Midterm presentation of A Coupled Transport and Chemical Model for Durability Predictions of Cement Based Materials

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Outline

Objective and motivation

Objective

- Present the status of the work within, A Coupled Transport and Chemical Model for Durability Predictions of Cement Based Materials
- Present input/output parameters for reactive mass transport modeling in cement based materials

Motivation

- Improve the understanding of concrete degradation, from advanced reactive mass transport modeling
- Specify the contribution from reactive mass transport modeling to the service life prediction framework

Full project title: A Coupled Transport and Chemical Model for Durability Predictions of Cement Based Materials

Outline

Model overview

Reactive mass transport model in a service life prediction

Overview of the physical and chemical processes described in the coupled model

Mass Transport

Processes included in the mass transport model:

- Diffusion of ions
- Eletromigration
- Moisture transport
- Sorption hysteresis
- Diffusion of gasses

Chemical Equilibrium

Processes included in the chemical equilibrium module:

- Water reactions
- Pure phases
- Solid solution
- Surface complexation

Coupled model

PDE system solved with FEM

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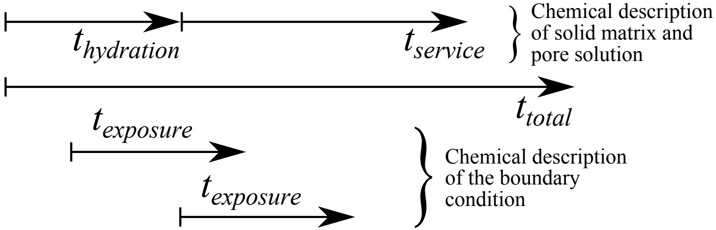
Model overview

Chemical equilibrium description in service life prediction

Different time aspects in chemical modeling

- Assumed time for hydration
- The time for the operating structure
- Changing boundary conditions initiated at different times



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Outline

Material model description

Parameters for the coupled system

Material parameters for mass transport calculation

- Tortuosity factor for porous material

Spatial and transient parameters for the finite element method

- Length of the system considered
- Spatial discritization
- Total time
- Time stepping length

Outline

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Material model description

Initial chemical values

Oxide composition for Reverse Bouge calculation of cement based material:

$$\text{Oxide[mass\%]} = \left[\mathrm{CaO;\ SiO_2;\ Al_2O_3;\ Fe_2O_3;\ SO_3;\ K_2O;\ Na_2O}\right]$$

Additional oxides may be added, e.g. MgO

Degree of hydration of clinker:

$$\alpha_i(t) = \left[\alpha_{\mathrm{C_3S}};\ \alpha_{\mathrm{C_2S}};\ \alpha_{\mathrm{C_3A}};\ \alpha_{\mathrm{C_2F}};\ \alpha_{\mathrm{C_4AF}};\ \alpha_{\mathrm{CS}};\ \alpha_{\mathrm{KS}};\ \alpha_{\mathrm{K_3NS_4}}\right]$$

Water to cement ratio:

$$w/c$$

Initial calculation determines, solid matrix composition, pore solution composition, saturation of porous system, porosity.

Outline

Boundary model description

Chemical description of the boundary environment

For water exposed boundary condition

- Ionic composition, e.g from Tronheim Fjord[1]

	Ca	Mg	Na	K	S	Cl	C
g/l	0.43	1.33	10.99	0.38	0.99	21.10	0.02

- Water temperature

For non-water exposed boundary or mixed, e.g splash zone

- Relative humidity, $RH(t)$
- Air temperature
- Direct tide variation measurements or averaged functions

[1] De Weerdt and Geiker 2012

Outline

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Physical property database

Physical properties for constituents

Database for physical constants of the constituents and phases:

- Ionic complexes
  - Diffusion coefficients
  - Electromigration coefficient
  - Valence
- Solid Species
  - Mole weight
  - Density
- Water and vapor diffusion coefficients

Fixed physical constants:

- Dielectricity for water
- Dielectricity in wacuum
- Farradays constant
- Density of water
- Vapour saturation density

