \) is the molar weight of water, \( R \) the universal gas constant, \( p^{g,H₂O} \) the vapour pressure and \( T \) the absolute temperature. The vapour pressure above a curved interface is described by Thompson’s law (also known as Kelvin’s law):

\[
p^{g,H₂O} = p^{g,H₂O,sat} \exp \left( -\frac{\gamma^{gI} M^{H₂O}}{\rho^l RT} \left( \frac{1}{r_1} + \frac{1}{r_2} \right) \right)
\] (3.71)
where $\gamma^{\text{fl}}$ is the surface tension at the water-air interface, $\gamma_1$ and $\gamma_2$ are the curvatures of the meniscus and $p_{g,H_2O,\text{sat}}$ is the saturation vapour pressure. $p_{g,H_2O,\text{sat}}$ can be obtained from the Clausius-Clapeyron relationship, but it is more convenient to use an approximate expression:

$$p_{g,H_2O,\text{sat}} = \exp \left( 65.8094 - \frac{7066.27}{T} - 5.976 \ln(T) \right)$$

which is valid within the range $263 \leq T \leq 323$ K and is hence suitable for most applications within the field of porous media.

The linear momentum equilibrium across a curved interface between two phases $\alpha$ and $\beta$ is given by the (Young-)Laplace equation:

$$p_\alpha - p_\beta = \gamma^{\text{fl}} \left( \frac{1}{r_1} + \frac{1}{r_2} \right)$$

For a water-air interface, the surface tension can be approximated by:

$$\gamma^{\text{fl}} = 7.59 \cdot 10^{-2} - 1.7 \cdot 10^{-4} (T - 273.15)$$

Combining relations (3.71) and (3.73) yields the Kelvin-Laplace equation:

$$p_{g,H_2O} = p_{g,H_2O,\text{sat}} \exp \left( -\frac{M_{H_2O}}{\rho \gamma^{\text{fl}} RT} p_c \right)$$

Using the above expressions (3.69), (3.70), (3.72) and (3.75), the capillary pressure $p_c$ can be computed from the mass balance for water (3.68), if the state variables $n$, $T$, $v^l$ and $v^s$ are known, and if an expression for $p_{g,H_2O}$ is provided.

3.4.4.3. Dry air mass balance

According to Dalton’s law the gas pressure can be written as the sum of partial pressures:

$$p_g = p_{g,O_2} + p_{g,H_2O}$$

For most building physics applications, it can safely be assumed that the gas pressure equals the atmospheric pressure and that this one is constant. Therefore, the partial air pressure becomes a dependent variable, and solving the air mass balance explicitly is not required.

3.4.4.4. Solid momentum balance

The solid momentum balance reads:

$$\varepsilon^s \rho^s \frac{D^s v^s}{Dt} = \nabla \cdot \sigma^s + \varepsilon^s \rho^s b^s$$
where $\sigma'$ is given by equation (3.49) and $b'$ is usually taken equal to the gravitational acceleration. The product $\varepsilon' \rho'$ is the apparent density, i.e. the mass of the solid divided by the total volume of matrix and pores.

3.4.4.5. Liquid water momentum balance

Hassanizadeh (1986) showed that the liquid water momentum balance transforms into Darcy’s law if viscous and second order effects are neglected, and if the permeability tensor $\kappa$ is invertible:

$$\varepsilon'(v' - \mathbf{v}) = -\frac{\kappa_{rel}}{\eta'}(\nabla p' - \rho'b)$$

(3.78)

with $\eta'$ the dynamic viscosity and $\kappa_{rel}$ the (dimensionless) relative permeability of the liquid, varying between zero and one. Equation (3.78) can be inserted in the mass balance for water (3.68) in order to eliminate $v'$.

3.4.4.6. Water vapour momentum balance

Hassanizadeh (1986) showed that the water vapour momentum balance transforms into Fick’s diffusion law if viscous and second order effects are neglected, and if the effective dispersion tensor $D_{g,H,O}$ is invertible:

$$J_{g,H,O} = -\rho_g D_{g,H,O} \nabla \left( \frac{p_{g,H,O}}{\rho_g} \right)$$

(3.79)

Again assuming that air is a binary mixture of dry air (superscript $O_2$) and water vapour and that water vapour can be considered as an ideal gas, and by making the additional assumptions that $\nabla M^g \approx 0$ and $M^g \approx M^{O_2}$ we can write (3.79) in terms of pressures:

$$J_{g,H,O} = -\rho_g M^{O_2} M^{H,O} D_{g,H,O} \nabla \left( \frac{p_{g,H,O}}{p^g} \right)$$

(3.80)

Under the assumption that the gas pressure equals the constant atmospheric pressure and considering the binary air mixture as an ideal gas allows writing

$$J_{g,H,O} = -\frac{M^{H,O}}{RT} D_{g,H,O} \nabla p_{g,H,O}$$

(3.81)

Equation (3.81) can be inserted in the mass balance for water (3.68).
3.4.4.7. Gas phase momentum balance

In analogy with equation (3.78), the momentum balance of the gas phase transforms into Darcy’s law if viscous and second order effects are neglected, and if the permeability tensor $\kappa$ is invertible:

$$
\varepsilon^g \left( \mathbf{v}^g - \mathbf{v} \right) = -\frac{\kappa^{gs}}{\eta^g} \left( \nabla p^g - \rho^g \mathbf{b} \right)
$$

(3.82)

with $\eta^g$ the dynamic viscosity and $\kappa^{gs}$ the (dimensionless) relative permeability of the gas, varying between zero and one. Since it was assumed that the gas pressure was constant and equal to the atmospheric pressure, the gradient term in equation (3.82) cancels. Equation (3.82) can be inserted in the mass balance for water (3.68) in order to eliminate $\mathbf{v}^g$.

3.4.4.8. Energy balance

The energy balance equation (3.39), expressed in terms of the internal energy $U^\alpha$, reads:

$$
\sum_\alpha \left( \frac{\partial \varepsilon^\alpha}{\partial t} \rho^\alpha \left( U^\alpha + \frac{1}{2} \mathbf{v}^\alpha \cdot \mathbf{v}^\alpha \right) + \nabla \cdot \left( \varepsilon^\alpha \rho^\alpha \left( U^\alpha + \frac{1}{2} \mathbf{v}^\alpha \cdot \mathbf{v}^\alpha \right) \mathbf{v}^\alpha \right) \right) = \nabla \cdot \left( -\mathbf{q} + \sum_\alpha \sigma^\alpha \cdot \mathbf{v}^\alpha \right)
$$

(3.83)

When dealing with phase change, it is more convenient to express the energy balance in the specific enthalpy $H^\alpha$, defined as:

$$
H^\alpha = U^\alpha + \frac{p^\alpha}{\rho^\alpha}
$$

(3.84)

where $p^\alpha$ is the hydrostatic part of the intrinsic partial stress tensor. If the specific enthalpy is considered a function of the absolute temperature $T$ and the intrinsic hydrostatic pressure $p^\alpha$, the differential reads:

$$
dH^\alpha = \frac{\partial H^\alpha}{\partial T} dT + \frac{\partial H^\alpha}{\partial p^\alpha} dp^\alpha = c_p^\alpha dT + \frac{\partial H^\alpha}{\partial p^\alpha} dp^\alpha \approx c_p^\alpha dT + \frac{1}{\rho^\alpha} dp^\alpha
$$

(3.85)

where $c_p^\alpha$ is the specific heat at constant pressure. Lewis and Schrefler (1998) showed that by applying relations (3.84) and (3.85), and by assuming that the terms related to viscous dissipation and mechanical work, caused by density variation due to temperature changes and caused by volume fraction changes can be neglected, the energy balance (3.83) can be converted into the following, more practical, format:

$$
\sum_\alpha \varepsilon^\alpha \rho^\alpha c_p^\alpha \frac{D^\alpha T}{Dt} + \nabla \cdot \mathbf{q} = -\varepsilon^g \rho^g \mathbf{v}^g \left( H^g - H^l \right)
$$

(3.86)
The gas mass balance equation can be used to eliminate the unknown rate \( r_{\text{rel}}^{\text{g}} \) at which phase change takes place. Equation (3.86) allows to determine the temperature \( T \).

### 3.4.5. Strong form of the equations

In the previous section, the 17-equation system was simplified to a large extent. The mass balance of dry air (1 eq.) does not need to be solved anymore. Furthermore the liquid (3 eqs.), vapour (3 eqs.) and gas momentum balance (3 eqs.) were substituted into the combined water mass balance equation. The resulting system contains 6 equations, namely the mass balance of the solid (1) and the water (1), the momentum balance of the solid (3) and the energy balance of the medium (1).

By making some additional simplifications, the system can be further reduced to a set of 5 reasonably simple equations. For stone-like material, deformations are usually small, and therefore it is justified to apply small deformation theory and to assume a constant porosity. Furthermore, we will focus on slow phenomena. Consequently convective and inertial terms can be disregarded. Solving the solid mass balance equation (3.65) is not required under these assumptions, and the solid momentum balance equation (3.77) becomes:

\[
\nabla \cdot \sigma^s + \varepsilon^s \rho^s \mathbf{b}^s = 0 \tag{3.87}
\]

The water balance equation (3.68) reads, after insertion of equations (3.78), (3.81) and (3.82):

\[
\frac{\partial (\varepsilon^l \rho^l + \varepsilon^g \rho^{g,H,O})}{\partial t} - \nabla \cdot \left( \rho^l \frac{K_{\text{rel}}}{\eta^l} (\nabla p^l - \rho^l \mathbf{b}) \right) + \nabla \cdot \left( \rho^{g,H,O} \frac{K_{\text{rel}}^g}{\eta^g} \rho^s \mathbf{b} \right) - \nabla \cdot \left( \frac{M_{H,O}}{RT} D^{g,H,O} \nabla p^{g,H,O} \right) = 0 \tag{3.88}
\]

Since the deformations were considered small, the hygromechanical coupling terms have vanished. If furthermore the gravity-driven flow is disregarded, the governing equation for mass transfer in an undeformable porous medium, as formulated by Janssen et al. (2007) is recovered.

\[
\frac{\partial (\varepsilon^l \rho^l + \varepsilon^g \rho^{g,H,O})}{\partial t} - \nabla \cdot (K^l \nabla p^l) - \nabla \cdot \left( \delta^{g,H,O} \nabla p^{g,H,O} \right) = 0 \tag{3.89}
\]

where \( \rho^l \frac{K_{\text{rel}}}{\eta^l} \) and \( \frac{M_{H,O}}{RT} D^{g,H,O} \) are denoted with \( K^l \) and \( \delta^{g,H,O} \), respectively. While equation (3.89) is only obtained from the general set of equations after introducing numerous approximations, Janssen et al. (2007) find it directly by writing a macroscopic mass balance for an infinitesimal volume of porous material. This illustrates that obtaining the set of
governing equations via the technique of volume averaging is cumbersome, but also that the methodology can successfully be applied to gain insight in the implicit assumptions in macroscopic theories.

Finally, the energy balance equation for the porous medium (3.86) can be further simplified. After inserting the mass balance equation for water vapour and rearranging, we have:

\[
\frac{\partial}{\partial t} \left( H^g - H^l \right) \varepsilon g \rho^{g, H,O} + \sum_{\alpha} \varepsilon ^{\alpha} \rho^{\alpha} c_p^{\alpha} (T - T_0) + \nabla \cdot \mathbf{q} + \nabla \cdot \left( H^g - H^l \right) \left( \varepsilon g \rho^{g, H,O} \mathbf{v}^g + \mathbf{J}^{g, H,O} \right) + \sum_{\alpha} \varepsilon ^{\alpha} \rho^{\alpha} c_p^{\alpha} \mathbf{v}^{\alpha} (T - T_0) = \sum_{\alpha} c_p^{\alpha} (T - T_0) \left( \frac{\partial \varepsilon^{\alpha} \rho^{\alpha}}{\partial t} + \nabla \cdot \varepsilon^{\alpha} \rho^{\alpha} \mathbf{v}^{\alpha} \right) \tag{3.90}
\]

where \( T_0 \) is a reference temperature, usually taken equal to 273.15 K. If the term on the right hand side is neglected, and if it is assumed that \( \mathbf{v}^l \ll \mathbf{v}^g \) and \( \mathbf{v}^l \ll \mathbf{v}^f \), we obtain:

\[
\frac{\partial}{\partial t} \left( H^g - H^l \right) \varepsilon g \rho^{g, H,O} + \sum_{\alpha} \varepsilon ^{\alpha} \rho^{\alpha} c_p^{\alpha} (T - T_0) + \nabla \cdot \mathbf{q} + \nabla \cdot \left( H^g - H^l \right) \left( \varepsilon g \rho^{g, H,O} \mathbf{v}^g + \mathbf{J}^{g, H,O} \right) + \sum_{\alpha} \varepsilon ^{\alpha} \rho^{\alpha} c_p^{\alpha} \left( \mathbf{v}^{\alpha} - \mathbf{v}^f \right) (T - T_0) = 0 \tag{3.91}
\]

Equations (3.78) and (3.82) can now be employed to eliminate \( \mathbf{v}^l \) and \( \mathbf{v}^g \), and \( \mathbf{J}^{g, H,O} \) is given by equation (3.81). Disregarding gravity-driven flow, the energy conservation equation of Janssen et al. (2007) is recovered.

\[
\frac{\partial}{\partial t} \left( H^g - H^l \right) \varepsilon g \rho^{g, H,O} + \sum_{\alpha} \varepsilon ^{\alpha} \rho^{\alpha} c_p^{\alpha} (T - T_0) \right) + \nabla \cdot \mathbf{q} - \nabla \cdot \left( H^g - H^l \right) \delta^{g, H,O} \nabla p^{g, H,O} + c^l_p (T - T_0) K^{l} \nabla p^{l} = 0 \tag{3.92}
\]

Janssen et al. (2007) showed that the coupled system of equations (3.89) and (3.92) can be cast in a simple format if \( \frac{\partial \rho^{g, H,O}}{\partial p_c} \) and \( \frac{\partial \rho^{g, H,O}}{\partial T} \) can be neglected and if it is assumed that \( \rho^{g, H,O} \) and \( \rho^g \) are small as compared to \( \rho^l \):

\[
c_{mm} \frac{\partial p_c}{\partial t} + c_{mc} \frac{\partial T}{\partial t} - \nabla \cdot \left( K_{mm} \nabla p_c + K_{mc} \nabla T \right) = 0 \tag{3.93}
\]

\[
c_{em} \frac{\partial p_c}{\partial t} + c_{ec} \frac{\partial T}{\partial t} - \nabla \cdot \left( K_{em} \nabla p_c + K_{ec} \nabla T \right) = 0 \tag{3.94}
\]

with
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\[
c_{mm} = n \rho_j \frac{\partial S^l}{\partial p_e}
\]

\[
c_{me} = 0
\]

\[
K_{mm} = K^l + \delta^{g,H_2O} \frac{M^{H_2O}}{\rho^l RT} p^{g,H_2O}
\]

\[
K_{me} = \delta^{g,H_2O} \frac{M^{H_2O}}{\rho^l RT^2} p^{g,H_2O} \left( \rho^l \left( H^g - H^l \right) - p_e \left( \frac{1}{\gamma^g} \frac{\partial \gamma^g}{\partial T} T - 1 \right) \right)
\]

and

\[
c_{em} = nc'_p \rho^l (T - T_0) \frac{\partial S^l}{\partial p_e}
\]

\[
c_{ee} = (1 - n) c'_p \rho^l S^l
\]

\[
K_{em} = c_p (T - T_0) K^l + \left( H^g - H^l \right) \delta^{g,H_2O} \frac{M^{H_2O}}{\rho^l RT} p^{g,H_2O}
\]

\[
K_{ee} = k + \left( H^g - H^l \right) \delta^{g,H_2O} \frac{M^{H_2O}}{\rho^l RT^2} p^{g,H_2O} \left( \rho^l \left( H^g - H^l \right) - p_e \left( \frac{1}{\gamma^g} \frac{\partial \gamma^g}{\partial T} T - 1 \right) \right)
\]

Equations (3.87), (3.95) and (3.96) are the final form of the system of equations.

### 3.5. Concluding remarks

In the first part of this chapter, the general set of governing equations for a multi-phase, multi-component system was derived. The derivations are similar to those of Hassanizadeh and Gray, but two important differences can be noted. First of all, all phases were considered as a multi-component mixture at the lower scale. The observation that the homogenized equations can be written in an identical format as the lower scale equations, has led to the insight that the homogenization procedure can be applied recursively. Although the practical use of this recurrent scheme is limited, it helps to interpret the physical meaning of the microscopic quantities, which were initially more or less postulated. The second difference with the work of Hassanizadeh and Gray lies in the notation. A comparison between and discussion of our notation and the original one is given in appendix C. The new notation is more consistent with the symbols used in the individual fields of heat and mass transfer and mechanics. Furthermore, all variables with a similar meaning are now denoted with the same symbol. Distinction between them can be made by means of the different types of overbars and/or superscripts.

In the second part of this chapter, the generic set of governing equations was specialized towards a tractable set of equations, applicable in the field of building physics.
Systematically, assumptions were listed, constitutive postulates defined and equations of state given. Finally, a set of equations describing the hygro-thermo-mechanical behaviour of continuous porous media was obtained. The system can be applied to study slow phenomena (no inertia), in absence of external pressure gradients (no convection or advection) under moderate temperature conditions (neither steam nor ice formation are taken into account). In the subsequent chapters we analyse how this theory can be applied for fractured porous media.
The theory outlined in the preceding chapter is a continuum theory, and, like all continuum theories, validity is lost if the requirements of smoothness and continuity are no longer met. This is for example the case if a fracture develops. Describing such discontinuous features requires a discrete extension of the continuum theory. This chapter focuses on the continuous-discontinuous description of the mechanical failure process. The next chapter treats the effect of the presence of a geometrical discontinuity on the hygro-thermal transport processes.

The idea to arrive at a better characterization of the whole failure process by combining continuous and discontinuous theories into a global framework has been successfully pursued by many authors (e.g. Ren and Bićanić 1997, Jirásek and Zimmermann 2001, Oliver et al. 2002), nevertheless some issues remain. It is for example not clear when a discrete crack should be introduced. Some authors introduce a traction-free discontinuity at the final stage of failure (e.g. Simone et al. 2003). In this case the continuum model governs the softening behaviour. Other authors make use of the cohesive zone assumption (Dugdale 1960; Barenblatt 1962). Here a traction-separation model governs the non-linear behaviour in the fracture process zone and the continuum can remain elastic at all times (e.g. Wells and Sluys 2001). Both approaches have in common that a single moment exists at which the continuum description is replaced by a discontinuous description. The distinct feature of the model proposed in the present chapter is that this transition takes place gradually. A damage-type cohesive law is developed that allows using the constitutive model for the continuum in the undamaged material bonds within the process zone, whereas the damaged part is considered traction-free. As damage grows, material bonds are broken and a macro-crack is formed. This conceptually different cohesive zone model is formulated irrespective of the underlying model for the undamaged material. The gradual transition ensures that the stress at a point varies in a continuous manner during the entire solution trajectory. This notion is known as ‘time continuity’, and was introduced by Papoulia et al. 2003 as a prerequisite for robustness of a continuous-discontinuous framework.

The chapter starts by a description of the enhanced kinematics of a fractured medium. Next, the theoretical background of the discrete model is discussed. Afterwards, the strong and the
weak formulation as well as the discretization and linearization procedure are presented, and the return mapping algorithm is laid out. The last section contains three academic examples, illustrating the capabilities of the proposed model.

4.1. Problem field

(i) The displacement field of a body containing a material interface is usually not smooth (weak discontinuity). (ii) In a fractured body, the displacement field exhibits a jump (strong discontinuity). (iii) The strain field around a crack tip in a perfectly brittle elastic medium is inversely proportional to the square root of the distance to the tip. These three examples illustrate that it is not always possible to approximate the real displacement or strain field by means of polynomial basis functions. Increasing the polynomial order leads to an improved approximation (p-refinement), as does the piecewise approximation with lower order polynomial functions (h-refinement). A third option consists in extending the basis with well-chosen linearly-independent functions that capture the characteristic feature of the real field. This idea has been forwarded by Melenk and Babuška and is the underlying concept of the Partition of Unity Finite Element Method (PUFEM, Melenk and Babuška 1996), the Generalized Finite Element Method (GFEM, Duarte et al. 2000) and the hp-cloud method (Duarte and Oden 1996).

Using the PU-philosophy, the displacement field $u$ can generally be written as:

$$u(x) = \hat{u}(x) + \sum_{j=1}^{m} \hat{u}_j(x) \varphi_j(x)$$

(4.1)

where $\hat{u}$ and $\hat{u}_j$ are smooth, continuous functions, $\varphi$ is the ‘enhanced’ approximation basis, describing the characteristic features of the displacement field, and $m$ is the number of terms in the enhanced basis. $\varphi$ does not need to be smooth nor continuous, only linear independence of the ‘standard’ approximation functions is required. The latter ones are used to approximate $\hat{u}$ and $\hat{u}_j$.

![Figure 4.1: (a) Body $\Omega$ crossed by a displacement discontinuity. Schematic representation of (b) the displacement field and (c) the corresponding strain field of a crossed 1D element.](image-url)
For a body $\Omega$ crossed by a displacement discontinuity $\Gamma_d$ (Figure 4.1a), the Heaviside step function $H_{\Gamma_d}$ can be used as enhanced approximation basis. The Heaviside function is equal to one for all points $x \in \Omega^-$ and zero for all other points $x \in \Omega^+$, where $\Omega = \Omega^- \cup \Omega^+$. The total displacement field (Figure 4.1b) is then given by:

$$u = \hat{u} + H_{\Gamma_d} \tilde{u} \tag{4.2}$$

The total strain field $\varepsilon^{tot}$ (Figure 4.1c) can be found by taking the symmetric gradient of the displacement field:

$$\varepsilon^{tot} = \nabla^s u = \nabla^s \hat{u} + H_{\Gamma_d} \nabla^s \tilde{u} + \delta_{\Gamma_d} \left( \tilde{u} \otimes \mathbf{n} \right)^s = \varepsilon + \delta_{\Gamma_d} \left( \tilde{u} \otimes \mathbf{n} \right)^s \tag{4.3}$$

where $\mathbf{n}$ is the normal to the discontinuity, $\varepsilon$ is the continuum part of the total strain field and $\delta_{\Gamma_d}$ is the Dirac delta distribution, centred at the discontinuity. The Dirac delta distribution is the derivative of the Heaviside step function and is nonzero only for the points at the discontinuity.

### 4.2. Cohesive zone model

#### 4.2.1. Motivation

Besides enhanced kinematics, a continuous-discontinuous framework can incorporate a cohesive zone model. Hereby, the material behaviour in the inelastic region ahead of the crack tip is modelled as a cohesive traction, acting on a fictitious extension of the crack surface. A large number of cohesive zone models can be found in literature. Many of them introduce a complete set of new material properties describing the tractions as a function of the separation of the crack surfaces. Another typical feature is that the tractions decrease with increasing crack opening. Both aspects are debatable. First, one could argue that the material in front of the crack tip is in general not different from the material in the bulk. Therefore a single set of material properties should exist, governing both the behaviour of the bulk and the failure process. Second, the decrease of the tractions with increasing crack opening is motivated by physical observations, but does not capture the underlying mechanism: (i) if two crack surfaces are further separated, the intact material bridges between both are stretched, leading to an increased tensile traction. (ii) Some bridges can not take this additional load and will snap through. If the second mechanism prevails, the overall effect is a reduction of the load carrying capacity, which is in agreement with classical cohesive zone models. The main advantage of modelling both mechanisms individually becomes evident when considering the case of unloading. Traditional cohesive zone models need to distinguish between a model for
loading ([\textbf{u}] \uparrow \Rightarrow \mathbf{t} \downarrow) and one for unloading ([\textbf{u}] \downarrow \Rightarrow \mathbf{t} \downarrow), exactly because the overall effect is modelled instead of the underlying mechanisms. A model that separates those can directly be applied for both cases.

The above criticism does not apply to all models. For instance, Oliver successfully derived a discrete model from a continuum model (Oliver 2000). The obvious advantage is that one set of parameters governs the entire material behaviour. Furthermore, his model can be applied for both loading and unloading. The drawback of the model lies in the mathematical nature of some parameters. In this section an alternative model is derived that shows some similarities with Oliver’s model, but is conceptually different.

### 4.2.2. Damage-based discrete constitutive equation

Consider an infinitesimal part of a plane \( dA \) with unit normal \( \mathbf{n} \) in a structure or structural component (Figure 4.2a). The tractions \( \mathbf{t} \) acting on this plane are obtained as

\[
\mathbf{t} = \sigma \mathbf{n}
\]  

(4.4)

where \( \sigma \) is the second order continuum stress tensor. Suppose that micro-cracks and -voids start to grow on this infinitesimal plane (Figure 4.2b). In that case, we can quantify the ratio between the damaged area and the total area with a scalar damage variable \( \omega \), ranging from zero to one. Zero damage corresponds to the undamaged bulk material, whereas \( \omega \) equals one upon complete separation along the crack plane. The bulk material will, in general, include pores, deficiencies and irregularities. All these ‘imperfections’ are randomly distributed in the material. As a result, they are not considered as ‘damage’ but rather as a characteristic of the continuum.

![Figure 4.2: Schematic representation of (a) an infinitesimal part of a plane with normal \( \mathbf{n} \) in a structure or structural component, (b) the cohesive zone with approximately 60% in-plane micro-damage and (c) the relation between damage, effective tractions and continuum stresses.](image)

Tractions can only be transferred via the undamaged material bonds. The linear momentum equilibrium for an infinitesimal part of the plane \( A \) states that the effective tractions in the
material bonds $t^{\text{eff}}$, acting on the undamaged part of the infinitesimal area $dA$, equal the homogenized stresses in the surrounding continuum, projected on the plane and acting on the area $dA$ (Figure 4.2c), or
\[
\sigma_n dA = t^{\text{eff}} (1 - \omega) dA \quad \text{for} \quad 0 \leq \omega \leq 1
\] (4.5)

Before any damage occurs, the effective tractions equal the continuum stresses (equation (4.4) with $\omega = 0$). As damage grows, the active area decreases and higher effective tractions are needed to maintain equilibrium with the continuum stresses. The increase in effective traction corresponds to the traction that was originally acting on the damaged part of the infinitesimal area $dA$, i.e. the tractions are redistributed. This redistribution causes additional deformations in the undamaged material bonds. Therefore, it is justified to additively decompose the effective traction into two terms, namely, (i) the original or ‘continuum’ traction, in magnitude equal to the projected continuum stress field acting on the undamaged part of the area $dA$, and (ii) the redistributed or ‘discrete’ traction giving rise to the elongation of the material bond:
\[
t^{\text{eff}} = \sigma_n + \gamma^{-1} Q [\tilde{u}]
\] (4.6)

where $Q$ is a second order tensor, describing the constitutive behaviour of the material bonds, $[\tilde{u}] = u|_{\Gamma_d} - u|_{\Gamma_d}$ is the displacement jump across the discontinuity $\Gamma_d$, $\gamma$ is a unit length (1 m) and follows from dimensional analysis. The tensor $Q$ relates the elongation of a material bond to the corresponding traction. In case material failure is studied, it can be argued that the material bond exhibits the same constitutive behaviour as the bulk material, and therefore, $Q$ can be taken equal to the acoustic tensor, i.e. the projection of the bulk behaviour onto the discontinuity plane:
\[
Q = nDn
\] (4.7)

with $D$ the 4th order constitutive tensor of the bulk material. In case interface failure is modelled, we can either use the acoustic tensor of the bond material (i.e. the glue) or - in absence of a bonding material - the acoustic tensor of the coupled system:
\[
Q = \left(\alpha Q_1^{-1} + (1 - \alpha) Q_2^{-1}\right)^{-1}
\] (4.8)

where $Q_1$ and $Q_2$ represent the acoustic tensors of both materials and $\alpha$ is a weighting factor, taken equal to $\alpha = \frac{1}{2}$. The meaning of $\alpha$ will be explained in more detail in the next chapter. The use of equation (4.8) implies a perfect bond between both materials. In case of two equal materials $Q = Q_1 = Q_2$, independent of $\alpha$. Equations (4.7) and (4.8) provide
simple estimates for $Q$ that can be applied to model a wide range of quasi-brittle materials. Instead of using the acoustic tensor, a constitutive tensor could be postulated (e.g. based on measurements), or alternatively, it could be obtained by means of homogenization from a more detailed simulation at a lower scale, i.e. by following a two-scale approach. In the remainder of the text the tensor $Q$ will be determined by equations (4.7) or (4.8).

Combining equations (4.4)-(4.6) finally yields the constitutive equation for the cohesive zone:

$$t = (1 - \omega) \left[ \sigma n + \gamma^{-1} Q [\ddot{u}] \right]$$

(4.9)

Equation (4.9) represents the gradual degradation from a continuum to a discrete state. Figure 4.3a illustrates this equation in a graphical way for a one-dimensional case with a specific choice of model parameters. Upon initiation of the crack, the crack width and the damage variable equal zero ($[\ddot{u}] = 0$; $\omega = 0$) and equation (4.4) is recovered: the material behaves as if no discontinuity were present. As damage grows, the relative contribution of the discrete component of the total traction gains importance over the continuum component (Figure 4.3a, dashed line). At rupture, the damage variable becomes one and the traction forces become zero. This corresponds to a traction-free discontinuity.

Figure 4.3: Schematic representation of the evolution of (a) the components of the traction vector as a function of the displacement jump and (b) the equivalent effective traction (dotted line) and the traction (solid line) as a function of damage during loading. In (a), total tractions are indicated with a solid line; the continuum part of the traction with a dashed line.

If the loading were reversed before rupture occurred, the damage would cease to grow, but equation (4.9) can still be used without modification to obtain the total traction vector. As the stress decreases, both crack width and total traction will decrease, and finally become zero.

### 4.2.3. Damage evolution

The proposed discrete constitutive equation needs to be supplemented with a proper damage criterion and a suitable damage evolution law.
Criteria for damage growth are either stress-based or strain-based. In a discrete setting, the corresponding criteria are traction-based or displacement jump-based. Considering that (i) the discrete law (equation (4.9)) depends on the equilibrium between the effective tractions in the undamaged material bonds and the homogenized stresses in the surrounding continuum matrix, and that (ii) the corresponding strain field is unbounded if localization occurs in a band of zero width, it is clear that a traction-based damage criterion is preferred in this formulation. In this study, a Rankine-type damage criterion is adopted:

\[ f(t_{\text{eff}}, \omega) = t_{\text{eff}, \text{eq}} - \kappa \]  

(4.10)

in which \( t_{\text{eff}, \text{eq}}(t_{\text{eff}}) \) is an equivalent effective traction, expressed as a function of the effective traction (equation (4.6)), and \( \kappa(\omega) \) is the residual strength of the damaged material.

Equivalent effective tractions leading to \( f > 0 \) are not allowed, since these would exceed the material strength. \( f = 0 \) thus represents the transition between admissible and non-admissible states. For mode I dominated failure, the following expression for the equivalent traction is found suitable:

\[ t_{\text{eff}, \text{eq}}(t_{\text{eff}}) = t_{\text{eff}} \cdot n \]  

(4.11)

For mixed-mode failure, one could e.g. employ the L2-norm of the effective traction vector, while for pure mode II, the magnitude of the tangential component could be a relevant measure. Mode II and mixed mode failure are not considered in the remainder of this thesis.

Inspired by the fact that many processes in nature, including failure, show exponential behaviour, the following expression for the material strength \( \kappa \) is proposed:

\[ \kappa(\omega) = f_i^0 + (f_i^1 - f_i^0) \frac{1 - \exp\left(- \frac{\omega}{\lambda}\right)^n}{1 - \exp\left(- \frac{1}{\lambda}\right)^n} \]  

(4.12)

with \( f_i^0 > 0 \) the tensile strength of the virgin bulk material (\( \omega = 0 \)), \( f_i^1 \geq 0 \) the residual tensile strength of the fully damaged bulk material (\( \omega = 1 \)), and \( \lambda \geq 0 \) and \( n \geq 0 \) numerical parameters related to hardening or softening. The term between the square brackets in equation (4.12) is normalized, as such that it ranges between zero (for \( \omega = 0 \)) and one (for \( \omega = 1 \)), and correspondingly, \( \kappa \) ranges between \( f_i^0 \) and \( f_i^1 \). A graphical illustration of equation (4.12) is depicted in Figure 4.3b.

Damage evolution is governed by the Kuhn-Tucker conditions (see also equation (3.54)):
\[ \dot{\omega} \geq 0, \ f \leq 0, \ \dot{\omega} f = 0 \quad (4.13) \]

The first condition states that damage can only grow. The second one imposes the restriction that every stress state must be admissible, i.e. that the effective equivalent traction \( t_{\text{eff}, \text{eq}} \) can not exceed the residual strength \( \kappa \) of the material. The third condition can be understood in two different ways, namely (i) that damage can only grow (\( \dot{\omega} \neq 0 \)) if the stress state is at the limit of the admissible domain (\( f = 0 \)) and (ii) that for the admissible stress states (\( f \neq 0 \)), damage growth can not take place (\( \dot{\omega} = 0 \)). The Kuhn-Tucker conditions must be supplemented with the consistency condition:

\[ \dot{\omega} \dot{f} = 0 \quad (4.14) \]

Equation (4.14) represents the additional constraints that (i) the stress state remains critical (\( \dot{f} = 0 \)) as long as the damage grows (\( \dot{\omega} \neq 0 \)), and vice versa, that (ii) damage growth ends (\( \dot{\omega} = 0 \)) as soon as the stress state becomes admissible (\( \dot{f} \neq 0 \)).

The damage evolution law is not explicitly given in terms of e.g. the equivalent traction. The updated values of the damage and the corresponding traction vector and crack width are obtained via return mapping, similar to plasticity. This algorithm will be discussed in more detail in section 4.3.6.

### 4.2.4. Determination of the mode I fracture energy

The fracture energy is defined as:

\[ G_f = \int_0^{\infty} t \cdot d[\tilde{u}] \quad (4.15) \]

Upon crack propagation, the traction can be expressed as:

\[ t = (1 - \omega) t_{\text{eff}} = (1 - \omega) \frac{\kappa}{m^\text{eq}} m \quad \text{with} \quad m^\text{eq} = t_{\text{eff}, \text{eq}}(m) \quad (4.16) \]

where \( m \) is a unit vector pointing in the direction of the traction vector and \( m^\text{eq} \) is the equivalent unit traction. For mode I dominated failure, the equivalent effective traction can be defined by expression (4.11), leading to \( m^\text{eq} = m \cdot n \). For mode II or mixed mode failure, \( t_{\text{eff}, \text{eq}} \) could for instance be modelled by the L2-norm of the traction vector, leading to \( m^\text{eq} = \|m\| = 1 \). Other definition can be chosen as well.

The displacement jump can be expressed as:

\[ [\tilde{u}] = \omega r Q^{-1} \frac{\kappa}{m^\text{eq}} m \quad (4.17) \]
Equation (4.17) is derived from (4.9), after eliminating $\sigma_n$ by means of (4.4) and $t$ by means of (4.16). Substituting equations (4.16) and (4.17) in (4.15), and assuming that $Q$ is independent of $\omega$, we obtain the general expression for the fracture energy $G_f$:

$$G_f = \left( \frac{m \cdot Q^{-1} m}{m^{eq}} \right) \gamma \int_{0}^{\gamma} (1 - \omega) \kappa \left( \kappa + \frac{\partial \kappa}{\partial \omega} \right) d\omega$$  \hspace{1cm} (4.18)

The mode I fracture energy $G_f^I$ is obtained by inserting $m^{eq} = m \cdot n$ into equation (4.18) and by taking into account that for pure mode I loading $m = n$:

$$G_f^I = \left( n \cdot Q^{-1} n \right) \gamma \int_{0}^{\gamma} (1 - \omega) \left( \omega \frac{\partial \kappa}{\partial \omega} + \kappa \right) \kappa d\omega$$ \hspace{1cm} (4.19)

If $\kappa$ is defined according to equation (4.12), an analytical expression can only be obtained after tedious manipulations, or, like it is done here, by using specialized software like Mathematica®:

$$G_f^I = - \frac{(n \cdot Q^{-1} n) \gamma}{2n(1 - \exp(\lambda^{-n}))^2} \left[ n(f^0 - f^I) \exp(\lambda^{-n}) \right]^2 + 2(f^0 - f^I \exp(\lambda^{-n}))(f^I - f^0) \exp(\lambda^{-n}) \lambda \left\{ n \Gamma[1, \frac{1}{n}, 0] + n \Gamma[1 + \frac{1}{n}, \lambda^{-n}] \right\} - 2 \Gamma[1, \lambda^{-n}] + 2 \lambda \Gamma[\frac{2}{n}, \lambda^{-n}] - \lambda n \Gamma[\frac{2 + n}{n}, \lambda^{-n}]$$

$$+ 2 \frac{1}{n} \left( f^I \exp(\lambda^{-n}) \right)^2 \lambda \left\{ n \Gamma[1 + \frac{1}{n}, 1 + \frac{1}{n}, 2 \lambda^{-n}] - 2 \Gamma[1, 2 \lambda^{-n}] \right\}$$

$$2 \frac{1}{n} \lambda \Gamma[\frac{2}{n}, 2 \lambda^{-n}] - 2 \frac{1}{n} \lambda n \Gamma[\frac{2 + n}{n}, 2 \lambda^{-n}]$$  \hspace{1cm} (4.20)

where $\Gamma[a, x]$ represents the upper incomplete gamma-function, defined as:

$$\Gamma[a, x] = \int_{-\infty}^{t} t^{a-1} \exp(-t) dt$$  \hspace{1cm} (4.21)

More practical results can be obtained by studying two limit cases for the variable $\lambda$. For $\lambda \to 0$, equation (4.12) reduces to:

$$\kappa(\omega) = f^I$$  \hspace{1cm} (4.22)

It implies a stepwise change of the material strength from $f^0$ to $f^I$ in the cohesive zone at the onset of damage. The corresponding mode I fracture energy is given by:

$$G_f^I = \frac{1}{2} (n \cdot Q^{-1} n) \gamma (f^I)^2$$  \hspace{1cm} (4.23)
For a given $f_i^1 < f_i^0$, equation (4.23) is the lower bound on the amount of dissipated energy, while for $f_i^1 > f_i^0$, it corresponds to the upper bound. For $f_i^1 = 0$, perfectly brittle failure without energy dissipation is obtained.

