STADIUM model

Technical basis

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The model is divided in 2 main modules:

- The transport module makes the species move during one time step,
- The chemistry module simulates the reactions between species in the pores and the hydrated paste.
Input parameters:
- Material properties
- Environment
- Geometry

- Input files: .txt, .xml
- Batch mode
- Interactive mode: Windows shell

Transport Module

Chemistry Module

End of calculation?

No

Yes

Model output

Next time step

- C/C++
- Multi-processor calculations
- Visual Studio

- Text files
Transport Module

Input parameters:
- Material properties
- Environment
- Geometry

- Coupled species diffusion
- Moisture/Temperature coupling
- Transport of main species
- Feedback effect
- Time-dependent transport properties (hydration)
- Time-dependent B.C.

Next time step

Transport Module

Chemistry Module

End of calculation?

Yes

Model output
\[ \mathbf{v}_l = -\frac{k_l}{\mu} \text{grad}(p_l) \]

\[ \mathbf{j}_v = -\theta_g \tau_g D_v^0 \text{grad}(\rho_v) \]

Averaging over REV

Assumption: diffusion-only movement of vapor

\[ \frac{\partial w}{\partial H} \frac{\partial H}{\partial t} + \frac{\partial w}{\partial T} \frac{\partial T}{\partial t} - \text{div}(D_{mH} \text{grad}(H) + D_{mT} \text{grad}(T)) = 0 \]
\[
S = \frac{1}{\beta (H^\delta - 1) + 1}
\]

\[
D_{mH} = \frac{k_s k_r^l \rho l R T}{\mu M_w} \frac{1}{H} + \frac{D_v^0 \kappa_s \tau_r^g M_w p_v^s}{\rho l R} \frac{(\phi - w)}{T}
\]

\[
k_r^l = \frac{1}{1 - a + a S^b}
\]
0.65 w/c opc concrete

Drying

Absorption

50-mm, 50% RH series
50-mm, 75% RH series
10-mm, 50% RH series
10-mm, 75% RH series
0.40 w/c opc concrete + dampproofer
The transport of ions in **STADIUM** is modeled using the extended Nernst-Planck equation with an advection and temperature term:

**Mass conservation equation:**

\[
\frac{\partial (wc_i)}{\partial t} + \text{div}(j_i) = 0
\]

**Flux of ions:**

\[
j_i = -D_i w \text{grad}(c_i) - \frac{D_i z_i F}{RT} wc_i \text{grad}(\psi) - D_i wc_i \text{grad}(\ln \gamma_i) - \frac{D_i c_i \ln(\gamma_i c_i)}{T} w \text{grad}(T) - c_i \nu_i
\]

**Variables:**

- Concentrations \(c_i\)
- Diffusion potential \(\psi\)
- Relative humidity \(H\)
- Temperature \(T\)
To complete the system of equations, the following relationships are considered:

\[ \text{Poisson: } \quad \text{div}(\tau w \text{ grad } \psi) + \frac{F}{\epsilon} w \left( \sum_{i=1}^{N} z_i c_i \right) = 0 \]

\[ \text{Heat conduction: } \quad \rho C_p \frac{\partial T}{\partial t} - \text{div}(\kappa \text{ grad}(T)) = 0 \]

The system of equations is solved using the finite element method:

- \text{N+3 unknowns: } N \times c_i + H + \psi + T
- \text{N+3 equations: } N \text{ conservation} + \text{Poisson} + \text{moisture} + \text{Heat}
Diffusion coefficient: \[ D_i = \tau_s \tau_r^r D_i^o \]

- \( \tau_s \): intrinsic tortuosity
- \( \tau_r^r \): relative tortuosity
- \( D_i^o \): self-diffusion coefficient = \( f(T) \)
Effect of saturation on tortuosity:

\[ \tau_l = \frac{D(s)}{D_{sat}} = \frac{\sigma(s)}{\sigma_{sat}} \]

