Manual for CemPy, ver. 0.11

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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 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 although python portability should guarantee compatibility to other platforms. The GUI on Windows systems was not tested and is the subject of next development.

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

2 Installation

The code is optimized for Ubuntu 8.04 and Python 2.5. Following libraries and python modules found in standard Ubuntu (or debian) packages are required

- libfftw-dev 2.1.3
- libboost-dev 1.34
- libboost-python-dev 1.34
- python2.5-dev
  - python-pmw 1.3.2-3
  - python-numeric 24.2-8
  - python-numeric-ext 24.2-8

3 Compiling

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. To compile and link, type

```
>> make
```

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

```
>> python cemh.py
```

4 GUI description

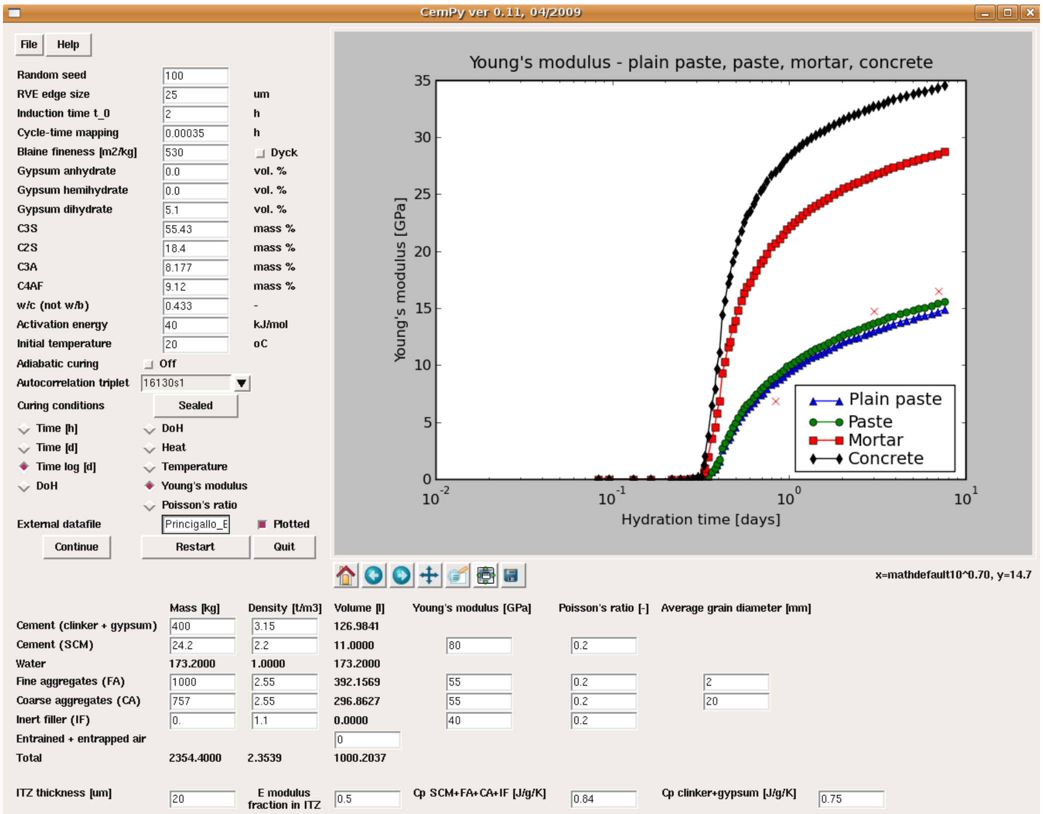

Figure 1: Typical GUI of CemPy

Fig. 1 shows a typical GUI layout. 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

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

where $t_0 \in \langle 0, 3\rangle$ h and $\beta \in \langle 4.0, 7.8\rangle$ h/cycle^2 for normal 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

$$G(d) = 1 - e^{-bd^n}, \ \lim_{d\to\infty} G(d) = 1, \tag{2}$$

$$b = 7.54 \cdot 10^{-4}\,\text{fineness} - 0.143, \tag{3}$$

$$n = -8.333 \cdot 10^{-4}\,\text{fineness} + 1.1175, \tag{4}$$

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

$$G(d) = 1 - e^{-bd^n}, \ \lim_{d\to\infty} G(d) = 1, \tag{5}$$

$$b = 1.74 \cdot 10^{-4}\,\text{fineness} - 0.029, \tag{6}$$

$$n = -3.1 \cdot 10^{-4}\,\text{fineness} + 1.2. \tag{7}$$

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

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.