For $\lambda \rightarrow +\infty$ equation (4.12) transforms into a simple, yet flexible, expression for $\kappa$:

$$
\kappa(\omega) = f_i^0 + (f_i^1 - f_i^0) \omega^0
$$

Using this expression, the fracture energy becomes:

$$
G_j' = (n \cdot Q^{-1} n) \gamma \frac{2n^2 (f_i^0)^2 + 2nf_i^0 f_i^1 + (n+1)(f_i^1)^2}{2(n+1)(2n+1)}
$$

In the special case that $f_i^1 = f_i^0 = f_i$, this expression reduces to:

$$
G_j' = (n \cdot Q^{-1} n) \gamma \frac{1}{2} f_i^2 = \frac{1}{2} f_i (\|\mathbf{u}_{\max}\| \cdot n)
$$

which corresponds to the classical case of linear softening in e.g. interface elements. $\|\mathbf{u}_{\max}\|$ is obtained from equation (4.17) with $\omega = 1$. Note that no softening parameters ($\lambda$ or $n$) are required in this case.

For intermediate values of $0 < \lambda < +\infty$, the fracture energy lies between the values obtained by equations (4.23) and (4.25).

### 4.2.5. Crack initiation and propagation

Finally, we need to define when a discontinuity should initiate or propagate. We have already shown that upon crack initiation, the discrete constitutive equation (equation (4.9)) reduces to traction equilibrium on the potential crack plane (equation (4.4)). In the same line of reasoning, the discrete damage criterion (equation (4.10)) corresponds to the following initiation criterion:

$$
f = \sigma_i - \kappa^0 \leq 0
$$

with $\sigma_i$ the $i^{th}$ principal stress and $\kappa^0 = \kappa(\omega = 0)$. If equation (4.27) is violated at a material point, a new crack segment is introduced with the normal pointing in the (critical) principal stress direction. Crack branching or merging is not considered.

Jirásek (1998) reported that a less tortuous crack path is obtained if the direction of the discontinuity is determined based on the non-local stress tensor $\mathbf{\sigma}$, calculated as a weighted average of stresses using a Gaussian weighting function $w$.
\[ \bar{\sigma} = \frac{\int_{\Omega} w \sigma d\Omega}{\int_{\Omega} w d\Omega} \quad \text{with} \quad w = \frac{1}{(2\pi)^{3/2} l^3} \exp \left( -\frac{r^2}{2l^2} \right) \]  

(4.28)

where \( r \) is the distance to the crack tip and \( l \) the influence length, taken approximately equal to three times the element size (Wells and Sluys 2001). The use of equation (4.28) does not introduce non-locality in the model. It is a method to smoothen the stress field in order to determine the principal directions more accurately. In case higher order finite elements are used, or for problems with a relatively homogeneous stress field, the difference between the principal directions obtained from the local and the non-local stress tensor is small.

In a two-dimensional setting, both curved and straight crack paths can be obtained, and \( C^0 \) crack path continuity can be easily enforced. In a three-dimensional setting, the crack path continuity requirement usually needs to be relaxed (Becker 2007). Although the proposed formulation is n-dimensional, only two-dimensional examples will be provided to illustrate the capabilities of the model.

### 4.3. Strong discontinuity formulation

#### 4.3.1. Strong form

The equilibrium equation reads (see equation (3.87)):

\[ \nabla \cdot \sigma^s + \varepsilon^s \rho^s \mathbf{b}^s = 0 \quad \text{in} \quad \Omega \]  

(4.29)

The natural boundary conditions are given by:

\[ \sigma^s \mathbf{n} = \mathbf{t}_1^s \quad \text{on} \quad \Gamma_2 \]

\[ \sigma^s \mathbf{n} = -\mathbf{t}_d^s \quad \text{on} \quad \Gamma_d^+ \]  

(4.30)

\[ \sigma^s \mathbf{n} = \mathbf{t}_d^- \quad \text{on} \quad \Gamma_d^- \]

where \( \sigma^s \) is the second order stress tensor of the solid phase, \( \mathbf{n} \) is the outward normal to the body, \( \mathbf{n} \) is the outward normal to \( \Omega^- \) on \( \Gamma_d^- \). The minus sign indicates that the direction of the tractions \( \mathbf{t}_d^- \) is opposite to the direction of \( \mathbf{n} \). Tensile tractions are taken positive.

The essential boundary conditions are:

\[ \mathbf{u} = \mathbf{u} \quad \text{on} \quad \Gamma_1 \]  

(4.31)

#### 4.3.2. Weak form

Weak equilibrium statement is written as:
\[ \int_\Omega w \cdot (\nabla \cdot \sigma' + \varepsilon' \rho' \mathbf{b}') \, d\Omega = 0 \quad (4.32) \]

which must hold for all admissible variations of displacement \( w = \mathbf{w} + H_{r_d} \tilde{\mathbf{w}} \). Following a Galerkin approach (i.e. taking the space of admissible variations the same as the actual displacements) leads, after standard manipulations, to the following set of variational statements:

\[
\int_\Omega \nabla^\top \mathbf{w} : \sigma' \, d\Omega = \int_\Omega \tilde{\mathbf{w}} : \varepsilon' \rho' \mathbf{b}' \, d\Omega + \int_{\Gamma_2} \tilde{\mathbf{w}} : \tilde{\mathbf{t}}_d \, d\Gamma + \int_{\Gamma_2} \tilde{\mathbf{w}} : \tilde{\mathbf{t}}'_d \, d\Gamma \\
= \int_\Omega H_{r_d} \nabla^\top \mathbf{w} : \sigma' \, d\Omega \\
\quad + \int_{\Gamma_2} H_{r_d} \tilde{\mathbf{w}} : \tilde{\mathbf{t}}_d \, d\Gamma + \int_{\Gamma_2} H_{r_d} \tilde{\mathbf{w}} : \tilde{\mathbf{t}}'_d \, d\Gamma \\
\quad + \int_{\Gamma_2} H^*_{r_d} \tilde{\mathbf{w}} : \tilde{\mathbf{t}}''_d \, d\Gamma \quad (4.33) \]

4.3.3. Discretized form

Nodes whose support is crossed by a discontinuity are assigned a regular and an enhanced set of degrees of freedom, denoted with \( a \) and \( b \), respectively. The discretized format of equation (4.2) then reads:

\[ \mathbf{u} = \mathbf{N}a + H_{r_d} \mathbf{N}b \quad (4.34) \]

where \( \mathbf{N} \) is the array containing the finite element shape functions. The same discretization is applied for the admissible variations \( w \):

\[ \mathbf{w} = \mathbf{N}c + H_{r_d} \mathbf{N}d \quad (4.35) \]

where \( c \) and \( d \) are the regular and enhanced set of nodal variations, respectively. Both the strain field and the gradient of the variational field can be discretized in a similar fashion using the interpolation matrix \( \mathbf{B} \). For elements with only regular degrees of freedom \( a \), the problem fields are discretized in the standard way.

The discretized format of the weak governing equations reads:

\[
\int_\Omega \mathbf{B}^\top \sigma' \, d\Omega = \int_\Omega \mathbf{N}^\top \varepsilon' \rho' \mathbf{b}' \, d\Omega + \int_{\Gamma_2} \mathbf{N}^\top \tilde{\mathbf{t}}_d \, d\Gamma \\
\int_\Omega H_{r_d} \mathbf{B}^\top \sigma' \, d\Omega = \int_\Omega H_{r_d} \mathbf{N}^\top \varepsilon' \rho' \mathbf{b}' \, d\Omega + \int_{\Gamma_2} H_{r_d} \mathbf{N}^\top \tilde{\mathbf{t}}_d \, d\Gamma + \int_{\Gamma_2} H^*_{r_d} \mathbf{N}^\top \tilde{\mathbf{t}}'_d \, d\Gamma \quad (4.36) \]

where we used the relations \( \mathbf{t}'_d = -\mathbf{t}'_d \) and \( H^*_{r_d} = 0 \).

4.3.4. Discretization of the constitutive relations

In absence of moisture, the partial stress tensor \( \sigma' \) equals the total stress tensor \( \sigma \) (see equation (3.48)). The total stress in the bulk material is expressed in terms of the nodal displacements as:
\[ \sigma' = \sigma = D\varepsilon = D\left( Ba + H_{x}Bb \right) \quad (4.37) \]

If the shape functions were able to exactly represent the displacement field, the true stress tensor could be computed by means of equation (4.37). In practice, the interpolation functions are a limited subset of the entire solution space, and equation (4.37) provides only an approximate value for the local stress tensor at a point. However, the proposed discrete model, as described in section 4.2, relies on the knowledge of the true local stress tensor to ensure a gradual transition from a continuum to a discrete state. Simply inserting the discretized expressions for displacement and stress in equation (4.9) could lead to inaccurate results, especially in the study of dynamic problems or in case a non-linear constitutive model for the bulk material is used. By casting the discrete traction law in a different format prior to discretization, the successful use of the method is no longer restricted to linear elastic, quasi-static simulations.

We first make a distinction between two types of transitions: namely (i) the transition to strong discontinuity kinematics (i.e. the insertion of a discontinuity in the displacement field) and (ii) the transition from a continuous to a discontinuous state as described by the cohesive model. The former corresponds to the moment at which the propagation criterion (equation (4.27)) at a point is violated and a strong discontinuity is inserted with zero damage \( \omega = 0 \); the latter relates to the process of damage evolution \( 0 < \omega \leq 1 \).

4.3.4.1. Transition to strong discontinuity kinematics

From equation (4.17) it is clear that a jump in the displacement field cannot exist in absence of damage \( \omega = 0 \). The use of strong discontinuity kinematics (with a Heaviside enrichment) is therefore not required. However, the displacement field does not need to be smooth, hence the strain field can exhibit a jump across the discontinuity, as long as equilibrium is satisfied:

\[ \left[ \sigma \right]n = 0 \quad (4.38) \]

A discontinuity in the strain field is termed a weak discontinuity. In the corresponding description of the displacement field, the distance function is usually used as enhanced basis function. In contrast with strong discontinuity kinematics, weak discontinuity kinematics does not give rise to integrals over the discontinuity in the weak form. Hence, using weak discontinuity kinematics at the onset of damage, it is not needed to provide an explicit expression for the cohesive traction if \( \omega = 0 \), and consequently the knowledge of the true stress tensor is not required. In section 4.3.5.3 we will return to this issue.
4.3.4.2. Transition from a continuous to a discontinuous state

Since the damage variable is nonzero during the transition, we can eliminate the continuum stress from equation (4.9) by means of equation (4.4):

\[
t = \left( \frac{1-\omega}{\gamma \omega} \right) Q \left[ \tilde{u} \right] \quad \text{with } 0 < \omega \leq 1
\]  

(4.39)

This expression allows computing the traction vector solely based on the displacement jump. The dependency on the continuum stress tensor is implicitly present.

At this point, it is worthwhile to make a comparison with another cohesive law used in a strong discontinuity context. Therefore, we replace the damage variable by \( \omega = \left( 1 + \gamma \left( 1 - \sigma \right) \right)^{-1} \), which yields:

\[
t = (1-\sigma) Q \left[ \tilde{u} \right] \quad \text{with } -\infty < \sigma \leq 1 \text{ m}^{-1}
\]  

(4.40)

Equation (4.40) has been obtained by Oliver (2000), by performing a strong discontinuity analysis of the isotropic damage model of Simo and Ju (1987). As compared to our formulation, two important differences have to be noted: (i) the dimensional damage variable \( \sigma \) ranging from \(-\infty \) m\(^{-1}\) to one m\(^{-1}\) is physically less relevant than the dimensionless variable \( \omega \) ranging from zero to one, and (ii) the singularity at \( \omega = 0 \) (in equation (4.39)) arises from an attempt to avoid errors introduced by the discretization, whereas the singularity at \( \sigma = -\infty \) m\(^{-1}\) (in equation (4.40)) results from the presence of a Dirac delta distribution in the strain field for strong discontinuity kinematics. Nevertheless, the use of weak discontinuity kinematics at the onset of failure removes the singularity in both theories.

4.3.5. Linearized and discretized form

4.3.5.1. Linearization of the discrete model

Since \( t = (1-\omega) t^{\text{eff}} \), we can write:

\[
\frac{dt}{d\left[ \tilde{u} \right]} = \frac{\partial t}{\partial \omega} \frac{d\omega}{d\left[ \tilde{u} \right]} + \frac{\partial t}{\partial t^{\text{eff}}} \frac{dt^{\text{eff}}}{d\left[ \tilde{u} \right]}
\]

(4.41)

For \( \omega = 0 \), the effective stress is given by equation (4.6), and the linearization procedure is rather standard. For \( 0 < \omega \leq 1 \), the effective stress can be derived from (4.39) and reads

\[
t^{\text{eff}} = \left( \gamma \omega^{-1} \right) Q \left[ \tilde{u} \right].
\]

In this case, equation (4.41) becomes:

\[
\frac{dt}{d\left[ \tilde{u} \right]} = \frac{\partial t}{\partial \omega} \frac{d\omega}{d\left[ \tilde{u} \right]} + \frac{\partial t}{\partial t^{\text{eff}}} \left( \frac{\partial t^{\text{eff}}}{\partial \omega} \frac{d\omega}{d\left[ \tilde{u} \right]} + \frac{\partial t^{\text{eff}}}{\partial \left[ \tilde{u} \right]} \right)
\]

(4.42)
and rearranging yields:

\[
\frac{d\mathbf{t}}{d[\mathbf{u}]} = \left( \frac{\partial \mathbf{t}}{\partial \mathbf{\omega}} + \frac{\partial \mathbf{t}^{\text{eff}}}{\partial \mathbf{\omega}} \right) \otimes \frac{d\mathbf{\omega}}{d[\mathbf{u}]} + \frac{\partial \mathbf{t}^{\text{eff}}}{\partial \mathbf{\omega}} \frac{d\mathbf{\omega}}{d[\mathbf{u}]} \tag{4.43}
\]

In the case of loading, the solution has to satisfy the loading function (4.10). The dependency of the loading function on the equivalent effective traction \(t^{\text{eff,eq}}\) and the residual strength \(\kappa\) allows writing:

\[
\frac{df}{d[\mathbf{u}]} = \frac{\partial f}{\partial t^{\text{eff,eq}}} \frac{dt^{\text{eff,eq}}}{d[\mathbf{u}]} + \frac{df}{\partial \kappa} \frac{d\kappa}{d[\mathbf{u}]} = 0 \tag{4.44}
\]

Expanding the derivatives yields:

\[
\frac{df}{d[\mathbf{u}]} = \frac{\partial f}{\partial t^{\text{eff,eq}}} \frac{dt^{\text{eff}}}{d[\mathbf{u}]} \left( \frac{\partial t^{\text{eff}}}{\partial \mathbf{\omega}} \otimes \frac{d\mathbf{\omega}}{d[\mathbf{u}]} \right) + \frac{df}{\partial \kappa} \frac{d\kappa}{d[\mathbf{u}]} = 0 \tag{4.45}
\]

After rearranging, equation (4.45) reads:

\[
\frac{df}{d[\mathbf{u}]} = \left( \frac{\partial f}{\partial t^{\text{eff,eq}}} \frac{dt^{\text{eff}}}{d[\mathbf{u}]} \right) \frac{d\mathbf{\omega}}{d[\mathbf{u}]} + \frac{df}{\partial \kappa} \frac{d\kappa}{d[\mathbf{u}]} = 0 \tag{4.46}
\]

Equation (4.46) provides an expression for \(\frac{d\mathbf{\omega}}{d[\mathbf{u}]}\) in the case of loading. By inserting this expression into (4.43) the general formulation for the consistent tangent is obtained:

\[
\frac{d\mathbf{t}}{d[\mathbf{u}]} = \frac{\partial \mathbf{t}^{\text{eff}}}{\partial \mathbf{\omega}} \otimes \frac{d\mathbf{\omega}}{d[\mathbf{u}]} + \frac{\partial \mathbf{t}^{\text{eff}}}{\partial \mathbf{\omega}} \frac{d\mathbf{\omega}}{d[\mathbf{u}]} \tag{4.47}
\]

For the case of unloading or reloading \(\frac{d\mathbf{\omega}}{d[\mathbf{u}]} = 0\), and (4.43) simplifies to:

\[
\frac{\partial \mathbf{t}}{\partial [\mathbf{u}]} = \frac{\partial \mathbf{t}^{\text{eff}}}{\partial [\mathbf{u}]} \tag{4.48}
\]

Inserting the model equations leads after some straightforward algebraic manipulations to:

\[
\frac{d\mathbf{t}}{d[\mathbf{u}]} = \left( \frac{1-\omega}{\gamma \omega} \right) \mathbf{Q} - \frac{1}{\gamma \omega} \frac{t^{\text{eff}}}{\kappa + \omega} \frac{d\mathbf{Q}}{d[\mathbf{u}]} \tag{4.49}
\]

where \(0 < \omega \leq 1\)

for the case of loading, and for unloading or reloading we find:

\[
\frac{\partial \mathbf{t}}{\partial [\mathbf{u}]} = \left( \frac{1-\omega}{\gamma \omega} \right) \mathbf{Q} \tag{4.50}
\]

where \(0 < \omega \leq 1\)
4.3.5.2. Linearization of the equilibrium equation

After linearization, the system of equations becomes:

\[
\begin{bmatrix}
K_{aa}^i & K_{ab}^i \\
K_{ba}^i & K_{bb}^i
\end{bmatrix}
\begin{bmatrix}
\delta \mathbf{a}^{i+1} \\
\delta \mathbf{b}^{i+1}
\end{bmatrix}
= 
\begin{bmatrix}
f_{\text{ext},a}^i \\
f_{\text{ext},b}^i
\end{bmatrix}
- 
\begin{bmatrix}
f_{\text{int},a}^i \\
f_{\text{int},b}^i
\end{bmatrix}
\]  
(4.51)

with

\[
K_{aa} = \int_\Omega B^T DB d\Omega
\]

\[
K_{ba} = K_{ab}^T = \int_\Omega H_{\Gamma_z} B^T DB d\Omega
\]

\[
K_{bb} = \int_\Omega H_{\Gamma_z} B^T DB d\Omega + \int_{\Gamma_z} H_{\Gamma_z} N^T T^* N d\Gamma
\]

\[
f_{\text{ext},a} = \int_\Omega N^T \varepsilon^* \rho^* \mathbf{b}^i d\Omega + \int_{\Gamma_z} N^T \mathbf{t}_1^* d\Gamma
\]

\[
f_{\text{ext},b} = \int_\Omega H_{\Gamma_z} N^T \varepsilon^* \rho^* \mathbf{b}^i d\Omega + \int_{\Gamma_z} H_{\Gamma_z} N^T \mathbf{t}_1^* d\Gamma
\]

\[
f_{\text{int},a} = \int_\Omega \mathbf{B}^T \sigma d\Omega
\]

\[
f_{\text{int},b} = \int_\Omega H_{\Gamma_z} \mathbf{B}^T \sigma d\Omega + \int_{\Gamma_z} H_{\Gamma_z} N^T \mathbf{t}^* d\Gamma
\]

The superscript \(i\) indicates the iteration counter in the global iterative procedure. The matrix \(T = \frac{dt}{d\mathbf{[u]}}\) is given by (4.49) in the case of loading, and (4.50) for the case of unloading and reloading.

4.3.5.3. Note on accuracy

For very small values of the damage variable, the use of equations (4.49) or (4.50) will have a negative impact on the condition number of the stiffness matrix. A pragmatic approach is followed. Equations (4.49) and (4.50) are used if the damage variable exceeds a predefined threshold \(\omega_{\text{crit}}\), where \(\omega_{\text{crit}}\) is a real positive number close to zero. Below \(\omega_{\text{crit}}\), it is more accurate to use the original expression (4.9) for the discrete law, where the local stress tensor is approximated as:

\[
\sigma_{\text{approx.}} = \frac{1}{2} (\sigma^- + \sigma^+)
\]  
(4.53)

In equation (4.53) \(\sigma^-\) and \(\sigma^+\) are the stress tensors, evaluated at the negative and positive side of the discontinuity. The tangent for \(0 \leq \omega < \omega_{\text{crit}}\) follows from the linearization of equation (4.9). Since the approximated expressions can be used for \(\omega = 0\), there is no need to employ weak discontinuity kinematics. The validity of this approximation is verified in section 4.4.3.
4.3.6. Return mapping

First, the system of equations (equation (4.51)) is solved using the previous converged value of the damage variable (trial state). Next, the effective traction is computed for each point on the discontinuity and the admissibility of the stress state is verified. If the damage criterion is satisfied, i.e. \( f \leq 0 \), the stress state is admissible and the trial state is the real state. However, if the damage criterion is violated (\( f > 0 \)), the damage variable needs to be updated.

The new damage variable can be found as the root of the damage criterion (equation (4.10)). Generally, \( \kappa \) can be a non-linear function of \( \omega \), and explicitly solving for \( \omega \) is not possible. Therefore a local iterative scheme should be applied (e.g. Newton-Raphson scheme):

\[
f^{j+1} = f^j + \frac{\partial f}{\partial \omega} \omega^{j+1} - \omega^j + R^2
\]

where the superscript \( j \) denotes the counter in the local iterative procedure. Omitting the terms of second order and higher (\( R^2 \)) and elaborating the derivative yields:

\[
f^{j+1} = f^j + \left( \frac{\partial t_{\text{eff.eq}}}{\partial \omega} \omega^{j+1} - \frac{\partial \kappa}{\partial \omega} \omega^j \right) (\omega^{j+1} - \omega^j)
\]

The term \( \frac{\partial \kappa}{\partial \omega} \) represents the change in residual strength of the material bonds during damage evolution, and can be obtained by derivation of equation (4.12), (4.22) or (4.24). The term \( \frac{\partial t_{\text{eff.eq}}}{\partial \omega} \) describes the variation of the effective stresses upon increasing damage. In the proposed discrete model, the evolution of damage is not explicitly given in terms of the equivalent traction. An expression for \( t_{\text{eff.eq}} \) can be obtained under the assumption that the total strain at the discontinuity \( \varepsilon_{\text{tot}} \) remains constant during a global iteration. In analogy with the additive decomposition of the effective traction vector (see equation (4.6)), the strain field at the discontinuity \( \varepsilon_{\text{tot}} \) is assumed to consist of two terms, namely, (i) a continuum strain component, related to the gradient of the displacement field and (ii) a discrete, strain-like term related to the displacement jump at the discontinuity:

\[
\varepsilon_{\text{tot}} = \varepsilon + \zeta (\bar{\mathbf{u}} \otimes \mathbf{n})
\]

Comparison with equation (4.3) points out that \( \varepsilon = \nabla \mathbf{u} + H_{\gamma} \nabla \mathbf{u} \) is the ‘continuum’ strain field and \( \zeta (\bar{\mathbf{u}} \otimes \mathbf{n}) \) with \( \zeta = \delta_{\gamma} \) is the ‘discrete’ contribution. The latter is theoretically unbound due to the presence of the Dirac delta function. In the spirit of strong discontinuity
analysis, we consider a discontinuity band of bandwidth \( h \), instead of a discontinuity plane with zero thickness. \( \zeta \) can then be defined as:

\[
\zeta = \begin{cases} 
0 & \text{if } x \notin \left[ -\frac{1}{2} h, \frac{1}{2} h \right] \\
\frac{1}{h} & \text{if } x \in \left[ -\frac{1}{2} h, \frac{1}{2} h \right]
\end{cases}
\]  

(4.57)

In the limit of \( h \rightarrow 0 \) we have \( \zeta = \delta_{i,j} \). Pre- and post-multiplying equation (4.56) with the stiffness \( D \) and the normal to the discontinuity \( n \), respectively, leads to:

\[
\mathbf{D}_{i,j} \sigma n + \zeta Q [\mathbf{u}] = 0
\]

(4.58)

where we made use of the constitutive relation \( \sigma = D \varepsilon \) (equation (4.37)) and the definition of the acoustic tensor. Rearranging yields:

\[
\mathbf{D}_{i,j} \sigma n = (1 - \zeta \gamma) \sigma n + \zeta \gamma \left( \sigma n + \gamma^{-1} Q [\mathbf{u}] \right)
\]

(4.59)

Note that the product \( \zeta \gamma \) is dimensionless. Using equations (4.4), (4.6) and (4.9) we obtain:

\[
\mathbf{D}_{i,j} \sigma n = (1 - \omega + \zeta \gamma \omega) \mathbf{t}^{\text{eff}}
\]

(4.60)

Under the assumption that \( \mathbf{e}^{\text{out}}_{i,j} \) is kept constant during a global iteration, the partial derivative of the effective traction vector with respect to damage can thus be expressed as:

\[
\frac{\partial \mathbf{t}^{\text{eff}}}{\partial \omega} = \left( \frac{1 - \zeta \gamma}{1 - \omega + \zeta \gamma \omega} \right) \mathbf{t}^{\text{eff}}
\]

(4.61)

Inserting equations (4.11) and (4.61) in (4.55) yields:

\[
\mathbf{f}^{j+1} = \mathbf{f}^j + \left( \frac{1 - \zeta \gamma}{1 - \omega^j + \zeta \gamma \omega^j} \right) \mathbf{t}^{\text{eff},\text{eq}} - \frac{\partial \kappa}{\partial \omega^j} \left( \omega^{j+1} - \omega^j \right)
\]

(4.62)

In the limit of \( h \rightarrow 0 \) we have \( \zeta = \delta_{i,j} \) and (4.62) becomes:

\[
\mathbf{f}^{j+1} = \mathbf{f}^j - \left( \frac{1}{\omega^j} \mathbf{t}^{\text{eff},\text{eq}} + \frac{\partial \kappa}{\partial \omega^j} \right) \left( \omega^{j+1} - \omega^j \right)
\]

(4.63)

We find the updated damage variable as the root of equation (4.63), after inserting the appropriate definition of the material strength \( \kappa \) (e.g. (4.12), (4.22) or (4.24)) and setting \( \mathbf{f}^{j+1} = 0 \). However, since this expression is singular for \( \omega = 0 \), we prefer using equation (4.62) with a value of \( \zeta > 1 \). This choice influences the rate of convergence of the local iterative procedure, not the global equilibrium state. \( \zeta \) only appears in the return mapping scheme, not in the tangent. Therefore, selecting a high value for \( \zeta \) does not render the system ill-conditioned. The updated damage variable obeys the Kuhn-Tucker conditions since \( \mathbf{f}^{j+1} = 0 \) and \( \Delta \omega > 0 \) if \( \zeta > 1 \).
4.3.7. Implementation

A general-purpose finite element code, written in Fortran 90, has been designed to solve the model equations. The program structure is modular. All common one, two and three dimensional element types are supported. Lagrangian elements are numerically integrated by means of standard quadrature rules (e.g. Gauss-Legendre), while element types expressed in barycentric coordinates employ specific schemes (e.g. Dunavant). The Visual Numerics® IMSL® Fortran Library is employed for basic algebraic operations and system solving.

For solving the system of equations, an iterative total incremental approach is followed. In each iteration, the system matrix and right hand side vector are composed, subsequently a Cholesky factorization or an LU-decomposition is performed, depending on the (non-)symmetry of the system matrix, next a direct solver is used to obtain the solution vector, and convergence of the iterative procedure is checked. In order to judge convergence, three different residuals are defined, namely (i) the force norm \( \| \mathbf{f}_{ext} - \mathbf{f}_{int} \| \), (ii) the energy norm \( | \mathbf{f}_{ext} \cdot \delta \mathbf{u} | \) and (iii) the displacement norm \( \| \delta \mathbf{u} \| \). For each residual both the absolute value and the scaled value with respect to the residual in the first iteration are checked against their respective threshold values. The latter ones are \( 10^{-4} \), \( 10^{-5} \) and \( 10^{-6} \) for the relative criteria and \( 10^{-6} \) for all absolute criteria. The solution vector is considered converged when for each of the three criteria, either the absolute or the relative residual, is below the threshold. In case one or more convergence criteria are violated, the iterative procedure is continued. A maximum allowed number of iterations is defined to provide a termination condition in case convergence problems arise. A value of 50 has been selected.

At the end of each converged time step, the crack initiation criterion (equation (4.27)) is verified in (i) the centre of mass of each integration zone and (ii) at every crack tip. At the point corresponding to the most severe violation of the initiation criterion a new crack is initiated or an existing crack is propagated. The direction is based on the non-local stress tensor (equation (4.28)). Multiple non-intersecting cracks per element are allowed. Cracks are inserted in the entire element at once, i.e. the crack tip is not allowed to be situated inside the element. This is a restriction of the current implementation, not of the proposed theory. After inserting a new crack segment, the time step is recomputed. We proceed to the next time step if either a stable crack pattern is obtained, or if the maximum number of new crack segments exceeds a predefined threshold. The default value for the threshold is 50. A more sophisticated threshold would be to impose an upper bound to the newly formed crack length (2D) or surface (3D). Such a threshold is invariant upon mesh refinement.
4.4. Academic examples

In this section three different numerical examples are presented. First, a uni-axial tension test on a three by three element mesh is studied. A full parametric study of the model is performed and the simplicity of the example allows observing the influence of the individual parameters. Next, aspects of mesh objectivity are analyzed by means of a four-point bending test. Finally, the applicability of the model in a multi-material setting is illustrated by means of a mode I double cantilever beam test.

4.4.1. Uni-axial tension

A 2D uni-axial tensile test is performed on a square sample with an edge length of 0.03 m (Figure 4.4). The sample is discretized with 9 square bilinear elements. Nodes on the left boundary are clamped in $x$-direction. Nodes at the right boundary are forced to move in $x$-direction at a fixed rate. Two additional constraints in $y$-direction prevent rigid body motions. A strong discontinuity with a normal pointing in the positive $x$-direction is inserted in the three middle elements. The discontinuity is damage-free at the beginning of the computations. Plane stress conditions are assumed. The Poisson’s ratio is taken equal to zero to simplify interpretation of the results. In a first analysis, an isotropic, linear elastic model for the bulk is adopted. The evolution of the residual strength is described by equation (4.24), i.e. $\lambda = +\infty$. The influence of changing the Young’s modulus, tensile strength, residual tensile strength at fracture and hardening exponent are studied. Table 4.1 gives an overview of the investigated parameters. Please note that $G_f^j$ is not an explicit model parameter, but is being calculated from equation (4.25).

![Figure 4.4: Uni-axial tensile test: geometry, mesh and boundary conditions.](image)
<table>
<thead>
<tr>
<th></th>
<th>$E$ [GPa]</th>
<th>$f_i^0$ [MPa]</th>
<th>$f_i^1$ [MPa]</th>
<th>$n$ [-]</th>
<th>$G_f^i$ [N/m]</th>
</tr>
</thead>
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<tr>
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<td>2.0</td>
<td>1.0</td>
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<td>1.0</td>
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<td>1.0</td>
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<td>3.0</td>
<td>4.5</td>
<td>1.0</td>
<td>712.5</td>
</tr>
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<td>1.0</td>
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</tr>
<tr>
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<td>4.5</td>
<td>0.2</td>
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<td>1.0</td>
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<td>5.0</td>
<td>535.2</td>
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Table 4.1: Investigated parameter combinations and resulting fracture energy (based on eq. (4.25)) for the uniaxial tensile test. Tests are subdivided in four groups (a-d). Corresponding results are shown in Figure 4.5a-d.

**Figure 4.5:** Uni-axial tensile test: sensitivity analysis of (a) Youngs modulus, (b) tensile strength, (c) residual tensile strength and (d) hardening exponent. All parameter combinations are listed in Table 4.1.
Figure 4.5a shows the influence of variations in stiffness. It is observed that the stiffer the material is, the more brittle it behaves. This is a direct consequence of the use of a stress-based damage criterion: the stiffness is inversely proportional with the required deformations to reach the ultimate strength. A higher tensile strength influences the peak load, but does not affect the slope of the loading and softening branch (Figure 4.5b). If tensile strength and residual tensile strength are given distinct values, both slope and shape of the softening branch are altered (Figure 4.5c). Choosing \( f_t^1 > f_t^0 \) leads to a more ductile response, whereas the opposite choice, \( f_t^1 < f_t^0 \), results in more brittle failure or even snap-back if \( f_t^1 < \left( \frac{n}{(n+1)} \right) f_t^0 \). Snap-back could not be illustrated in Figure 4.5c since the test is performed under displacement control. Figure 4.5d illustrates the effect of the softening parameter. If \( n > 1 \), the slope of the softening branch becomes more convex. A more concave shape is found for \( 0 < n < 1 \). Essential parameters \( E \) and \( f_t^0 \) can be identified experimentally from a uni-axial tensile test. Secondary parameters \( f_t^1 \) and \( n \) require inverse analysis. In chapter 7, inverse parameter identification will be applied in several of the presented examples.

<table>
<thead>
<tr>
<th>( k_w )</th>
<th>( f_t^0 )</th>
<th>( f_t^1 )</th>
<th>( n )</th>
<th>( G_f^l )</th>
</tr>
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<tbody>
<tr>
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<td>[MPa]</td>
<td>[MPa]</td>
<td>[-]</td>
<td>[N/m]</td>
</tr>
<tr>
<td>(e)</td>
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<td>3.0</td>
<td>3.0</td>
<td>1.0</td>
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<td></td>
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<td>3.0</td>
<td>3.0</td>
<td>1.0</td>
</tr>
</tbody>
</table>

Table 4.2: Investigated parameter combinations and resulting fracture energy (according to equation (4.25)) for the uni-axial tensile test. Corresponding results are shown in Figure 4.6e.

Figure 4.6: Uni-axial tensile test: influence of (e) parameter \( k_w \) of the bulk material model. All parameter combinations are listed in Table 4.2. Figures (f) and (g) illustrate conceptually the pre- and post-peak state of the material, respectively.
In the second analysis an isotropic damage model was used to model the degradation of the bulk material (see chapter 3, section 3.4.3.2). The model parameter $k_w$ was varied, and the remaining parameters $\lambda_w$ and $E$ were selected as such that the continuous-discontinuous transition point coincides with the transition point in a linear elastic analysis with $E = 10$ GPa and $f^0_t = 3$ MPa (Table 4.2). The damaged stiffness at the transition point is therefore the same, i.e. 10 GPa, for all simulations. Since, (i) the slope of the softening branch is determined by the stiffness of the bulk and (ii) the damage in the bulk does not develop further beyond the transition point, the obtained post-peak response for the damage model is identical to the one for the linear elastic model (Figure 4.6e). By varying $f^1_t$ and $n$, or by adopting different expressions for $\kappa$ (instead of equation (4.24)), the shape of the softening branch can be altered.

The amount of dissipated energy during the tensile test now consists of two parts. On the one hand the energy dissipated in the continuum, prior to the formation of a discrete crack. On the other hand the energy dissipated as the discrete crack forms. The latter component is the fracture energy, as obtained from equation (4.25), and is not affected by the pre-peak non-linearity (Table 4.2). The dissipated energy in the pre-peak regime is associated with the damage process in the bulk material, and is adequately described by a bulk (or continuum) damage variable (Figure 4.6f). The post-peak energy is associated with the formation of a discrete fracture. Since fractures are planar structures, a discrete damage variable is the most appropriate to describe the damage process in the localization zone (Figure 4.6g).

### 4.4.2. Four-point bending

A four-point bending test on a notched beam is used to prove mesh objectivity of the response. The same test will be studied in chapter 7 and compared with measurements. The beam has a length of 0.24 m and cross-sectional dimensions 0.048 m x 0.024 m (height x depth). The notch has a width of 0.004 m, a depth of 0.008 m and a circular tip. The distance between the two supports is 0.2 m and between the loading points 0.1 m. In this example, the bulk material is considered linear elastic and isotropic. The evolution of the residual strength according to equation (4.24) is used. A Young’s modulus of 10 GPa, a Poisson’s ratio of 0.2, a tensile strength of 3 MPa, a residual tensile strength of 2 MPa and a softening exponent of 0.6 were selected. The simulations were performed in 2D under plane stress assumptions. Meshes were constructed for two element types, namely bilinear quadrilaterals (Q4) and linear triangles (T3), and for three levels of mesh refinement (572, 1596 and 5604 dofs,
respectively). The six meshes are depicted in Figure 4.7. A new crack segment is introduced at the end of a load step, if the failure criterion is violated at the crack tip. In this way, crack path continuity is easily enforced. Afterwards global equilibrium is again evaluated. The procedure is repeated until the initiation criterion is no longer met. New crack segments cross the entire element at once.

Displacement control was applied.

![Figure 4.7: Four-point bending test: geometry, meshes and boundary conditions.](image)

The results of the mesh sensitivity analysis are presented in Figure 4.8 as ‘force (F)’ versus ‘crack mouth opening displacement (CMOD)’ diagrams. CMOD is measured at the bottom surface of the specimen, across the notch. Comparing the three structured meshes based on quadrilateral elements (Figure 4.8a) it is seen that the meshes with 1596 and 5604 dofs yield almost the same response. The mesh with 572 dofs is too coarse to capture the actual behaviour. For the meshes based on triangular elements, load drops are observed in the softening branch each time a new crack segment is introduced (Figure 4.8b). The presence of load drops is related to the constant strain property of the T3-element. Since we use a linear elastic constitutive relation, the stress field is constant over the element as well. Therefore, the stress field in the cohesive zone is not decaying gradually, but in a stepwise manner. Upon propagation, the stress field undergoes a stepwise change, and a load drop is observed. Upon mesh refinement, the number of elements over the cohesive zone increases, allowing a more accurate representation of the stress field in the cohesive zone. As a result, the number of load drops increases, but their magnitude decreases. The mesh with 5604 dofs yields the same response as the two finest meshes with quadrilateral elements.
The computations were repeated with smaller load steps. At coinciding loading points an identical response was obtained. For this example the size of the load step did not influence the robustness of the algorithm. If a nonlinear model is chosen to represent the bulk damage behaviour, like in the comparative tests in chapter 7, an upper bound to the load step exists.

