Manual for CemPy, ver. 0.15

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Any suggestions or help to port the software to other platforms are welcomed and appreciated.

1 Introduction

The CEMHYD3D hydration program [Bentz, 2005] inspired me to write more user-friendly version for civil engineers. The majority of the C/C++ code was created at NIST, USA by D.P. Bentz and E.J. Garboczi, who are greatly acknowledged. The hydration routines are extended further for the prediction of elastic properties at the level of cement paste, mortar and concrete. Graphical user interface (GUI) should be intuitive enough to use the program. The code is tested on linux / Ubuntu 8.04 - Ubuntu 10.04, although python portability should guarantee compatibility to other platforms as well. The GUI on Windows systems was not tested and is subject of further possible development.

Only Portland systems are treated correctly in this code. Although some extensions to silica fume and slag exists, they are still under development at NIST. If you want to simulate blended cements, it might be worthy to use the latest CEMHYD3D version directly without the GUI support [Bentz, 2005].

2 Installation

The code is now optimized for Ubuntu 18.04 and Python 3.6. The python module Tkinter is responsible for GUI. Modified CEMHYD3D code v 3.0 in C/C++ [Bentz, 2005] is wrapped and exposed as a module to the python. Other libraries and python versions might work but have not been tested throughfully. The following libraries and python modules, found in the standard Ubuntu (or debian) packages, are required

- python3.6
- libboost1.65
- python3 tk
- python3 Pmw
- python3 numeric
- python3 numeric-ext
- python3 matplotlib

3 Compiling

Download the zip archive and unzip to a directory. Maintain the structure of associated *math*, *homog* and *tinyxml* directories. If necessary, modify paths to them in the beginning of the Makefile. To compile and link, type

```
>> make
```

which creates *.o files, links them and creates two shared libraries *.so. To run the GUI, use a command

```
>> python cem.py
```

Optionally, it is possible to clean out the object files

```
>> make clean
```

4 GUI description

Fig. 1 shows a typical GUI layout of the CemPy interface. A short description of input fields follows. The RVE size could range from 10 μm, but more appropriate is the size of 50 μm, for very precise calculations even 100 μm. Since cellular automata cycles mean no meaningful scale of hydration time, time-mapping equation is introduced in the form

$$\text{time} = t_0 + \beta \, \text{cycle}^2, \tag{1}$$

where $t_0 \in \langle 0, 3 \rangle$ h and $\beta \in \langle 4.0, 7.8 \rangle$ h/cycle^2 for ordinary Portland cements [Šmilauer and Krejčí, 2009]. Blaine fineness roughly corresponds to cement grade[1]

Cement grade	Blaine fineness [m^2/kg]
CEM I 32.5	240 – 400
CEM I 42.5	280 – 450
CEM I 52.5	400 – 600

The particle size distribution of cement grains is approximated by Rosin-Rammler cumulative distribution $G(d)$, fitted to a NIST reference database for Dyckerhoff cements, see [Bentz, 2005], with the results