Predefined chemical database models

State of the art

Chemical degradation of the solid matrix

	Reactions
Pure phases	
Portlandite	$Ca(OH)_2 + 2H^+ \longleftrightarrow Ca^{2+} + 2H_2O$
Silica(am)	$SiO_2 + 2H_2O \longleftrightarrow H_4SiO_4$
Magnesite	$MgCO_3 + H^+ \longleftrightarrow Mg^{2+} + HCO_3^-$
Brucite	$Mg(OH)_2 + 2H^+ \longleftrightarrow Mg^{2+} + H_2O$
OH-Hydrotalcite	$Mg_4Al_2(OH)_{14} : 3H_2O \longleftrightarrow$ $4Mg^{2+} + 2Al(OH)_4^- + 6OH^- + 3H_2O$
CO_3-Hydrotalcite	$Mg_4Al_2(OH)_{14}CO_3 : 2H_2O \longleftrightarrow$ $4Mg^{2+} + 2Al(OH)_4^- + CO_3^{2-} + 4OH^- + 2H_2O$
Syngenite	$K_2Ca(SO_4)_2H_2O \longleftrightarrow Ca^{2+} + 2K^+ + 2SO_4^{2-} + H_2O$
Gypsum	$CaSO_4 : 2H_2O \longleftrightarrow Ca^{2+} + SO_4^{2-} + 2H_2O$
Calcite	$CaCO_3 \longleftrightarrow CO_3^{2-} + Ca^{2+}$
Anhydrite	$CaSO_4 \longleftrightarrow Ca^{2+} + SO_4^{2-}$
Thaumasite	$(CaSiO_3)_2(CaSO_4)_2(CaCO_3)_2(H_2O)_{30} \longleftrightarrow$ $6Ca^{2+} + 2H_3SiO_4^- + 2CO_3^{2-} + 2SO_4^{2-} + 2OH^- + 26H_2O$
$C_4A\bar{C}H_{11}$	$(CaO)_3Fe_2O_3(CaCO_3) : 11H_2O \longleftrightarrow$ $4Ca^{2+} + 2Fe(OH)_4^- + CO_3^{2-} + 4OH^- + 5H_2O$
$C_4F\bar{C}H_{11}$	$(CaO)_3Al_2O_3(CaCO_3) : 11H_2O \longleftrightarrow$ $4Ca^{2+} + 2Al(OH)_4^- + CO_3^{2-} + 4OH^- + 5H_2O$
CAH_{10}	$CaAl_2(OH)_8 : 6H_2O \longleftrightarrow Ca^{2+} + 2Al(OH)_4^- + 6H_2O$
$Al(OH)_3(am)$	$Al(OH)_3 + OH^- \longleftrightarrow Al(OH)_4^-$
Gibsite	$Al(OH)_3 + 3H^+ \longleftrightarrow Al^{3+} + 3H_2O$
$Fe(OH)_3(am)$	$Fe(OH)_3(am) + 3H^+ \longleftrightarrow Fe^{3+} + 3H_2O$
$Fe(OH)_3(cr)$	$Al(OH)_3(cr) + 3H^+ \longleftrightarrow Fe^{3+} + 3H_2O$
Solid Solution	
	C-S-H (ss)
TobH	$(CaO)_{0.66}(SiO_2)(H_2O)_{1.5} + 1.32H^+ \longleftrightarrow$ $0.66Ca^{2+} + H_4SiO_4 + 0.16H_2O$
TobD	$(CaO)_{0.83}(SiO_2)_{0.66}(H_2O)_{1.83} + 1.66H^+ \longleftrightarrow$ $0.83Ca^{2+} + 0.66H_4SiO_4 + 1.34H_2O$
JenH	$(CaO)_{1.33}(SiO_2)(H_2O)_{2.16} + 2.66H^+ \longleftrightarrow$ $1.33Ca^{2+} + H_4SiO_4 + 1.49H_2O$
JenD	$(CaO)_{1.5}(SiO_2)_{0.66}(H_2O)_{2.5} + 3.00H^+ \longleftrightarrow$ $0.66Ca^{2+} + H_4SiO_4 + 0.16H_2O$