Figure 4.8: Four-point bending test: load-displacement curves obtained with meshes based on (a) Q4 and (b) T3 elements.

4.4.3. Double cantilever beam

As a final example, a comparison between the proposed cohesive zone model and classical interface elements is presented by means of a mode I double cantilever beam test (DCB). A composite beam of 0.0025 m length and 0.0005 m height is subjected to a vertical load at one corner, and restrained at two other corners (see Figure 4.9).
The beam consists of two layers with equal height: a softer upper layer on a stiffer base layer. Both layers have a Poisson’s ratio of 0.3 and a tensile strength of 1 MPa. The stiffness of the base layer is 10 GPa. The stiffness of the upper layer is taken 5, 10, 20 and 50 times lower. The material interface is modelled in two different ways. First using the proposed cohesive zone model \( (E = 10 \text{ GPa}; \nu = 0; f^0_t = 1 \text{ MPa}; f^1_t = 1 \text{ MPa}; \lambda = +\infty; n = 1) \). This choice of parameters yields a linear softening behaviour with a fracture energy of 50 N/m (Figure 4.10a). Alternatively, interface elements employing a linear softening law are used (Figure 4.10b). Although the use of a dummy stiffness can be avoided by e.g. initially constraining the interfaces (Camacho and Ortiz 1996), we make use of classical Coulomb interface elements with a penalty stiffness of \( 10^6 \text{ GPa} \). This value is large enough to provide a reasonable stiffness but small enough to avoid numerical problems, such as spurious traction oscillations (Schellekens and de Borst 1992). The tensile strength and fracture energy are taken 1 MPa and 50 N/m, respectively. The beam consists of 125 bilinear elements for the X-FEM simulation and 150 bilinear elements for the simulation with interface elements. Both meshes have 300 dofs. Plane stress conditions are assumed.
In Figure 4.11a, the applied load $F$ is plotted against the vertical displacement of the loading point. Dashed lines represent the solution with interface elements, solid lines are used for the X-FEM results. As expected, it is observed that the overall response is not depending on the modelling technique for the material interface. A small difference in slope of the softening branch is found with increasing difference in stiffness between the two layers. This is related to the way the equivalent traction is defined in the discrete model, namely as the normal component of the effective traction vector. In the Coulomb interface element, damage evolution is governed by the norm of the displacement jump vector (normal and tangential). In the presence of shear (or a tangential jump) along the interface, damage will grow faster in the interface formulation. The importance of the shear contribution increases with increasing difference in stiffness between both layers. The good agreement between the response of the proposed cohesive zone model and of classical interface elements indicates that the introduction of the approximation for the local stress tensor at zero damage (equation (4.53)) is justified.
4.5. Concluding remarks

A general strategy to model the mechanical behaviour of quasi-brittle materials is proposed. The formulation employs the partition of unity (PU) concept and introduces a new cohesive zone model, capturing the transition between the initial continuum state and the final discrete state and ensuring equilibrium between the effective tractions in the undamaged material bonds and the stresses in the continuum at every stage of the failure process. The discrete equation can be used in combination with basically any continuum constitutive model, yielding a continuous-discontinuous material model that can describe the entire failure process. Besides the study of fracture processes in bulk material, the discrete model can also be applied to examine delamination or interface failure. In contrast with classical interface elements, no dummy stiffness is required.

The predictive capabilities of the model crucially depend on the characteristics of the continuum model and the appropriate choice of the damage criterion. The pre-peak behaviour is entirely governed by the continuum model. The post-peak behaviour results from the interplay between the continuum model and the selected damage criterion, whereby the former applies to the material in the undamaged material bridges, and the latter controls the failure of the remaining material bridges. It was shown that for mode I, realistic trends can already be obtained based on a simple mechanical model (linear elasticity) and failure criterion (Rankine). In chapter 7, a comparison with experimental results will be performed, illustrating that also quantitatively correct results can be obtained with the proposed model.
5. Hygro-thermal behaviour of discontinuous porous media

Geometrical discontinuities, like material interfaces and fractures, not only have an impact on the stress distribution and the mechanical behaviour, but also strongly affect transport processes. Consider for instance the case of moisture transport in a fractured porous medium. The fracture acts as a preferential flow channel and flow along the discontinuity can take place more easily. In contrast, flow across the gas-filled part of the fracture is hindered since the major transport mechanism in absence of an external pressure gradient, namely capillary suction, can not take place. Flow across the water-filled part of the fracture is on the other hand hardly affected by the presence of the discontinuity.

In this chapter, the problem of modelling the impact of geometrical discontinuities on transport processes is addressed. Pursuing a continuous-discontinuous approach, different transport models are attributed to fracture and matrix. Hereby, the fracture-induced anisotropic behaviour is automatically incorporated.

The chapter starts by motivating the use of a discontinuous description of the temperature and pressure field (section 5.1). Next, the need for a discrete cohesive zone model is discussed (5.2.1), a detailed derivation of the discrete thermal constitutive equation for a damaged material interface is given (5.2.2), and the discrete hygro-thermal constitutive equations are presented (5.2.3). Additionally, special attention is given to the exchange of heat and mass between the bulk material and the environment via the fracture (5.2.4). In section 5.3 the governing equations for hygro-thermal transport processes are transformed into a format suitable for computer implementation. Finally, the characteristic features of the proposed model are illustrated by means of several academic examples (section 5.4).

5.1. Problem field

Moisture transport in fractured porous media has been studied by several authors. Larsson et al. (1996) proposed to describe the pressure field in a shear band under undrained conditions by a regularized Dirac delta distribution. In contrast, Armero and Callari (1999) keep the pressure field continuous, but introduce a discontinuity in the mass flux across the
discontinuity. The jump in the flux is proportional to the mass accumulating in the fracture. Segura and Carol (2004) studied the hydraulic behaviour of joints. They suggest that a jump in hydraulic head can occur across the discontinuity and drive transverse flow. In the same year, De Borst et al. introduced a strong discontinuity in the pressure field, merely motivated by the analogy with the decomposition of the displacement field. In subsequent papers, the idea of a discontinuous pressure field is again abandoned; instead a weak discontinuity in the pressure field is used (Réthoré et al. 2007 and 2008).

The literature on heat flow in fractured porous media is rather limited. Usually fractures are considered adiabatic, i.e. no energy is exchanged with the surrounding porous material. In a recent paper by Fagerström and Larsson (2008), heat exchange between fracture and the surrounding matrix is considered. To that extent, the temperature field is decomposed using a Heaviside function, but the opportunity to develop a strong discontinuity is not exploited in their examples.

In reality, all parts of a fractured porous medium behave as independent components, but share a common history. They can reach a different stress state, moisture content and temperature distribution, depending on the specific conditions they are subjected to. Mathematically, mutual independence of the different parts can be achieved by inserting a strong discontinuity in every problem field. As a result, all state variables can exhibit a jump across a discontinuity, but only in case the circumstances invoke a discontinuous state. For instance, the existence of a temperature gradient across a fractured porous medium is a necessary, but not a sufficient condition for a temperature jump to occur: only in case a gradient across the gas-filled crack is invoked, the temperature of both crack surfaces will become different, given that a gas-filled crack has a non-zero thermal resistance.

![Figure 5.1](image_url): Schematic representation of the (a) capillary pressure and (b) temperature field over a crossed 1D element of length L.
In analogy with the decomposition of the displacement field (chapter 4), the capillary pressure field $p_c$ is decomposed as:

$$p_c = \hat{p}_c + H_{\tau_d} \bar{p}_c$$

and for the temperature field $T$ we have:

$$T = \hat{T} + H_{\tau_d} \bar{T}$$

where $\hat{p}_c$, $\bar{p}_c$, $\hat{T}$ and $\bar{T}$ are smooth, continuous functions on $\Omega$ and $H_{\tau_d}$ is the Heaviside step function, used as enhanced approximation basis.

A discontinuous description of the pressure and temperature field might seem contra-intuitive, since both fields are continuous in reality. The apparent contradiction can be explained by realizing that the pressure or temperature jump occurs over the width of the discontinuity. Hence, the actual fields exhibit a finite gradient across the discontinuity, not a jump. A discontinuous mathematical description is therefore not conflicting with the physical reality.

### 5.2. Cohesive zone model

#### 5.2.1. Motivation

The approach to model transport in a fractured porous medium is closely related to the way in which the fracture process is modelled. In the previous chapter, the continuous-discontinuous strategy to describe failure was put forward. Herein, a continuum model governs the mechanical material behaviour up to the onset of localization. At that moment, a cohesive segment is inserted. The behaviour of this segment, described by the proposed cohesive zone model, is initially identical to the continuum behaviour. As the damage process proceeds, the cohesive segment gradually develops into a strong discontinuity, i.e. a fracture. The same strategy is applicable to model transport processes in fractured porous media. Initially, a continuum transport model can be employed. When a cohesive segment is inserted, the use of an appropriate discrete transport model should ensure that the behaviour remains identical to the continuum behaviour. As damage develops, the cohesive zone gradually develops into a fracture, and correspondingly, the discrete transport model gradually develops into a model that describes transport in and across a fracture. Herein lays the main difference with the mechanical discrete cohesive zone model. Tensile forces can not be transmitted across a true discontinuity. Transport across a discontinuity can however take place - just via a different transport mechanism. For example, heat transfer across a gas-filled crack can take place by
means of conduction, convection and radiation. Mass transfer can occur by means of
advective and diffusive flow.

Since a fracture forms a connection between the environment and the bulk material, mutual
interaction occurs. The continuous-discontinuous modelling concept, proposed in the
preceding chapter, therefore needs to be extended to incorporate the possible interaction with
the environment via the fractured part of the interface. In the following, the derivation of the
discrete damage-based constitutive equation for heat transfer at a damaged material interface
will be discussed in detail. By assuming the same material at both sides of the interface, the
discrete model for fracture is obtained. The derivation of the coupled hygro-thermal discrete
model is similar, and therefore only the main results will be presented.

5.2.2. Damage-based discrete constitutive equation for heat transfer

5.2.2.1. General derivation

Consider a partially fractured material interface (Figure 5.2a). The amount of damage can be
described with a scalar damage variable $\omega$ ranging from zero to one. Two pathways for heat
transfer can be distinguished, namely (i) directly via the undamaged material bonds and (ii)
indirectly via the damaged region.

![Figure 5.2: (a) Schematic representation of the damaged material interface. Flux equilibrium at the positions (b) $\Gamma_d^-$, (c) $\Gamma_d^+$ and (d) $\Gamma_d^+$.](image)

The derivation for the discrete cohesive zone model starts from energy conservation, written
for three different positions, namely $\Gamma_d^-$, $\Gamma_d^+$ and $\Gamma_d$, which are the interfaces between $\Omega^-$
and the cohesive zone, $\Omega^+$ and the cohesive zone, and the material interface (Figure 5.2a). For an infinitesimal part of $\Gamma_d$ with area $dA$ and normal $\mathbf{n}$, we can write (Figure 5.2b):

$$\left( q^- \cdot \mathbf{n} + (1-\omega) q_{\Gamma_d} \cdot \mathbf{n} + \omega q_{\Gamma_d} \cdot \mathbf{n} \right) dA = 0$$

(5.3)

where $q^-$ is the heat flux flowing from $\Omega^-$ towards the interface, $q_{\Gamma_d}$ the flux flowing in the material bond towards the interface, and $\mathbf{q}_{\Gamma_d}$ the flux flowing from the fracture towards the interface.

In analogy with the decomposition of the effective traction vector in the mechanical cohesive zone model (see equation (4.6)), we will decompose the effective flux $q_{\Gamma_d}^{\text{eff}} = q_{\Gamma_d} \cdot \mathbf{n}$ in two components, namely (i) a component proportional to the temperature gradient, in magnitude equal to the continuum flux in $\Omega^-$ at an infinitesimal distance from $\Gamma_d$ and (ii) a discrete component, proportional to the temperature jump between $\Gamma_d$ and $\Gamma_d$. At this stage, the latter component can be seen as a correction term, to compensate for the difference between $q_{\Gamma_d}^{\text{eff}}$ and the continuum term. Later, it will become clear that both are always equal for undamaged interfaces. The discrete term is therefore damage-related, as is the development of a temperature jump. The effective flux is given by:

$$-q_{\Gamma_d}^{\text{eff}} = -q_{\Gamma_d} \cdot \mathbf{n} = q^- \cdot \mathbf{n} + \gamma^{-1} \alpha^{-1} K_{\Gamma_d} \left( T_{\Gamma_d} - T_{\Gamma_d} \right)$$

(5.4)

where $K_{\Gamma_d}$ is the discrete permeability of the material bond. In analogy with mechanics, $K_{\Gamma_d}$ can be modelled as $\mathbf{n} \cdot K_{\Omega^+} \mathbf{n}$. Alternatively, $K_{\Gamma_d}$ can be postulated or it can be obtained from a lower scale simulation. The minus sign in equation (5.4) is a consequence of the convention that energy source terms are positive. $\gamma$ is one unit meter and follows from dimensional analysis. $T_{\Gamma_d}$ and $T_{\Gamma_d}$ are the temperatures at $\Gamma_d$ and $\Gamma_d$, respectively. $\alpha$ indicates the relative position of the material interface in the cohesive zone (see Figure 5.2). The default value is $\alpha = 0.5$.

Substitution of (5.4) into (5.3) and rearranging leads to:

$$q^- \cdot \mathbf{n} = (1-\omega) \left( q^- \cdot \mathbf{n} + \gamma^{-1} \alpha^{-1} K_{\Gamma_d} \left( T_{\Gamma_d} - T_{\Gamma_d} \right) \right) - \omega \mathbf{q}_{\Gamma_d} \cdot \mathbf{n}$$

(5.5)

Analogously, the equilibrium at $\Gamma_d$ yields (Figure 5.2d):

$$q^+ \cdot \mathbf{n} = (1-\omega) \left( q^+ \cdot \mathbf{n} + \gamma^{-1} (1-\alpha)^{-1} K_{\Gamma_d} \left( T_{\Gamma_d} - T_{\Gamma_d} \right) \right) - \omega \mathbf{q}_{\Gamma_d} \cdot \mathbf{n}$$

(5.6)
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The flux-equilibrium in the material bonds at the material interface \( \Gamma_d \), reads (Figure 5.2c):

\[
q_{\Gamma_d}^{\text{eff}} + q_{\Gamma_d}^{\text{eff}} = q_{\Gamma_d} \cdot n + q_{\Gamma_d} \cdot n = 0
\]  

Equation (5.7) allows determining the interface temperature \( T_{\Gamma_d} \). To that extent we first insert the expressions for the effective flux (equation (5.3) for \( \Gamma_d \)) into equation (5.7):

\[
\left( q \cdot n + \gamma^{-1} \alpha^{-1} K_{\Gamma_d} \left( T_{\Gamma_d} - T_{\Gamma_d} \right) \right) + \left( q^* \cdot n + \gamma^{-1} (1 - \alpha)^{-1} K_{\Gamma_d} \left( T_{\Gamma_d} - T_{\Gamma_d} \right) \right) = 0
\]  

(5.8)

\( q \cdot n \) can be eliminated by means of equation (5.5) and \( q^* \cdot n \) by means of (5.6), leading to:

\[
T_{\Gamma_d} = \gamma^{-1} \left( \alpha^{-1} K_{\Gamma_d} T_{\Gamma_d} + (1 - \alpha)^{-1} K_{\Gamma_d} T_{\Gamma_d} \right) - \omega \left( \bar{q}_{\Gamma_d} \cdot n + \bar{q}_{\Gamma_d} \cdot n \right)
\]  

(5.9)

After substituting result (5.9) in equation (5.5), the discrete flux at \( \Gamma_d \) becomes:

\[
q^* \cdot n = (1 - \omega) \left( q^* \cdot n + \gamma^{-1} K_{\Gamma_d} \left( T_{\Gamma_d} - T_{\Gamma_d} \right) \right) + \left( 1 - \omega \right) \omega \left( 1 - \alpha \right)^{-1} K_{\Gamma_d} \left( \left( 1 - \alpha \right)^{-1} K_{\Gamma_d} + (1 - \alpha)^{-1} K_{\Gamma_d} \right)^{-1} \left( \bar{q}_{\Gamma_d} \cdot n + \bar{q}_{\Gamma_d} \cdot n \right) - \omega \bar{q}_{\Gamma_d} \cdot n
\]  

(5.10)

where \( K_{\Gamma_d} = \left( \alpha K_{\Gamma_d}^{-1} + (1 - \alpha) K_{\Gamma_d}^{-1} \right)^{-1} \) is the combined discrete permeability. In the case of two equal materials \( K_{\Gamma_d} = K_{\Gamma_d} \), the combined discrete permeability \( K_{\Gamma_d} \) equals the material permeability, independent of the value for \( \alpha \).

After eliminating the interface temperature \( T_{\Gamma_d} \), the discrete flux at \( \Gamma_d^+ \) reads:

\[
q^* \cdot n = (1 - \omega) \left( q^* \cdot n + \gamma^{-1} K_{\Gamma_d} \left( T_{\Gamma_d} - T_{\Gamma_d} \right) \right) + \left( 1 - \omega \right) \omega \left( 1 - \alpha \right)^{-1} K_{\Gamma_d} \left( \left( 1 - \alpha \right)^{-1} K_{\Gamma_d} + (1 - \alpha)^{-1} K_{\Gamma_d} \right)^{-1} \left( \bar{q}_{\Gamma_d} \cdot n + \bar{q}_{\Gamma_d} \cdot n \right) - \omega \bar{q}_{\Gamma_d} \cdot n
\]  

(5.11)

Expressions (5.10) and (5.11) are the general expressions for the discrete thermal cohesive zone model of a material interface. Adding (5.10) and (5.11) together yields:

\[
\omega \left( q^* \cdot n + q^+ \cdot n \right) = -\omega^2 \left( \bar{q}_{\Gamma_d} \cdot n + \bar{q}_{\Gamma_d} \cdot n \right) = -\omega \bar{q}_{\Gamma_d}
\]  

(5.12)

where

\[
\bar{q}_{\Gamma_d} = \omega \left( \bar{q}_{\Gamma_d} \cdot n + \bar{q}_{\Gamma_d} \cdot n \right)
\]  

(5.13)
represents the heat source per unit area of the planar cohesive zone. \( \bar{q}_{\Gamma_d} \) is positive if energy is transferred from the fracture towards the cohesive zone. Equation (5.12) has to hold for every value of \( \omega \), therefore:

\[
q^- \cdot n + q^+ \cdot n = -\bar{q}_{\Gamma_d}
\]  

(5.14)

which represents the global energy equilibrium over the cohesive region. Time dependent terms are absent since an interface does not have a volume, and consequently does not possess a capacity. This does not imply that the heat flow along the fracture has to be stationary. The fracture has a width and consequently also a volume. The energy conservation law, written for the domain of the fracture, will therefore contain time-dependent terms. The interaction between the fracture domain and the surrounding porous medium takes place via the exchange fluxes \( \bar{q}_{\Gamma_d}^- \) and \( \bar{q}_{\Gamma_d}^+ \). Simplified conservation equations for the fracture domain will be given in section 5.2.4.

5.2.2.2. Isolated micro-crack or cavity

In an isolated micro-crack or cavity, external sources of energy are absent. Therefore, the flux via the damaged part of \( \Gamma_d^- \) to the cavity must be equal to the flux from the cavity to \( \Gamma_d^+ \), or more precisely \( \bar{q}_{\Gamma_d}^- \cdot n = -\bar{q}_{\Gamma_d}^+ \cdot n \equiv \bar{q}_{\Gamma_d} \cdot n \). In this case, expressions (5.10) and (5.11) simplify to:

\[
(q^- \cdot n = (1-\omega)(q^- \cdot n + \gamma^{-1}K_{\Gamma_d}(T_{\Gamma_d}^- - T_{\Gamma_d}^+)) - \omega \bar{q}_{\Gamma_d} \cdot n)
\]  

(5.15)

and

\[
q^+ \cdot n = (1-\omega)(q^+ \cdot n + \gamma^{-1}K_{\Gamma_d}(T_{\Gamma_d}^+ - T_{\Gamma_d}^-)) + \omega \bar{q}_{\Gamma_d} \cdot n
\]  

(5.16)

Summing both expressions and rearranging yields:

\[
\omega(q^- \cdot n + q^+ \cdot n) = 0
\]  

(5.17)

which, again, has to hold for every value of \( \omega \). Therefore \( -q^- = q^+ = q \), and the discrete thermal cohesive zone model in case of a cavity reads:

\[
q \cdot n = (1-\omega)(q \cdot n + \gamma^{-1}K_{\Gamma_d}[T]) + \omega \bar{q}_{\Gamma_d} \cdot n
\]  

(5.18)

This expression clearly states that the total flux (left hand side) consists of (i) a flux through the undamaged material bonds (right hand side, first term) and (ii) a flux through the micro-crack or cavity (right hand side, second term). The flux trough the undamaged material bonds
consists of a continuum and a discrete component. The physical meaning of both terms can be understood by rearranging equation (5.18):

\[
\omega q \cdot n = (1 - \omega) \gamma^{-1} K_{\Gamma_d} [T] + \omega \tilde{q}_{\Gamma_d} \cdot n
\]  

(5.19)

Equation (5.19) clearly shows that a temperature jump cannot occur ([T] = 0) in absence of damage (\(\omega = 0\)). When damage is present, the thermal flux that was originally flowing through the damaged part of the interface (\(\omega q \cdot n\)) is redistributed. A part of this flux is exchanged with the micro-crack or cavity via the fractured part of the interface (\(\omega \tilde{q}_{\Gamma_d} \cdot n\)). The remaining heat flows through the undamaged material bridge. The magnitude of the latter is proportional to the temperature difference across the material bridge.

5.2.2.3. Adiabatic fracture

If it is assumed that no heat is exchanged between the material and the fracture or \(\tilde{q}_{\Gamma_d} \cdot n = \tilde{q}_{\Gamma_d} \cdot n = 0\), we obtain the academic limit case of an adiabatic fracture. Even in vacuum, this situation does not occur since heat exchange by means of radiation does not require a medium. Considering an adiabatic fracture therefore only has theoretical value. In this case, expressions (5.10) and (5.11) reduce to:

\[
q^- \cdot n = (1 - \omega) \left( q^- \cdot n + \gamma^{-1} K_{\Gamma_d} \left( T_{\Gamma^{-}_d} - \tilde{T}_{\Gamma^-_d} \right) \right)
\]  

(5.20)

and

\[
q^+ \cdot n = (1 - \omega) \left( q^+ \cdot n + \gamma^{-1} K_{\Gamma_d} \left( T_{\Gamma^+_d} - \tilde{T}_{\Gamma^+_d} \right) \right)
\]  

(5.21)

Equation (5.17) also holds in this case. Therefore \(-q^- = q^+ = q\), and the discrete thermal cohesive zone model in case of an adiabatic fracture reads:

\[
q \cdot n = (1 - \omega) \left( q \cdot n + \gamma^{-1} K_{\Gamma_d} [T] \right)
\]  

(5.22)

The similarity with the discrete mechanical cohesive zone model is obvious (compare with equation (4.9)). This could be expected since the mechanical model was derived under the assumption that no tensile tractions could be transferred across the damaged parts of the fracture. For the mechanical model, this assumption is however justified.

5.2.3. Damage-based discrete constitutive equation for coupled heat and mass transfer

In case coupled heat and mass transfer is considered, the equilibrium at \(\Gamma^{-}_d\) and \(\Gamma^+_d\) can be expressed, in a similar format as equations (5.5) and (5.6):
Hygro-thermal behaviour of discontinuous porous media

\[
\begin{align*}
\mathbf{g}^- \cdot \mathbf{n} &= (1 - \omega) \left[ \mathbf{g}^- \cdot \mathbf{n} + \gamma^{-1} \mathbf{K}_{\Gamma_d} \begin{pmatrix} p_{c,\Gamma_d} - p_{c,\Gamma_d} \\ T_{\Gamma_d} - T_{\Gamma_d} \end{pmatrix} \right] - \omega \left[ \overline{\mathbf{g}}_{\Gamma_d} \cdot \mathbf{n} \right] \\
\mathbf{q}^- \cdot \mathbf{n} &= (1 - \omega) \left[ \mathbf{q}^- \cdot \mathbf{n} + \gamma^{-1} (1 - \alpha)^{-1} \mathbf{K}_{\Gamma_d} \begin{pmatrix} p_{c,\Gamma_d} - p_{c,\Gamma_d} \\ T_{\Gamma_d} - T_{\Gamma_d} \end{pmatrix} \right] - \omega \left[ \overline{\mathbf{q}}_{\Gamma_d} \cdot \mathbf{n} \right]
\end{align*}
\]

(5.23)

and

\[
\begin{align*}
\mathbf{g}^+ \cdot \mathbf{n} &= (1 - \omega) \left[ \mathbf{g}^+ \cdot \mathbf{n} + \gamma^{-1} \mathbf{K}_{\Gamma_d} \begin{pmatrix} p_{c,\Gamma_d} - p_{c,\Gamma_d} \\ T_{\Gamma_d} - T_{\Gamma_d} \end{pmatrix} \right] - \omega \left[ \overline{\mathbf{g}}_{\Gamma_d} \cdot \mathbf{n} \right] \\
\mathbf{q}^+ \cdot \mathbf{n} &= (1 - \omega) \left[ \mathbf{q}^+ \cdot \mathbf{n} + \gamma^{-1} (1 - \alpha)^{-1} \mathbf{K}_{\Gamma_d} \begin{pmatrix} p_{c,\Gamma_d} - p_{c,\Gamma_d} \\ T_{\Gamma_d} - T_{\Gamma_d} \end{pmatrix} \right] - \omega \left[ \overline{\mathbf{q}}_{\Gamma_d} \cdot \mathbf{n} \right]
\end{align*}
\]

(5.24)

where

\[
\mathbf{K}_{\Gamma_d} = \begin{bmatrix} K_{mm,\Gamma_d} & K_{me,\Gamma_d} \\ K_{em,\Gamma_d} & K_{ee,\Gamma_d} \end{bmatrix}
\]

and

\[
\mathbf{K}_{\Gamma_d} = \begin{bmatrix} K_{mm,\Gamma_d} & K_{me,\Gamma_d} \\ K_{em,\Gamma_d} & K_{ee,\Gamma_d} \end{bmatrix}
\]

(5.25)

are the coupled permeability/conductivity matrices. The first subscript of the entries in the matrices denotes the equation in which these terms appear (\( m \) for mass balance, \( e \) for energy balance) and the second subscript indicates their corresponding variable (\( m \) for the variable related to mass transport, namely the capillary pressure \( p_c \), \( e \) for the variable related to energy transport, namely the temperature \( T \)). In equations (5.23) and (5.24) \( \mathbf{g}^- \) and \( \mathbf{g}_{\Gamma_d}^- \) are mass fluxes flowing from \( \Omega^- \) and from the fracture towards the interface \( \Gamma_d^- \), \( \mathbf{g}^+ \) and \( \mathbf{g}_{\Gamma_d}^+ \) are mass fluxes flowing from \( \Omega^+ \) and from the fracture towards the interface \( \Gamma_d^+ \), and \( p_{c,\Gamma_d^-} \), \( p_{c,\Gamma_d^+} \) and \( p_{c,\Gamma_d} \) are capillary pressures at \( \Gamma_d^- \), \( \Gamma_d^+ \) and \( \Gamma_d \), respectively. All other symbols have the same meaning as before. After eliminating the unknowns at the material interface \( \Gamma_d \) by means of the interface equilibrium, equation (5.23) becomes:

\[
\begin{align*}
\mathbf{g}^- \cdot \mathbf{n} &= (1 - \omega) \left[ \mathbf{g}^- \cdot \mathbf{n} + \gamma^{-1} \mathbf{K}_{\Gamma_d} \begin{pmatrix} p_{c,\Gamma_d} - p_{c,\Gamma_d} \\ T_{\Gamma_d} - T_{\Gamma_d} \end{pmatrix} \right] \\
&+ (1 - \omega) \omega \alpha^{-1} \mathbf{K}_{\Gamma_d} \left( \alpha^{-1} \mathbf{K}_{\Gamma_d} + (1 - \alpha)^{-1} \mathbf{K}_{\Gamma_d} \right)^{-1} \left[ \mathbf{g}_{\Gamma_d}^- + \mathbf{g}_{\Gamma_d}^+ \right] \cdot \mathbf{n} - \omega \left[ \overline{\mathbf{g}}_{\Gamma_d} \cdot \mathbf{n} \right]
\end{align*}
\]

(5.26)

where the coupled tensor \( \mathbf{K}_{\Gamma_d} \) is defined as:

\[
\mathbf{K}_{\Gamma_d} = \left( \alpha^{-1} \mathbf{K}_{\Gamma_d}^{-1} + (1 - \alpha)^{-1} \mathbf{K}_{\Gamma_d}^{-1} \right)^{-1}
\]

(5.27)

Equation (5.24) reads after the same manipulations:
From equations (5.26) and (5.28) we obtain the identity:

\[
\begin{align*}
\mathbf{g}^* \cdot \mathbf{n} + \mathbf{q}^+ \cdot \mathbf{n} &= (1 - \omega) \left( \mathbf{g}^* \cdot \mathbf{n} + \gamma^{-1} \mathbf{q}^+ \cdot \mathbf{n} \right) + (1 - \omega) \omega (1 - \alpha)^{-1} \mathbf{K}_{\gamma^*} \left( (1 - \alpha)^{-1} \mathbf{K}_{\gamma^*} + (1 - \alpha)^{-1} \mathbf{K}_{\gamma^*} \right)^{-1} \left( \mathbf{g}_{\gamma^*} + \mathbf{q}_{\gamma^*} \right) \cdot \mathbf{n} - \omega \mathbf{q}_{\gamma^*} \cdot \mathbf{n}
\end{align*}
\]

Expression (5.29) is the equivalent of equation (5.12) in the purely thermal model. It is obvious that equations (5.10) and (5.11) are a special case of equations (5.26) and (5.28). An extension to include more fields is trivial.

### 5.2.4. Simplified models for heat and mass transfer across micro-cracks, cavities and fractures

We make a distinction between the cohesive zone, i.e. the region in which \( 0 < \omega < 1 \), and the fracture (\( \omega = 1 \)). The cohesive zone is characterized by micro-cracks and cavities of different sizes. Depending on the amount of damage, the cavities and micro-cracks are isolated features, or are partially interconnected. In contrast to a cohesive zone, a fracture is considered a single, fully-connected, macroscopic entity. The distinction between cohesive zone and fracture is important in the modelling of heat and mass transfer. Because of the relatively large size of a fracture, gradients in temperature and pressure can exist along the length of the fracture and invoke flow in this direction. For the smaller micro-cracks and cavities in the cohesive zone, it can be argued that gradients across the fracture are more relevant than the in-plane gradients. Furthermore, the volume of the micro-cracks and cavities in the cohesive zone is much smaller than the one of the fracture. Therefore, neglecting capacity of the fluid inside the micro-cracks and cavities can be defended, as a first approximation. However, this assumption is debatable for fractures, certainly if they are filled with a fluid like water. A final difference between fracture and cohesive zone is that a fracture is generally partially filled with gas and partially with liquid, while the small scale of micro-cracks and cavities allows to consider them filled with a mixture of gas and liquid. In a fracture we look at both phases separately, and at the meniscus between them. The flow of the fluid phase is governed by differences in liquid pressure, while the flow of the gas phase happens under gradients in gas pressure. At the meniscus, both have to be in equilibrium with
the surface tension along the meniscus. In the cohesive zone, the flow of the liquid-gas mixture is driven by capillary pressure gradients.

Below, a simplified model for coupled heat and mass transfer across the cohesive zone is given. The use of fracture flow models within the proposed framework is briefly discussed. Fracture flow models are not considered in the examples in the remainder of this thesis.

5.2.4.1. Mass flow across micro-crack or cavity

Mass can be transferred across a micro-crack or cavity by means of liquid flow or vapour diffusion. The magnitude of the liquid flux is assumed proportional to a pressure gradient:

\[ \mathbf{g}^{l,H_2O} = -K^l \mathbf{\nabla} p^{l,H_2O} \]  

(5.30)

where \( K^l \) is the liquid permeability of the medium. Under the assumption that the gas pressure equals the (constant) atmospheric pressure, the gradient of the sum of liquid pressure and capillary pressure equals zero, hence:

\[ \mathbf{g}^{l,H_2O} = K^l \mathbf{\nabla} p_c \]  

(5.31)

The governing equation for vapour transport by means of diffusion reads:

\[ \mathbf{g}^{g,H_2O} = -\delta^{g,H_2O} \mathbf{\nabla} p^{g,H_2O} \]  

(5.32)

where \( \delta^{g,H_2O} \) is the vapour permeability of the medium. Using the Kelvin-Laplace relation (equation (3.75)), we can transform equation (5.32) into:

\[ \mathbf{g}^{g,H_2O} = -\delta^{g,H_2O} \mathbf{\nabla} \left( p^{g,H_2O,\text{sat}} \exp \left( -\frac{M^{H_2O}}{\rho^l R T p_c} \right) \right) \]  

(5.33)

Expanding the gradient term, under the assumption that \( \rho^l \) is independent of \( p_c \) and \( T \) (see equation (3.63)), yields:

\[ \mathbf{g}^{g,H_2O} = -\delta^{g,H_2O} \left\{ \frac{\partial p^{g,H_2O,\text{sat}}}{\partial T} \exp \left( -\frac{M^{H_2O}}{\rho^l R T p_c} \right) \mathbf{\nabla} T - \frac{M^{H_2O}}{\rho^l R T} p^{g,H_2O} \left( \mathbf{\nabla} p_c + \frac{\partial p_c}{\partial T} - \frac{p_c}{T} \right) \mathbf{\nabla} T \right\} \]  

(5.34)

The Clausius-Clapeyron relation allows writing:

\[ \frac{\partial p^{g,H_2O,\text{sat}}}{\partial T} = p^{g,H_2O,\text{sat}} \frac{M^{H_2O}}{RT^2} (H_g - H^l) \]  

(5.35)

Furthermore, the partial derivative of the Laplace equation (3.73) reads:

\[ \frac{\partial p}{\partial T} = \left( \frac{1}{r_1} + \frac{1}{r_2} \right) \frac{\partial \gamma^{g^l}}{\partial T} = \left( \frac{1}{r_1} + \frac{1}{r_2} \right) \gamma^{g^l} \left( \frac{1}{\gamma^{g^l}} \frac{\partial \gamma^{g^l}}{\partial T} \right) = p_c \left( 1 \frac{\partial \gamma^{g^l}}{\partial T} \right) \]  

(5.36)

Inserting expressions (5.35) and (5.36) in equation (5.34) and rearranging gives:
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\[
\mathbf{g}_q^{g,H_2O} = -\delta^{g,H_2O} \left( \frac{M^{H_2O}}{\rho' RT} p^{g,H_2O} \nabla p_c + \frac{M^{H_2O}}{\rho' RT^2} p^{g,H_2O} \left( \rho' (H^g - H^i) - p_c \left( \frac{T}{\gamma^{\text{wg}}} \frac{\partial \gamma^{\text{wg}}}{\partial T} - 1 \right) \right) \nabla T \right) \tag{5.37}
\]

Using a finite difference approximation for the capillary pressure and temperature gradient in the normal direction to the cavity or micro-crack, the total flux from the micro-crack or cavity towards \( \Gamma^+_d \) is given by:

\[
\bar{\mathbf{g}}_{\Gamma^+_d} \cdot \mathbf{n} = \left( g^{l,H_2O} + g^{g,H_2O} \right) \left[ \mathbf{n} \right]_{\Gamma^+_d} = k_{mm,\Gamma^+_d} \left( p_{e,\Gamma^+_d} - p_{c,\Gamma^+_d} \right) - k_{me,\Gamma^+_d} \left( T_{\Gamma^+_d} - T_{\Gamma^+_d} \right) \tag{5.38}
\]

with

\[
k_{mm,\Gamma^+_d} = \left( \left[ \mathbf{u}^l \right] \cdot \mathbf{n} \right)^{-1} \left( \mathbf{n} \cdot \left( \mathbf{K}^l + \delta^{g,H_2O} \frac{M^{H_2O}}{\rho' RT} p^{g,H_2O} \right) \mathbf{n} \right) \]

\[
k_{me,\Gamma^+_d} = \left( \left[ \mathbf{u}^l \right] \cdot \mathbf{n} \right)^{-1} \left( \mathbf{n} \cdot \delta^{g,H_2O} \mathbf{n} \frac{M^{H_2O}}{\rho' RT^2} p^{g,H_2O} \left( \rho' (H^g - H^i) - p_c \left( \frac{T}{\gamma^{\text{wg}}} \frac{\partial \gamma^{\text{wg}}}{\partial T} - 1 \right) \right) \right) \tag{5.39}
\]

where the capillary pressures on \( \Gamma^-_d \) and \( \Gamma^+_d \) are denoted with \( p_{e,\Gamma^-_d} \) and \( p_{c,\Gamma^-_d} \), and the temperatures with \( T_{\Gamma^-_d} \) and \( T_{\Gamma^+_d} \), respectively, and where \( \left[ \mathbf{u}^l \right] \cdot \mathbf{n} \) is the width of the micro-crack or cavity in the direction of the normal to the discontinuity. Equation (5.38) is applied as a boundary condition on the damaged part of the cohesive zone \( (\partial A) \). Since this area is not yet created in absence of damage, the singularity at \( \left[ \mathbf{u}^l \right] = 0 \) for \( k_{mm,\Gamma^+_d} \) and \( k_{me,\Gamma^+_d} \) does not pose a problem. As damage develops, the crack width becomes non-zero (equation (4.17)) and the area associated with (5.38) as well.