[1] Lecture notes, R. Dillmann: Zement, Universität Duisburg - Essen

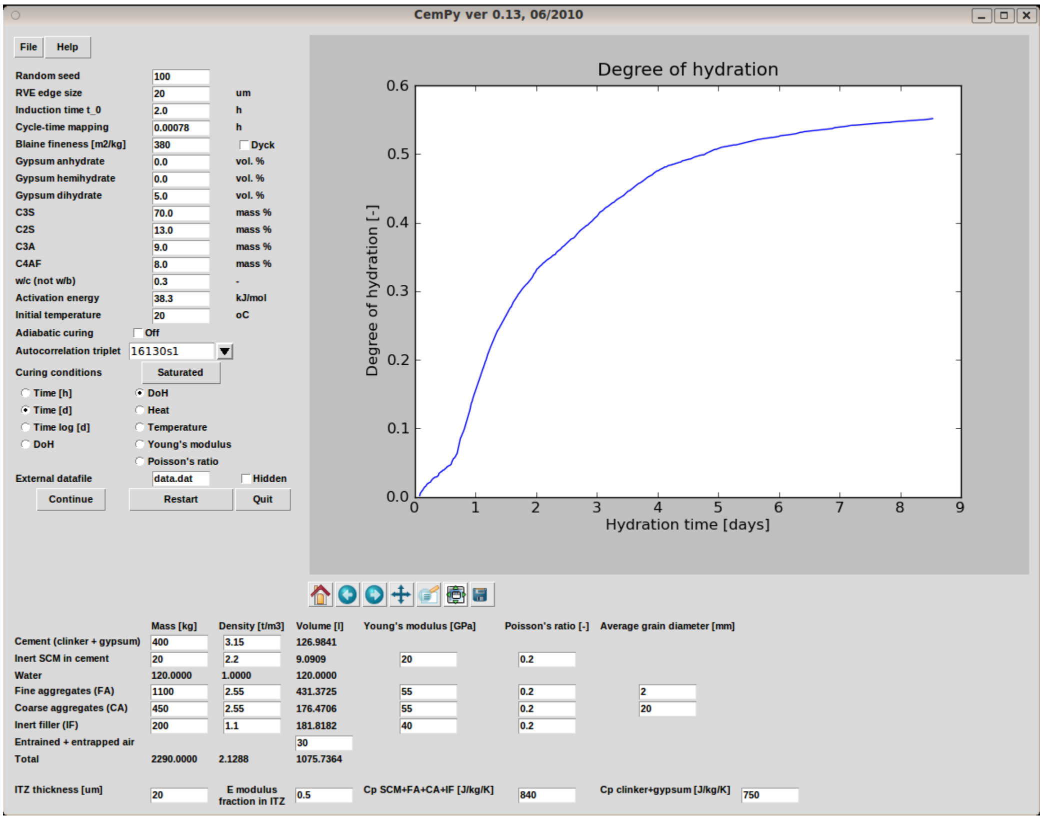

Figure 1: Typical GUI of CemPy

$$G(d) = 1 - e^{-bd^n}, \quad \lim_{d\to\infty} G(d) = 1, \tag{2}$$
$$b = 7.54 \cdot 10^{-4}\,\text{fineness} - 0.143, \tag{3}$$
$$n = -8.333 \cdot 10^{-4}\,\text{fineness} + 1.1175, \tag{4}$$

where d [μm] is the particle diameter and Blaine fineness is expressed in [m^2/kg]. The alternative Rosin-Rammler distribution was proposed in [van Breugel, 1997] in the form

$$G(d) = 1 - e^{-bd^n}, \quad \lim_{d\to\infty} G(d) = 1, \tag{5}$$
$$b = 1.74 \cdot 10^{-4}\,\text{fineness} - 0.029, \tag{6}$$
$$n = -3.1 \cdot 10^{-4}\,\text{fineness} + 1.2. \tag{7}$$

Two options (Dyck, Breu) are given in GUI. Fig. 2 gives the idea of two particle size distributions.

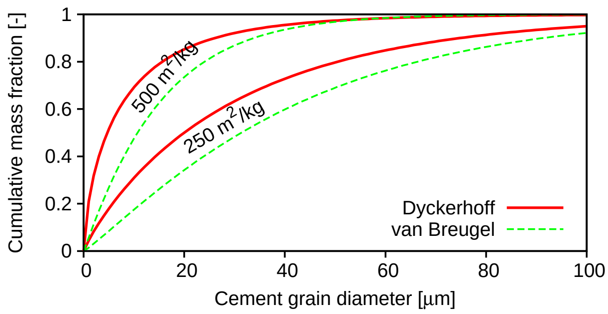

Figure 2: Particle size distribution according to NIST cement database for Dyckerhoff cements and van Breugel [van Breugel, 1997]

Gypsum dihydrate represents typically 5.0 vol. % of cement. Activation energy corresponds roughly to 40 kJ/mol [Kada-Benameur et al., 2000]. Autocorrelation functions to segment clinker minerals have a negligible effect on degree of hydration or homogenized elastic properties and may be selected arbitrarily.

Points from external datafile can be plotted inside a graph. Two columns from specified file are read in the same units. For example, time vs. Young's modulus will have columns in [h] and [GPa].

Once calculation runs, changing values in GUI has no effect, even when changed upon pause. Please use the quit button to terminate correctly two python threads. If not, the thread will keep going and must be killed externally.

4.1 Extension to elasticity

Methodology for a multiscale elastic homogenization is described in [Šmilauer, 2006] and Fig. 3. Used analytical homogenization methods include Mori-Tanaka [Mori and Tanaka, 1973], self-consistent [Hill, 1965] and N-Layered spheres [Hervé and Zaoui, 1993]. Necessary input data include air entrained and entrapped voids. They are taken into account at the level of cement paste in the homogenization process. Typical Young modulus for aggregates is between 50 and 90 GPa [Mehta and Monteiro, 1993].

The microstructure of cement paste is filtered through percolation algorithm to assess only connected solid phases. Resulting effective moduli on all scales correspond to dynamic moduli. Static moduli will be lower, especially in the beginning of hydration. This phenomenon is discussed in [Torrenti and Benboudjema, 2005] and origins in limited cohesion among solids. Dynamic moduli can be considered as an upper bound.