	Reactions
Solid Solution	
	AFm(1) (ss)
C_2AH_8	$Ca_2Al_2(OH)_{10} : 3H_2O \longleftrightarrow 2Ca^{2+} + 2Al(OH)_4^- + 2OH^- + 3H_2O$
C_2FH_8	$Ca_2Fe_2(OH)_{10} : 3H_2O \longleftrightarrow 2Ca^{2+} + 2Fe(OH)_4^- + 2OH^- + 3H_2O$
	AFm(2) (ss)
C_4AH_{13}	$Ca_4Al_2(OH)_{14} : 6H_2O \longleftrightarrow 4Ca^{2+} + 2Al(OH)_4^- + 6OH^- + 6H_2O$
C_4FH_{13}	$Ca_4Fe_2(OH)_{14} : 6H_2O \longleftrightarrow 4Ca^{2+} + 2Fe(OH)_4^- + 6OH^- + 6H_2O$
	AFm(3) (ss)
C_2ASH_8	$(CaO)_2Al_2O_3SiO_2 : 8H_2O \longleftrightarrow 2Ca^{2+} + 2Al(OH)_4^- + H_3SiO_4^- + OH^- + 2H_2O$
C_2FSH_8	$(CaO)_2Fe_2O_3SiO_2 : 8H_2O \longleftrightarrow 2Ca^{2+} + 2Fe(OH)_4^- + H_3SiO_4^- + OH^- + 2H_2O$
	AFm(4) (ss)
$C_4A\bar{S}H_{12}$	$(CaO)_3Al_2O_3(CaSO_4) : 12H_2O \longleftrightarrow 4Ca^{2+} + 2Al(OH)_4^- + SO_4^{2-} + 4OH^- + 6H_2O$
$C_4F\bar{S}H_{12}$	$(CaO)_3Fe_2O_3(CaSO_4) : 12H_2O \longleftrightarrow 4Ca^{2+} + 2Fe(OH)_4^- + SO_4^{2-} + 4OH^- + 6H_2O$
	Hydrogarnets (ss)
C_3AH_6	$(CaO)_3Al_2O_3 : 6H_2O \longleftrightarrow 3Ca^{2+} + 2Al(OH)_4^- + 4OH^-$
C_3FH_6	$(CaO)_3Fe_2O_3 : 6H_2O \longleftrightarrow 3Ca^{2+} + 2Fe(OH)_4^- + 4OH^-$
	AFm(5) (ss)
$C_4A\bar{C}_{0.5}H_{12}$	$(CaO)_3Al_2O_3(Ca(OH)_2)_{0.5}(CaCO_3)_{0.5} : 11.5H_2O \longleftrightarrow 4Ca^{2+} + 2Al(OH)_4^- + 0.5CO_3^{2-}$ $+ 5OH^- + 5.5H_2O$
$C_4A\bar{F}_{0.5}H_{12}$	$(CaO)_3Fe_2O_3(Ca(OH)_2)_{0.5}(CaCO_3)_{0.5} : 11.5H_2O \longleftrightarrow 4Ca^{2+} + 2Fe(OH)_4^- + 0.5CO_3^{2-}$ $+ 5OH^- + 5.5H_2O$
	AFt(1) (ss)
Al-Ettringite	$Ca_6Al_2(SO_4)_3(OH)_{12} : 26H_2O \longleftrightarrow 6Ca^{2+} + 2Al(OH)_4^- + 3SO_4^{2-} + 4OH^- + 26H_2O$
Fe-Ettringite	$Ca_6Fe_2(SO_4)_3(OH)_{12} : 26H_2O \longleftrightarrow 6Ca^{2+} + 2Fe(OH)_4^- + 3SO_4^{2-} + 4OH^- + 26H_2O$
	AFt(1) (ss)
Al-Ettringite	$Ca_6Al_2(SO_4)_3(OH)_{12} : 26H_2O \longleftrightarrow 6Ca^{2+} + 2Al(OH)_4^- + 3SO_4^{2-} + 4OH^- + 26H_2O$
Tricarboaluminate	$Ca_6Al_2(CO_3)_3(OH)_{12} : 26H_2O \longleftrightarrow 6Ca^{2+} + 2Al(OH)_4^- + 3CO_3^{2-} + 4OH^- + 26H_2O$