During unloading, the crack closes again, but a non-zero contact resistance should remain. Therefore the permeabilities (5.39) have to be constrained by:

\[
\frac{1}{k_{mm,\Gamma^+_d}} = \max \left( \min \left( \frac{1}{k_{\text{history}}^{\text{mm,}\Gamma^+_d}}, \frac{1}{k_{\text{contact}}^{\text{mm,}\Gamma^+_d}} \right), \frac{1}{k_{mm,\Gamma^+_d}} \right) \tag{5.40}
\]

\[
\frac{1}{k_{me,\Gamma^+_d}} = \max \left( \min \left( \frac{1}{k_{\text{history}}^{\text{me,}\Gamma^+_d}}, \frac{1}{k_{\text{contact}}^{\text{me,}\Gamma^+_d}} \right), \frac{1}{k_{me,\Gamma^+_d}} \right)
\]

where the superscript ‘history’ indicates the minimum permeability (i.e. maximum resistance) ever reached and ‘contact’ is the contact permeability. The value of the latter term depends on the characteristics of the contact between the materials at both sides of the discontinuity, i.e. the (mis-)match between both pore systems. As a first approximation, the inverse of the vapour resistance of the porous medium (in the case of fracture) or of the combined vapour
resistance (in the case of a material interface) can be selected. A good estimate for the vapour permeability of the micro-crack or cavity $n \cdot K^g n$ is the vapour conductivity for air (approximately $\delta_v \approx 1.87 \cdot 10^{-10}$ s at 293 K and at atmospheric pressure). The magnitude of the liquid permeability of the micro-crack or cavity $n \cdot K^l n$ is expected to be small, and can be neglected.

5.2.4.2. Heat flow across micro-crack or cavity

A micro-crack or cavity can be seen as two parallel surfaces, exchanging heat by means of conduction, convection and radiation. Furthermore, the enthalpy flux must be taken into account if mass exchange takes place between both surfaces. The heat flux across a micro-crack or cavity can be approximated by:

$$
\bar{q}_{T_g} \cdot n = -k_{T_g} \left( T_{T_g} - T_{T_g} \right) + c^l \left( T_m - T_0 \right) g^{lH,O} \cdot n + \left( c^g \left( T_m - T_0 \right) + \left( H^g - H^l \right) \right) g^{gH,O} \cdot n 
$$

where $c^l$ and $c^g$ are the isobaric specific heat of the liquid and the gas, $T_m = \frac{1}{2} \left( T_{T_g} + T_{T_g} \right)$ is the average of the surface temperatures, $T_0$ is a reference temperature, $g^{lH,O}$ and $g^{gH,O}$ are defined in the previous paragraph, and $k_{T_g}$ is the effective thermal conductivity, given by:

$$
\frac{1}{k_{T_g}} = \max \left( \frac{1}{k_{T_g}}, \frac{1}{k_{T_g}} \right) \left[ \frac{\left( \lambda^g + \left( \lambda^l - \lambda^g \right) S^l \right) \bar{u} \cdot n + \frac{C_b F_T}{1 - e_{T_g} - 1}}{1 - 1}_{e_{T_g}} \right]^{-1} 
$$

where $k_{T_g}$ the minimum thermal conductivity (i.e. maximum thermal resistance) ever reached, $k_{T_g}$ a contact conductivity upon crack closure, $\bar{u} \cdot n$ the width in the direction of the normal to the discontinuity, $\lambda^l$ and $\lambda^g$ the conductivities of liquid and gas in the micro-crack, $S^l$ the degree of liquid saturation, $C_b = 5.67 \text{ W/m}^2\text{K}^4$ the black body constant, $e_{T_g}$ and $e_{T_g}$ the emission factors of both crack surfaces, and $F_T$ the temperature factor, given by:

$$
F_T \approx \left( \frac{T_m}{100} \right)^3
$$

For dry air at 273 K and at atmospheric pressure $\lambda^g \approx 0.025 \text{ W/(mK)}$ and $c^g \approx 1024 \text{ J/(kgK)}$, while for water vapour under the same conditions, $\lambda^g \approx 0.016 \text{ W/(mK)}$ and $c^g \approx 1860 \text{ J/(kgK)}$. For liquid water $\lambda^l \approx 0.561 \text{ W/(mK)}$ and $c^l \approx 4180 \text{ J/(kgK)}$. 

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5.2.4.3. Flow along a fracture

For completeness, we mention that the proposed continuous-discontinuous approach can also be combined with most fracture flow models found in literature. Segura and Carol (2008) present a model describing diffusive flow along a fracture, taking into account dynamic effects like the time-dependent evolution of the crack width and the capacity. Vandersteen (2003) derived a model for fluid flow in a fracture, based on a simplified version of the Navier-Stokes equations. These and other models take into account the flow from fracture to matrix. The latter terms correspond to \( \bar{g}_{r_j} \cdot n \) and \( \bar{g}_{r_j} \cdot n \) in the proposed discrete transport model. To incorporate the fracture flow model into the proposed continuous-discontinuous framework, two options exist. In the monolithic approach, \( \bar{g}_{r_j} \cdot n \) and \( \bar{g}_{r_j} \cdot n \) are substituted by the fracture flow model equations. According to Roels et al. (2003), the large contrast in permeability between fracture and matrix might however lead to convergence problems for this strategy. They suggest using a staggered approach, where the matrix flow and the fracture flow are solved independently, and the exchange fluxes \( \bar{g}_{r_j} \cdot n \) and \( \bar{g}_{r_j} \cdot n \) are updated iteratively.

5.3. Strong discontinuity formulation

5.3.1. Strong form

The strong form of the mass conservation law is given by (equations (3.93)):

\[
c_{mm} \frac{\partial P_c}{\partial t} + c_{me} \frac{\partial T}{\partial t} + \nabla \cdot g = 0 \text{ in } \Omega, \text{ with } g = -\left( K_{mm} \nabla p_c + K_{me} \nabla T \right)
\]  
(5.44)

Conservation of energy reads (equations (3.94)):

\[
c_{em} \frac{\partial P_c}{\partial t} + c_{ee} \frac{\partial T}{\partial t} + \nabla \cdot q = 0 \text{ in } \Omega, \text{ with } q = -\left( K_{em} \nabla p_c + K_{ee} \nabla T \right)
\]  
(5.45)

where \( c \) are capacity terms. The first subscript again denotes the equation in which these terms appear (\( m \) for mass balance, \( e \) for energy balance) and the second subscript indicates their corresponding variable (\( m \) for the capillary pressure \( p_c \), \( e \) for the temperature \( T \)).

The natural boundary conditions are given by:

\[
g \cdot \bar{n} = -\bar{g}_{r_j} \quad \text{and} \quad q \cdot \bar{n} = -\bar{q}_{r_j} \quad \text{on } \Gamma_2
\]
\[
g \cdot n = -g^+ \cdot n \quad \text{and} \quad q \cdot n = -q^+ \cdot n \quad \text{on } \Gamma^+_d
\]
\[
g \cdot n = g^- \cdot n \quad \text{and} \quad q \cdot n = q^- \cdot n \quad \text{on } \Gamma^-_d
\]  
(5.46)
The essential boundary conditions are:
\[ p_c = \bar{p}_c \quad \text{and} \quad T = \bar{T} \quad \text{on} \quad \Gamma_1 \quad (5.47) \]

In the subsequent two sections we focus on the energy conservation law and illustrate the transformation into the weak form and the subsequent discretization. The manipulations for the mass conservation law are identical and are not elaborated upon.

### 5.3.2. Weak form

The weak form of the system (5.45) is given by:
\[
\int_\Omega (c_{em} \frac{\partial \rho}{\partial t} + c_{ec} \frac{\partial T}{\partial t} + \nabla \cdot \mathbf{q}) \, d\Omega = 0 \quad (5.48)
\]

which must hold for all admissible variations \( w = \tilde{w} + H_{T,J} \tilde{\mathbf{w}} \) of temperature \( T \). Following a Galerkin approach leads, after standard manipulations, to the following set of variational statements:
\[
\int_\Omega \tilde{w} \left( c_{em} \frac{\partial \rho}{\partial t} + c_{ec} \frac{\partial T}{\partial t} \right) \, d\Omega - \int_\Omega \nabla \tilde{w} \cdot \mathbf{q} \, d\Omega \\
= -\int_{\Gamma_s} \tilde{w} \mathbf{q}^- \cdot n \, d\Gamma - \int_{\Gamma_J} \tilde{w} \mathbf{q}^+ \cdot n \, d\Gamma + \sum_{\Gamma_s} \tilde{w} \mathbf{q}^- \cdot n \, d\Gamma
\]

\[
\int_{\Omega_{T,J}} \tilde{w} \left( c_{em} \frac{\partial \rho}{\partial t} + c_{ec} \frac{\partial T}{\partial t} \right) \, d\Omega - \int_{\Omega_{T,J}} H_{T,J} \nabla \tilde{w} \cdot \mathbf{q} \, d\Omega \\
= -\int_{\Gamma_s} H_{T,J} \tilde{w} \mathbf{q}^- \cdot n \, d\Gamma - \int_{\Gamma_J} H_{T,J} \tilde{w} \mathbf{q}^+ \cdot n \, d\Gamma + \sum_{\Gamma_s} \tilde{w} \mathbf{q}^- \cdot n \, d\Gamma
\]

where we employed the boundary conditions (5.46).

### 5.3.3. Discretized form

#### 5.3.3.1. Discretization in time

Using a finite difference scheme to perform discretization in time, equation (5.49) becomes:
\[
\int_\Omega \tilde{w}_t \left( c_{em} \left( p_c - p_c' \right) + c_{ec} \left( T - T' \right) \right) \, d\Omega - \int_\Omega \nabla \tilde{w} \cdot \mathbf{q} \, d\Omega \\
= -\int_{\Gamma_s} \tilde{w}_t \mathbf{q}^- \cdot n \, d\Gamma - \int_{\Gamma_J} \tilde{w}_t \mathbf{q}^+ \cdot n \, d\Gamma + \sum_{\Gamma_s} \tilde{w}_t \mathbf{q}^- \cdot n \, d\Gamma
\]

\[
\int_{\Omega_{T,J}} \tilde{w}_t \left( c_{em} \left( p_c - p_c' \right) + c_{ec} \left( T - T' \right) \right) \, d\Omega - \int_{\Omega_{T,J}} H_{T,J} \nabla \tilde{w} \cdot \mathbf{q} \, d\Omega \\
= -\int_{\Gamma_s} H_{T,J} \tilde{w}_t \mathbf{q}^- \cdot n \, d\Gamma - \int_{\Gamma_J} H_{T,J} \tilde{w}_t \mathbf{q}^+ \cdot n \, d\Gamma + \sum_{\Gamma_s} \tilde{w}_t \mathbf{q}^- \cdot n \, d\Gamma
\]

where the superscript \( t \) denotes a value at the previous converged time step and \( \Delta t \) is the adopted time step.
5.3.3.2. Discretization in space

5.3.3.2.1. Discretization of the problem fields

Discretization in space is performed using finite elements. Nodes whose support is crossed by a discontinuity are assigned a regular and an enhanced set of degrees of freedom, denoted by \( a \) and \( b \), respectively. The discretized format of the capillary pressure field (5.1) reads:

\[
p_c = N \cdot a_m + H_{\Gamma_\delta} N \cdot b_m
\]

(5.51)

and for the temperature field (5.2) we obtain:

\[
T = N \cdot a_e + H_{\Gamma_\delta} N \cdot b_e
\]

(5.52)

where \( N \) is the vector containing the finite element shape functions. The same interpolation is assumed for both capillary pressure and temperature. Following a Galerkin approach, an identical discretization is performed for the variational field \( w \). The gradient of the problem fields and the corresponding variational fields can be discretized in a similar fashion using the interpolation matrix \( B \). For elements with only regular degrees of freedom \( a \), the problem fields are discretized in the standard way.

5.3.3.2.2. Discretization of the constitutive relations

In chapter 3, the constitutive relation for heat transfer was expressed in the following format:

\[
q = -(K_{en} \nabla p_c + K_{ce} \nabla T)
\]

(5.53)

The minus sign indicates that heat flows from high to low temperatures. After replacing the gradient terms by the corresponding discretized terms (5.51) and (5.52), equation (5.53) becomes:

\[
q = -(K_{en} \left( B a_m + H_{\Gamma_\delta} B b_m \right) + K_{ce} \left( B a_e + H_{\Gamma_\delta} B b_e \right))
\]

(5.54)

5.3.3.2.3. Discretization of the cohesive zone model

Equation (5.54) is an approximation of the true local heat flux at a point. The proposed discrete model, as described in section 5.2, relies on the knowledge of the true local flux vector. As illustrated in chapter 4 this conflict can be resolved without approximation if \( \omega_{crit} \geq \omega \geq 1 \), where \( \omega_{crit} \) is a real positive number, close to zero. In that case, the flux vector can be eliminated from the cohesive zone model. The reduced format of the coupled hygro-thermal model reads:
\[
\begin{align*}
\mathbf{g}^+ \cdot \mathbf{n} &= \left(1 - \frac{\omega}{\omega_c}\right) \gamma^{-1} \begin{bmatrix}
K_{mm}\Gamma_d & K_{me}\Gamma_d \\
K_{em}\Gamma_d & K_{ee}\Gamma_d
\end{bmatrix}
\begin{bmatrix}
p_{c,\Gamma_d} - p_{c,\Gamma_2} \\
T_{\Gamma_d} - T_{\Gamma_2}
\end{bmatrix} \\
&\quad \left(1 - \frac{\omega}{\omega_c}\right)(1 - \alpha)^{-1} K_{\Gamma_d} \left(\alpha^{-1} K_{\Gamma_d} + (1 - \alpha)^{-1} K_{\Gamma_2}\right)^{-1}
\begin{bmatrix}
\bar{\mathbf{g}}_{\Gamma_d} \\
\bar{\mathbf{q}}_{\Gamma_d}
\end{bmatrix} - \begin{bmatrix}
\mathbf{g}^+ \cdot \mathbf{n} \\
\mathbf{q}^+ \cdot \mathbf{n}
\end{bmatrix}
\end{align*}
\] (5.55)

For small values of the damage variable \((0 \leq \omega < \omega_{crit})\), the denominator of equation (5.55) would go to zero, leading to large errors in the solution field. Therefore it is more accurate to employ the original equation (5.28), using an approximate value for the heat and mass flux:

\[
\begin{align*}
\mathbf{q}^+ &= -\frac{1}{2} \left(\mathbf{q}\big|_{\Gamma_d} + \mathbf{q}\big|_{\Gamma_2}\right) \quad \text{ (5.56)} \\
\mathbf{g}^+ &= -\frac{1}{2} \left(\mathbf{g}\big|_{\Gamma_d} + \mathbf{g}\big|_{\Gamma_2}\right) \quad \text{ (5.57)}
\end{align*}
\]

where the vertical bar indicates that the continuum flux should be evaluated at the position indicated by the subscript.

5.3.3.2.4. Discretized form

After inserting equations (5.51), (5.52) and (5.54) in (5.50), the discretized format of the weak governing equations reads:

\[
\begin{align*}
\frac{1}{\Delta t} \int_{\Omega} \mathbf{N}^T c_{en} \mathbf{N} d\Omega + \int_{\Omega} \mathbf{B}^T \mathbf{K}_{em} \mathbf{B} d\Omega \right) \mathbf{a}_m - \frac{1}{\Delta t} \int_{\Omega} \mathbf{N}^T c_{em} \mathbf{N} d\Omega \right) \mathbf{a}_m' \\
\quad \left(1 - \frac{\omega}{\omega_c}\right)(1 - \alpha)^{-1} K_{\Gamma_d} \left(\alpha^{-1} K_{\Gamma_d} + (1 - \alpha)^{-1} K_{\Gamma_2}\right)^{-1}
\begin{bmatrix}
\bar{\mathbf{g}}_{\Gamma_d} \\
\bar{\mathbf{q}}_{\Gamma_d}
\end{bmatrix} - \begin{bmatrix}
\mathbf{g}^+ \cdot \mathbf{n} \\
\mathbf{q}^+ \cdot \mathbf{n}
\end{bmatrix}
\end{align*}
\]

(5.58)
where we used equation (5.14) and $H_{r_j} = 0$.

### 5.3.4. Linearized and discretized form

The discretized system of equations (5.58) can be linearized in the classical way. Linearization of the cohesive zone model is trivial, since the damage variable does not depend on capillary pressure nor on temperature. Full linearization leads to an optimal convergence rate, but in this particular case also to a non-symmetric system of equations. Omitting the terms related to the linearization of the non-linear material properties renders the system symmetric again. Hereby, the computational cost per iteration is reduced, but the convergence rate decreases as well. According to Janssen et al. (2007), the former effect dominates for 2D and 3D computations, and therefore partial linearization is preferred. The resulting coupled system of equations becomes:

$$
\begin{bmatrix}
K_{a_{ua}}^i & K_{b_{ua}}^i & K_{a_{ub}}^i & K_{b_{ub}}^i \\
K_{a_{va}}^i & K_{b_{va}}^i & K_{a_{vb}}^i & K_{b_{vb}}^i \\
K_{a_{ua}}^i & K_{b_{ua}}^i & K_{a_{ub}}^i & K_{b_{ub}}^i \\
K_{a_{va}}^i & K_{b_{va}}^i & K_{a_{vb}}^i & K_{b_{vb}}^i 
\end{bmatrix}
\begin{bmatrix}
\delta a_{m}^{i+1} \\
\delta b_{m}^{i+1} \\
\delta a_{e}^{i+1} \\
\delta b_{e}^{i+1}
\end{bmatrix}
= \begin{bmatrix}
f_{ext,a}^i \\
f_{ext,b}^i \\
f_{int,a}^i \\
f_{int,b}^i 
\end{bmatrix}
- \begin{bmatrix}
f_{int,a}^i \\
f_{int,b}^i \\
f_{int,a}^i \\
f_{int,b}^i 
\end{bmatrix}
= (5.59)
$$

where the superscript $i$ indicates the iteration counter in the global iterative procedure.

The terms of one block of the $K$-matrix are given by:

$$
K_{a_{ua}}^i = \frac{1}{\Delta t} \int_{\Gamma_{a}} N^T c_{em} N d\Omega + \int_{\Gamma_{a}} B^T K_{em} B d\Omega - \int_{\Gamma_{a}} N^T \frac{\partial \overline{q}_{1s}}{\partial \overline{P}_c} d\Gamma - \int_{\Gamma_{a}} N^T \frac{\partial \overline{q}_{1s}}{\partial \overline{P}_c} d\Gamma
$$

(5.60)
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\[ K^{i}_{a,b} = \frac{1}{\Delta t} \int_{\Omega} H_{r_d} N^T c_{em} N d\Omega + \int_{\Omega} H_{r_d} B^T K_{em} B d\Omega \]
\[ -\int_{r_d} H_{r_d} N^T \frac{\partial q_{r_d}}{\partial p_c} d\Gamma - \int_{r_d} H_{r_d} N^T \frac{\partial q_{r_d}}{\partial p_c} d\Gamma \]

\[ K^{i}_{b,a} = \frac{1}{\Delta t} \int_{\Omega} H_{r_d} N^T c_{em} N d\Omega + \int_{\Omega} H_{r_d} B^T K_{em} B d\Omega \]
\[ + \int_{r_d} H_{r_d} N^T \frac{\partial q^* \cdot n}{\partial p_c} d\Gamma - \int_{r_d} N^T \frac{\partial q_{r_d}}{\partial p_c} d\Gamma \]

\[ K^{i}_{b,b} = \frac{1}{\Delta t} \int_{\Omega} H_{r_d} N^T c_{em} N d\Omega + \int_{\Omega} H_{r_d} B^T K_{em} B d\Omega \]
\[ + \int_{r_d} H_{r_d} H_{r_d} N^T \frac{\partial q^* \cdot n}{\partial p_c} d\Gamma - \int_{r_d} H_{r_d} H_{r_d} N^T \frac{\partial q_{r_d}}{\partial p_c} d\Gamma \]

The terms for the other blocks are obtained by varying the subscripts \( e \) and \( m \). Matrix entries with an \( e \) as first subscript contain \( q^* \) and \( \overline{q}_{r_d} \), if the first subscript is an \( m \), \( q^* \) and \( \overline{g}_{r_d} \) should be present. A second subscript \( e \) corresponds to partial derivatives with respect to \( T \), for \( m \) the partial derivative should be taken with respect to \( p_c \). The entries in the external force vector read:

\[ f^{i}_{ext,a} = \int_{r_d} N^T \overline{g} d\Gamma \]
\[ f^{i}_{ext,b} = \int_{r_d} H_{r_d} N^T \overline{q} d\Gamma \]
\[ f^{i}_{ext,c} = \int_{r_d} N^T \overline{q} d\Gamma \]
\[ f^{i}_{ext,h} = \int_{r_d} H_{r_d} N^T \overline{q} d\Gamma \]

The entries of the internal force vector are given by:

\[ f^{i}_{int,a} = \frac{1}{\Delta t} \int_{\Omega} N^T \left( S^i_{m} - S^i_{e} \right) d\Omega - \int_{\Omega} B^T g^i d\Omega - \int_{r_d} N^T \overline{g} d\Gamma \]
\[ f^{i}_{int,b} = \frac{1}{\Delta t} \int_{\Omega} H_{r_d} N^T \left( S^i_{m} - S^i_{e} \right) d\Omega - \int_{\Omega} H_{r_d} B^T g^i d\Omega + \int_{r_d} H_{r_d} N^T \left( g^* \cdot n \right) d\Gamma \]
\[ f^{i}_{int,c} = \frac{1}{\Delta t} \int_{\Omega} N^T \left( S^i_{e} - S^i_{c} \right) d\Omega - \int_{\Omega} B^T q^i d\Omega - \int_{r_d} N^T \overline{q} d\Gamma \]
\[ f^{i}_{int,h} = \frac{1}{\Delta t} \int_{\Omega} H_{r_d} N^T \left( S^i_{e} - S^i_{c} \right) d\Omega - \int_{\Omega} H_{r_d} B^T q^i d\Omega + \int_{r_d} H_{r_d} N^T \left( q^* \cdot n \right) d\Gamma \]

In equation (5.62), \( S_m \) and \( S_e \) are mass and energy conservation terms, given by:

\[ S_m = w \]
where \( w \) is the moisture content, \( c_0 \) is the heat capacity of the porous medium at the reference temperature and \( c_f = 4180 \text{ J/kgK} \) is the isobaric specific heat of liquid water. These terms were first introduced by Celia et al. (1990) in order to avoid errors due to linearization.

To clarify this, we focus on the mass conservation term. The moisture content \( w \) is equal to the product of the porosity \( n \), the liquid density \( \rho' \) and the saturation \( S'^{i} \). For the change of the moisture content over time, we can therefore write:

\[
\frac{\partial w}{\partial t} = \frac{\partial (n\rho'S'^{i})}{\partial t} = \left( n\rho' \frac{\partial S'^{i}}{\partial p_c} \right) \frac{\partial p_c}{\partial t} = c_{mn} \frac{\partial p_c}{\partial t} \quad (5.65)
\]

where porosity and density are considered independent of the capillary pressure \( p_c \). Applying a finite difference scheme to approximate the time derivative yields:

\[
\frac{w_{j+1}^{i} - w_j^{i}}{\Delta t} \quad \text{and} \quad \frac{c_{mn}^{i} p_{c,j+1}^{i} - p_{c,j}^{i}}{\Delta t} \quad (5.66)
\]

If \( c_{mn} \) were independent of \( p_c \), both expressions would be equivalent. However, the relation between moisture saturation and capillary pressure is known to be highly nonlinear. Therefore the finite difference approximation in \( p_c \) introduces a serious error, as compared to the approximation in the variable \( w \). Nevertheless, \( p_c \) is the primary variable of the mass balance equation, and using the expression in \( p_c \) has certain algorithmic advantages. Celia et al. (1990) therefore proposed to use a mixed mode formulation in an iterative scheme:

\[
c_{mn}^{i} p_{c,j+1}^{i} - p_{c,j}^{i} + \frac{w_{j+1}^{i} - w_j^{i}}{\Delta t} \quad (5.67)
\]

where \( i \) is the iteration counter in the global iterative procedure. The first term appears in the left hand side of the system of equations (a.o. in \( K'_{a,a}^{i} \) in (5.59)). After substituting \( w_{j+1}^{i} \) by the symbol \( S'^{i}_{m} \) and \( w_j^{i} \) by \( S'^{i}_{m} \), the second term is found on the right hand side of the system of equations (a.o. in \( f_{int,a}^{i} \) in (5.62)). Upon convergence, only the latter term remains. A similar reasoning has been followed in the derivation of equation (5.64).

### 5.3.5. Implementation

The model equations have been implemented in the general purpose finite element code described in section 4.3.7. The coupled system of equations is solved in a staggered way, as will be explained in detail in section 6.1. For each sub-system, an iterative total incremental
approach is employed. Like for the mechanical system of equations, three residuals are defined per sub-system, namely $\| f_{ex} - f_{int} \|$, $\| f_{int} \cdot \delta x \|$ and $\| \delta x \|$, where $x$ represents either $p_c$ or $T$. The solution is considered converged if for each residual either the absolute or the relative value is below a predefined threshold. The threshold values are $10^{-4}$, $10^{-5}$ and $10^{-6}$ for the relative criteria and $10^{-6}$ for all absolute criteria. For solving the system of equations, the Cholesky factorization routine and the direct solver from the Visual Numerics® IMSL® Fortran Library are employed.

5.4. Academic examples

In this section three different numerical examples are presented. The first two deal with heat transfer, the last one with a moisture diffusion problem. Coupled problems are deferred to chapter 7 and 8. In the first example, the transient thermal behaviour of a fractured porous medium is studied. The influence of the damage parameter and the heat capacity are investigated. Next, a similar test is performed on a two-layer composite material. It is shown that impact of damage on the dynamic thermal response depends on the layer order. In a final example the methodology to impose boundary conditions along an arbitrarily oriented discontinuity is verified by means of a preferential penetration example.

5.4.1. Heat transfer in a fractured porous medium

Transient heat transfer is studied on a 2D square sample with edge length of 0.03 m (Figure 5.3). The sample is discretized with 9 square bilinear elements (Q4). A strong discontinuity with normal pointing in the positive $x$-direction is inserted in the three middle elements. Initially the temperature of the sample is uniform and equals 283 K. The temperature of the nodes on the left boundary is kept constant in time ($T_l = 283$ K). The right boundary is exposed to an indoor environment at 293 K. The resulting heat flux is proportional to the difference in temperature between the sample boundary and the environment, and is consequently varying over time. A heat transfer coefficient of $h_t = 8$ W/(m²K) is selected.

$$\bar{q}_{f_2} = h_t (T_i - T)$$ (5.68)

We investigate the influence of the heat capacity ($c'_p = 0$ or 500 J/(kgK)) and the amount of interface damage ($\omega = 0, 0.1$ or $1$) on the thermal behaviour. A mass density of $\rho' = 2000$ kg/m³ and thermal conductivity of $k' = 0.4$ W/mK were used. In this example, we want to focus on the influence of damage on the magnitude of the temperature jump across
the discontinuity under steady-state and under transient conditions. To simplify interpretation of the results, the fracture is assumed adiabatic \((\mathbf{q}_d \cdot \mathbf{n} = \mathbf{q}_d \cdot \mathbf{n} = 0)\). In the subsequent example (section 5.4.2), more realistic thermal behaviour of the fracture will be considered.

\[
\mathbf{q}_d = h_i (T_i - T) \quad \text{and} \quad \mathbf{q}_d = 0.
\]

**Figure 5.3:** Heat transfer in a fractured porous medium: geometry, mesh and boundary conditions.

\[(a) \ \omega = 0 \% \quad (b) \ \omega = 10 \% \quad (c) \ \omega = 100 \% \]

**Figure 5.4:** Heat transfer in a fractured porous medium: temperature profiles at selected points in space (left column) and temperature evolution at selected points in time (right column) for three different amounts of damage at the interface: (a) \(\omega = 0 \%\), (b) 10 \% and (c) 100 \%. Solid lines indicate steady-state simulations \((c_p^s = 0 \text{ J/kgK})\); dashed lines correspond to transient simulations \((c_p^s = 500 \text{ J/kgK})\).
Figure 5.4 summarizes the results of the simulations. In the right column, temperature profiles over the width of the sample are given at selected points in time ($t = 0, 15, 30$ and $60$ s). In the left column, the temperature evolution over time is shown for four different locations, namely at the left sample boundary ($x = 0$ m) at both sides of the discontinuity ($x = 0.015$ m) and at the right sample boundary ($x = 0.03$ m).

Figure 5.4a shows the results for a damage-free discontinuity. At every instance in time, the temperature profile is continuous across the sample. This indicates that an undamaged interface does not possess thermal resistance. Under steady-state conditions, the temperature at the right sample boundary can be computed analytically from the energy equilibrium:

$$
T_{ss} = T_i + \frac{h_i}{d + k_s} \left( T - T_i \right)
$$

For the given material properties and geometry, a temperature of 286.75 K is obtained. The same value is found in the steady-state simulation. The transient simulation tends asymptotically towards the equilibrium state.

Upon increasing the amount of interface damage, the part of the cross-sectional area that participates in the heat transfer decreases and consequently the thermal resistance of the interface increases. Correspondingly, the temperature difference over the sample increases and a temperature jump develops across the interface (Figure 5.4b). Again, we notice that the transient simulation tends asymptotically towards the steady state temperature distribution.

Figure 5.4c illustrates the fully fractured case. Since the fracture is considered adiabatic in this simulation, a fully damaged crack acts as a perfect heat barrier. Therefore, the left part of the sample remains at the initial temperature, while the right part of the sample strives towards thermal equilibrium with the environment. The temperature jump across the discontinuity eventually becomes equal to the temperature difference between $T_i$ and $T$.

### 5.4.2. Heat transfer in a composite

Heat transfer in a two-layer composite material is studied to illustrate that the proposed discrete model is capable of capturing dynamic effects. For a given amount of damage at the interface, it is shown that its influence on the dynamic thermal behaviour is not fixed, but depends on the properties of both layers and the layer order.

We consider a 2D square sample with edge length of 0.3 m (Figure 5.5). The sample is discretized with 9 square bilinear elements (Q4). A strong discontinuity with normal pointing in the positive $x$-direction is inserted in the three middle elements, separating material 1 (left)...
from material 2 (right). Both materials have a mass density of \( \rho = 2000 \text{ kg/m}^3 \). The thermal conductivity \( k^i \) and the heat capacity \( c^i_{p,i} \) of each layer are varied in each simulation. We will investigate both perfect and imperfect contact between both materials. The imperfect contact is simulated by assuming 10\% interface damage. The thermal behaviour of the air-filled cavities between both materials is modelled according to (5.41). We assume \( e_{r_j} = e_{r_j} = 0.9 \), \( R_e = 0 \) and \( n = 2 \cdot 10^{-3} \text{ m} \). Mass transport is not considered in this example. All investigated cases are summarized in Table 5.1. Initially the temperature of the composite sample is uniform and equals 283 K. The left boundary is exposed to an exterior environment with a periodically varying temperature \( T_e = 283 + 10 \sin(2\pi t/86400) \), corresponding to a simplified day-night cycle \( (h_e = 23 \text{ W/(m}^2\text{K})\)).

\[
\bar{q}_{\Gamma_2} = h_e (T_e - T) \tag{5.70}
\]

The right boundary is in contact with an indoor environment at a constant temperature \( T_i = 293 \text{ K} \) \( (h_i = 8 \text{ W/(m}^2\text{K)} \), see equation (5.68)).

![Figure 5.5: Heat transfer in a two-layer composite material: geometry, mesh and boundary conditions.](image)

<table>
<thead>
<tr>
<th>( c_{p,1} )</th>
<th>( k^1 )</th>
<th>( \omega )</th>
<th>( c_{p,2} )</th>
<th>( k^2 )</th>
<th>( A_j )</th>
<th>( \phi_i )</th>
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<td>1.86</td>
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</tbody>
</table>

Table 5.1: Investigated parameter combinations and resulting amplitude and phase shift. Tests are subdivided in two groups (a, b). Corresponding results are shown in Figure 5.6a,b.
We simulate ten cycles, sufficient to reach periodic response of the two-layer composite system. The last cycle is used to compute the amplitude $A_i$ and the phase angle $\phi_i$ of the fluctuating temperature at the inner surface. The last two columns of Table 5.1 summarize the results. The temperature variation at the inner surface for the last cycle is shown in Figure 5.6.

**Figure 5.6**: Heat transfer in a two-layer composite material: temperature fluctuations at the inner surface. Both layers have different (a) capacity or (b) conductivity. Solid and dashed lines correspond to simulations with a damage-free and 10% damaged interface, respectively. All parameter combinations are listed in Table 5.1.

First, we focus on the impact of the amount of interface damage. It is clear that increasing the damage leads to smaller temperature fluctuations (Table 5.1) and a higher average temperature (Figure 5.6) on the inner surface. This is evident, since additional damage corresponds to supplementary contact resistance. But, because the additional damage alters the dynamic behaviour of the system, an extra phase shift is observed as well, although no capacity is added (see section 5.2.4).

It is well known that the dynamics of a layered system depends on the layer order. From Table 5.1, we observe that the effect of an increase in damage is not prescribed, but also depends on the layer order. Having a capacitive material at the outside suppresses the damage-induced damping and phase shift to some extent (group a). The mutual position of a conductive and a resistive layer does not have a pronounced impact on the effect of the damage on the damping. Damage causes a larger phase shift if the more conductive material is placed at the outside (group b).

### 5.4.3. Moisture uptake via a fracture

As a final example, we verify the methodology to impose boundary conditions along an internal discontinuity. Therefore, we compare the results obtained with the proposed methodology (X-FEM) to a simulation where the discontinuity is explicitly modelled and where the boundary conditions are imposed in the classical manner (FEM). To ensure that the
simplicity of the example does not mask potential inaccuracies, we now focus on a highly nonlinear moisture transport problem.

For the X-FEM simulation, we consider a small 2D bar of 0.008 m length and $10^{-5}$ m height (Figure 5.7). The bar is discretized with 259x1 bilinear elements. The central element has a width of $10^{-5}$ m. The element width gradually increases towards both ends of the bar. The width of the elements at the endpoints is $10^{-4}$ m. A strong discontinuity is inserted in the middle element. Two discontinuity orientations are considered: (i) with normal pointing in the positive $x$-direction and (ii) with a normal 30 degrees tilted with the positive $x$-direction.

The left half of the X-FEM mesh (i.e. $\Omega^-$) is used in the reduced FEM simulation. The internal discontinuity becomes an external boundary on which boundary conditions can be imposed.

![Figure 5.7](image-url)

**Figure 5.7:** Moisture uptake via a fracture: geometry, meshes and boundary conditions.

![Figure 5.8](image-url)

**Figure 5.8:** Moisture uptake via a fracture: (a) moisture saturation $S$ and (b) liquid permeability (solid line) and vapour permeability (dashed line) as a function of the logarithm of the capillary pressure of the material used in the simulation.
Figure 5.9: Moisture uptake via a fracture: comparison between degrees of saturation obtained via FEM and X-FEM simulations with Neumann boundary conditions for two different fracture orientations, namely (a) coinciding with or (b) inclined with respect to the symmetry axis of the geometry. The diagonal line corresponds to a perfect match.

Figure 5.10: Moisture uptake via a fracture: evolution of saturation profiles in time obtained via (a) FEM and (b) X-FEM simulations with Neumann boundary conditions for a fracture coinciding with the symmetry axis of the geometry.

The sample is initially considered oven-dry, corresponding to $p_c = 10^6$ Pa. The material properties are illustrated in Figure 5.8. First, Neumann boundary conditions are imposed along the internal discontinuity.

$$\mathbf{g} \cdot \mathbf{n} = \beta (\overline{p_c} - p_c)$$  \hspace{1cm} (5.71)

A transition coefficient of $\beta = 10^{-6}$ s/m is used. A capillary pressure $p_c = 10$ Pa is assumed in the fracture, which represents a liquid-filled fracture. Figure 5.9 compares degrees of saturation obtained via FEM and X-FEM simulations for seven points in space ($x = \{0.00005, 0.0001, 0.0002, 0.0005, 0.001, 0.002, 0.005\}$ m), at every second over the first interval of 30 s. It can be seen that the X-FEM results coincide with the FEM reference solution, regardless the discontinuity orientation. The maximum relative error between both is 0.1 %
for the vertical fracture and 0.01 % for the inclined fracture. In Figure 5.10 saturation profiles along the bar at different points in time are depicted for both the FEM and the X-FEM simulation of the vertical fracture. A good agreement between both methods is observed.

![Figure 5.10](image1.png)

**Figure 5.10:** Saturation profiles along the bar at different points in time for both the FEM and the X-FEM simulation of the vertical fracture.

Next, Dirichlet boundary conditions are studied ($\bar{p}_c = 10$ Pa). In the proposed X-FEM formulation, Dirichlet boundary conditions cannot be imposed directly along the fracture. Nevertheless, by setting the transition coefficient $\beta$ in equation (5.71) theoretically equal to $+\infty$, a penalty-type formulation for imposing Dirichlet boundary conditions is obtained. High values for $\beta$ lead to a low constraint violation, but can render the system of equations to be ill-posed. A value of $\beta = 10^{-2}$ s/m was selected. Figure 5.11 shows degrees of saturation obtained via FEM and X-FEM simulations for seven points in space ($x = \{0.00005, 0.0001, 0.0002, 0.0005, 0.001, 0.002, 0.005\}$ m), at every second over the first interval of 30 s. Again, both approaches yield superimposed results, regardless of the discontinuity orientation. The maximum relative error between both is 0.9 % for the vertical fracture and 0.8 % for the inclined fracture. Selecting a value of $\beta = 10^{-1}$ s/m reduces the relative error to 0.1 % and 0.06 %, respectively.