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

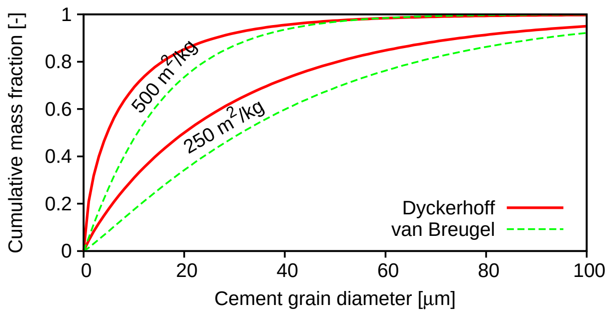

Figure 2: Particle size distribution according to NIST cement database for Dyckerhoff cements and van Breugel [van Breugel, 1997]

4.1 Extension to elasticity

Methodology for a multiscale elastic homogenization is described in [Šmilauer, 2006]. 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.

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.

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References

[Bentz, 2005] Bentz, D. P. (2005). CEMHYD3D: A Three-Dimensional Cement Hydration and Microstructure Development Modeling Package. Version 3.0. Technical report, NIST Building and Fire Research Laboratory, Gaithersburg, Maryland.

[van Breugel, 1997] van Breugel, K. (1997). *Simulation of hydration and formation of structure in hardening cement-based materials*. Ph.D. thesis, Delft University Press.

[Hervé and Zaoui, 1993] Hervé, E. and Zaoui, A. (1993). N-layered Inclusion-based Micromechanical Modelling. *Int. J. Engng Sci.*, 31:1–10.

[Hill, 1965] Hill, R. (1965). Theory of mechanical properties of fiber-strengthened materials. - III: Self-consistent model. *J. Mech. Phys. Solids*, 13:189–198.

[Kada-Benameur et al., 2000] Kada-Benameur, H., Wirquin, E., and Duthoit, B. (2000). Determination of apparent activation energy of concrete by isothermal calorimetry. *Cem. Concr. Res.*, 30(2):301–305.

[Mehta and Monteiro, 1993] Mehta, P. and Monteiro, P. (1993). *Concrete - Microstructure, Properties and Materials*. Prentice-Hall, Englewood Cliffs, New Jersey.

[Mori and Tanaka, 1973] Mori, T. and Tanaka, K. (1973). Average stress in matrix and average elastic energy of materials with misfitting inclusions. *Acta Metallurgica*, 21(5):1605–1609.

[Newkirk, 1952] Newkirk, T. F. (1952). The alkali phases in Portland cement clinker. In *Proc. of the 3rd Int. Symp. on the Chem. of Cem., London*, pages 151 – 171.

[Šmilauer, 2006] Šmilauer, V. (2006). *Elastic properties of hydrating cement paste determined from hydration models*. PhD thesis, ČVUT in Prague, Faculty of Civil Engineering.

[Princigallo et al., 2003] Princigallo, A., Lura, P., van Breugel, K., and Levita, G. (2003). Early development of properties in a cement paste: A numerical and experimental study. *Cem. Concr. Res.*, 33(7):1013 – 1020.

[Torrenti and Benboudjema, 2005] Torrenti, J. M. and Benboudjema, F. (2005). Mechanical threshold of cementitious material at early age. *Materials and Structures*, 38:299 – 304.

[Šmilauer and Krejčí, 2009] Šmilauer, V. and Krejčí, T. (2009). Multiscale model for temperature distribution in hydrating concrete. *Journal for Multiscale Computational Engineering*, 0(0):accepted.