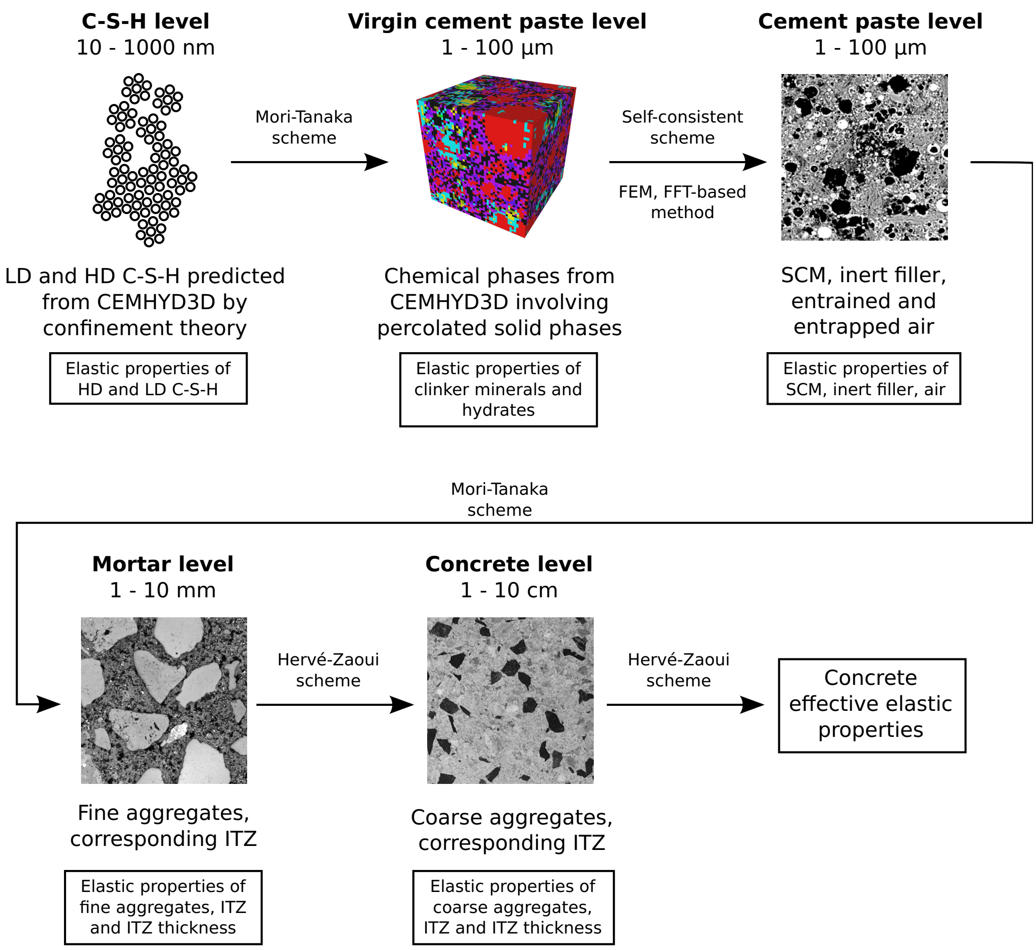

Figure 3: Adopted multiscale elastic homogenization approach

The un/drained conditions play important role in the paste elasticity. Undrained conditions represent bulk modulus of water as 2.18 GPa and prevent any water migration from the sample due to its compression. Such situation is typical for ultrasonic velocity, mature cement paste and low w/c. On the other hand, young paste and high w/c lead to drained conditions. The user has to replace the line in *cemhydmat.cpp* according what he needs

- PhaseFrac[1], 0.001, 0.499924 - for undrained conditions with capillary water bulk modulus $k = 2.18$ GPa (by default)
- PhaseFrac[1], 0.001, 0.001 - for drained conditions with $k = 0.0003$ GPa

5 Example

Following example shows the simulation from [Princigallo et al., 2003]. The real water content was 43.3 kg per 100 kg of cement ($w/c = 0.433$), Blaine fineness 530 m^2/kg. Mineral composition was obtained according to NewKirk [Newkirk, 1952] which gives $C_3S = 55.43$, $C_2S = 18.4$ in contrast to Bogue $C_3S = 53.7$, $C_2S = 19.71$. The difference is subtle and has negligible influence on the simulation. Sealed cement paste was placed at 20 °C. In the simulation, 400 kg per cubic meter of concrete is assumed. Silica and other solid components in cement paste are treated as secondary cementitious material (SCM). The example contains three files

- Princigallo.inp - main input file
- Princigallo_DoH.dat - degree of hydration determined from isothermal calorimetry
- Princigallo_E.dat - Young's modulus determined from mechanical tests

In this particular case, plain cement cement paste refers to water and cement only, paste contains in addition entrained + entrapped air + secondary cementitious material. Elastic values for mortar and concrete are fictitious.

Load the Princigallo.inp input file from the menu File-¿Load input data. Run the simulation. Compare experimental degree of hydration or evolution of Young's modulus directly in the plot window with the simulation.

Acknowledgement

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