**5.5. Concluding remarks**

It was shown that the influence of damage on the coupled heat and mass transfer in porous media can be modelled by means of an extension of the continuous-discontinuous strategy, developed in the previous chapter. Without introducing additional parameters, the continuum transport models were employed to describe heat and mass flow across fractures and material
interfaces. The hygro-thermal cohesive zone model is directly linked to the mechanical cohesive zone model by means of the damage variable $\omega$. In absence of damage, the continuum behaviour is recovered. It was shown that boundary conditions can be successfully imposed along the damaged part of the internal discontinuity. Neumann boundary conditions can be exactly enforced, while for Dirichlet boundary conditions a penalty-type formulation is employed. The methodology proved to be applicable for quasi-static, periodic and transient problems, both for linear and non-linear material models.
6. Numerical methods

In this chapter, numerical methods to simplify the implementation of and to optimise the solution strategy for coupled, discontinuous theories are developed. The first two algorithms are designed to solve coupled systems of equations more efficiently, without sacrificing accuracy. They decrease the computational cost by adjusting the solution scheme to the specific temporal and spatial characteristics of the individual equations and to their mutual degree of coupling. A second set of algorithms is devised to overcome some issues related to discontinuous theories, especially X-FEM. Amongst others, a new strategy to insert discontinuities into finite elements and a technique to perform accurate integration over elements containing discontinuities are presented.

6.1. Solution strategy for the coupled system

6.1.1. Staggered solution scheme

Typical problems in porous media are described by a strongly coupled and highly nonlinear system of equations. The equations can be integrated simultaneously (monolithic approach) or a staggered scheme can be employed. The latter often leads to computational savings resulting from smaller problem sizes and possible symmetry in the sub-problems (Vijalapura and Govindjee 2005, Schrefler et al. 1997, Turska and Wisniewski 1994). Furthermore, staggered schemes are generally better conditioned\(^3\), and therefore a higher accuracy can be obtained. Finally, they allow optimizing the solution strategy for each individual sub-problem separately. This is particularly appealing since each sub-problem imposes different requirements on mesh resolution and time step size. However, since all sub-problems are coupled, data must be exchanged among them, and therefore neither mesh nor time stepping method can be altered freely. In the next two sections, we propose a strategy to reconcile the different spatial and temporal requirements of the individual sub-problems, exploiting the advantages of a staggered solution scheme.

---

\(^3\) If no special measures are taken. If scaling operations are applied in the monolithic approach, the condition number can be reduced to a similar or lower level as for the individual sub-problems in the staggered approach.
6.1.2. Time integration using dynamic sub-stepping

6.1.2.1. Concept

In order to reconcile the differences in temporal requirements of the different sub-systems in the staggered solution scheme, a dynamic sub-stepping technique has been developed. The basic concept is to adapt the time step size for each sub-system separately, according to the specific requirements of that sub-system for that particular point in time. To ensure that the coupling between the sub-systems is properly taken into account, time steps are not allowed to have arbitrary magnitude, but are round down to selected discrete values. At corresponding time steps, data can be exchanged. At every point in time, a sub-system is solved using (i) computed data from the sub-systems that are also solved at that point in time, and (ii) interpolated data for the other sub-systems (Figure 6.1).

![Figure 6.1: Schematic representation of the adaptive sub-stepping technique. Black dots denote points in time where a system is solved. Dotted lines denote exchange of computed data; dash-dotted lines denote exchange of interpolated data.](image_url)

6.1.2.2. Initialization

Before starting the computation, the maximum size $\Delta t_i$ of each global time step $i$ for the solution of the coupled system and the maximum allowed number of iterations $n_i \text{max}$ for each sub-problem are selected. The global time step size is often determined by the output frequency (post-processing). Limiting the number of iterations to $n_i \text{max}$ guarantees that the algorithm eventually stops in case convergence problems arise. Afterwards, the simulation should be repeated with a reduced time step, from the last converged state on.

Each sub-problem $s$ is initially solved with an ‘educated guess’ for the time step $\Delta t_{s,1}$, which is a fraction $\alpha_{s,1}$ of the (first) global time step $\Delta t_i$:

$$\Delta t_{s,1} = \alpha_{s,1} \Delta t_i$$

(6.1)
If making an educated guess is not possible, it is recommended to select the same time step for all systems of equations. We assume that the scale factor $\alpha_{s,j}$ obeys:

$$\alpha_{s,j} = m^{-n_{s,j}}$$  \hspace{1cm} (6.2)

with $m$ and $n_{s,j}$ integer values that satisfy $m \geq 1$ and $0 \leq n_{s,j} \leq n_{s,\text{max}}$. Equation (6.2) restricts the magnitude of the time step to certain discrete values. If e.g. a value $m = 2$ is selected, the allowed time step sizes are $\frac{1}{2}$, $\frac{1}{4}$, $\frac{1}{8}$, ... of the global time step size (see also Figure 6.1). The constraint $n_{s,j} \leq n_{s,\text{max}}$ is added to impose a lower limit to the time step size. This constraint should be regarded as a means to prevent that the time step becomes infinitely small in case convergence problems arise.

6.1.2.3. Solving a global time step

The $i+1$th global time step starts at $t_i$ and ends at $t_{i+1}$:

$$t_{i+1} = t_i + \Delta t_{i+1}$$ \hspace{1cm} (6.3)

Each subsystem is solved with a time step smaller than or equal to the global time step.

$$\Delta t_{s,j+1} = \alpha_{s,j+1} \Delta t_{i+1} \text{ with } \alpha_{s,j+1} \leq 1$$ \hspace{1cm} (6.4)

We again restrict the magnitude of the time step to certain discrete values, by assuming the following format for the scale factor $\alpha_{s,j+1}$:

$$\alpha_{s,j+1} = m^{-n_{s,j+1}}$$ \hspace{1cm} (6.5)

with $n_{s,j+1}$ an integer value that satisfies $0 \leq n_{s,j+1} \leq n_{s,\text{max}}$. In total, sub-system $s$ requires $m^{n_{s,j+1}}$ sub-steps to solve one global time step. If a sub-step counter $k_s$, varying between 1 and $m^{n_{s,j+1}}$, is defined, the current point in time $t_s$ for sub-system $s$ is found as:

$$t_s = t_i + k_s \Delta t_{s,j+1}$$ \hspace{1cm} (6.6)

In order to solve a sub-system $t$, data $X_s$ are required from all coupled sub-systems $s$. Since the time step size of the other sub-systems might be different, the data must be obtained from available data at non-corresponding points in time. If the latest available data corresponds to a point in time before or at the current time ($t_s \leq t_i$), these data are directly used. If the latest available data correspond to a point in time after the current time ($t_s > t_i$), data at the current time are obtained via linear interpolation:
where the symbol $X^k_s$ stands for data $X$ from sub-system $s$ at the $k^{th}$ sub-step for that system and $\mod(\bullet)$ denotes the modulo of the value between the brackets after division by one. It was verified whether higher convergence rates could be obtained by using extrapolated data for $t_s \leq t_t$. This was generally not the case. For weakly coupled sub-systems, the choice between ‘last available’ or ‘extrapolated’ data does hardly have an affect on the converged result or the convergence rate. For strongly coupled sub-systems, the intensive data-exchange necessitates that both systems are solved at equal points in time, and therefore the situation in which extrapolated data could potentially be used does not occur. For intermediate situations, the smaller time step size of sub-system $s$ is associated with the non-linear nature of the coefficients of the system matrix. A linear extrapolation might provide a better estimate for $X^k_s$, but, since $X$, fluctuates until sub-system $s$ reaches convergence, it does not lead to a reduction of the number of iterations for sub-system $t$. Because the benefit from using extrapolated data was not clear from the investigated examples, the last available data are used in the dynamic sub-stepping scheme.

Stage 0 (initial situation)

Stage 1 ($k_1 = 1; k_2 = 1$)

Stage 2 ($k_1 = 2; k_2 = 1$)

Stage 3 ($k_1 = 3; k_2 = 2$)

Figure 6.2: Schematic representation of the dynamic sub-stepping algorithm for two coupled sub-systems. Circular markers denote points in time where a system is solved. The colour of the marker corresponds to the availability of the data: black markers for converged steps, white for future time steps, and mixed black/white for data which are currently iterated upon. Dotted lines denote the exchange of computed data; dash-dotted lines the exchange of interpolated data.
As an example consider the two coupled sub-systems schematically depicted on Figure 6.2, Stage 0. The time step size of sub-system 1 (1 s) is initially smaller than the one of sub-system 2 (2 s). Both are smaller than the global time step of 4 s. Both sub-systems are assumed to be non-linear, and hence to require an iterative solution technique.

We start by solving the first time step of both sub-systems (Figure 6.2, Stage 1, \( k_1 = 1; k_2 = 1 \)). If both sub-systems are coupled, solving sub-system 1 requires data from sub-system 2 and vice-versa. The last available data from sub-system 2, namely at \( t_2 = 0 \) s, are used to perform one iteration for \( t_1 = 1 \) s of sub-system 1. Next, the first time point for sub-system 2 \( (k_2 = 1) \), namely \( t_2 = 2 \) s, is computed. Hereby, the last available data from sub-system 1 (at \( t_1 = 1 \) s) is used. We proceed with the next iteration for sub-system 1, still for \( t_1 = 1 \) s. Now, data from sub-system 2 are available both at \( t_2 = 0 \) s and at \( t_2 = 2 \) s. Therefore, interpolated data can be used for this iteration (see equation (6.7)). Afterwards, the next iteration of sub-system 2 can be performed using the latest available date from sub-system 1. We continue this process until convergence is reached. We only iterate on non-converged sub-systems.

After convergence is reached for all sub-systems, we proceed with the next time step for sub-system 1 \( (k_1 = 2) \). The solution for sub-system 2 was obtained using data from sub-system 1 corresponding to an earlier time step, namely at \( t_1 = 1 \) s. Therefore, we will continue iterating on time step \( t_2 = 2 \) s \( (k_2 = 1) \), but now using the updated data from sub-system 1 (Figure 6.2, Stage 2, \( k_1 = 2; k_2 = 1 \)). We keep on computing steps for sub-system 1 and updating sub-system 2 until both are solved at a coinciding point in time \( (t_1 = t_2 = 2) \). Afterwards, we can proceed with the next step for both sub-systems (Figure 6.2, Stage 3, \( k_1 = 3; k_2 = 2 \)).

Keeping track of the time step sizes, the last available data and the data on which these rely for each individual system, might seem complicated. Nevertheless, the algorithmic treatment is straightforward, even for a large number of coupled sub-systems, if a counter \( k = 1 \ldots m^n \) is defined, where \( n = \max(n_s) \). The step to solve in sub-system \( s \) is then given by:

\[
k_s = \left\lceil k \left( m^{n_s} - n_s \right) \right\rceil
\]

(6.8)

where \( \left\lceil \cdot \right\rceil \) denotes a mapping of the quantity between the brackets to the next higher integer value. In order to store the data, three vectors are required: one to store the converged data from the last global time step, one to store the last converged data from the sub-step and one
to store the non-converged values. The first vector is only required to be able to re-compute the global time step in case convergence problems arise.

6.1.2.4. Updating the time step size

Adaptive time-stepping algorithms, found in literature, usually express the new time step size $\Delta t_{s,i+1}$ for a sub-system $s$ as a function of the current time step size $\Delta t_{s,i}$ and a relative scale factor $\beta_{s,i+1}$. The latter one depends on e.g. the required number of iterations $ni_s$ to reach the required level of convergence for that sub-problem in the current time step:

$$\Delta t_{s,i+1} = \beta_{s,i+1} \Delta t_{s,i} \quad \text{and} \quad \beta_{s,i+1} = f(ni_s, \ldots)$$

(6.9)

The factor $\beta_{s,i+1}$ is a strictly positive real number. $\beta_{s,i+1} < 1$ implies a reduction of the current time step size, whereas $\beta_{s,i+1} > 1$ denotes that the current time step can be enlarged. When $\beta_{s,i+1} = 1$ the time step does not require modification, hence the current value is the ‘optimal’ value. We propose to determine the relative scale factor $\beta_{s,i+1}$ from:

$$\beta_{s,i+1} = f(ni_s, \ldots) = \min\left(1 + \left(\frac{\beta_{s,\min}}{\beta_{s,\max}} - 1\right) \frac{\min(ni_s, ni_{s,red}) - ni_{s,opt}}{ni_{s,red} - ni_{s,opt}}, \beta_{s,\max}\right)$$

(6.10)

where $\min(\bullet, \bullet)$ denotes the minimum of the two values between the brackets, $\beta_{s,\min}$ and $\beta_{s,\max}$ are the lower and upper bound to $\beta_{s,i+1}$, respectively, $ni_{s,opt}$ is the desired (or optimal) number of iterations, $ni_{s,red}$ is the number of iterations above which $\beta_{s,i+1}$ does not reduce further, and $c_s$ is a shape parameter larger than zero (Figure 6.3a).

In analogy with the definition of the scale factor $\alpha_s$ (equation (6.5)), we define $\beta_{s,\min}$ and $\beta_{s,\max}$ as:

$$\beta_{s,\min} = m^{-n_{s,\text{down}}}$$

$$\beta_{s,\max} = m^{n_{s,\text{up}}}$$

(6.11)

where $n_{s,\text{down}}$ and $n_{s,\text{up}}$ are the maximum number of steps down or up on the ladder of allowed time step sizes, respectively. The main advantage of adopting equation (6.10) is that the optimal number of iterations can be set explicitly, independent of the other parameters. In many adaptive time stepping algorithms (e.g. Roels et al. 2006), the optimal number of iterations is an implicit function of other parameters. Therefore, it is unclear to which step size these algorithms are implicitly driving the problem.
The relative scale factor $\beta_{s,i+1}$ is a real number that can continuously vary between the imposed bounds $\beta_{s,min}$ and $\beta_{s,max}$. The sub-stepping algorithm is expressed in terms of an absolute scale factor $\alpha_{s,i+1}$ with respect to the global time step, and can only take certain discrete values. $\beta_{s,i+1}$ can be transformed into $\alpha_{s,i+1}$ by means of:

$$\alpha_{s,i+1} = m^{-n_{s,i+1}} \text{ with } n_{s,i+1} = \min\left(\frac{-\log(\min(\alpha_{s,i+1},1))}{\log(m)}, n_{s,max}\right)$$  (6.12)

Figure 6.3b illustrates equation (6.12) in a graphical way for a specific choice of the parameters.

Figure 6.3: (a) New continuum scale factor versus number of iterations of the previous converged time step for the adaptive time-stepping algorithm according to equation (6.10). (b) Conversion of the relative scale factor $\beta$ into the absolute scale factor $\alpha$, by means of equation (6.12).

Adapted time step sizes for a specific sub-system are based on the total number of iterations required to solve the global time step, divided by the number of sub-steps during that global step, i.e. the average number of iterations per sub-step of that sub-system. Therefore, time step sizes can only be updated at the end of each global time step.
6.1.2.5. Academic example

Proving rigorously that the proposed algorithm (i) converges and (ii) reduces the computational cost is beyond the scope of this thesis. Instead, we will illustrate the main characteristics of the algorithm based on a two-equation example in the unknowns $x$ and $y$:

$$
\begin{bmatrix}
  a & b \\
  c & d
\end{bmatrix}
\begin{bmatrix}
  x \\
  y
\end{bmatrix} =
\begin{bmatrix}
  e \\
  f
\end{bmatrix}
$$

(6.13)

where $a$ and $d$ are non-zero coefficients, and $b$, $c$, $e$, and $f$ can have arbitrary values. The coefficients in the matrix on the left hand side can depend on $x$ and $y$. The coefficients in the right hand side vector only depend on the time $t$. Equation (6.13) can be solved using a staggered solution scheme:

$$
x^{j+1} = \left( a^{j+1} \right)^{-1} \left( e - b^{j+1} y^j \right)
$$

$$
y^{j+1} = \left( d^{j+1} \right)^{-1} \left( f - c^{j+1} x^{j+1} \right)
$$

(6.14)

where $j$ is an iteration counter. The notation $d^{j+1}$ indicates that the coefficient $d$ is evaluated using $x^{j+1}$ and $y^j$. For this simple example, where each sub-system is a single equation, the staggered solution scheme is a standard Gauss-Seidel method.

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Table 6.1: Staggered solution for two non-linear systems of equations with different degrees of coupling - results without sub-stepping.
We assume \( a = 2(x+1), \ b = 0, \ d = 10(2+y), \ e = 8t \) and \( f = 10t \). Furthermore, we assume three different values for the coupling coefficient \( c \), namely 0, 0.1 and 10, corresponding to uncoupled, weakly coupled and strongly coupled equations. Table 6.1 shows for the three different cases the intermediate values for \( x \) and \( y \) during the iterative procedure of the first time step (1 s). The solution is considered converged if the square of the difference between two consecutive approximations is below \( 5 \cdot 10^{-5} \).

From the uncoupled case, it is clear that both equations show non-linear behaviour. This is however more pronounced for the equation in the unknown \( x \). If a weak coupling between both equations is taken into account, the solution for \( y \) slightly changes, but no additional iterations are required. If both equations are strongly coupled, the non-linear nature of equation 1 has a significant effect on the number of iterations to reach convergence for \( y \).

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**Table 6.2:** Staggered solution for two non-linear systems of equations with different degrees of coupling - results with sub-stepping.
In case $n_{i_{\text{max}}}$ would be less than 13, both equations would be recomputed with a reduced time step. In case the optimal number of iterations would be less then 13 for both systems, the time step size for equation 1 would be reduced. In the strong coupling case, the time step for both equations would be reduced. The algorithm thus tends to maintain similar time stepping for strongly coupled equations, while for weakly or uncoupled equations both time step sizes can be independent, and can be adapted to the characteristics of the equation. Table 6.2 shows for the three different cases the intermediate values for $x$ and $y$ for $t = 1$, using sub-stepping.

In this example, the absolute computational cost to solve system 1 has increased by reducing the time step with a factor two. Nevertheless, the objectives, namely reducing the average number of iterations per sub-step and improving the accuracy of the solution, have been met. The average number of iterations per sub-step reduced from 14 to $(10+12)/2=11$, and it can be verified that the absolute residual, i.e. $|ax + by - e|$, has decreased from $2.02 \cdot 10^{-2}$ to $1.42 \cdot 10^{-2}$. In the uncoupled and weakly coupled case, the computational cost to solve equation 2 has only slightly increased (one extra iteration). Herein lies the main advantage of the proposed algorithm. Since all equations can be computed with a different time step size, a reduction of the step size for one equation only affects that particular equation and the strongly coupled equations. All weakly coupled or independent equations keep their original time stepping scheme. For each sub-step where an equation is not solved, additional iterations are performed using the latest available data from all systems. If this equation is independent from the others, one iteration will be sufficient to reach convergence (Table 6.2, $c = 0$, equation 2, $k = 2$). If some degree of coupling with other equations exists, the iterative procedure should be continued until the residual again becomes smaller than the threshold (Table 6.2, $c \neq 0$, equation 2, $k = 2$). The required number of iterations is related to the strength of the coupling, and has an influence on the size of the next time step.

### 6.1.3. Adaptive spatial integration using nodal storage

In general, a high mesh resolution is only needed in a part of the domain. This specific region is not necessarily the same for all sub-problems and it is usually not stationary in time. Adaptive meshing techniques (Schrefler et al. 2006) are appealing for individual problems, but in the context of coupled problems, they significantly complicate the overall solution scheme. An alternative approach consists in applying a higher order integration scheme in the regions where a higher accuracy is permanently or temporarily needed, and a low order scheme in the remaining part of the domain (Janssen and Carmeliet 2006). All sub-problems
are solved using the same underlying finite element mesh. The integration schemes are chosen based on the current needs of every specific sub-problem. A problem arises if information, e.g. material history, is stored at integration point level. Changing the integration scheme implies that these data must be transferred from the old to the new set of integration points. Such a mapping operation is based on interpolation, and therefore results in smoothing of the original field. Since the mapping operation is performed at element level, the error of a single mapping operation is small and vanishes upon mesh refinement (Wells 2001). However, in case successive mapping operations are carried out, it can be expected that the accuracy of the solution field is affected. To avoid this, a technique is developed in which all model variables are stored at the nodes of the finite element. The nodal data can be interpolated to the position of the integration point. As will be seen, this technique introduces an approximation error. Also this error vanishes upon mesh refinement.

**Figure 6.4:** Schematic representation of the two key-concepts of the storage strategy: (a) evaluation and storing all model variables at the element nodes, and (b) interpolating the stored quantities to the integration point.

Generally, we can write for a variable $\zeta_i$ at node $i$ of an element:

$$\zeta_i = f\left(\mathbf{X}, \dot{\mathbf{X}}, \nabla \mathbf{X}, \ldots \right)$$

where $\mathbf{X}$, $\dot{\mathbf{X}}$ and $\nabla \mathbf{X}$ are the primal variables of the system of equations and their time and spatial derivatives, respectively. The primal variables $\mathbf{X}$ are usually $C^0$-continuous across element boundaries. Therefore, the gradient field $\nabla \mathbf{X}$ is usually discontinuous across element boundaries, and since $\zeta_i$ depends on that field, $\zeta_i$ will not have a unique value at a node. Instead, at each node, we will obtain - and store - as many values as there are elements sharing that node (Figure 6.4a). Once we have the nodal values, interpolation towards the integration point can be performed in the standard way, using the finite element shape functions:

$$\zeta(\xi) = \sum_i N_i(\xi) \zeta_i$$

(6.16)
where $\xi$ is the natural coordinate of the position of the integration point and $N_i$ are the finite element shape functions associated with node $i$ (Figure 6.4b).

Theoretically, the nodal storage strategy (N-storage) has many advantages over the classical integration point storage technique (IP-storage). The main advantage is that the integration scheme can be altered freely, without additional calculations. Furthermore, the memory requirements are of the same order of magnitude as for IP-storage, but do not vary in time. N-storage is also beneficial in post-processing, since the quantities available at the nodes are the ones that are used in the computations. Additional mapping is not required.

Despite these advantages, the successful use of N-storage depends on the magnitude of the error that is introduced by using it. A major source of inaccuracy is the use of the interpolated nodal gradient field instead of the actual gradient field. The magnitude of the error can be expressed as:

$$e = \mathbf{B}X - N(B_{\text{nodal}}X)$$  \hspace{1cm} (6.17)

where $\mathbf{B}X$ denotes the gradient, evaluated at an integration point; $B_{\text{nodal}}X$ denotes the gradient, evaluated at a node; and $N$ interpolates the nodal gradient towards the integration point. By taking the L2-norm of the error and normalizing it, we get an objective error indicator:

$$e \equiv \frac{\| \mathbf{B}X - N(B_{\text{nodal}}X) \|}{\| \mathbf{B}X \|} \leq e_{\text{max}}$$  \hspace{1cm} (6.18)

The error $e$ can be computed explicitly from known quantities at each point in time. If the error exceeds a predefined threshold $e_{\text{max}}$, mesh refinement ($h$ or $p$-refinement) is needed to capture the occurring phenomena correctly.

In the field of mechanics, it is well known that there exist ‘optimal stress locations’ that coincide with the integration points of the lowest order Gauss-Legendre scheme that is sufficient to correctly integrate the finite element shape function (Barlow 1976a,b). At these points, the evaluated strain (the derivations were performed using linear elasticity, and hence stress and strain are proportional) is the same as the value that would be obtained if a one order higher shape function would have been used. In order to reach the same accuracy, N-storage requires a mesh with a higher polynomial order ($p$-refinement) or with a smaller element size ($h$-refinement). From the point of view of computational cost, IP-storage is thus always preferable. The use of N-storage can only be recommended in those situations where the approximation error can be avoided, i.e. the locally evaluated and the nodally interpolated
data should be equal. This is e.g. the case for variables that are a linear combination of the primal variables of the system of equations, their temporal derivatives and some constants. This is also the case for a number of common element types, like lines (1D), linear triangles (2D) or tetrahedrons (3D).

6.2. **Generic algorithms for X-FEM**

6.2.1. **Simplified element partitioning strategy**

In the extended finite element method, the quadrature rule is altered for elements intersected by a discontinuity. In order to adequately integrate the discontinuous field, integration is performed separately over the regions at both sides of the discontinuity. The methodology to partition the original element into two integratable sub-regions has been laid out in an early paper on X-FEM (Dolbow et al. 2000) and has not been altered since. This ‘standard’ methodology is schematically illustrated in Figure 6.5 for a bilinear element (Q4). Consider the element geometry and the direction and position of the discontinuity shown in Figure 6.5a. The first step consists in finding the intersections of the discontinuity and the element boundaries. At those intersections, situated in between the element nodes, local nodes are inserted (Figure 6.5b). Next, the arbitrarily shaped domains at both sides of the discontinuity need to be converted into integratable sub-regions. To that extent, triangulation is employed, and additional local nodes are inserted (Figure 6.5c). It is emphasized that no degrees of freedom are associated with the additional local nodes. They are only necessary to describe the underlying mesh over which integration is performed.

![Figure 6.5: Standard element partitioning strategy for X-FEM.](image)

The complexity of the standard approach grows rapidly in case three-dimensional calculations are undertaken, or in case multiple discontinuities per element are considered. A simplified element partitioning strategy has been designed that reduces the complexity without affecting generality. Figure 6.6 illustrates the methodology for a bilinear element (Q4). Consider the...
Since the element geometry is known, is it straightforward to split it into simplices (Figure 6.6b). A simplex is an n-dimensional analogue of a triangle: in 1D it is a point, in 2D a triangle, and in 3D a tetrahedron. Usually, a geometry can be split into simplices in several ways. It is recommended to avoid subdivisions that generate highly skewed simplices. To that extent, a quadrilateral is e.g. split along its shortest diagonal. More sophisticated criteria could involve the orientation of the discontinuity in relation to the orientation of the element boundaries, but unavoidably require more preparatory calculations. Since the goal is to design a straightforward and generic methodology, simple rules based on solely the element geometry are favoured. The second step of the partitioning algorithm consists in finding the intersections of the discontinuity and the boundaries of each simplex. Local nodes are inserted at those intersections situated in between the simplex nodes (Figure 6.6c). The resulting sub-regions have a shape that allows direct integration (i.e. for which quadrature rules exist),
therefore triangulation is not required. However, triangulation can optionally be performed if
the quality of the resulting integration regions would not match predefined quality
requirements (e.g. limited skewness), or, if preference is given to use only triangular (2D) or
tetrahedral (3D) elements (Figure 6.6d). The proposed algorithm is fully recursive. Therefore,
determining the quadrature rules for elements that contain multiple cracks does not pose any
added complexity (Figure 6.6e).
Comparing both partitioning algorithms, we can roughly state that the standard algorithm
starts by increasing the complexity of the geometry (by splitting), followed by a reduction of
the complexity (via triangulation). The proposed algorithm does the opposite: it starts by
reducing the complexity (by splitting into simplices) and it subsequently performs the
splitting operation on the simplified geometry. Therefore, the proposed algorithm leads to a
lower number of integration zones, and can be implemented in a more straightforward manner
- even in \( n \)-dimensions. As an example, Figure 6.7 shows the partitioned mesh for a planar
fracture in a mesh build up from hexahedrons for (a) the standard approach and (b) the
simplified approach. Figure 6.7a is adopted from Sukumar et al. (2000). The reduced
complexity of the partitioned mesh in the simplified approach is clearly visible.

\( \text{(a) standard partitioning strategy} \quad \text{(b) simplified partitioning strategy} \)

\( \text{Figure 6.7: 3D crack propagation with (a) the standard and (b) the simplified element partitioning strategy.} \)
\( \text{Figure (a) has been adopted from Sukumar et al. (2000).} \)

In a different context, namely generating structured finite element models from solid models
(or CAD models), a similar algorithm has been proposed by Belytschko et al. (2003).
Recently, Becker (2007) described a partitioning procedure in 3D which is analogue to the
proposed algorithm. However, to the authors’ knowledge, the generic character of the
proposed strategy and the recursive properties have not been recognized before.
6.2.2. Generic reverse mapping algorithm

In the process of partitioning the finite element, via either the standard or the proposed simplified approach, we are confronted with the following sub-problem: given the global coordinates (e.g. Cartesian coordinates) of a point within an element, determine the corresponding natural coordinates. We will term this operation ‘reverse mapping’. The opposite relation, namely determining the global coordinates from the natural coordinates is realized by a straightforward mapping operation:

\[ x = \sum_i N_i(\xi) x_i \] (6.19)

where \( x_i \) is the global coordinate vector of the nodes of the element, \( \xi \) is the natural coordinate vector of the point for which the global coordinate vector \( x \) need to be found, and \( N_i \) is the finite element shape function associated with node \( i \).

Reverse mapping essentially comes down to writing equation (6.19) explicitly in terms of the natural coordinates. For linear shape functions (lines in 1D, triangles in 2D, tetrahedrons in 3D) the reverse relationship can be derived analytically. For higher order shape functions a single point in the global coordinate system corresponds to multiple points in the natural coordinate system, since an \( n \)-th order function has \( n \) roots. Only one out of them is situated within the reference element, since the mapping is unique. Finding the correct roots is however cumbersome and the formulation differs per element type. To overcome these drawbacks, a computationally efficient iterative reverse mapping algorithm was developed:

\[ (0) \text{ initialization} \quad \xi_0 = \xi_{cm} \]

\[ (1) \text{ forward mapping} \quad \xi_k \rightarrow x_k \]

\[ (2) \text{ increment} \quad \Delta \xi_k = \left(J^T\right)^{-1} \left(x - x_k\right) \quad \text{if} \quad \|\Delta \xi_k\| > (\Delta_{max})^2 \]

\[ (3) \text{ update} \quad \xi_{k+1} = \xi_k + \Delta \xi_k \]

\[ (4) \text{ exit} \quad \xi = \xi_{k+1} \]

where \( \xi_{cm} \) are the natural coordinates of the centre of mass of the reference element, \( \xi_k \) is the \( k \)-th approximation of the natural coordinate vector corresponding to the global coordinate vector \( x \), \( J \) is the Jacobian matrix of the element and \( \Delta_{max} \) is the tolerance on the natural coordinates. The value of \( \Delta_{max} \) depends on the precision of the computer. If a value of \( \Delta_{max} = 10^{-15} \) is selected on a 32bit system, convergence is achieved within 4-5 iteration steps. The algorithm does not depend on the element type, nor the number of spatial dimensions.
6.2.3. Accurate sub-integration by higher order mapping

In this last section, a potential source of errors during the numerical integration of non-simplex elements crossed by a discontinuity is identified and a general solution strategy is proposed. The error consists in over-integrating the domain at one side of the discontinuity, and under-integrating the domain at the other side. This is caused by not properly taking into account the presence of non-linear terms in the mapping between the reference element of the global element and the global element itself (Figure 6.8).

![Figure 6.8: Integration error due to disregarding the effect of non-linear terms in the mapping between reference and global element. (a) Quadrature sub-cell. (b) Reference element of the finite element illustrated in (c).](image)

To clarify the source of the error, consider a straight discontinuity segment in a bilinear element. The discontinuity can be described by the general equation of a line in 2D:

\[ ax + by = c \]  

(6.20)

where \( a \), \( b \) and \( c \) are polynomial coefficients and \( x \) and \( y \) are Cartesian coordinates. Within the bilinear element, we can express the coordinates \( x \) and \( y \) as a function of the nodal coordinates \( x_i \) and \( y_i \), using the mapping given by equation (6.19):

\[
a \left( \sum_{i=1}^{4} N_i(\xi, \eta) x_i \right) + b \left( \sum_{i=1}^{4} N_i(\xi, \eta) y_i \right) = c
\]  

(6.21)

Inserting the expressions for the bilinear shape functions into equation (6.21) yields:

\[
A \xi \eta + B \xi + C \eta + D = c
\]  

(6.22)

with

\[
A = \frac{1}{4} \sum_{i=1}^{4} (ax_i + by_i) \xi \eta_i
\]

\[
B = \frac{1}{4} \sum_{i=1}^{4} (ax_i + by_i) \xi
\]

\[
C = \frac{1}{4} \sum_{i=1}^{4} (ax_i + by_i) \eta
\]

(6.23)
\[ D = \frac{1}{4} \sum_{i=1}^{4} (ax_i + by_i) \]

Equation (6.22) represents a straight line in the reference element if the coefficient \( A \) equals zero, thus:

\[ A = a(x_1 - x_2 + x_3 - x_4) + b(y_1 - y_2 + y_3 - y_4) = 0 \]  \hspace{1cm} (6.24)

For the non-trivial case \((a, b \neq 0)\), constraint (6.24) implies:

\[ x_1 - x_2 = x_4 - x_3 \quad \text{and} \quad y_1 - y_2 = y_4 - y_3 \]  \hspace{1cm} (6.25)

Only quadrilaterals fulfilling these two conditions, like a parallelogram, map straight lines onto straight lines, regardless the values for \(a\), \(b\) and \(c\). If conditions (6.25) are violated, most straight line segments in the global finite element space correspond to curved segments in the reference space. The quadrature sub-cells in the reference domain usually have linear boundaries. The mismatch between the curved and the straight boundary segment will result in an incorrect evaluation of the integral contributions to the weak form of the governing equation (Figure 6.8).

**Figure 6.9:** Removal of the integration error by higher order mapping. (a) Quadrature sub-cell. (b) Reference element of the finite element illustrated in (c).

The error can be avoided by imposing geometrical conformity between the border of the mapped quadrature sub-cell and the curved segment corresponding to the discontinuity. In the given example this can be realized by using a serendipity element (Q8) as quadrature sub-cell. In general, the integration error can be avoided if the polynomial used in the mapping from the quadrature sub-cell to the reference element is complete up to an order which is at least the same as the highest order term appearing in the mapping from reference to global element. For a 3-noded triangular element (T3), the highest order term is linear, hence the mapping to the reference element can be performed with shape functions which are complete up to the first order. For a bilinear quadrilateral (Q4) and a 6-noded triangular element (T6) we require second order completeness. For Q8 and the 9-noded quadrilateral (Q9) we require third and fourth order completeness, respectively. The same observations hold in 3D.
The magnitude of the possible integration error depends on the constraint violation (see equation (6.25)), the position and direction of the discontinuity ($a$, $b$ and $c$) and the function to be integrated. To illustrate that the error can be significant, even in simple cases, we study an academic example. Consider a bilinear element with coordinates (0,0), (2,0), (1,1) and (0,1), crossed by a vertical line segment at $x = 0.5$ (Figure 6.10). We integrate a unit quantity over the domain at the left side of the discontinuity. The result should be equal to the unit quantity times the considered area, being $1 \times 0.5 \text{ m}^2 = 0.5 \text{ m}^2$. Using a bilinear quadrature sub-cell (Q4) with a 2x2 Gauss-Legendre integration scheme, we obtain $0.542 \text{ m}^2$, corresponding to an absolute error of 8.3%. Using a serendipity sub-cell (Q8) with the same 2x2 integration scheme leads however to the correct result of $0.5 \text{ m}^2$. The example points out that the integration error in skewed meshes should not automatically be neglected.

6.3. Concluding remarks

The use of a staggered solution scheme allows directing the computational effort to the parts where it is needed. Each equation can be individually tailored to increase efficiency and improve accuracy. Two types of measures were proposed. In order to resolve discrepancies between the characteristic time of the phenomena described by the different equations, we rely on dynamic time stepping, whereby the selected time step is round down to certain discrete values. The time step is individually adapted per sub-system to incorporate the degree of non-linearity of the problem at hand and the strength of the coupling with other fields. Discrepancies in required spatial resolution are traditionally tackled by either adaptive meshing or by means of adaptive integration. The latter solution allows solving all equations on the same mesh, and therefore the coupling between the equations can be realized via the nodes. A common problem is related to the transfer of information stored at the integration points from the old to the new positions. As an alternative to the classical mapping strategy, nodal storage is proposed. Nodal storage allows changing the integration scheme freely, but
proved to suffer from an approximation error. The magnitude of the error can be reduced by means of mesh refinement ($h$ or $p$-refinement). Since comparable levels of accuracy can be obtained at a lower computational cost using the classical mapping strategy, the latter one is preferred in most practical situations. In some specific situations, e.g. when first order elements are used, the approximation error vanishes, and nodal storage can be used successfully.

The second part of the chapter deals with modifications to the standard X-FEM approach. For regular meshes, the proposed splitting strategy reduces the complexity of the implementation, and allows controlling element quality more easily. On skewed meshes, the combination with a higher order mapping scheme provides significantly more accurate results than the classical X-FEM methodology.
7. Experimental - computational verification

In the current chapter, we assess the performance of the continuous-discontinuous framework by means of comparison with experimental data. Two materials have been selected, namely Meule, a sandstone, and masonry. The tests on Meule allow investigating aspects of crack propagation. The tests on masonry serve at analyzing issues related to material interfaces.

7.1. Tests on Meule sandstone

In this section two verification tests on Meule sandstone are presented. First a uni-axial tensile test is studied. It illustrates the capability of the model to simulate crack propagation in a heterogeneous porous medium and the resulting anisotropic behaviour. Next, four-point bending tests on notched beams of three different sizes are analyzed. The latter simulations are conducted using the same parameters as for the uni-axial tensile test. The simulations are performed on both oven-dry and saturated material. It is shown that the model can reproduce the experimentally observed size effect. The good agreement with the experimental data gives an indication that the model properly captures the underlying physical phenomena. Prior to the verification study, some general characteristics of Meule sandstone are presented.

7.1.1. Material characteristics

The grès à Meules, or simply Meule, is a fluviial sandstone from the grès à Voltzia formation in the Vosges, France, deposited during the Trias, i.e. 200-250 million years ago (Gall and Grauvogel-Stamm 2005). The fluvial origin gives the sandstone its layered structure: thick red layers alternate with thin black layers (Figure 7.1a). Fracture planes along such a black layer reveal the presence of micas (illite). The stone is composed of quartz grains (74%) and contains an amount of clay (like smectite, illite and kaolinite) and other secondary mineralization, like feldspar (Van de Abeele et al. 2002). The bonding material is primarily silica. The name ‘Meule’ is probably related to its primary application as base material for mill stones (French: meule). This type of sandstone has also been frequently applied as a building material, e.g. to construct the tower of the Cathedral of Strasbourg (Figure 7.1b).
Figure 7.1: (a) Layered structure of Meule sandstone. (b) Tower of the Cathedral of Strasbourg, France, constructed primarily from Meule sandstone.