Source: Larsen et al., RILEM pro-051 2006
Effect of hydration on tortuosity:

\[ H(t) = \frac{a}{1 + (a - 1)e^{-\alpha(t-t_0)}} \]
Effect of dissolution/precipitation on tortuosity:

\[ H(\phi) = e^{\frac{4.3}{Vp}(\phi - \phi_0)} \]
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Numerical methods:

• All equations are coupled to each other (e.g. temperature influences moisture and diffusion),
• The equations are solved using FEM,
• 1D and 2D versions are available.
• Euler implicit time-stepping.
• Adaptative time-stepping.
Chemistry Module

Input parameters:
- Material properties
- Environment
- Geometry

Transport Module

Chemistry Module

End of calculation?
- Local Equilibrium Assumption
- Dissolution/precipitation
- Solid solutions
- Chemical/Pitzer database in separate text file
- Effect of temperature on chemistry

Model output
The chemical reactions are modeled according to dissolution/precipitation equilibrium relationships:

- **Dissolution/precipitation:**

  \[ K_m = \prod_{i=1}^{N} c_i^{\nu_{mi}} \gamma_j^{\nu_{mi}} \quad \text{with} \quad m = 1, \ldots, M \]

In the case of chlorides, the formation of Friedel’s salts is modeled according to an ionic exchange relationship:

- **Friedel’s salts formation:**

  \[ \left[ \frac{\text{AF}^+}{m} - \text{SO}_4^{2-} \right] + 2\text{Cl}^- \rightleftharpoons \left[ \frac{\text{AF}^+}{m} - 2\text{Cl}^- \right] + \text{SO}_4^{2-} \]

- **Relationship:**

  \[ K_{\text{Cl}/\text{SO}_4} = \frac{\{\text{Cl}\}^2 [\text{AFmSO}_4]}{\{\text{SO}_4\} [\text{AFmCl}]} \]
C-S-H model:

- Berner’s approach: C-S-H $\rightarrow$ $\text{CaH}_2\text{SiO}_4 + 1.65 \text{Ca(OH)}_2$
- $K_{ps} = f(C/S)$ for $\text{CaH}_2\text{SiO}_4$ and $\text{Ca(OH)}_2$
**INPUT TO CHEMISTRY MODULE**

- Mix composition
- Cement chemistry
- SCMs chemistry
- Chemistry database

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**CALCULATED PARAMETERS**

- Hydrated cement paste composition
- Pore solution composition
At the end of calculations, the model provides the following information:

- Space and time distribution of species concentrations,
- Space and time distribution of mineral contents,
- Space and time distribution of temperature and humidity,
- Analysis of the main variables to get: total calcium, sulfur and chloride content.
- Space and time distribution of pH.
- Chloride content at specific depth to estimate the time to initiate corrosion for different rebar depths.
Sulfate exposure

- Paste sample
- Thickness: 25 mm
- Sealed except on top
- Hydration: 28 days (fog room)

- Volume of solution: 30 L
- Regularly renewed to maintain stable conditions
- Exposure duration: 12 months
- Solutions: 50 mM Na$_2$SO$_4$
Sulfate exposure

Microprobe sulfur profile
Sulfate exposure

Microprobe calcium profile
Chloride profiles: wetting/drying cycles vs. immersed

- Solution: 0.5 M NaCl
- Cycles: 3 days in solution, 4 days drying at 50% RH
- Duration: 2.5 years
C3S paste exposed to pure water

25 L Tank

25 mm

↑ 1.2 mm

CBP/SIMCO  Hanford Training, August 2014  26
C3S paste exposed to pure water

Sound C₃S paste

Leached C₃S paste
C3S paste exposed to pure water – Ca profiles

- **2 days**
  - Simulation
  - Microprobe

- **4 days**
  - Simulation
  - Microprobe

- **7 days**
  - Simulation
  - Microprobe
C3S paste exposed to pure water – Si profiles

2 days

4 days

7 days
Questions?