VCCTL Software: Overview and Opportunities

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Particle Size Distribution

Methods developed by Dale Bentz & Paul Stutzman (NIST)

...X-ray element maps ...

... segmented image ...

... measure autocorrelation functions on majority phases
How VCCTL Simulates Hydration

- Microstructure is mapped on a 3-D digital image.
- Each voxel represents a discrete volume of material.
- Voxels act as independent agents that follow rules for
Microstructure is mapped on a 3-D digital image.

Each voxel represents a discrete volume of material.

Voxels act as independent agents that follow rules for

Dissolve
How VCCTL Simulates Hydration

- Microstructure is mapped on a 3-D digital image.
- Each voxel represents a discrete volume of material.
- Voxels act as independent agents that follow rules for:
  - Dissolve
  - Diffuse
  - React
VCCTL Software Interface

Material Inventory

- Edit or create a cement
  - Name: cement140
  - Upload data from a ZIP file for the cement:
  - Cement data

- Mass fractions of sulfates
  - Dihydrate: 0.0039
  - Hemihydrate: 0.022
  - Anhydrite: 0.016

- Edit or create a fly ash
VCCTL Software Interface

Step 1: Prepare mix

Binder
- Choose a cement: cement140
- Modify phase distribution in the clinker
- Modify calcium sulfate amounts in the cement
- Add SCM to the binder

Curing Conditions

Thermal
- Conditions:
  - isothermal
  - semi-adiabatic
  - adiabatic
- Initial temperature: 25.0 °C
- Aggregate

Mix

<table>
<thead>
<tr>
<th>Mass fraction</th>
<th>Volume fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Binder</td>
<td>0.1724 0.1307</td>
</tr>
<tr>
<td>Water</td>
<td>0.0776 0.1897</td>
</tr>
<tr>
<td>Water/Binder ratio</td>
<td>0.45 0.2658</td>
</tr>
<tr>
<td>Add Coarse Aggregate</td>
<td>0.30 0.2658</td>
</tr>
<tr>
<td>Change properties</td>
<td></td>
</tr>
<tr>
<td>Add Fine Aggregate</td>
<td>0.45 0.4138</td>
</tr>
<tr>
<td>Change properties</td>
<td></td>
</tr>
<tr>
<td>Air</td>
<td>0.04</td>
</tr>
</tbody>
</table>

Aging

- Hydrate for 28.0 days
- Or stop at degree of hydration: 1.0
- Use time conversion
  - Time conversion factor: 3.5E-4 h/cycle²
- Use a calorimetry file
- Use a chemical shrinkage file

Saturation conditions

- saturated
- sealed

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Exploring influence of curing conditions and test conditions on a durability design parameter

Linking Microstructure to Properties

Microstructure ➔ Elastic Moduli (FE) ➔ D-EMT ➔ 28 d Strength
Some Industry Success Stories

- German cement manufacturer used VCCTL to diagnose field problems with excessively high 28 d compressive strength and explore ways to correct it by adjusting clinker chemistry (alite/belite ratio). **3 week study saved ≈ $1M**

- German cement manufacturer used VCCTL to determine the amount of additional clinker grinding required to achieve the same strength development in a cement with lower lime saturation factor (**more economical production**)

- International cement manufacturer reported a cost savings by using VCCTL of ≈ **$750K over several weeks**. Details of the project were not provided to NIST.

- SCG in Thailand (**details coming up**)

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It is fundamentally important to predict the processing time under different conditions of external temperature and mixture proportions.

Doing this experimentally is time consuming and expensive.
Temperature Effects on Fresh Concrete

Role of T, w/c, and cement:aggregate ratio
Temperature Effects on Fresh Concrete

Setting modeled by fraction of interconnected solids in the paste microstructure
Temperature Effects on Fresh Concrete

VCCTL predictions of minimum processing time for two concretes as a function of temperature.
Temperature Effects on Fresh Concrete

Experimental validation of VCCTL predictions of minimum processing time for two concretes
Temperature Effects on Fresh Concrete

Temperature not generally constant in the field:

- Ambient temperature changes during the day
- Heat of hydration raises material temperature

VCCTL can handle these temperature effects, but requires estimates of the heat transfer coefficient between the concrete and atmosphere.

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