### 7.1.2. Uni-axial tensile test

#### 7.1.2.1. Experimental setup

Uni-axial tensile tests were performed on dogbone-shaped specimens (Figure 7.2a). Two different loading directions were investigated: parallel and orthogonal to the direction of the mica-layers. The samples have a height of 0.095 m. The cross section in contact with the loading platens measures 0.045 m x 0.014 m (width x thickness) and gradually reduces to 0.03 m x 0.014 m (width x thickness) at the smallest point. A fixed connection between samples and test equipment is realized by means of glue. In this way, rigid body rotations are prevented and the stress state is more uniform as compared to the use of rotating boundary conditions (Van Vliet 2000). This simplifies comparison with numerical simulations. The tests were conducted under displacement control. Two extensometers with measurement basis of 0.02 m were mounted at opposite sides of the specimen. The load was controlled as such that the average extension would increase with a constant rate of 0.02 mm/min. A sampling rate of 0.5 pt/s was chosen.

Figure 7.2: Uni-axial tensile test on Meule sandstone: (a) geometry of the dog-bone specimen, and (b) experimentally determined stress-strain relationship for two loading directions.
Figure 7.2b shows the measured stress-strain response for two different loading directions. Stresses are hereby understood as the measured force in the load cell, divided by the cross sectional area at the notch. Strains are defined as the average of the measured elongation from both extensometers, divided by the length of the measurement basis. Three tests were conducted for each loading direction. In two tests, the crack initiated at one side of the specimen and propagated towards the other end. The data shown in Figure 7.2b correspond to the four tests where cracks initiated at both sides of the specimen at the same time, and propagated in a symmetric way towards the middle.

Several observations can be made. Sandstone shows considerable anisotropic behaviour, most likely as a consequence of its layered structure. Nevertheless, the initial stiffness does not seem to depend on the loading direction, indicating that the stiffness of the mica-rich layers must be of the same order of magnitude as of the quartz-rich layers. The load bearing capacity for the orthogonal loading direction is approximately one third less than for parallel loading conditions. Therefore it can be assumed that mica-rich layers have a lower strength. Also the softening response is found to depend on the loading direction. For the orthogonally loaded specimens, failure occurs in a brittle manner. The weaker mica-rich layer acts hereby as a preferential crack path. For the other loading direction, a more tortuous crack path is formed, and correspondingly, a more ductile response is obtained.

7.1.2.2. Numerical analysis

The layered structure of the sandstone triggers transversely isotropic behaviour, i.e. the material behaviour orthogonal to the layering differs from the in-plane behaviour. Anisotropy can be modelled either by using a suitable anisotropic continuum material model or by explicitly modelling the layering. The former methodology has the advantage that coarser meshes can be applied since individual layers do not need to be modelled. The drawback of applying a homogenized material model is however that they are generally not capable to predict a different failure mechanism depending on the loading direction (van der Meer and Sluys 2009). Moreover, comparing the dimensions of the sample (width $L = 0.045$ m) with the inter-layer distance (c.t.c. $\ell \approx 0.009$ m, see further), it is seen that the separation of scales principle ($\ell \ll l \ll L$) does not hold. Therefore, we will model the sandstone layers explicitly, rather than using an anisotropic material model.
Figure 7.3: Uni-axial tensile test on Meule sandstone: geometry, (refined) meshes and boundary conditions used in the numerical simulations. Mesh (a) is used for the orthogonal loading case, mesh (b) in the parallel case. The real sample is rotated over 90 degrees.

The dimensions of the computational model correspond to the theoretical dimensions of the test specimen, whereby the symmetry of test setup and failure pattern is exploited (Figure 7.3). The thickness of the layers was obtained in several steps. First the test specimen was wetted in order to increase the visual contrast between both layer types. Next, the number of layers per specimen was counted. Division by the corresponding dimension of the specimen provided the average centre-to-centre distance (0.009 m). The thickness of each layer was manually measured using a so-called crack meter. The average values of all layers of all (six) specimens were round to the nearest multiple of 0.0005 m. This procedure leads to a thickness of 0.0015 m for the mica-rich layer and 0.0075 m for the quartz-rich layer. Layers were assumed to be symmetrically distributed over the specimens. For the specimens in which symmetric failure took place, this assumption is valid.

The geometry is discretized with bilinear elements (Q4). In the notch area, the mica-rich layers where meshed with at least 3 elements over their thickness to properly take into account the material behaviour. Quartz-rich layers have at least 8 elements over their thickness. Interfaces between both layers types coincide with element boundaries. For each loading direction, a coarse and a refined mesh was generated. In the parallel loading condition the coarse mesh had 1123 elements versus 2180 elements for the refined mesh. The meshes for the orthogonal loading conditions count 862 and 2166 elements, respectively.
At the top boundary, a monotonically increasing vertical displacement is imposed \((\bar{u}_y = 0.02 \text{ mm/min})\), while the horizontal motion is constrained \((\bar{u}_x = 0)\). The bottom boundary is fully constrained \((\bar{u}_x = \bar{u}_y = 0)\). The displacement of the nodes along the symmetry axis is constrained in horizontal direction \((\bar{u}_x = 0)\).

The anisotropy in the mechanical response is assumed to originate from the layered structure. The material behaviour of each layer can, as a first approximation, be considered isotropic. Both materials are modelled with the Weibull-based isotropic damage model (section 3.4.3.2). This model takes five input parameters, namely the Young’s modulus \(E\), the Poisson’s ratio \(\nu\), the damage threshold \(r_0\), and the Weibull parameters \(\lambda_w\) and \(k_w\). Since it was observed that the initial response of the sandstone is independent of the layer orientation, the elastic properties \((E \text{ and } \nu)\) can be assumed equal for both layers. Furthermore, the measured stress-strain relationship is from the onset non-linear, i.e. the damage process starts from the moment the first load is applied. Therefore the damage threshold \(r_0\) can be set to zero for both materials. From the 2x5 input parameters, required to model the continuum material behaviour of the sandstone specimen, only six \((2+2x2)\) remain to be determined.

The discrete fracture process is governed by the proposed cohesive zone model (section 4.2). Herein, the residual strength of the material is modelled by equation (4.12) and depends on four parameters, namely the strength \(f^0_i\) at which softening starts, the strength \(f^1_i\) of the last piece of material within the cohesive zone that fails, and the parameters \(\lambda\) and \(n\) who describe the evolution of the material strength from \(f^0_i\) to \(f^1_i\). The strength \(f^0_i\) physically corresponds to the stress level at which the redistribution mechanisms are locally exhausted and thus to the maximum stress at a material point. For the Weibull-based softening law, the maximum stress can be determined analytically as a function of the Weibull parameters only:

\[
\sigma_{\text{max}} = f^0_i = \lambda_w \left( \frac{1}{k_w} \right)^{1/k_w} \exp \left( -\frac{1}{k_w} \right) \text{ if } r_0 = 0
\]

\(f^0_i\) is therefore a dependent variable. The discrete crack model thus requires 2x3 additional parameters, bringing the total number of parameters of the continuous-discontinuous material model for sandstone to 12.

The identification process is performed in several steps. The initial tangent of the measured stress-strain curve provides an estimate for the Young’s modulus, namely 12 GPa. A Poisson’s ratio of 0.15 is assumed, but the simulations were found to be insensitive to
(reasonable) variations of this parameter. The parameters \( k_w \) and \( \lambda_w \) can not be directly identified from the measurements. Both are however related to the measured peak load by means of equation (7.1). \( \lambda_w \) can therefore be considered a dependent variable. Simulations of the loading branch have been conducted for several values of \( k_w \). The values for which the best correspondence with the measurements was found were selected. Next, the parameters for the discrete model were identified. The residual strength \( f_{r}^{i} \) can be obtained from the total elongation of the sample at failure by means of equation (4.17) (with \( \omega = 1 \) and \( \kappa = f_{r}^{0} \)). The remaining two parameters, \( \lambda \) and \( n \), govern the slope of the softening branch. The set of parameters providing the best agreement with the measurements was selected.

Further refinement of the estimated parameters \( k_w, \lambda_w, f_{r}^{i}, \lambda \) and \( n \) was done using inverse analysis by means of the Levenberg-Marquardt algorithm (Levenberg 1944, Marquardt 1963, Carmeliet 1999). Herein, the difference between the simulated and measured stress at a given strain is minimized, by iteratively updating the model parameters according to:

\[
\Delta \beta = (J^T J + \zeta \text{diag}(J^T J))^{-1} J^T (y^{\text{exp}} - y^{\text{sim}}(\beta)) \quad \text{with} \quad J_i = \frac{\partial y^{\text{sim}}}{\partial \beta} \approx \frac{\Delta y^{\text{sim}}}{\Delta \beta}
\]

(7.2)

where \( \beta \) is the vector containing the model parameters, \( d\beta \) is the update of \( \beta \), \( y^{\text{exp}} \) and \( y^{\text{sim}} \) are the measured and the simulated response, respectively, \( J \) is the Hessian matrix, containing the derivatives of the simulated response to the model parameters, and \( \zeta \) is a damping factor. A large value for the damping factor brings the algorithm closer to the steepest descent method, while for small values, the Gauss-Newton algorithm is recovered. The latter one yields optimal convergence if a good initial estimate for the model parameters is provided. Since the initial guess yields a response close to the measured response, it can be assumed that the model parameters are close to the optimal set of parameters. Therefore, a small value of \( \zeta = 5 \) was selected. An overview of the obtained model parameters is given in Table 7.1.

<table>
<thead>
<tr>
<th></th>
<th>( E ) [GPa]</th>
<th>( \nu ) [-]</th>
<th>( \lambda_{w} ) [MPa]</th>
<th>( k_{w} ) [-]</th>
<th>( f_{r}^{i} ) [Pa]</th>
<th>( \lambda ) [-]</th>
<th>( n ) [-]</th>
</tr>
</thead>
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<td>Quartz</td>
<td>12.0</td>
<td>0.15</td>
<td>2.780</td>
<td>0.355</td>
<td>65000</td>
<td>0.002</td>
<td>0.25</td>
</tr>
<tr>
<td>Mica</td>
<td>12.0</td>
<td>0.15</td>
<td>0.191</td>
<td>0.227</td>
<td>9500</td>
<td>0.0002</td>
<td>0.25</td>
</tr>
</tbody>
</table>

Table 7.1: Model parameters for the layers of Meule sandstone.
7.1.2.3. Results and discussion

Figure 7.4: Uni-axial tensile test on Meule sandstone: measured stress-strain diagrams for both loading directions (solid lines) and corresponding simulations for two different mesh resolutions (dashed/dotted lines).

From Figure 7.4 it is clear that mesh-objective results are obtained, although a non-regularized isotropic damage model has been used to describe the bulk material behaviour. The proposed strategy, in which a cohesive zone is locally inserted at a point when the stress at that point reaches its peak value, successfully regularizes the problem. The regularization stems from the fact that softening is entirely governed by the mesh-objective cohesive zone model. The bulk material starts unloading instead of softening after the peak stress has been reached and a cohesive zone has been inserted. The amount of continuum damage at the peak of the constitutive stress-strain relation can be obtained as:

\[ d_{\text{max}} = 1 - \exp \left( -\frac{1}{k_w} \right) \]  

(7.3)

Inserting the model variables \( k_w \) from Table 7.1 into equation (7.3) yields \( d_{\text{mica}}^{\text{max}} = 0.985 \) and \( d_{\text{sand}}^{\text{max}} = 0.940 \) for mica and Meule, respectively. Figure 7.5 depicts the damage distribution in the investigated specimens at final rupture. The obtained damage values do not exceed the theoretical limits, illustrating the fact that the bulk material did not reach a stress state beyond the peak in the constitutive relation. It can be clearly observed that damage mainly localizes in the mica-layers. Under parallel loading conditions, also a large region of the sand layers becomes damaged. This is one reason for the higher energy dissipation for this configuration. The other reason is the difference in (discrete) mode I fracture energy (Equation (4.20)).
A good agreement between measurements and simulations was found for both loading directions (Figure 7.4). Nevertheless, two remarkable differences are to be noted, both related to the use of constant material properties within each material layer. First, it can be seen that the post-peak response for the simulation of the orthogonal loading conditions shows a characteristic load drop after the peak load, which is not observed in the measurements. This load drop corresponds to the failure of the outermost quartz-layer. The remaining part of the softening branch is then governed by the behaviour of the second quartz layer. In reality, the material properties change gradually and therefore these load drops are smoothed out. A second difference with the measurements is the absence of long softening tails. In the simulation final rupture occurs at a unique threshold value, while in nature failure is a stochastic phenomenon. Moreover, a real crack surface is seldom smooth. Therefore some load can still be transferred by means of friction or hooking resistance.

The good agreement between simulations and measurements could be anticipated since three out of seven parameters in the continuous-discontinuous material model for each layer are not directly related to measurable quantities, and were selected as such that a good agreement was obtained. The question should be asked how many parameters are minimally needed to properly describe the anisotropic mechanical behaviour of a layered material. A classical, regularized, continuum damage model, like e.g. a gradient enhanced damage model (Peerlings et al. 1996), that exhibits linear elastic loading and linear softening behaviour requires five parameters (two elastic constants, one gradient parameter and two parameters in the softening
law). We employ only two additional parameters to describe all pre- and post-peak non-linearity in a layer. From this point of view, the number of model parameters can be considered adequate. In order to remove the doubt that the model has enough degrees of freedom to accommodate to any response, we will simulate a series of four-point bending tests in the next paragraph, using the same set of material parameters, and compare the simulated response against measurements.

7.1.3. Four-point bending tests

7.1.3.1. Experimental setup

Four-point bending tests are performed on notched beams of Meule sandstone (Figure 7.6). Two different moisture contents and three different beam sizes are considered. The geometry and dimensions of the reference beam are identical to the one studied in section 4.4.2, namely, a length of 0.24 m and cross-sectional dimensions 0.048 m x 0.024 m (height x depth). The notch has a width of 0.004 m, a depth of 0.008 m and a circular tip. The distance between the two supports is 0.2 m and between the loading points 0.1 m. The two other beams are respectively half and double the size of the reference beam. All tests were conducted under displacement control. To this extent, an extensometer with measurement basis of either 0.0125 m (for the small beam and the reference beam) or 0.025 m (for the largest beam) was placed over the notch, on the bottom surface of the sample (Figure 7.6b). The load was controlled as such that the crack mouth opening displacement (CMOD) increases at a constant rate of 0.1 mm/min. A sampling rate of 20 pts/s was chosen.

Figure 7.6: 4-point bending tests on Meule sandstone: (a) overview test setup for the reference beam and zoom on the notched sandstone beam with extensometer in place.
7.1.3.2. Numerical analysis

The simulations are performed in 2D under plane strain assumptions. The geometry of the computational models is identical to the theoretical dimensions of the test specimens (Figure 7.7). The layers are modelled in a similar way as for the uni-axial tensile test (c.t.c. 0.009 m). Structured meshes consisting of 524, 1424 and 2572 bilinear elements (Q4) were employed to discretize the small, medium and large beam, respectively. Each mesh is more refined towards the notch section to capture the stress concentration. The element sizes in the central area are similar to the ones employed in the uni-axial tensile test, for which mesh objectivity was shown. At the loading points, a vertical displacement at a fixed rate was prescribed ($\dot{u}_y = 0.1 \text{ mm/min}$). The supports of the testing machine are metal cylindrical bars without bearing. They can be adequately modelled by means of a Coulomb friction model:

$$F_x = \mu F_y$$  \hspace{1cm} (7.4)

where the horizontal frictional force $F_x$ is obtained as the product of the (static) friction coefficient $\mu$ and the vertical compressive force on the support $F_y$. The static friction coefficient between fine-grained sandstone and steel is $\mu = 0.94$ according to Avallone et al. (2006). In order to prevent rigid body motion, the motion of the left support was restricted in horizontal direction ($\dot{u}_x = 0$), while the Coulomb model is applied on the right support. At both supports, the motion in vertical direction is restricted ($\dot{u}_y = 0$). The test is simulated with the material model and parameters described in the previous section. A time step of one second is selected.

![Figure 7.7: Four-point bending test on Meule sandstone: geometry, meshes and boundary conditions employed in the numerical simulations.](image)
7.1.3.3. Results and discussion

Figure 7.8: Four-point bending test on Meule sandstone: (a) measured and simulated nominal stress versus strain relation for the three investigated beam sizes at 0 % saturation. (b) Same, but for saturated specimens. (c) Dimensionless peak values of the nominal strength versus dimensionless beam size for the investigated beam sizes at 0 % and 100 % saturation.

In Figure 7.8a and b, measured and simulated nominal stresses $\sigma_N$ are plotted as a function of the strain for all beam sizes. Hereby, the strain is obtained as the measured displacement by the extensometer, divided by the length of the measurement basis. The nominal stress is the maximum stress in the mid-plane of a vertical cross-section through the beam and can be obtained analytically from the measured load $F$ as:

$$\sigma_N = \frac{3}{2} \frac{l_{up} - l_{load}}{h^2 w} F$$  \hspace{1cm} (7.5)

where $h$ is the height of the cross-section at the position of the notch, $w$ is the specimen width, and $l_{up}$ and $l_{load}$ are the distances between the supports and the loading points, respectively. The simulations for the dry material (Figure 7.8a) assume $p_i = 10^8$ Pa, while $p_c = 10$ Pa was considered representative for saturated material (Figure 7.8b). A Biot coefficient of 0.6 was assumed, leading to a hygric stress of 1.6 MPa.

From the measurements, it is seen that the bigger, but otherwise identical, test specimens fail at a lower nominal stress levels than smaller specimens (Figure 7.8). This is frequently
observed in brittle materials and is called the deterministic size effect (Bažant and Planas 1998). It originates from the release of (elastically) stored energy of a specimen or structure into the fracture front. The required energy to propagate a crack one unit area is constant for a material, i.e. the fracture energy. The larger the specimen, the more energy can be elastically stored in it, and the larger the potential for the initiation and propagation of cracks. Besides the deterministic size effect, several other sources of size effect exist as well. The stochastic distribution of micro-cracks, voids and defects in the specimen and the randomness of the material strength give for instance rise to the so-called probabilistic or statistical size effect (Carmeliet and Hens 1994, Bažant and J. Planas 1998). For small specimens the stochastic variation can be relatively large, and a large scatter on the measurement data can arise. The scatter normally decreases with increasing specimen size. This effect is not observed in the measurements.

The deterministic size effect is present, both for dry and saturated specimens (Figure 7.8a and b). The maximum load bearing strength of the saturated specimens is approximately three times lower than the one of the dry material. The strain at which the peak nominal stress occurs is hardly affected by the degree of saturation.

The data depicted in Figure 7.8a and b are represented in a dimensionless way on a log-log scale in Figure 7.8c. The nominal stress at the peak load is made dimensionless by division with a factor \( Bf \), where \( B \) is a dimensionless constant and \( f \) is the tensile strength. The factor \( Bf \) is taken equal to the maximum normalized stress found in the experiments (7 MPa at \( S_l = 0\% \) and 3.3 MPa at \( S_l = 100\% \)). The beam size is normalized by means of the height \( h_0 \) of the cross-section at the position of the notch of the reference beam. The dimensionless nominal strength shows a clear decreasing trend with increasing specimen size. The amount of size effect is not altered by the degree of saturation. For comparison, the size effect law (SEL) according to the formulation of Shah (1990) is given as well:

\[
\frac{\sigma_N}{Bf} = \left(1 + \frac{h}{h_0}\right)^{-0.5}
\]  

(7.6)

This relation exhibits a smooth transition from the theoretical limit strength on the one hand to the decreasing relation between nominal strength and specimen size according to linear elastic fracture mechanics (LEFM) on the other hand.

From Figure 7.8, it can be observed that a good agreement between measurements and simulations is found for all three beam sizes and for both saturation levels. Since this analysis has been conducted based on the same material model as the uni-axial tensile test, this result
gives some confidence that the determined model parameters are linked to physical material characteristics.

7.2. Tests on masonry

In this section, we assess the capability of the continuous-discontinuous framework to capture the behaviour of material interfaces. Two types of verification tests are presented. First a uniaxial tensile test on a mortar joint embedded between two bricks is studied. Detailed experimental results for this case have been published by van der Pluijm (1997). It is shown that based on the measured properties, all but one of the model parameters can be determined. The sensitivity of the response to the remaining variable is assessed, and it is shown that the variation in the mechanical response is smaller than the experimental scatter. The second example focuses on the hygric behaviour of mortar joints. A detailed study of an uptake experiment on a single mortar joint between two bricks has been conducted by Derluyn et al. (2008). It is shown that using the measured properties, the experimental results can be captured. Nevertheless, the good agreement relies heavily on the magnitude of the interface permeability.

7.2.1. Material characteristics

Masonry is a composite material consisting of individual units, bound together by mortar. Common unit materials are ceramic bricks or concrete blocks. The units are usually assembled according to a regular (periodic) pattern, and consequently most masonry structures exhibit orthotropic properties. Due to the periodic arrangement of the two phases, preferential cracking orientations exist, usually along the mortar joints. Lawrence and Cao (1987) studied the mechanisms of bond development between mortar and brick. They conclude that the brick-mortar bond is essentially mechanical in nature, i.e. the fine-grained mortar penetrates into the pore system of the brick during bricklaying and after curing both materials are interconnected. A detailed study of the various factors affecting the bond strength was carried out by Groot (1993). His study reveals the importance of moisture transport between mortar and brick, since it affects the curing process. For instance, mortar cured on dry bricks exhibits a higher porosity and a lower bond strength. Recently, Derluyn et al. (2008) showed that the curing conditions also have a twofold effect on the moisture permeability. On the one hand, the hygric properties of the mortar joint are modified, and on the other hand, a hygric resistance arises at the interface layer.
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7.2.2. Uni-axial tensile test

7.2.2.1. Experimental setup

In the period 1990-1995, van der Pluijm and co-workers have carried out an extensive amount of deformation controlled tensile tests on masonry specimens. In order to assess the proposed mechanical continuous-discontinuous model for material interfaces, we use the data of their 1995 test series on wire-cut clay bricks (brand: Joosten) with general purpose mortar (1 part CEM I 32.5 R, 1 part lime, 6 parts dry sand), as reported in van der Pluijm (1997). The masonry specimens consist of two brick units of 0.1 x 0.05 m (W x H), connected to each other by means of a mortar joint of 0.0125 m thickness (Figure 7.9). They are equipped with four LVDT’s to control the increase of the deformation over the localization area, i.e. the brick mortar interface, during the test. The LVDT gauge length was 0.03 m.

Figure 7.9: Uni-axial tensile test on masonry: (a) Tensile testing arrangement (van der Pluijm 1997) and (b) shape of the masonry test specimens.

The composite specimen is glued between the loading platens of the tensile test equipment (Figure 7.9). The top platen is part of a parallelogram, restraining possible rotations. Any non-uniform crack opening (e.g. because the crack starts at one side of the specimen) will be caught up by the test setup, giving rise to a bump in the softening branch in the stress-strain plot and an overestimation of the fracture energy (Van Vliet 2000, Hordijk 1992).

Figure 7.10a shows the measured stress-elongation curves for all 33 reported tests. It is apparent that a large scatter was found. Van der Pluijm (1997) determined for each test three quantities, namely the stiffness $E$, the tensile strength $f_t$ and the mode I fracture energy $G_{II}^t$.

Average values of 2.371 GPa, 0.4 MPa and 5.5 N/m were reported, respectively. In Figure 7.10b-d the three measured quantities for all 33 tests are presented as frequency distributions. Stiffness and tensile strength appear as asymmetric stochastic distributions. The fracture energy does not exhibit a clear trend; a large coefficient of variation was found (70%), and no real physical significance can be attributed to the average value.
Experimental - computational verification

Figure 7.10: Uni-axial tensile test on masonry: (a) experimentally determined stress-displacement curves (van der Pluijm 1997), and frequency distributions for three derived quantities (b) $E$, (c) $f_t$ and (d) $G^f_j$. In (b-d) the average value (avg.) and the coefficient of variation (cv) obtained by van der Pluijm (1997) are given as well.

For this particular test series, van der Pluijm reports that no clear correlation could be found between the measured mode I fracture energy and tensile strength, but that the former tends to increase with the latter (Figure 7.11a). Therefore it is unclear from the measurements whether the fracture energy should be considered as a dependent or an independent variable. In the proposed cohesive zone model, the fracture energy is assumed to depend on the model parameters (see section 4.2.4):

$$G_f^i = G_f^i (E, f_t, \ldots)$$

(7.7)

In analogy with equation (4.26), the fracture energy is now assumed to be proportional to the square of the tensile strength and inversely proportional to the stiffness:

$$G_f^i = \alpha \frac{f_t^2}{2E}$$

(7.8)

In Figure 7.11b the measured mode I fracture energy is plotted against the factor $f_t^2/2E$, calculated based on the measured tensile strength and the corresponding, measured, secant stiffness. The secant stiffness is the damaged stiffness corresponding to the moment at which the peak load has been reached and is tabulated in van der Pluijm (1997) for every
investigated test specimen. A clear correlation ($R^2 = 0.75$) is found for $\alpha = 0.058$, indicating that $G_i$ can indeed be considered a dependent variable (Figure 7.11b).

**Figure 7.11:** (a) Measured tensile bond strength versus mode I fracture energy for clay brick masonry with 1:1:6 mortar. (b) Mode I fracture energy versus $f_t^2 / 2E$.

### 7.2.2.2. Numerical analysis

In this section the experiments of van der Pluijm are simulated, using the data given in the paper. Only the upper left quarter of the masonry specimen is modelled (Figure 7.12). Hereby, it is implicitly assumed that symmetric failure occurs. The specimen is meshed with 1250 bilinear elements (Q4). The motion of the nodes on the symmetry axes of the model is restricted in the direction orthogonal to the axes. The motion of the nodes on the top boundary is restricted in horizontal direction ($\vec{u}_x = 0$). In vertical direction, a monotonically increasing displacement is imposed. Since time-dependent effects are not considered, the rate can be freely chosen. A value of $\vec{u}_y = 10^{-5}$ m/s is adopted.

**Figure 7.12:** Uni-axial tensile test on masonry: geometry, mesh and boundary conditions for the numerical simulation.
Linear elastic constitutive behaviour is assumed for both brick and mortar (equation (3.51)). Linear elasticity requires two parameters, namely the stiffness and the Poisson’s ratio. In the 1995 test series, a Young’s modulus of 16.605 GPa was found for Joosten brick under tensile loading conditions. For the Young’s modulus of mortar, the average measured value of 2.4 GPa can be used. Poisson’s ratios were not reported in van der Pluijm (1997). Following Massart (2003), a value of 0.15 for brick and 0.20 for mortar are adopted.

Interface failure is included in the simulation by means of the proposed cohesive zone model (section 4.2). Four parameters need to be determined, namely the initial and the residual tensile strength of mortar ($f^0_t$ and $f^1_t$) and the softening parameters $\lambda$ and $n$. The bond strength of the interface is taken equal to the average measured tensile strength (0.4 MPa). The residual tensile strength can be determined from the maximum crack width. Unfortunately, all 33 stress displacement curves were shown on a single graph in van der Pluijm (1997), which complicates the visual determination of the maximum crack width. The curves seem to cluster into two groups (Figure 7.10a). One group has (i) higher peak load, (ii) a residual load level at the end of the test, and (iii) the softening branch of the stress-displacement curve exhibits a bump, characteristic for non-uniform crack growth. The other group has (i) a lower peak load, (ii) a zero load level at the end of the test and (iii) a more monotonic softening branch. The maximum crack widths for the latter group cluster around $3.5 \times 10^{-5}$ to $4.0 \times 10^{-5}$ m. Using equation (4.17) with $\omega = 1$, $[\mathbf{u}] \cdot \mathbf{n} = 3.75 \times 10^{-5}$ m and $\kappa = f^1_t$, a value of 0.16 MPa is found for the residual tensile strength. The two remaining parameters, namely $\lambda$ and $n$, determine the way in which the strength in the material bridges decreases, but can not be determined unambiguously from the experiments. Only one of the two parameters can be freely chosen. The other one follows from the constraint that the resulting fracture energy (equation (4.20)) must correspond to the measured value. For reasons mentioned earlier, we prefer determining the fracture energy from equation (7.8), rather than directly from the measurements. Using the factor $\alpha = 0.058$, and the average of the measured values for the tensile strength $f_t$ (0.4 MPa) and the secant stiffness (1.2 MPa), a value of 3.8 N/m is found. Simulations are conducted for two extreme combinations of $\lambda$ and $n$ to assess the sensitivity for a particular choice. The set \{ $\lambda = 0.5; n = 0.0561$ \} yields an almost vertical asymptote at the onset of softening. The set \{ $\lambda = 1.0; n = 0.0798$ \} corresponds to the maximum value for $\lambda$ for which a parameter $n$ can be determined as such that the correct amount of energy is dissipated.
7.2.2.3. Results and discussion

Figure 7.13: Simulated stress-displacement curves for masonry specimens loaded under tension for (a) two extreme combinations of $\lambda$ and $n$, and (b) two realizations of a stochastic distribution of the tensile strength. The shaded area represents the range of the experimental results.

Figure 7.13a compares the numerical simulations with the experimental data. It is clear that the overall response agrees well with the measurements. Different parameter combinations of $\lambda$ and $n$ alter the shape of the softening branch to a small extent, nevertheless all curves remain well within the experimental range. The observed pre-peak non-linearity in the experiments is not present in the numerical simulations. This stems from the fact that the bond strength is a stochastic variable (see Figure 7.10c), while it was treated as a deterministic variable in the simulations. Figure 7.13b shows the same simulation, but now the initial bond strength is modelled as an uncorrelated random field according to a normal probability distribution with mean value 0.4 MPa and standard deviation 30%. Although the assumption of a symmetric failure mode is no longer valid in this case, the simulation is conducted on the same geometry as for the previous analysis. In this way, the failure mode is predetermined, and the differences in the response are a direct consequence of the randomness of the properties. As can be seen, pre-peak non-linearity is now present to a small extent, and some variation in the peak load can also be observed.

From the preceding analysis, it can be concluded that the proposed model has a potential to simulate interface failure in masonry. Nevertheless, it is clear that the behaviour of a material interface is, even under controlled laboratory conditions, determined by stochastic effects. A complete stochastic analysis is a necessary next step in order to assess the impact of variations of the material properties on the obtained response. The continuous-discontinuous modelling strategy could be employed for this purpose.
7.2.3. Water uptake in masonry

7.2.3.1. Experimental setup

Derluyn et al. (2008) have investigated moisture transport across a brick-mortar interface by means of water uptake experiments on simple masonry specimens. The investigated specimens consisted of two bricks \( W \times H = 0.07 \times 0.03 \) m, connected by means of a mortar joint of 0.01 m thickness (Figure 7.14). Since the transport properties are known to be dependent on the curing conditions, two test series have been conducted. In the first series, the bricks were dried before the mortar was applied, while in the second series, the bricks were initially saturated. The masonry specimens were subjected to water uptake perpendicular to the direction of the mortar joint. During the test, X-ray images were taken at regular time intervals, from which the position of the moisture front could be extracted. The moisture front is defined as the position where the degree of saturation equals 50 %.

![Figure 7.14: (a) test setup for the water uptake experiment, and (b) X-ray output image after 5 minutes of uptake.](image)

7.2.3.2. Numerical analysis

Since moisture uptake orthogonal to the material interface is studied, and since the material properties were reasonably homogeneous over the width of the test specimen, a one-dimensional analysis is performed. To this extent, a mesh with 898 linear elements is constructed. The element size ranges from \( 8.67 \times 10^{-6} \) m near the bottom surface and the material interfaces, until \( 1.75 \times 10^{-4} \) m inside the brick material. Initially oven dry conditions are assumed \( (p_v = 10^{10} \text{ Pa}) \). A Dirichlet boundary condition of \( p_v = 10 \text{ Pa} \) is imposed at the bottom to represent the direct contact with liquid water. At the top of the specimen, evaporation to an indoor environment at 293.15 K and 70 % relative humidity can take place (surface transfer coefficient \( \beta_l = 18.5 \times 10^{-9} \text{ kg/(m}^2\text{s}) \)).
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The material properties, required in the numerical simulation, are the (wetting) moisture retention curve and the moisture permeability for brick as well as for mortar under the two considered curing conditions. Additionally, the discrete damage variable and the relative interface position needs to be determined. In Derluyn et al. (2008) the measured continuum moisture properties were reported (see Figure 7.15).

![Figure 7.15](image1.png)

**Figure 7.15:** (a) Moisture content and (b) moisture permeability as a function of capillary pressure for the brick material (solid line) and for mortar cured on both dry (dashed line) and wet brick (dotted line) (Derluyn et al. 2008).

Since the mortar penetrates into the brick material, it is justified to assume that the interface permeability will be mainly determined by the mortar permeability. As a first approximation, the relative position of the material interface (see section 5.2) is therefore assumed to lie entirely in the mortar layer ($\alpha = 1$).

![Figure 7.16](image2.png)

**Figure 7.16:** Microscopic images of the brick-mortar interface for (a) dry and (b) wet curing conditions (Derluyn et al. 2008).

The damage variable represents the fraction of the contact area where the hydraulic contact between brick and mortar is not perfect, e.g. because of the presence of compaction pores. Derluyn et al. (2008) present 2D microscopic images of (a part of) the material interface, from which the impact of the curing conditions on the bond quality can be clearly observed (Figure
Nevertheless, the quantitative determination of the damage variable should be based on e.g. 3D tomographic data. Lacking such detailed information, we will determine the damage variable via inverse analysis and critically evaluate its magnitude in light of Figure 7.16.

7.2.3.3. Results and discussion

Figure 7.17: Comparison between the measured and simulated propagation of the moisture front in the masonry specimen for (a) dry and (b) wet curing conditions. Markers correspond to measured data. The dashed and solid line represent simulations with a perfect (\( \omega = 0 \)) and a damaged material (\( \omega \neq 0 \)) interface, respectively.

Figure 7.17 compares the measured and simulated propagation of the moisture front. The best agreement between both was found by using a damage variable of 0.5 % and 0.35 % for dry and wet curing conditions, respectively. The quality of the agreement strongly depends on the magnitude of the damage variable. This variable is theoretically related to the reduced area over which perfect contact takes place. Therefore, the larger value found for the dry curing conditions can be explained by the presence of compaction pores. However, especially under dry curing conditions, the value of the damage variable is significantly less than what could be expected from Figure 7.16a.

Figure 7.18: Schematic representation of different phenomena at the brick-mortar interface layer. The gray colour represents mortar. The orange blocks represent the brick material with larger characteristic pore size.

The discrepancy between the expected amount of interface damage and the value determined via inverse analysis is due to the inability of the model to capture the true underlying physical phenomena. The interpenetration of mortar into the brick pore system is e.g. not properly
taken into account, and moisture can e.g. not flow around a microscopic barrier, like a compaction pore or a region with a low permeability (Figure 7.18). Including these effects requires determining the interface permeability from a micro-scale model, rather than using a weighted coupled permeability ($\alpha = 1$). Using the correct permeability in the model can restore the physical meaning of the damage variable. This can be illustrated by means of equation (5.19), written in terms of capillary pressures instead of temperatures:

\[
g \cdot n = \left( \frac{1 - \omega}{\omega} \right) \gamma^{-1} K_{mn,rf} \left[ p_c \right] + \bar{g}_{rf} \cdot n
\]  

(7.9)

Increasing the damage variable $\omega$ leads to a decrease of the factor $(1 - \omega)/\omega$. The same response, i.e. same fluxes and pressures, can only be obtained if the discrete permeability $K_{mn,rf}$ increases. Assume for example that a damage variable of 33.3% is obtained from experimental analysis of the material interface, instead of the value 0.5% mentioned earlier. In this case, the term $(1 - \omega)/\omega$ decreases from 199 to 2, and therefore a nearly 100 times higher permeability is needed to obtain the same response. Knowing that the permeabilities of mortar and brick vary over 7 and 10 orders of magnitude, respectively, and that the difference between both permeabilities is almost 4 orders of magnitude at saturation and nearly 2 orders of magnitude in the dry state (see Figure 7.15), a change over 2 orders of magnitude at the interface layer is not unrealistically high. Consequently, it can be expected that the values of the damage variable regain their physical meaning, by deriving the interface permeability from a lower scale model.

A possible validation test for the current mono-scale model could consist in testing a composite specimen with an artificial imperfection at the contact layer. This can be achieved by applying a kaolin layer at the entire interface, with exception of a number of spots with known position and dimensions. At these spots, an impermeable layer (e.g. metal paint) can be applied. The kaolin layer creates a perfect contact between both surfaces. The ratio of the impermeable area over the total interface area yields the damage variable. The transport properties are the ones of the bulk materials.

### 7.3. Concluding remarks

We have assessed the performance of the continuous-discontinuous framework by means of a comparison with experimental data. In the first part of this chapter the main focus was on the correct prediction of material failure. The layered sandstone Meule was selected as exemplary material. First, the mechanical properties of the two types of layers were determined based on
uni-axial tensile tests parallel and orthogonal to the layer direction. Since the highly anisotropic behaviour could be captured by a single parameter set, it can be assumed that the model captures at a macroscopic level the underlying physical failure mechanism. Next, four-point bending tests on dry and saturated Meule beams were studied. Using the same set of material properties, it was shown that the experimentally observed size effect could be reproduced in both cases.

In the second part of this chapter, we focused on masonry to assess the ability of the framework to model material interfaces. In a first test, the mechanical behaviour of the interface was studied. The material properties and experimental results were taken from a study by van der Pluijm (1997). A good agreement was found. Nevertheless, it became clear that successful modelling of interface behaviour requires a stochastic instead of deterministic approach. In a second example the performance of the discrete hygric model was investigated. Although the model could reproduce the experimental data, the use of a more advanced model to determine the permeability of the material interface (instead of a coupled permeability) is recommended in order to capture the physics of the problem in a better way.

