

Manual for CemPy, ver. 0.10

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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 and is 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 used

- 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, run

```
>> make
```

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

>> python cemh.py

4 GUI description

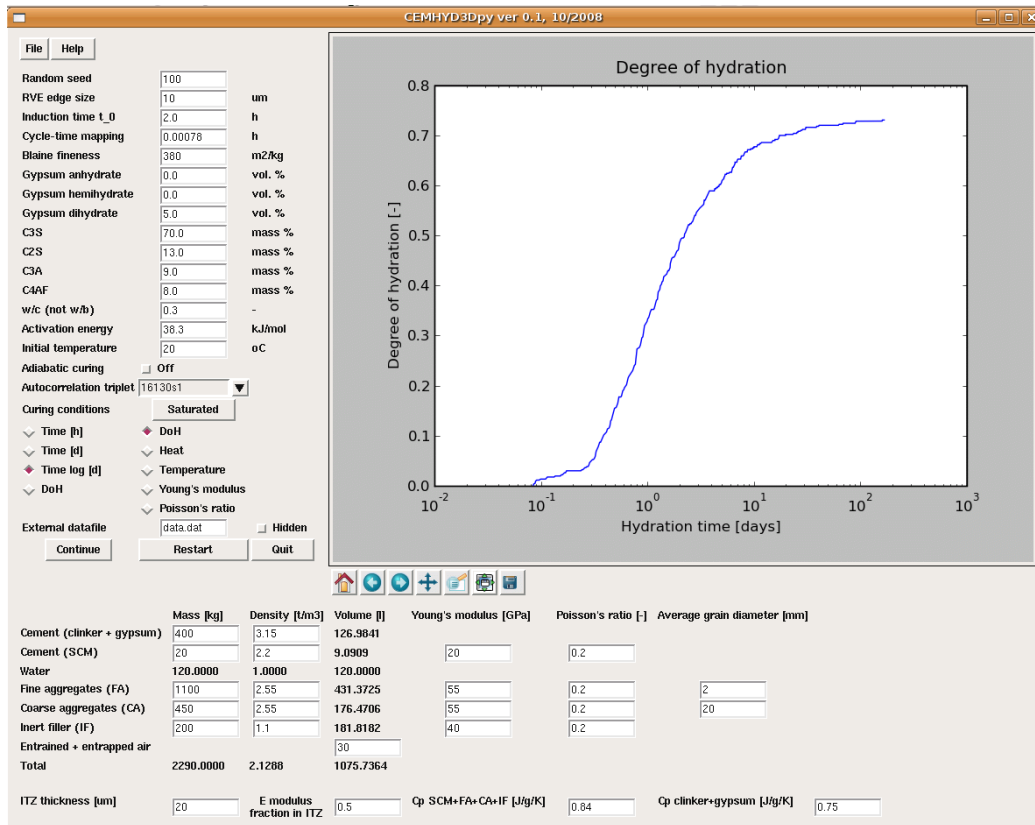


Figure 1: Typical GUI of CEMHYD3Dpy

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 precise calculations 100 μm . Cycle-time mapping is found in the ranges $t_0 \in \langle 0, 3 \rangle$ h and $\beta \in \langle 4.0, 7.8 \rangle$ h/cycle² for normal portland cements [Šmilauer and Krejčí, 2009]. Blaine fineness roughly corresponds to cement grade¹

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

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

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

$$G(d) = 1 - e^{-bd^n}, \quad \lim_{d \rightarrow \infty} G(d) = 1, \quad (1)$$

$$n = -8.333 \cdot 10^{-4} \text{ fineness} + 1.1175, \quad (2)$$

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

where d [μm] is the particle diameter and Blaine fineness is expressed in [m^2/kg].

Gypsum dihydrate possesses 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.

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].

Methodology for a multiscale elastic homogenization is described in [Šmilauer, 2006]. Necessary input data include air entrained voids with a typical size range 10 μm - 1 mm. They are taken into account at the level of cement paste in the homogenization process. Entrapped voids possess sizes between 1 and 10 mm but remain placed in the cement paste rather than on aggregate surface [Neville, 1997]. Entrapped voids are considered also at the level of cement paste, Hervé-Zaoui scheme can not account for them at the scale of mortar (not additional hollow sphere). Typical Young modulus for aggregates is between 70 and 90 GPa [Mehta and Monteiro, 1993].

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.

Acknowledgement

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