Lothenbach, CemData07

Predefined chemical database models

State of the art

Chloride binding models

	Reactions
Pure phases:	
Kuzel's salt	$Ca_4Al_2(SO_4)_{0.5}Cl(OH)_{12}:6H_2O \longleftrightarrow 4Ca^{2+} + 2Al(OH)_4^- + 4OH^- + 0.5SO_4{}^{2-} + 6H_2O$
Solid solution:	
	C_4AH_{13} + Friedel's salt (ss)
Friedel's salt	$Ca_4Al_2Cl_2(OH)_{12}:4H_2O \longleftrightarrow 4Ca^{2+} + 2Al(OH)_4^- + 4OH^- + 2Cl^- + 4H_2O$
C_4AH_{13}	$Ca_4Al_2(OH)_{14}:6H_2O \longleftrightarrow 4Ca^{2+} + 2Al(OH)_4^- + 6OH^- + 6H_2O$
	$C_4A\bar{C}H_{11}$ + Friedel's salt (ss)
Friedel's salt	$Ca_4Al_2Cl_2(OH)_{12}:4H_2O \longleftrightarrow 4Ca^{2+} + 2Al(OH)_4^- + 4OH^- + 2Cl^- + 4H_2O$
$C_4A\bar{C}H_{11}$	$(CaO)_3Al_2O_3(CaCO_3):11H_2O \longleftrightarrow 4Ca^{2+} + 2Al(OH)_4^- + CO_3^{2-} + 4OH^- + 5H_2O$

Lothenbach + Balonis

Predefined chemical database models

State of the art

Input for surface reaction sites

	Reactions
Pure phases	
C-S-H	$Ca_2Si_2O_5(OH)_2 + H^+ + H_2O \longleftrightarrow 6\,Ca^{2+} + 2\,H_4SiO_4$
Surface reactions	Silanol sites
SurfChar_1	$\equiv SiOH \longleftrightarrow \equiv SiO^- + H^+$
SurfChar_2	$\equiv SiOH + Ca^{2+} \longleftrightarrow \equiv SiOCa^+ + H^+$
SurfBrid_1	$\equiv SiOH + \equiv SiOH + Ca^{2+} \longleftrightarrow \equiv SiOCaOSi\equiv + 2\,H^+$
SurfBrid_2	$\equiv SiOH + Ca^{2+} + H_2O \longleftrightarrow \equiv SiOCaOH\equiv + 2\,H^+$
SurfBrid_3	$\equiv SiOH + \equiv SiOH + H_4SiO_4 \longleftrightarrow \equiv SiOSi(OH)_4OSi\equiv + 2\,H_2O$

Nonat + Hosokawa

Electrical double layer, thickness of double layer.

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Model output and links

Output values from model and links to other projects

Model output:

- Pore solution
  - Ionic concentration
  - PH
  - Ionic strength
- Solid phase composition
- Porosity
- Water/vapor saturation

Links to present projects

- Any porous media diffusion model
  - Physical and chemical input for this type of model
- Corrosion model
  - Initiation modeling
  - Corrosion cell modeling

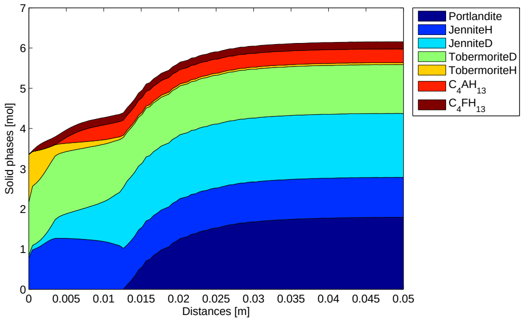
Links to future projects

- Atomistic modeling
- Crack modeling

Simulation results

Reactive mass transport model in a service life prediction

Example of model output, showing phase changes with pure water boundary conditions



Show phase development

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Conclusion

Conclusion of the midterm status of the project

- State of the art modules within, for the coupled model:
  - Continuum mechanical transport theories
  - Chemical equilibrium modeling
- Reactive transport modeling is applicable in the framework of service life prediction
  - Theoretical and numerical implementation
- Open and general format,
  - Use at different purposes and cross disciplinary, e.g. within research topics or consulting
  - easy to adapt future findings within, material constants, chemical reactions, etc.