In general, we can conclude that the proposed mechanical model captures the experimentally observed trends very well, both for material and interface failure. The ability of the hygric model to represent transport across a material interface has been shown as well, but due to the high degree of non-linearity, the behaviour is very sensitive to the value of the coupled permeability. The thermal component of the model has not been studied due to a lack of adequate experimental data. However, since (i) the governing equations describing thermal and hygric transport processes in porous materials are of the same type and since (ii) the thermal properties, i.e. the coefficients in the governing equations, generally exhibit less non-linearity than their hygric counterparts, a good performance can be expected.
8. Case study

In this chapter, we move away from the academic examples and the basic tests on small-size laboratory specimens investigated so far. The goal is to show that the proposed theory can be successfully applied to study practical applications. As an example, we investigate the behaviour of an outside render on a masonry wall under different types of loading. It is shown that the model is capable to reproduce several common failure modes encountered in reality.

8.1. Problem description

In literature, many problems regarding failure in outside plaster render have been reported. Two different failure patterns are illustrated in Figure 8.1. For both, drying shrinkage can be identified as the main cause of damage.

![Figure 8.1: Moisture induced failure: (a) orthogonal crack pattern corresponding to the joints of the underlying masonry wall; (b) random crack pattern, independent of the underlying masonry wall. Adaptation from: Blaich (1999).](image)

The crack pattern shown in Figure 8.1a, matches the position of the joints of the underlying masonry wall. This situation can be encountered when the render is applied on a wet wall. During the drying process, the moisture saturation in the surface layer of the brick material decreases more rapidly than in the render. Therefore, drying-induced shrinkage is more pronounced in the brick material, and gives rise to the development of tensile stresses in the render, especially across the mortar joints. If the render is not reinforced, this might lead to the observed failure pattern. Other adverse factors are e.g. a limited thickness of the render or
a large discrepancy between the shrinkage properties of brick and render. Applying the render on a brick wall with incompletely pointed (butt) joints also increases the risk of failure. The crack pattern on Figure 8.1b does not show any correlation with the structure of the underlying masonry wall. Here, failure is caused by drying-induced shrinkage of the render itself. Damage of this type can be expected when the render material (i) is sensitive to shrinkage, (ii) has low strength, and (iii) is applied as a thin layer.

Figure 8.2: (a) Orthogonal crack pattern corresponding to the joints of the underlying insulation panels. Adaptation from: Blaich (1999). (b) Severe delamination due to poor connection between render and wall. Adaptation from: www.missionsjc.com/preservation.

Apart from hygric sources of damage, also a difference in thermal expansion coefficient between wall and render can lead to failure. Again, both structured and random failure patterns can be encountered (Figure 8.2). Orthogonal cracks usually arise during cold periods, when thermal shrinkage leads to high tensile stresses, especially across the joints. This situation for example occurs if the render is applied on a thermal insulation layer with a higher thermal expansion coefficient (Figure 8.2a). Figure 8.2b shows severe damage, resulting from de-cohesion between render and wall. Thermal expansion of the render, in combination with a poor connection between render and wall, causes the render to bend out and detach from the wall. Random cracks emerge at the surface if the local curvature becomes too high. Finally, buckling of the render can occur, whereby large parts of the render fall off. By good craftsmanship and a deliberate choice of the applied materials, all presented damage cases can be easily avoided.

8.2. Numerical study

The concise overview in the previous section revealed that the specific failure mode is not fixed, but depends on the interplay between geometrical factors, material behaviour and external conditions. Among the geometrical factors, incompletely pointed (butt) joints and the
application of a relatively thin plaster layer were mentioned. Low strength of the render and a mismatch in hygric, thermal or mechanical material properties between render and underlying wall were identified as main material-related grounds for failure. Finally, the external conditions force the material to change state, e.g. to heat up, and, depending on geometry and the materials employed, the development of a specific failure pattern might be triggered. With the proposed continuous-discontinuous modelling technique, it is possible to investigate this interaction. To that extent, a simplified numerical study is conducted on a part of a masonry wall with an outside render. The considered wall is an example of bad craftsmanship. Therefore, different failure patterns might arise depending on the external conditions, allowing to illustrate the capabilities of the proposed modelling strategy.

8.2.1. Computational model

8.2.1.1. Geometry

We consider a two-dimensional, periodic cell in a vertical cross section of a double-wythe masonry wall (Figure 8.3). Three-dimensional effects are not accounted for. The wall is composed of bricks (L x W x H = 0.21 x 0.1 x 0.05 m) with a 0.01 m mortar joint between them. The wall is not pointed. At the outside, a mineral-based plaster of 0.01 m thickness is applied. The inside surface is left unfinished. Insulation material is not present.

8.2.1.2. Spatial discretization

Two different meshes have been created, with 2945 and 978 bilinear elements (Q4), respectively. The former is to be used in the analyses where moisture transfer plays a role, while the latter is designed for cases where heat transfer is dominant. The material interface between render and brick is modelled by means of the proposed cohesive zone approach i.e. the mechanical behaviour is governed by equation (4.9) and the hygro-thermal behaviour by
equation (5.26). The brick-mortar interface coincides with an element boundary. Since no interface element or cohesive zone is added, interface damage is precluded. In order to verify this assumption, the stress at each point of the interface was continuously monitored. It never exceeded the bond strength and therefore this modelling approach is valid.

8.2.1.3. Boundary conditions
At the symmetry axes of the model, the displacements are restricted in y-direction \( \bar{u}_y = 0 \) and no-flux boundary conditions are imposed for heat and mass transfer \( \bar{g} = \bar{q} = 0 \). In order to prevent rigid body motion, the displacement in horizontal direction of the bottom-left node of the computational model is restricted \( \bar{u}_x = 0 \). Gravitational effects are neglected. This implies that the compressive load of the brickwork above the investigated periodic cell is not taken into account. The in- and outside surface are exposed to climatic boundary conditions (equations (5.68)), i.e. they can exchange mass with the environment by means of evaporation or condensation \( \beta_i = 18.5 \times 10^{-9} \text{ kg/(m}^2\text{s}) \); \( \beta_e = 140.0 \times 10^{-9} \text{ kg/(m}^2\text{s}) \)), and heat by means of convection and radiation \( h_i = 8 \text{ W/(m}^2\text{K}) \); \( h_e = 23 \text{ W/(m}^2\text{K}) \)). Latent heat exchange with the surroundings is accounted for. No rain is considered. The indoor environment is assumed to have a constant temperature of 293.15 K and a relative humidity of 50 %. The temperature and relative humidity of the outdoor climate depend on the investigated case.

The brick-render interface is initially considered damage-free \( \omega = 0 \). If interface damage develops during the simulation, the damaged area is modelled as a gas-filled micro-crack whose hygro-thermal behaviour is governed by equations (5.38) and (5.41). The same behaviour is assumed for the cavity behind the outside render.

8.2.1.4. Material model
All materials are considered linear elastic and isotropic (equation (3.51)). Hygric effects are taken into account by means of the effective stress principle (equations (3.49) and (3.50)). Thermal expansion or contraction is modelled as a thermal strain component:

\[
\varepsilon_r = \alpha^T (T - T_0)
\]

(8.1)

where \( \alpha^T \) is the thermal expansion coefficient and \( T_0 \) the reference temperature. The total strain is the sum of the elastic and the thermal strain.

The material properties for brick and mortar cured on dry brick, as presented in chapter 7, are used in the analysis. The hygric material properties of the render are assumed to be identical to the ones of mortar. Its thermal properties, mechanical stiffness and thermal expansion
coefficient are average quantities, obtained from various literature sources. The mechanical strength of the render is assumed to develop gradually towards its final value of 4 MPa. This is a simplified way to describe the hardening during hydration. In practice all properties will gradually change during hardening, but insufficient experimental data were found to include this in the simulation. The Biot-coefficient is estimated to be 0.6. An overview of the most relevant properties for the three materials is given in Table 8.1.

<table>
<thead>
<tr>
<th>Property</th>
<th>Units</th>
<th>Brick</th>
<th>Mortar</th>
<th>Render</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$</td>
<td>GPa</td>
<td>16.605</td>
<td>2.371</td>
<td>10.0</td>
</tr>
<tr>
<td>$\nu$</td>
<td></td>
<td>0.15</td>
<td>0.2</td>
<td>0.15</td>
</tr>
<tr>
<td>$f_t$</td>
<td>MPa</td>
<td>2.0</td>
<td>0.4</td>
<td>$4 - 3 \exp \left( -2 \times 10^{-4} t \right)$</td>
</tr>
<tr>
<td>$b^+$</td>
<td></td>
<td>0.6</td>
<td>0.6</td>
<td>0.6</td>
</tr>
<tr>
<td>$\alpha^\ell$</td>
<td>1/K</td>
<td>1.2e-5</td>
<td>10.4e-6</td>
<td>16.4e-6</td>
</tr>
<tr>
<td>$w_{cap}$</td>
<td>kg/m$^3$</td>
<td>130.0</td>
<td>97.0</td>
<td>97.0</td>
</tr>
<tr>
<td>$\mu$</td>
<td></td>
<td>32.0</td>
<td>451.0</td>
<td>451.0</td>
</tr>
<tr>
<td>$\rho^c$</td>
<td>kg/m$^3$</td>
<td>2086.5</td>
<td>2232.0</td>
<td>849.0</td>
</tr>
<tr>
<td>$c_p^c$</td>
<td>J/kgK</td>
<td>900.0</td>
<td>840.0</td>
<td>900.0</td>
</tr>
<tr>
<td>$k^c$</td>
<td>W/mK</td>
<td>$1.0 + 0.611S$</td>
<td>$1.95 + 0.2977S$</td>
<td>$0.48 + 1.02S$</td>
</tr>
</tbody>
</table>

Table 8.1: Overview of the employed material properties for brick, mortar and render.

8.2.1.5. Numerical aspects

The crack initiation or propagation criterion (equation (4.10)) is checked at each point in time at the centre of mass of every finite element, and at the endpoint(s) of existing discontinuities. The latter choice ensures crack path continuity. The propagation direction is based on the non-local stress tensor (equation (4.28)). New discontinuity segments are inserted using the simplified partitioning strategy explained in section 6.2.1. The number of discontinuities per element is restricted to one. Integration of the fractured elements makes use of the proposed higher order mapping technique (section 6.2.3).

8.2.2. Render applied on a saturated masonry wall

To simulate the behaviour of a wet render, applied on a saturated wall, we assume an initial capillary pressure of $10^4$ Pa for both ($S \gg 99 \%$). The outside temperature is taken equal to the inside temperature to ensure that the resulting damage pattern is not caused by the development of differential thermal stresses. An outside relative humidity of 85% is assumed. Figure 8.4 illustrates the resulting failure pattern after one day of drying and the equilibrium state (after 100 days).
In the first hours of drying, the saturation in the surface layer of the render decreases rapidly. Hereby, hygric stresses develop, exceeding the tensile strength of the young material. As a result a distributed network of fine surface cracks is formed (Figure 8.4a).

Additionally, moisture diffuses from the brick, via the render towards the surface. Because of the difference in moisture properties, the degree of saturation at the brick-render interface will decrease faster in the brick than in the render. The brick deforms during the drying process, and subjects the render to tensile loading and bending. Because the joints were not fully pointed, a small cavity exists. This cavity locally hinders the supply of moisture from the bulk of the wall towards the surface. Therefore, drying of the render is not uniform, and a shrinkage-induced stress concentration arises at the position of the joint. Both effects add up and cause crack initiation (Figure 8.4a).

As the drying proceeds, the stresses in the render resulting from the restrained shrinkage increase, and one of the existing cracks propagates further. The crack in the render creates a pathway between the cavity and the outside environment. Moisture might enter via this channel, expose the brick-render interface to wetting and trigger an acceleration of the degradation process (Figure 8.4b).
8.2.3. Render applied on a dry masonry wall

A dry masonry wall is modelled by assuming an initial capillary pressure of $10^8$ Pa ($S \approx 1\%$). The render is wet when it is applied, and therefore an initial capillary pressure of $10^4$ Pa ($S \gg 99\%$) is chosen. The boundary conditions towards the outside environment are similar to the ones in the previous example, namely a temperature of 293.15 K and a relative humidity of 85%. We only assume that the outdoor wind speed is higher, resulting in a higher surface transfer coefficient ($\beta_\epsilon = 280.0 \times 10^{-9}$ kg/(m²s)), Figure 8.5 illustrates the resulting failure pattern after 1 min, 20 min, 3 h and 12 h of drying.

![Deformed configuration of a wet render, applied on a dry masonry wall after 1 min, 20 min, 3 h and 20 h of drying. Deformations are magnified with a factor 1000. Colours correspond to the degree of saturation. Dashed lines indicate material boundaries. Cracks are overlayed with black lines to increase visibility.](image)

**Figure 8.5:** Deformed configuration of a wet render, applied on a dry masonry wall after 1 min, 20 min, 3 h and 20 h of drying. Deformations are magnified with a factor 1000. Colours correspond to the degree of saturation. Dashed lines indicate material boundaries. Cracks are overlayed with black lines to increase visibility.

The difference in vapour pressure between the surface of the saturated render and the surrounding air triggers the drying process. Already after one minute, the drying-induced hygric stress reaches the tensile strength of the fresh material and small surface cracks appear (Figure 8.5a). Furthermore, the large difference in capillary pressure between brick and render causes drying at the reverse side of the render. The drying-induced shrinkage of the render is hindered by the stiffer brick material. As a result, a series of parallel cracks is initiated orthogonal to the brick-render material interface (Figure 8.5a).

As the drying proceeds a large number of surface cracks appear (Figure 8.5b). As mentioned earlier, only one crack per element is allowed in the simulations. Without this restriction, several hundreds of small surface cracks would appear (not shown). These are better described by means of a continuum damage variable (like in section 7.1). Nevertheless, it is seen that also with a linear elastic continuum model, the correct failure mode is recovered.

After 3 hours of drying, the crack pattern at the surface is fully formed (compare Figure 8.5c and d). As the drying proceeds, the bending in the render vanishes and the cracks will close.
8.2.4. Render on a dimensionally unstable wall after cooling

The third type of damage is usually encountered when the render is applied on a wall with a high thermal expansion coefficient. In order to investigate the capability of the model to reproduce the correct damage pattern, we will assume an expansion coefficient of $5.0 \times 10^{-5} \text{ K}^{-1}$ for the brick material instead of $1.2 \times 10^{-5} \text{ K}^{-1}$. The cross section is exposed to an outside temperature of 273.15 K. The wall is initially at 283.15 K. The indoor and outdoor relative humidity are taken equal to ensure that the resulting damage pattern is solely due to the development of thermal stresses. Figure 8.6 illustrates the resulting failure pattern at thermal equilibrium. Note that the deformed configuration of the integration zones, not of the elements, is plotted. The diagonal in every finite element, crossed by a crack or an interface, is a consequence of employing the simplified partitioning strategy (section 6.2.1).

![Figure 8.6: Deformed configuration of a render on a dimensionally unstable wall after cooling. Deformations are magnified with a factor 1000. Colours correspond to temperature.](image)

From Figure 8.6 the dimensional instability of the brick under thermal loading can be clearly seen: at the inside wall surface the brick expands, while thermal contraction is observed at the outside surface. In reality, the entire wall would be subjected to bending. This three-dimensional effect is however not accounted for in the simulation. The deformation of the brick is introduced into the render and triggers crack initiation at its inside surface, at the height of the mortar joint. Afterwards, the crack has propagated towards the outside surface of the render. This implies that crack growth is not caused by the thermal stresses in the render. The latter stresses reach a maximum at the outside surface, and therefore, they would trigger a crack propagating from outside to inside. The mortar joint at the outer side of the wall is also loaded under tension by the deformation of the brick. Decreasing the temperature further, would trigger also damage in the brick-mortar interface.
8.2.5. Render with poor bond to the wall after heating

The poor connection between render and wall is modelled by assuming an initial amount of damage of 1% for the brick-render cohesive zone. We assume that the temperature of the environment equals 313.15 K (40°C). The wall is initially at 293.15 K (20°C). Again, the outside relative humidity is taken equal to the inside relative humidity to exclude the effect of differential hygric stresses. Figure 8.7 illustrates the resulting failure pattern after heating.

![Deformed configuration of a render with a poor connection to the wall, exposed to heating.](image_url)

**Figure 8.7:** Deformed configuration of a render with a poor connection to the wall, exposed to heating. Deformations are magnified with a factor 1000. Colours correspond to temperature.

Although the interface was initially only slightly damaged, delamination was already triggered under moderate thermal loading conditions ($\Delta T < 20$ °C). Moreover, the amount of delamination is restricted due to the limited height of the considered (periodic) cell. In reality, it can take place over a large area and might finally lead to spalling of the render.

8.3. Concluding remarks

Although the simulations do not cover the full complexity of real-life applications, they clearly illustrate the potential of the proposed methodology. Complicated interactions between heat and mass transfer on the one hand, and mechanical behaviour on the other hand can be studied. As discrete cracks are formed, either within the material or along material interfaces, new pathways and new surfaces are created. The pathways alter the transport properties of the material in an anisotropic way. Via the new surfaces, the bulk of the material will start to interact with the adjacent environment. All these aspects are of key-importance in the study of physical degradation processes of porous materials.
9. Conclusions and perspectives

9.1. Main results and conclusions

The objective of this work was to develop and experimentally validate an efficient numerical model for simulating the behaviour and the degradation of porous building materials exposed to combined mechanical and hygro-thermal loading. A careful literature survey pointed out that the best way to proceed consisted in combining continuous and discontinuous models in a common framework. The development of this combined model was dealt with in chapters 4 and 5. Different strategies to render the computations, based on the proposed model, more efficient and reliable were presented in chapter 6. Chapter 7 was concerned with comparing the model results with experimental data. For each of these aspects, the approach and the main results are summarized below.

9.1.1. Model development

The cornerstone of this work is the development of a new type of cohesive zone model. The model is based on the assumption that a cohesive zone consists of a cracked and a non-cracked part. The material behaviour in the non-cracked part is governed by the bulk model for the continuum, projected onto the plane of the discontinuity. The cracked part is considered an external boundary of the material on which appropriate boundary conditions are imposed. In combination with the fundamental conservation equations of linear momentum, mass and energy, the general expression for the cohesive zone model is obtained.

Using this model, we can describe the entire failure process of a porous medium - starting from the initial diffuse damage growth, over the subsequent formation of a failure band up to its final evolution into a macroscopic discrete crack - in a single macroscopic framework, without introducing artificial parameters or parameters with a debatable physical significance. Hereby, the development of a discrete crack affects all considered fields (e.g. displacements, pressure and temperature) in a generic way. It has been demonstrated that the formulation holds both for material failure and interface failure.
Chapter 9

9.1.2. Numerical efficiency and accuracy

Numerical efficiency is crucial in conducting multi-field simulations. The high number of degrees of freedom involved renders this particular type of simulation extremely demanding. A staggered solution scheme offers the best framework to optimize the computational effort. It allows responding to the different spatial and temporal requirements of the individual sub-problems. Two measures are proposed to increase efficiency. To reconcile the different temporal requirements, an adaptive sub-cycling scheme has been developed. The simulations are conducted using the optimal time step for each individual sub-problem, taking into account both the non-linearity of the problem itself and the strength of the coupling to the other considered sub-problems. To reconcile the different spatial requirements, adaptive integration is employed. Adapting the integration scheme poses a problem if information is stored at the integration points. Indeed, the position of the integration points changes over time. The position of the nodes is however fixed, and since the primary unknowns in a finite element simulation are nodal values, an algorithm was designed that allowed storing the material history at the position of the nodes as well. This methodology allows to freely adapt the integration scheme to the required spatial discretization. However, the required number of degrees of freedom to reach the same level of accuracy as with the traditional storage at the integration points is theoretically higher for the proposed algorithm. Only in certain cases, e.g. when linear finite elements are used, the advantages of the novel algorithm can be fully exploited.

Besides increasing efficiency, we also did an effort to reduce the added complexity of considering fractures as discrete geometrical entities. A simplified, recursive splitting strategy has been proposed. Furthermore, it has been shown that it is required to use higher order shape functions in the mapping of the sub-domain onto the global domain, in order to prevent integration errors. The novel algorithms contribute to a more efficient and accurate solution strategy for multi-field continuous-discontinuous simulations.

9.1.3. Comparison with experimental data

A model is necessarily a simplification of reality. In the proposed modelling approach, the fracture process zone is not modelled explicitly, but lumped onto the fracture plane and indirectly taken into account by the cohesive zone model. In the latter, the change of the material structure in the undamaged material bonds is only considered in an averaged way. The validity of these assumptions has been verified both for the case of material failure and for the case of interface failure by comparison with experiments on layered sandstone and
masonry, respectively. It was shown that by explicitly modelling the layered nature of the selected sandstone, the anisotropic mechanical behaviour and failure pattern could be captured. Furthermore, the experimentally observed size effect could be reproduced. This indicates that the true physical processes underlying the failure mechanism are properly captured by the proposed model and that the selected model parameters are closely related to physical properties.

The model for interface failure was used to analyse a uni-axial tensile test on a dry masonry specimen. The corresponding experimental results show a large amount of scatter, revealing the stochastic nature of the bond between brick and mortar. Although the model predictions agree well with the average measurement data, a full statistical analysis is required to assess the relevance of this result. Finally, water uptake across a brick-mortar interface was studied. The potential of the model to reproduce the experimental results was demonstrated. Nevertheless, the need for a more accurate determination of the interface permeability was identified.

9.2. Recommendations for further research

The recommendations for further research are subdivided into two categories. The first category, termed level I, is an immediate extension of the work presented in this thesis. The proposed research areas require novel input, but fit in the proposed framework. In contrast, level II recommendations necessitate conceptual changes.

9.2.1. Level I

9.2.1.1. Extension to mode II

The cohesive zone model, as proposed in chapter 4, is based on mode I failure. An extension towards mode II requires two interconnected changes. First of all the initiation criterion (equation (4.27)) needs to be modified. For mode I, a Rankine criterion was applied. For pure mode II, a Tresca criterion would be suitable. In order to model the more general case of mixed mode failure, employing a Mohr-Coulomb, Drucker-Prager or Von Mises failure criterion could be considered. The second modification is related to the loading function governing the growth of the damage variable. This implies adopting a novel definition of the equivalent effective traction (equation (4.11)), that incorporates the tangential component of the traction vector. The choices for the initiation criterion and the loading function are closely related: the loading function should evaluate zero at the instant a new discontinuity segment is inserted.
9.2.1.2. Crack tip enrichment

Although theoretically a crack tip can be situated at an arbitrary location within a finite element, it is not unusual to propagate cracks in an element-by-element manner (e.g. Wells and Sluys 2001). In that way, the crack tip is always situated on an element boundary and a zero opening at the crack tip can easily be enforced by not enriching the nodes on the crack tip support. Nevertheless, this methodology does not allow an accurate prediction of the stress field in the element ahead of the crack tip, and consequently, the moment at which crack propagation will occur, is not predicted correctly.

The classical technique to arrive at a better approximation of the near-tip stress field is to apply a Westergaard enrichment to all nodes within a pre-defined range around the crack tip (e.g. Dolbow et al. 2000). The Westergaard functions describe the stress field around a sharp crack tip in an elastic medium, and consequently, they can only reproduce the ‘exact’ analytical solution in that particular situation. Furthermore, the dimensions of the enriched region have to be carefully selected. If the region is chosen too large, linear dependency of the enrichment function and the standard shape function can cause convergence problems. Choosing a too small region leads to an inaccurate stress prediction.

It is clear that simulating the near-tip stress field is not straightforward, even in an elastic medium. Therefore, it might prove useful to opt for a less ‘exact’, but more generic and robust alternative. The idea is to enrich the nodes belonging to all supports intersected or touched by the crack. For the nodes belonging to the intersected supports the traditional Heaviside enrichment can still be selected. For the nodes on the crack tip support, we can use a new tip-enrichment function based on the angle $\theta \ (-\frac{\pi}{2} \leq \theta \leq \frac{\pi}{2})$ with the fictitious extension of the discontinuity (see Figure 9.1), which is discontinuous along the support and continuous in the element ahead of the crack tip. Examples of such functions are:

\[ \varphi = \frac{1}{2} + \frac{\theta}{\pi} \]  

or

\[ \varphi = \frac{1 + \sin(\theta)}{2} \]

An enrichment like (9.1) or (9.2) allows the support to be ‘kinked’, which results in a significant improvement of the kinematics of the crack tip element, as compared to the case where the support nodes are not enriched. The predicted stress field is not exact, but the approximation improves upon mesh refinement.
9.2.1.3. Chemical degradation

As mentioned in the introduction, degradation can be of physical, chemical or biological nature. The approach, proposed in this thesis, has been applied to describe physical degradation based on hygro-thermo-mechanical loading conditions. A logical extension would be to incorporate chemical damage processes as well. Both direct and indirect chemical degradation can be considered. The former consists in the chemical degeneration of the material matrix, e.g. dissolution of calcium carbonate by hydrogen chloride. The latter can occur when e.g. dissolved ions crystallize inside the porous material. The corresponding change in surface tension, the crystal pressure, might lead to the generation of stress levels exceeding the material strength and the initiation of (micro-)cracks. Indirect chemical degradation can be modelled using Biot-theory (e.g. Poupeleer 2007), direct chemical decay via distinguishing between initial porosity and chemical porosity (e.g. Bangert et al. 2003). The impact of fractures on the distribution of the concentration of the salt ions in the fluid and on the crystal pressure can be incorporated using the proposed discrete modelling strategy.

9.2.2. Level II

9.2.2.1. Incorporation of topology changes

Solving a problem that involves discrete crack propagation involves two separate stages. In a first stage, the boundary value problem is solved, and an updated displacement field is obtained. In the second stage, the admissibility of the stress state is checked, and cracks are initiated or propagated accordingly. These two steps are repeated until a stable crack pattern is found. This strategy is radically different from a continuum approach to failure, where the damage pattern and the displacement field are updated simultaneously. In this manner, a consistent tangent can be derived and a Newton-Raphson type solution strategy can be
employed, leading to high convergence rates. Designing a similar approach for discrete crack propagation could lead to a significant reduction of the associated computational cost. A possible strategy consists in considering the initiation of a crack as a change in topology. Branching of cracks, or crack bridging are other examples of topological changes. The current topology, in other words the current crack pattern, can be stored nodally by means of a level-set approach (Osher and Fedkiw 2003). At each node we therefore have unknowns related to the displacement field and to the topology. In analogy with a continuum approach to failure, a two-stage solution procedure can now be employed. First, a trial step is computed, based on the last converged variables and the current boundary conditions. In all subsequent iterations, the admissibility of the stress state is verified at each integration point, and, when needed, the topology variables are updated via return mapping. Since stress equilibrium and the evolution of the crack pattern are considered simultaneously, linearization can be applied, and high convergence rates can be obtained. Furthermore, by making use of the level set approach, the description of bridging or branching should not pose any difficulties. Remaining challenge is the elegant numerical integration of a discontinuous function.

### 9.2.2.2. Extension to multi-scale

In the proposed theory, the interface properties are derived from the properties of the materials sharing the interface (see equations (4.8) and (5.27)). This assumption is only valid for perfect contact between both. A more realistic approach takes into account the specific characteristics of the contact area. Consider e.g. moisture transport across a brick-mortar interface (see section 7.2.3). The difference in characteristic pore size between the two materials is reflected in the bulk properties of the materials. However, the mismatch between the pore systems at the interface is not accounted for in the proposed model, neither is the penetration of one material (the mortar) into the pore system of the other material (the brick). To incorporate these and other phenomena, the interface properties should be derived from a lower-scale interface model. This can be a finite element model, or an analytical model. The former can be embedded in a multi-scale framework by means of e.g. the coupled volume technique (Gitman 2006) or computational homogenization (Suquet 1985), while the latter relies on mathematical homogenization (e.g. Mori and Tanaka 1973).
A. Macroscopic balance equations

Specific balance laws for a component $\pi$ in a phase $\alpha$ are obtained by (i) transforming the microscopic properties $\psi^\pi$, $i^\pi$, $j^\pi$, $f^\pi$ and $g^\pi$ (see Table 3.1) into macroscopic properties by using the averaging operator (3.12) and the relations (3.28) and (3.29), and (ii) inserting them into the general macroscopic balance equation (3.26). The corresponding constraints are obtained from (3.27).

A.1. Mass balance

The macroscopic properties are given by:

$$\bar{\psi}^{a,\pi} = 1$$

$$\bar{f}^{a,\pi} = \frac{1}{\varepsilon^a \rho^{a,\pi}} \int dV \, \psi^a \bar{r}^a \gamma^a dV$$

$$\bar{g}^{a,\pi} = 0$$

and

$$\mathbf{N} \cdot \mathbf{i}^{a,\pi} = 0$$

$$g^{a\beta,\pi} = \frac{1}{\varepsilon^a \rho^{a,\pi}} \sum_{\beta=1}^{n} \int dA \, \bar{w}^{a\beta} (\mathbf{w}^{a\beta} - \mathbf{v}^\pi) \cdot \mathbf{n}^{a\beta} dA$$

The mass balance equation for a component $\pi$ in phase $\alpha$ becomes:

$$\frac{\partial (\varepsilon^a \rho^{a,\pi})}{\partial t} + \nabla \cdot (\varepsilon^a \rho^{a,\pi} \bar{\mathbf{v}}^{a,\pi}) = \varepsilon^a \rho^{a,\pi} (\bar{r}^{a,\pi} + r^{a\beta,\pi})$$

Subjected to the restrictions:

$$\sum_{\pi} \varepsilon^a \rho^{a,\pi} \bar{r}^{a,\pi} = 0 \quad \forall \alpha$$

and

$$\sum_{\alpha} \varepsilon^a \rho^{a,\pi} r^{a\beta,\pi} = 0 \quad \forall \pi$$
A.2. Momentum balance

The macroscopic properties are given by:

\[
\Psi^{\alpha,\pi} = \bar{v}^{\alpha,\pi}
\]

\[
\mathbf{f}^{\alpha,\pi} = \frac{1}{\varepsilon^{\alpha} \rho^{\alpha,\pi}} \int_{dV} \theta^{\pi} \left( \bar{r}^{\pi} v^{\pi} + \bar{b}^{\pi} \right) \gamma^{\alpha} dv
\]

\[
= \bar{r}^{\alpha,\pi} \bar{v}^{\alpha,\pi} + \bar{r}^{\pi} \left( \bar{v}^{\pi} - \bar{v}^{\alpha,\pi} \right) + \left( \bar{r}^{\pi} - \bar{r}^{\alpha,\pi} \right) \left( \bar{v}^{\pi} - \bar{v}^{\alpha,\pi} \right) + \bar{b}^{\pi}
\]

\[
\mathbf{f}^{\alpha,\pi} = 0
\]

\[
\mathbf{g}^{\alpha,\pi} = \bar{b}^{\alpha,\pi}
\]

and

\[
\mathbf{N} \cdot \mathbf{i}^{\alpha,\pi} = \frac{1}{dA} \int_{dA} n^{\alpha\beta} \left[ \sigma^{\pi} - \theta^{\pi} \left( v^{\pi} - \bar{v}^{\alpha,\pi} \right) \otimes \left( v^{\pi} - \bar{v}^{\alpha,\pi} \right) \right] \gamma^{\alpha} da
\]

\[
= \mathbf{N} \cdot \mathbf{\sigma}^{\alpha,\pi}
\]

\[
g^{\alpha\beta,\pi} = \frac{1}{\varepsilon^{\alpha} \rho^{\alpha,\pi}} \int_{dV} \sum_{\beta \neq \alpha} \left( \theta^{\pi} v^{\pi} \otimes (w^{\alpha\beta} - v^{\pi}) \right) \cdot n^{\alpha\beta} da
\]

\[
= \frac{1}{\varepsilon^{\alpha} \rho^{\alpha,\pi}} \sum_{\beta \neq \alpha} \int_{dA} \theta^{\pi} \bar{v}^{\alpha,\pi} \otimes (w^{\alpha\beta} - v^{\pi}) \cdot n^{\alpha\beta} da
\]

\[
+ \frac{1}{\varepsilon^{\alpha} \rho^{\alpha,\pi}} \sum_{\beta \neq \alpha} \int_{dA} \theta^{\pi} \left( v^{\pi} - \bar{v}^{\alpha,\pi} \right) \otimes (w^{\alpha\beta} - v^{\pi}) + \sigma^{\pi} \cdot n^{\alpha\beta} da
\]

\[
= r^{\alpha\beta,\pi} \bar{v}^{\alpha,\pi} + b^{\alpha\beta,\pi}
\]

The momentum balance equation for a component \( \pi \) in phase \( \alpha \) becomes:

\[
\frac{\partial \left( \varepsilon^{\alpha} \rho^{\alpha,\pi} \bar{v}^{\alpha,\pi} \right)}{\partial t} + \nabla \cdot \left( \varepsilon^{\alpha} \rho^{\alpha,\pi} \bar{v}^{\alpha,\pi} \otimes \bar{v}^{\alpha,\pi} \right) - \nabla \cdot \sigma^{\alpha,\pi}
\]

\[
= \varepsilon^{\alpha} \rho^{\alpha,\pi} \left( \bar{r}^{\alpha,\pi} \bar{v}^{\alpha,\pi} + \bar{b}^{\alpha,\pi} \right) + \varepsilon^{\alpha} \rho^{\alpha,\pi} \left( r^{\alpha\beta,\pi} \bar{v}^{\alpha,\pi} + b^{\alpha\beta,\pi} \right) + \varepsilon^{\alpha} \rho^{\alpha,\pi} \bar{b}^{\alpha,\pi}
\]

Subjected to the restrictions:

\[
\sum_{\pi} \varepsilon^{\alpha} \rho^{\alpha,\pi} \left( \bar{r}^{\alpha,\pi} \bar{v}^{\alpha,\pi} + \bar{b}^{\alpha,\pi} \right) = 0 \quad \forall \alpha
\]

(A.5)

and

\[
\sum_{\alpha} \varepsilon^{\alpha} \rho^{\alpha,\pi} \left( r^{\alpha\beta,\pi} \bar{v}^{\alpha,\pi} + b^{\alpha\beta,\pi} \right) = 0 \quad \forall \pi
\]

(A.6)
A.3. Energy balance

The macroscopic properties are given by:

\[
\begin{align*}
\bar{\psi}^{a,\pi} &= \frac{1}{\epsilon^{a,\pi}} \rho^{a,\pi} \int dV \bar{q}^{\pi} \left( U^{\pi} + \frac{1}{2} \mathbf{v}^{\pi} \cdot \mathbf{v}^{\pi} \right) \gamma^{a} dv \\
&= U^{\pi} + \frac{1}{2} \mathbf{v}^{\pi} \cdot \mathbf{v}^{\pi} + \mathbf{\bar{w}}^{a,\pi} \cdot \mathbf{\bar{v}}^{a,\pi} \\
&= \bar{U}^{\pi} + \frac{1}{2} \mathbf{\bar{v}}^{a,\pi} \cdot \mathbf{\bar{v}}^{a,\pi} \\
\bar{f}^{a,\pi} &= \frac{1}{\epsilon^{a,\pi}} \rho^{a,\pi} \int dV \bar{q}^{\pi} \left( \bar{U}^{\pi} + \frac{1}{2} \mathbf{\bar{v}}^{a,\pi} \cdot \mathbf{\bar{v}}^{a,\pi} + \frac{\mathbf{\bar{b}}^{a,\pi} \cdot \mathbf{\bar{v}}^{a,\pi} + h^{\pi}}{\rho^{a,\pi}} \right) \gamma^{a} dv \\
&= \frac{\mathbf{\bar{b}}^{a,\pi} \cdot \mathbf{\bar{v}}^{a,\pi} + h^{\pi}}{\rho^{a,\pi}} \\
\bar{g}^{a,\pi} &= \frac{1}{\epsilon^{a,\pi}} \rho^{a,\pi} \int dV \bar{q}^{\pi} \left( \mathbf{\bar{b}}^{a,\pi} \cdot \mathbf{\bar{v}}^{a,\pi} + h^{\pi} \right) \gamma^{a} dv \\
&= \frac{\mathbf{\bar{b}}^{a,\pi} \cdot \mathbf{\bar{v}}^{a,\pi} + h^{\pi}}{\rho^{a,\pi}} \\
\end{align*}
\]

and

\[
\mathbf{N} \cdot \mathbf{i}^{a,\pi} = \frac{1}{dA} \int_{dA} n^{a} \left[ \sigma^{a} \cdot \mathbf{v}^{\pi} - q^{\pi} \right] - \frac{1}{2} \left( \sigma^{a} \cdot \mathbf{v}^{\pi} - q^{\pi} \right) \left( \mathbf{\bar{v}}^{a,\pi} \cdot \mathbf{\bar{v}}^{a,\pi} \right) \gamma^{a} da \\
= \frac{1}{dA} \int_{dA} n^{a} \left[ \sigma^{a} - q^{\pi} \left( \mathbf{\bar{v}}^{a,\pi} \cdot \mathbf{\bar{v}}^{a,\pi} \right) \right] \gamma^{a} da \\
- \frac{1}{dA} \int_{dA} n^{a} \left[ \mathbf{q}^{\pi} - \sigma^{a} \left( \mathbf{\bar{v}}^{a,\pi} \cdot \mathbf{\bar{v}}^{a,\pi} \right) - q^{\pi} \left( \bar{U}^{\pi} - \bar{U}^{\pi} \right) \right] \gamma^{a} da \\
= \mathbf{N} \cdot \left( \sigma^{a} \cdot \mathbf{\bar{v}}^{a,\pi} - q^{a,\pi} \right)
\]
The energy balance equation for a component \( \pi \) in phase \( \alpha \) becomes:

\[
\frac{\partial}{\partial t} \left( \varepsilon^\alpha \rho^\alpha,\pi \left( \bar{U}^\pi + \frac{1}{2} \bar{V}^\alpha,\pi \cdot \bar{V}^\alpha,\pi \right) \right) + \nabla \cdot \left( \varepsilon^\alpha \rho^\alpha,\pi \bar{V}^\alpha,\pi \left( \bar{U}^\pi + \frac{1}{2} \bar{V}^\alpha,\pi \cdot \bar{V}^\alpha,\pi \right) \right) = -\nabla \cdot \left( \sigma^\alpha,\pi \bar{V}^\alpha,\pi - q^\alpha,\pi \right) - \varepsilon^\alpha \rho^\alpha,\pi \left( r^\alpha,\pi \left( \bar{U}^\pi + \frac{1}{2} \bar{V}^\alpha,\pi \cdot \bar{V}^\alpha,\pi \right) + \bar{b}^\alpha,\pi \cdot \bar{V}^\alpha,\pi + \bar{h}^\alpha,\pi \right)
\]

\[(A.7)\]

Subjected to the restrictions:

\[
\sum_{\pi} \varepsilon^\alpha \rho^\alpha,\pi \left( r^\alpha,\pi \left( \bar{U}^\pi + \frac{1}{2} \bar{V}^\alpha,\pi \cdot \bar{V}^\alpha,\pi \right) + \bar{b}^\alpha,\pi \cdot \bar{V}^\alpha,\pi + \bar{h}^\alpha,\pi \right) = 0 \quad \forall \alpha \quad (A.8)
\]

And

\[
\sum_{\pi} \varepsilon^\alpha \rho^\alpha,\pi \left( r^\alpha,\pi \left( \bar{U}^\pi + \frac{1}{2} \bar{V}^\alpha,\pi \cdot \bar{V}^\alpha,\pi \right) + \bar{b}^\alpha,\pi \cdot \bar{V}^\alpha,\pi + h^\alpha,\pi \right) = 0 \quad \forall \pi \quad (A.9)
\]
A.4. Entropy balance

The macroscopic properties are given by:

\[ \varphi_{a,\pi} = S_{-a,\pi} \]

\[ f_{a,\pi} = \frac{1}{\epsilon_{a} \rho_{a,\pi}} \int_{V} q^{\pi} \left( \tilde{p}^{\pi} S^{\pi} + \tilde{s}^{\pi} \right) \gamma^{a} dv \]

\[ = \tilde{r}^{\pi} S_{-a,\pi} + \tilde{f}_{a,\pi} \left( S^{\pi} - S_{-a,\pi} \right) + \left( \tilde{p}^{\pi} - \tilde{p}_{a,\pi} \right) \left( S^{\pi} - S_{-a,\pi} \right) + \tilde{s}^{\pi} \]

\[ f_{a,\pi} = \Phi_{a,\pi} \]

\[ g_{a,\pi} = S_{a,\pi} \]

and

\[ \mathbf{N} \cdot \mathbf{i}_{a,\pi} = \frac{1}{dA} \int_{dA} n^{ab} \left[ \phi^{\pi} - q^{\pi} \left( S^{\pi} - S_{-a,\pi} \right) \left( v^{\pi} - v_{\pi,\pi} \right) \right] \gamma^{a} da \]

\[ = \mathbf{N} \cdot \mathbf{\phi}_{a,\pi} \]

\[ g_{a,\pi} = \frac{1}{\epsilon_{a} \rho_{a,\pi}} \int_{V} \sum_{\beta=1}^{\pi} \int_{dA} \left( q^{\pi} S^{\pi} \left( w^{ab} - v^{\pi} \right) + \phi^{\pi} \right) \cdot n^{ab} da \]

\[ = \frac{1}{\epsilon_{a} \rho_{a,\pi}} \int_{V} \sum_{\beta=1}^{\pi} \int_{dA} \left( q^{\pi} S_{-a,\pi} \left( w^{ab} - v^{\pi} \right) + \phi^{\pi} \left( S^{\pi} - S_{-a,\pi} \right) \left( w^{ab} - v^{\pi} \right) + \phi^{\pi} \right) \cdot n^{ab} da \]

\[ = r^{ab,\pi} S_{-a,\pi} + s^{ab,\pi} \]

The entropy balance equation for a component \( \pi \) in phase \( \alpha \) becomes:

\[ \frac{\partial}{\partial t} \left( \epsilon_{a} \rho_{a,\pi} S_{-a,\pi} \right) + \nabla \cdot \left( \epsilon_{a} \rho_{a,\pi} \mathbf{v} S_{-a,\pi} \right) - \nabla \cdot \phi^{\pi,\pi} \]

\[ = \epsilon_{a} \rho_{a,\pi} \left( \tilde{r}_{a,\pi} S_{-a,\pi} + \tilde{s}_{a,\pi} \right) + \epsilon_{a} \rho_{a,\pi} \left( r^{ab,\pi} S_{-a,\pi} + s^{ab,\pi} \right) + \epsilon_{a} \rho_{a,\pi} \left( \Phi_{a,\pi} + S_{a,\pi} \right) \]

(A.10)

Subjected to the restrictions:

\[ \sum_{\pi} \epsilon_{a} \rho_{a,\pi} \left( \tilde{r}_{a,\pi} S_{-a,\pi} + \tilde{s}_{a,\pi} \right) = 0 \quad \forall \alpha \]

(A.11)

and

\[ \sum_{\alpha} \epsilon_{a} \rho_{a,\pi} \left( r^{ab,\pi} S_{-a,\pi} + s^{ab,\pi} \right) = 0 \quad \forall \pi \]

(A.12)
Specific mean macroscopic balance laws for a phase $\alpha$ are obtained by adding up the corresponding macroscopic balance law for all components $\pi$ in phase $\alpha$ (equation (3.26) combined with Table 3.2), hereby taking into account the physical constraints (3.27).

**B.1. Mass balance**

After rearranging, the mass balance equation for component $\pi$ in phase $\alpha$ reads:

$$\frac{\partial}{\partial t}(\varepsilon^\alpha \rho^\alpha c^\alpha,\pi) + \nabla \cdot \left( \varepsilon^\alpha \rho^\alpha c^\alpha,\pi \mathbf{v}^\alpha \right) + \nabla \cdot \mathbf{J}^\alpha,\pi = \varepsilon^\alpha \rho^\alpha c^\alpha,\pi \left( \overline{\mathbf{p}}^\alpha,\pi + r^{\alpha\beta,\pi} \right)$$

(B.13)

Subjected to the restrictions:

$$\sum_{\pi} \varepsilon^\alpha \rho^\alpha c^\alpha,\pi \overline{r}^\alpha,\pi = 0 \quad \forall \alpha$$

(B.14)

and

$$\sum_{\pi} \varepsilon^\alpha \rho^\alpha c^\alpha,\pi r^{\alpha\beta,\pi} = 0 \quad \forall \pi$$

(B.15)

Summation over all components $\pi$ and taking into account that molecular interactions do not give rise to a net increase of mass yields the averaged mass balance equation for phase $\alpha$:

$$\frac{\partial}{\partial t}(\varepsilon^\alpha \rho^\alpha) + \nabla \cdot (\varepsilon^\alpha \rho^\alpha \mathbf{v}^\alpha) = \varepsilon^\alpha \rho^\alpha r^{\alpha\beta}$$

(B.16)

with

$$r^{\alpha\beta} = \sum_{\pi} \varepsilon^\alpha \rho^\alpha r^{\alpha\beta,\pi}$$

(B.17)

and subjected to:

$$\sum_{\alpha} \varepsilon^\alpha \rho^\alpha r^{\alpha\beta} = 0$$

(B.18)

Using the definition of material time derivative (3.22), equation (B.16) becomes:

$$\frac{D^{\alpha}}{Dt} \varepsilon^\alpha \rho^\alpha + \varepsilon^\alpha \rho^\alpha \nabla \cdot \mathbf{v}^\alpha = \varepsilon^\alpha \rho^\alpha r^{\alpha\beta}$$

(B.19)
B.2. Momentum balance

After rearranging, the momentum balance equation for component \( \pi \) in phase \( \alpha \) reads:

\[
\frac{\partial}{\partial t}(\varepsilon^\alpha \rho^a c^{\alpha,\pi} v^a) + \nabla \cdot \left( \varepsilon^\alpha \rho^a c^{\alpha,\pi} v^a \otimes v^a \right) - \nabla \cdot \left( (\sigma^{\alpha,\pi} - \varepsilon^\alpha \rho^a c^{\alpha,\pi} v_d^{\alpha,\pi} \otimes v_d^{\alpha,\pi}) \right) \\
+ \frac{\partial}{\partial t}(\varepsilon^\alpha \rho^a c^{\alpha,\pi} v_d^{\alpha,\pi}) + \nabla \cdot (\varepsilon^\alpha \rho^a c^{\alpha,\pi} v_d^{\alpha,\pi} \otimes v^a) + \nabla \cdot (\varepsilon^\alpha \rho^a c^{\alpha,\pi} v_d^{\alpha,\pi} \otimes v_d^{\alpha,\pi})
\]

\[= \varepsilon^\alpha \rho^a c^{\alpha,\pi} \left( (\bar{r}^{\alpha,\pi} (v_d^{\alpha,\pi} + v^a) + \bar{b}^{\alpha,\pi}) + (r^{\alpha,\pi} (v_d^{\alpha,\pi} + v^a) + b^{\alpha,\pi}) \right) + \varepsilon^\alpha \rho^a c^{\alpha,\pi} \bar{b}^{\alpha,\pi}
\]

Subjected to the restrictions:

\[
\sum_\pi \varepsilon^\alpha \rho^a c^{\alpha,\pi} \left( (\bar{r}^{\alpha,\pi} (v_d^{\alpha,\pi} + v^a) + \bar{b}^{\alpha,\pi}) \right) = 0 \quad \forall \alpha
\]

and

\[
\sum_\alpha \varepsilon^\alpha \rho^a c^{\alpha,\pi} \left( (r^{\alpha,\pi} (v_d^{\alpha,\pi} + v^a) + b^{\alpha,\pi}) \right) = 0 \quad \forall \pi
\]

Summation over all components \( \pi \) and taking into account that molecular interactions do not give rise to a net increase of momentum yields the averaged momentum balance equation for phase \( \alpha \):

\[
\frac{\partial}{\partial t}(\varepsilon^\alpha \rho^a v^a) + \nabla \cdot (\varepsilon^\alpha \rho^a v^a \otimes v^a) - \nabla \cdot \sigma^a = \varepsilon^\alpha \rho^a (r^{\alpha,\pi} v^a + b^{\alpha,\pi}) + \varepsilon^\alpha \rho^a b^a
\]

with

\[
\sigma^a = \sum_\pi \left( \sigma^{\alpha,\pi} - \varepsilon^\alpha \rho^a c^{\alpha,\pi} v_d^{\alpha,\pi} \otimes v_d^{\alpha,\pi} \right)
\]

\[
b^a = \sum_\pi c^{\alpha,\pi} \bar{b}^{a,\pi}
\]

\[
b^{\alpha,\pi} = \sum_\pi c^{\alpha,\pi} \left( r^{\alpha,\pi} v_d^{\alpha,\pi} + b^{\alpha,\pi} \right)
\]

and subjected to:

\[
\sum_\alpha \varepsilon^\alpha \rho^a \left( r^{\alpha,\pi} v^a + b^{\alpha,\pi} \right) = 0
\]

Rearranging equation (B.23) using equation (B.16) leads to:

\[
\varepsilon^\alpha \rho^a \frac{D^a v^a}{Dt} - \nabla \cdot \sigma^a = \varepsilon^\alpha \rho^a \left( b^{\alpha,\pi} + b^a \right)
\]
B.3. Energy balance

After rearranging, the energy balance equation for component \( \pi \) in phase \( \alpha \) reads:

\[
\frac{\partial}{\partial t} \left( \varepsilon^a \rho^a c_{a,\pi} \left( U^\pi^a + \frac{1}{2} \mathbf{v}_d^{a,\pi} \cdot \mathbf{v}_d^{a,\pi} + \frac{1}{2} \mathbf{v}^a \cdot \mathbf{v}^a \right) \right) + \frac{\partial}{\partial t} \left( e^a \rho^a c_{a,\pi} \left( \frac{1}{2} \mathbf{v}_d^{a,\pi} \cdot \mathbf{v}_d^{a,\pi} \right) \right) + \nabla \cdot \left( e^a \rho^a c_{a,\pi} \mathbf{v}^a \left( \mathbf{U}^\pi^a + \frac{1}{2} \mathbf{v}_d^{a,\pi} \cdot \mathbf{v}_d^{a,\pi} + \frac{1}{2} \mathbf{v}^a \cdot \mathbf{v}^a \right) \right) \\
- \nabla \cdot \left( \left( \sigma^{a,\pi} - e^a \rho^a c_{a,\pi} \left( \mathbf{v}_d^{a,\pi} \otimes \mathbf{v}_d^{a,\pi} \right) \right) \mathbf{v}^a + \sigma^{a,\pi} \mathbf{v}_d^{a,\pi} \right) + \nabla \cdot \left( e^a \rho^a c_{a,\pi} \left( \frac{1}{2} \mathbf{v}_d^{a,\pi} \cdot \mathbf{v}_d^{a,\pi} \right) \mathbf{v}_d^{a,\pi} \right) \\
+ \nabla \cdot \left( e^a \rho^a c_{a,\pi} \mathbf{v}^a \left( \frac{1}{2} \mathbf{v}_d^{a,\pi} \cdot \mathbf{v}_d^{a,\pi} \right) \right) + \nabla \cdot \left( e^a \rho^a c_{a,\pi} \mathbf{v}^a \left( \frac{1}{2} \mathbf{v}_d^{a,\pi} \cdot \mathbf{v}_d^{a,\pi} \right) \right)
\]

Subjected to the restrictions:

\[
\sum_{\pi} e^a \rho^a c_{a,\pi} \left( \frac{\theta_{a,\pi}}{\theta_{a,\pi}} \left( U^\pi^a + \frac{1}{2} \left( \mathbf{v}_d^{a,\pi} + \mathbf{v}^a \right) \cdot \left( \mathbf{v}_d^{a,\pi} + \mathbf{v}^a \right) \right) \right) = 0 \quad \forall \alpha \tag{B.28}
\]

and

\[
\sum_{\alpha} e^a \rho^a c_{a,\pi} \left( \theta_{a,\pi} \left( U^\alpha^a + \frac{1}{2} \left( \mathbf{v}_d^{a,\pi} + \mathbf{v}^a \right) \cdot \left( \mathbf{v}_d^{a,\pi} + \mathbf{v}^a \right) \right) \right) = 0 \quad \forall \pi \tag{B.29}
\]

Summation over all components \( \pi \) and taking into account that molecular interactions do not give rise to a net increase of energy yields the averaged energy balance equation for phase \( \alpha \):

\[
\frac{\partial}{\partial t} \left( e^a \rho^a \left( U^a + \frac{1}{2} \mathbf{v}^a \cdot \mathbf{v}^a \right) \right) + \nabla \cdot \left( e^a \rho^a \left( U^a + \frac{1}{2} \mathbf{v}^a \cdot \mathbf{v}^a \right) \mathbf{v}^a \right) - \nabla \cdot \left( \sigma^a \cdot \mathbf{v}^a - \mathbf{q}^a \right) \\
= e^a \rho^a \left( \theta^a \left( U^a + \frac{1}{2} \mathbf{v}^a \cdot \mathbf{v}^a \right) \right) + \nabla \cdot \left( e^a \rho^a \left( \frac{1}{2} \mathbf{v}_d^{a,\pi} \cdot \mathbf{v}_d^{a,\pi} \right) \mathbf{v}_d^{a,\pi} \right) + \nabla \cdot \left( e^a \rho^a \mathbf{v}^a \left( \frac{1}{2} \mathbf{v}_d^{a,\pi} \cdot \mathbf{v}_d^{a,\pi} \right) \right) \\
+ e^a \rho^a \mathbf{b}^a \cdot \left( \mathbf{v}_d^{a,\pi} + \mathbf{v}^a \right) + \mathbf{h}^a 
\]

with

\[
U^\alpha = \sum_{\pi} c_{a,\pi} \left( U^\pi^a + \frac{1}{2} \mathbf{v}_d^{a,\pi} \cdot \mathbf{v}_d^{a,\pi} \right) \tag{B.31}
\]
Appendix B

\[ q^\alpha = \sum \left( \sigma^{\alpha,\pi} - \epsilon^\alpha \rho^\alpha \epsilon^{\alpha,\pi} \left( \overline{U}^{\alpha,\pi} + \frac{1}{2} \mathbf{v}_d^{\alpha,\pi} \cdot \mathbf{v}_d^{\alpha,\pi} \right) \right) \mathbf{v}_d^{\alpha,\pi} - q^{\alpha,\pi} \]

\[ h^{\alpha\beta} = \sum c^{\alpha,\pi} \left( v^{\alpha\beta,\pi} \left( \overline{U}^{\alpha,\pi} - \mathbf{U}^\alpha + \frac{1}{2} \mathbf{v}_d^{\alpha,\pi} \cdot \mathbf{v}_d^{\alpha,\pi} \right) + b^{\alpha\beta,\pi} \cdot \mathbf{v}_d^{\alpha,\pi} + h^{\alpha\beta,\pi} \right) \]

\[ h^\alpha = \sum c^{\alpha,\pi} \left( \overline{b}^{\alpha,\pi} \cdot \mathbf{v}_d^{\alpha,\pi} + \overline{h}^\alpha \right) \]

and subjected to:

\[ \sum \epsilon^\alpha \rho^\alpha \left( r^{\alpha\beta} \left( \mathbf{U}^\alpha + \frac{1}{2} \mathbf{v}^\alpha \cdot \mathbf{v}^\alpha \right) + b^{\alpha\beta} \cdot \mathbf{v}^\alpha + h^{\alpha\beta} \right) + \epsilon^\alpha \rho^\alpha \left( b^\alpha \cdot \mathbf{v}^\alpha + h^\alpha \right) = 0 \]  \hspace{1cm} (B.32)

Rearranging equation (B.30) using equations (B.16) and (B.23) leads to:

\[ \epsilon^\alpha \rho^\alpha \frac{D^\alpha U^\alpha}{Dt} - \mathbf{\sigma}^\alpha \cdot \nabla \cdot \mathbf{v}^\alpha + \nabla \cdot \mathbf{q}^\alpha = \epsilon^\alpha \rho^\alpha \left( h^{\alpha\beta} + h^\alpha \right) \]  \hspace{1cm} (B.33)
B.4. Entropy balance

After rearranging, the entropy balance equation for component $\pi$ in phase $\alpha$ reads:

$$
\frac{\partial (\epsilon^\alpha \rho^\alpha c^\alpha \pi S^{-\alpha,\pi})}{\partial t} + \nabla \cdot \left( \epsilon^\alpha \rho^\alpha c^\alpha \pi v^\alpha S^{-\alpha,\pi} \right) - \nabla \cdot \left( \Phi^\alpha - \epsilon^\alpha \rho^\alpha c^\alpha \pi v^\alpha S^{-\alpha,\pi} \right) = \epsilon^\alpha \rho^\alpha c^\alpha \pi \left( \bar{r}^{-\alpha,\pi} S^{-\alpha,\pi} + \bar{s}^{-\alpha,\pi} \right) + \epsilon^\alpha \rho^\alpha c^\alpha \pi \left( \bar{\Phi}^\alpha + \bar{s}^{-\alpha,\pi} \right) \tag{B.34}
$$

Subjected to the restrictions:

$$
\sum_\pi \epsilon^\alpha \rho^\alpha c^\alpha \pi \left( \bar{r}^{-\alpha,\pi} S^{-\alpha,\pi} + \bar{s}^{-\alpha,\pi} \right) = 0 \quad \forall \alpha \tag{B.35}
$$

and

$$
\sum_\alpha \epsilon^\alpha \rho^\alpha c^\alpha \pi \left( r^{\alpha\beta,\pi} S^{-\alpha,\pi} + s^{\alpha\beta,\pi} \right) = 0 \quad \forall \pi \tag{B.36}
$$

Summation over all components $\pi$ and taking into account that molecular interactions do not give rise to a net increase of entropy yields the averaged entropy balance equation for phase $\alpha$:

$$
\frac{\partial (\epsilon^\alpha \rho^\alpha S^\alpha)}{\partial t} + \nabla \cdot \left( \epsilon^\alpha \rho^\alpha v^\alpha S^\alpha \right) - \nabla \cdot \phi^\alpha = \epsilon^\alpha \rho^\alpha \left( r^{\alpha\beta} S^\alpha + s^{\alpha\beta} \right) + \epsilon^\alpha \rho^\alpha \left( \Phi^\alpha + s^\alpha \right) \tag{B.37}
$$

with

$$
S^\alpha = \sum_\pi c^{\alpha\pi} S^{-\alpha,\pi}
$$

$$
\phi^\alpha = \sum_\pi \left( \phi^{\alpha\pi} - \epsilon^\alpha \rho^\alpha c^{\alpha\pi} v^\alpha S^{-\alpha,\pi} \right)
$$

$$
s^{\alpha\beta} = \sum_\pi c^{\alpha\pi} \left( r^{\alpha\beta,\pi} \left( S^{-\alpha,\pi} - S^\alpha \right) + s^{\alpha\beta,\pi} \right) \tag{B.38}
$$

$$
\Phi^\alpha = \sum_\pi c^{\alpha\pi} \bar{\Phi}^{\alpha\pi}
$$

$$
s^\alpha = \sum_\pi c^{\alpha\pi} S^{\alpha\pi}
$$

and subjected to:

$$
\sum_\alpha \epsilon^\alpha \rho^\alpha \left( r^{\alpha\beta} S^\alpha + s^{\alpha\beta} \right) = 0 \tag{B.39}
$$

Rearranging equation (B.37) using equations (B.16) leads to:

$$
\epsilon^\alpha \rho^\alpha \frac{D^\alpha S^\alpha}{Dt} - \nabla \cdot \phi^\alpha = \epsilon^\alpha \rho^\alpha \left( s^{\alpha\beta} + s^\alpha \right) + \epsilon^\alpha \rho^\alpha \Phi^\alpha \tag{B.40}
$$
C. Nomenclature

In chapter 3 a modified nomenclature for porous media has been introduced. It is mainly based on the notation used in a series of papers from Hassanizadeh and Gray (1986). The modifications serve three objectives, namely (i) simplifying, (ii) improving consistency and (iii) complying with internationally established symbols. As an example, consider the supply of momentum. In the original nomenclature it was denoted with $g$ or $\hat{t}$, depending on whether the origin of the supply was external to the system or at molecular level, respectively. In the modified nomenclature, supply of momentum is always denoted with the letter $b$ (standard notation in the field of mechanics). All quantities from molecular origin are marked with a curved overbar. Supply of momentum with a molecular origin is therefore denoted by $b$. Similar notational changes have been made regarding the supply of energy ($h$ and $\tilde{h}$ instead of $h$ and $\dot{q}$) and the supply of entropy ($s$ and $\tilde{s}$ instead of $b$ and $\dot{\phi}$). Other notational changes are related to the consistent use of overbars. As mentioned earlier, quantities with a molecular origin receive a concave-up overbar. The mathematical volume averaging operator is denoted with a horizontal overbar, and ‘collected’-variables with a concave-down overbar. Collected variables are a group of variables with a clear physical meaning that have been assigned a specific symbol (see e.g. equation (3.31)). Newly defined variables do not get any overbars. This notation allows to carefully analyse how a variable is obtained. The most complicated example is probably $\overline{b^\pi_\alpha}$. This variable is obtained from the molecular supply of momentum $b$ to species $\pi$, which was then combined with some other variables in order to preserve its meaning (concave-down overbar) and finally volume averaged over the phase $\alpha$. The corresponding symbol in the work of Hassanizadeh and Gray is $\overline{\tilde{t}^\alpha}$. Here, confusion might arise regarding the interpretation of the double horizontal overbar. A detailed overview comparing the original and the modified notation is given below.
### C.1. Microscopic balance equations

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<td>external supply of energy to species $\pi$</td>
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<tr>
<td>$\dot{q}^\alpha$</td>
<td>$\tilde{h}^\pi$</td>
<td>molecular supply of energy to species $\pi$</td>
<td>J/(kg s)</td>
</tr>
<tr>
<td>$S^\alpha$</td>
<td>$S^\pi$</td>
<td>specific entropy of species $\pi$</td>
<td>J/(kg K)</td>
</tr>
<tr>
<td>$\phi^\alpha$</td>
<td>$\phi^\pi$</td>
<td>surface flux vector of entropy of species $\pi$</td>
<td>J/(K m² s)</td>
</tr>
<tr>
<td>$b^\alpha$</td>
<td>$s^\pi$</td>
<td>external supply of entropy to species $\pi$</td>
<td>J/(kg s K)</td>
</tr>
<tr>
<td>$\dot{\phi}^\alpha$</td>
<td>$\tilde{s}^\pi$</td>
<td>molecular supply of entropy to species $\pi$</td>
<td>J/(kg s K)</td>
</tr>
<tr>
<td>$\Gamma^\alpha$</td>
<td>$\Gamma^\pi$</td>
<td>internal supply of entropy to species $\pi$</td>
<td>J/(kg K s)</td>
</tr>
</tbody>
</table>
### C.2. Macroscopic balance equations

<table>
<thead>
<tr>
<th>H&amp;G</th>
<th>Chapter 3</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \tilde{\psi}^\alpha )</td>
<td>( \Phi^\alpha,\pi )</td>
<td>typical thermodynamic property of species ( \pi ) in phase ( \alpha ), macroscopic counterpart of ( \psi^\pi )</td>
<td>*</td>
</tr>
<tr>
<td>( \bar{I}^\alpha )</td>
<td>( i^\alpha,\pi )</td>
<td>surface flux vector of a mean macroscopic thermodynamic quantity ( \psi^\pi )</td>
<td>(* kg)/(m(^2) s)</td>
</tr>
<tr>
<td>-</td>
<td>( \bar{f}^\alpha )</td>
<td>macroscopic effect of molecular interaction inside a phase on ( \tilde{\psi}^\alpha,\pi )</td>
<td>*/s</td>
</tr>
<tr>
<td>-</td>
<td>( g^{\alpha\beta,\pi} )</td>
<td>macroscopic effect of phase interaction on ( \tilde{\psi}^\alpha,\pi )</td>
<td>*/s</td>
</tr>
<tr>
<td>-</td>
<td>( \tilde{F}^\alpha )</td>
<td>internal supply of a macroscopic thermodynamic quantity ( \tilde{\psi}^\alpha,\pi )</td>
<td>*/s</td>
</tr>
<tr>
<td>-</td>
<td>( \tilde{G}^\alpha )</td>
<td>external supply of a macroscopic thermodynamic quantity ( \tilde{\psi}^\alpha,\pi )</td>
<td>*/s</td>
</tr>
<tr>
<td>( \bar{r}^\alpha )</td>
<td>( \bar{r}^\alpha,\pi )</td>
<td>macroscopic supply of mass related to molecular interaction</td>
<td>s(^{-1})</td>
</tr>
<tr>
<td>( \bar{\rho}^\alpha )</td>
<td>( r^{\alpha\beta,\pi} )</td>
<td>macroscopic supply of mass related to phase interaction</td>
<td>s(^{-1})</td>
</tr>
<tr>
<td>( \hat{R}^\alpha )</td>
<td>( \bar{r}^\alpha,\pi + r^{\alpha\beta,\pi} )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \bar{V}^\alpha )</td>
<td>( \dot{\Phi}^\alpha,\pi )</td>
<td>average velocity of species ( \pi ) in phase ( \alpha )</td>
<td>m/s</td>
</tr>
<tr>
<td>( \bar{\sigma}^\alpha )</td>
<td>( \sigma^{\alpha,\pi} )</td>
<td>macroscopic partial stress tensor of species ( \pi ) in phase ( \alpha )</td>
<td>N/m(^2)</td>
</tr>
<tr>
<td>( \bar{g}^\alpha )</td>
<td>( \dot{\bar{b}}^{\alpha,\pi} )</td>
<td>resulting macroscopic external supply of momentum to species</td>
<td>m/s(^2)</td>
</tr>
<tr>
<td>( \bar{t}^\alpha )</td>
<td>( \dot{\bar{b}}^{\alpha,\pi} )</td>
<td>macroscopic supply of momentum related to molecular interaction</td>
<td>m/s(^2)</td>
</tr>
<tr>
<td>( \bar{m}^\alpha )</td>
<td>( b^{\alpha\beta,\pi} )</td>
<td>macroscopic supply of momentum related to phase interaction</td>
<td>m/s(^2)</td>
</tr>
<tr>
<td>( \hat{t}^\alpha )</td>
<td>( \dot{\bar{b}}^{\alpha,\pi} + b^{\alpha\beta,\pi} )</td>
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<td></td>
</tr>
<tr>
<td>( \bar{E}^\alpha )</td>
<td>( \bar{U}^\alpha )</td>
<td>macroscopic specific internal energy of species ( \pi ) in phase ( \alpha )</td>
<td>J/kg</td>
</tr>
<tr>
<td>( -\bar{q}^\alpha )</td>
<td>( q^{\alpha,\pi} )</td>
<td>macroscopic surface flux vector of heat of species ( \pi ) in phase ( \alpha )</td>
<td>J/(m(^3) s)</td>
</tr>
</tbody>
</table>
C.3. Mean macroscopic balance equations

<table>
<thead>
<tr>
<th>H&amp;G</th>
<th>Chapter 3</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\overline{\psi}^f)</td>
<td>(\psi^\alpha)</td>
<td>typical macroscopic thermodynamic property of phase (\alpha)</td>
<td>*</td>
</tr>
<tr>
<td>(\overline{I}^f)</td>
<td>(i^\alpha)</td>
<td>surface flux vector of a mean macroscopic thermodynamic quantity (\psi^\alpha)</td>
<td>(* kg)/m² s</td>
</tr>
<tr>
<td>(\overline{G}^f)</td>
<td>(g^\alpha)</td>
<td>external supply of a mean macroscopic thermodynamic quantity (\psi^\alpha)</td>
<td>*/s</td>
</tr>
<tr>
<td>-</td>
<td>(g^{\alpha\beta})</td>
<td>mean macroscopic effect of phase interaction on (\psi^\alpha)</td>
<td>*/s</td>
</tr>
<tr>
<td>-</td>
<td>(f^\alpha)</td>
<td>internal supply of a mean macroscopic thermodynamic quantity (\psi^\alpha)</td>
<td>*/s</td>
</tr>
<tr>
<td>(\hat{R}^f)</td>
<td>(r^{\alpha\beta})</td>
<td>mean macroscopic supply of mass related to phase interaction</td>
<td>s⁻¹</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
<td>Unit</td>
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<td>--------</td>
<td>-------------</td>
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<td></td>
</tr>
<tr>
<td>$\overline{v}^f$</td>
<td>average velocity of all species in phase $\alpha$</td>
<td>m/s</td>
<td></td>
</tr>
<tr>
<td>$\overline{\sigma}^f$</td>
<td>mean macroscopic partial stress tensor of phase $\alpha$</td>
<td>N/m²</td>
<td></td>
</tr>
<tr>
<td>$b^\alpha$</td>
<td>mean macroscopic external supply of momentum to phase $\alpha$</td>
<td>m/s²</td>
<td></td>
</tr>
<tr>
<td>$\hat{T}^f$</td>
<td>mean macroscopic supply of momentum related to phase interaction</td>
<td>m/s²</td>
<td></td>
</tr>
<tr>
<td>$\overline{E}^\alpha$</td>
<td>macroscopic specific internal energy of phase $\alpha$</td>
<td>J/kg</td>
<td></td>
</tr>
<tr>
<td>$-\overline{q}^f$</td>
<td>mean macroscopic surface flux vector of heat of phase $\alpha$</td>
<td>J/(m² s)</td>
<td></td>
</tr>
<tr>
<td>$h^\alpha$</td>
<td>mean macroscopic external supply of energy to phase $\alpha$</td>
<td>J/(kg s)</td>
<td></td>
</tr>
<tr>
<td>$\hat{Q}^f$</td>
<td>mean macroscopic supply of energy related to phase interaction</td>
<td>J/(kg s)</td>
<td></td>
</tr>
<tr>
<td>$\overline{S}^f$</td>
<td>mean macroscopic specific entropy of phase $\alpha$</td>
<td>J/(kg K)</td>
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</tr>
<tr>
<td>$-\overline{\phi}^f$</td>
<td>mean macroscopic surface flux vector of entropy of phase $\alpha$</td>
<td>J/(K m² s)</td>
<td></td>
</tr>
<tr>
<td>$s^\alpha$</td>
<td>mean macroscopic external supply of entropy to phase $\alpha$</td>
<td>J/(kg s K)</td>
<td></td>
</tr>
<tr>
<td>$\hat{\phi}^f$</td>
<td>mean macroscopic supply of entropy related to phase interaction</td>
<td>J/(kg s K)</td>
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</tr>
<tr>
<td>$\Gamma^f$</td>
<td>mean macroscopic internal supply of entropy to phase $\alpha$</td>
<td>J/(kg K s)</td>
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</tbody>
</table>
References


References


References


References


R. Woltman, Beiträge zur Hydraulischen Architektur, Dritter Band, Johann Christian Dietrich, Göttingen, 1794.


Continuous-discontinuous modelling of hygrothermal damage processes in porous media
by P. Moonen

Degradation of porous materials usually does not have a single identifiable cause, but results from the complex interaction between different types of degradation mechanisms. In the study at hand, both experimental and numerical methods are employed to gain insight herein.

A novel continuous-discontinuous concept to model physical degradation of porous materials is put forward. It enforces a gradual transition between the continuous state before fracture occurs and the discontinuous state afterwards. The formulation covers both diffuse damage processes in the bulk material as well as the initiation and propagation of discrete cracks. Furthermore it describes in a generic way the impact of the development of a fracture on the transport of mass and energy in the porous material.

Strategies to solve the resulting model equations in an optimal and accurate way are developed as well. Hereby, the advantages of a staggered solution scheme were exploited to respond dynamically to the specific needs of the different coupled systems of equations. The new algorithms allow minimizing the computational cost by optimizing both the temporal and the spatial resolution of the solution, without sacrificing accuracy.

Simulations based on the continuous-discontinuous framework were compared to experimental data and a good agreement was found. Therefore the proposed methodology can be applied with confidence to tackle a wide range of potential applications.
Continue-discontinue modellering van hygro-thermische schadeprocessen in poreuze media door P. Moonen

Degradatie van poreuze materialen heeft vaak niet één enkele oorzaak, maar is het gevolg van de complexe wisselwerking tussen verschillende schadeprocessen. In deze studie worden zowel numerieke als experimentele technieken aangewend om hierin meer inzicht te verwerven.

Een continue-discontinue raamwerk voor het modelleren van fysische degradatie van poreuze materialen wordt naar voren geschoven. Het verzekert de continue overgang tussen twee toestanden, namelijk de continue toestand vooraleer breuk optreedt, en de discontinue toestand achteraf. De formulering omvat zowel de initiële diffuse schadeprocessen verspreid over zones in het materiaal, als de initiatie en groei van discrete scheuren. Daarenboven beschrijft het model op generieke wijze de impact van de ontwikkeling van een scheur op het transport van massa en energie in het poreuze materiaal.

Strategieën om de resulterende modelvergelijkingen zo optimaal en accuraat mogelijk op te lossen werden eveneens ontwikkeld. Daarbij werden de mogelijkheden van een getrapt oplossingsschema optimaal benut om dynamisch in te spelen op de individuele vereisten van de verschillende gekoppelde stelsels vergelijkingen. De nieuwe algoritmes laten toe om de benodigde rekentijd te minimaliseren door de discretisatie van de oplossing in zowel tijd als ruimte te optimaliseren, zonder daarbij aan nauwkeurigheid op te offeren.

Simulaties, gebaseerd op het continue-discontinue raamwerk, werden vergeleken met experimentele data, en een goede overeenkomst werd teruggevonden. Daarom wordt het mogelijk de voorgestelde methodologie ook in de praktijk succesvol aan te wenden.
Propositions

- Experimental and numerical research are complementary. They are both valuable, but without one another incomplete.

- Creative solutions can only be found if you don’t confine yourself to state-of-the-art knowledge.

- The beginning of wisdom is the ability to call things by their right names.
  [Chinese proverb accredited to K'ung Fu Tzu (Confucius)]

- Developing a theory goes hand in hand with developing the vocabulary to discuss it.

- The way a question is asked limits and disposes the ways in which any answer to it - right or wrong- may be given.
  [Susanne K. Langer]

- Knowledge complicates matters.

These propositions are considered opposable and defendable and as such have been approved by the promoters J. Carmeliet and L.J. Sluys.
Stellingen

- Experimenteel en numeriek onderzoek zijn complementair. Ze zijn beide waardevol, maar op zichzelf onvolledig.

- Men kan niet tot creatieve oplossingen komen indien men zich blind staart op de gevestigde kennis.

- Wijsheid begint bij de eigenschap om zaken bij hun correcte naam te noemen. [Chinees gezegde toegekend aan K'ung Fu Tzu (Confucius)]

- Het ontwikkelen van een theorie gaat nauw samen met het ontwikkelen van de taal om ze te bespreken.

- De vraagstelling beperkt en bepaalt de manier waarop - al dan niet correct - geantwoord kan worden. [Susanne K. Langer]

- Kennis is ballast.

Deze stellingen worden opponeerbaar en verdedigbaar geacht en zijn als zodanig goedgekeurd door de promotoren J. Carmeliet en L. J. Sluys.
Curriculum Vitae

July 31, 1980  Born in Leuven, Belgium, as Peter Moonen
              St. Pieterscollege Leuven, Belgium
1998 - 2003  Advanced studies, Civil engineering - architecture, highest distinction
              K.U. Leuven, Belgium
2003 - 2005  research affiliate at K.U. Leuven, Belgium
2006 - 2008  research affiliate at T.U. Delft, The Netherlands
2009 - current  research affiliate at ETH Zürich, Switzerland