

Manual for CEMHapp v.1.0



Version 1.0

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The CEMHapp was developed in Python 2.7.6 and tested on Mac OS X 10.9.2, Ubuntu Linux 13.04, and Windows 7.



Please promote our work by refereeing to the publications [2] and [5]. Suggestions or help to port this software to other operating systems are appreciated.

1 Introduction

The affinity hydration model accommodates all stages of cement hydration under isothermal temperature at 25°C. The rate of hydration reads

$$\frac{dDoH}{dt} = \bar{A}_{25}(DoH), \quad (1)$$

where $\bar{A}_{25}(DoH)$ corresponds to the chemical affinity [time⁻¹]. The affinity for isothermal temperature can be obtained experimentally; specifically, the isothermal calorimetry measures a heat flow $q(t)$, which gives the hydration heat $Q(t)$ after integration. Cervera et al. [1] proposed an analytical form of the normalized affinity, which was further refined by Gawin et al. [3]. In this work, a slightly modified formulation, proposed in [5], is taken into account

$$\bar{A}_{25}(DoH) = \beta_1 \left(\frac{\beta_2}{DoH_\infty} + DoH \right) \cdot (DoH_\infty - DoH) \cdot \exp\left(-\eta \frac{DoH}{DoH_\infty}\right), \quad (2)$$

where β_1 and β_2 are parameters to be adjusted, η is the micro-diffusion of free water through formed hydrates, and DoH_∞ is the ultimate degree of hydration. These parameters express isothermal hydration at 25°C. When hydration proceeds under varying temperature T [K], \bar{A}_{25} can be scaled via Arrhenius equation

$$\bar{A}_T = \bar{A}_{25} \cdot \exp\left[\frac{E_a}{R} \cdot \left(\frac{1}{298.15} - \frac{1}{T}\right)\right], \quad (3)$$

where R [Jmol⁻¹K⁻¹] is the universal gas constant and E_a [Jmol⁻¹] is the activation energy. The evolution of DoH is obtained through numerical integration since there is no analytical exact solution. The affinity hydration model performs well on OPC and blended cements. The model's validation and application is available in [2].

The goal of this cross-platform software is to provide an intuitive graphical user interface (GUI) and freely promote the affinity hydration model. The GUI has been tested on Mac OS X 10.9.2, Windows 7, and Linux Ubuntu 13.04.

2 Installation

- **Mac OS X 10.9.2:** copy the CEMHapp.app from CEMHapp.dmg to your application folder and run it.
- **Windows 7:** install the application (CEMapp.msi) and run CEMHapp.exe.
- **Linux Ubuntu 13.04:** run the command » `python CEMHapp.py` from Terminal.

The source code was written in Python 2.7.6 and the python module PyQt4 is responsible for the GUI. Other libraries and python versions might work but they have not been tested. The following libraries and python modules are required: a) python 2.7.6, b) matplotlib 1.3.1, c) numpy 1.8.0, and d) PyQt 4.10.4.

3 GUI description

The typical GUI layout of the CEMHapp is shown in Fig. 1.

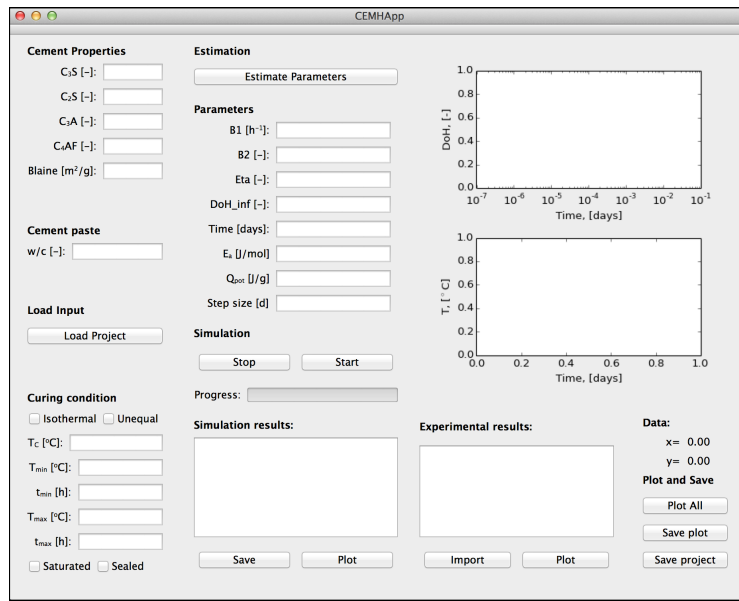


Figure 1: Typical CEMHapp GUI on Mac OS X 10.9.2.

The input fields C_3S , C_2S , C_3A , and C_4AF relate to the compound composition of cement; whereas $Blaine$ is the fineness of cement in m^2/kg and w/c is the water-cement ratio of the cement paste. In case the sum of cement compounds exceeds 95%, a warning message is shown and the *Estimate parameters* button will not proceed with calculations.

The curing conditions can be set to isothermal or unequal. The former considers constant curing temperature T_c [$^{\circ}C$]; while the latter considers

$$T(t) = (\bar{T} - T_{max}) \cdot \cos(2\pi(t - h_{min}/24)) + \bar{T} \quad (4)$$

where T_{min} and T_{max} are the minimum and maximum temperature of the day, h_{min} and h_{max} are the corresponding time when T_{min} and T_{max} occur, and \bar{T} is the average temperature.

The parameters β_1 , β_2 , and η and DoH_∞ , see Eq. (2), can be adjusted by the user or estimated (*Estimate parameters* button) by

$$\beta_1 = 0.738C_3S^{-0.206} \cdot C_2S^{-0.128} \cdot C_3A^{0.161}, \quad (5)$$

$$\beta_2 = (-0.0767C_4AF + 0.0184) \cdot B_f/350\beta_1, \quad (6)$$

$$\eta = 10.95C_3S + 11.25C_2S - 4.10C_3A - 0.892. \quad (7)$$

Eqs. (5)-(7) were converted from Lin and Meyer [7] since the model considered in the CEMHapp proceeds at 25°C instead of 20°C.

The theoretical value of DoH_∞ is limited to $\frac{w/c}{0.40} \leq 1.0$ (sealed condition), or $\frac{w/c}{0.36} \leq 1.0$ (saturated condition) due to unavailable capillary space for accommodating hydration products [4]. Recent publications [5, 7] show that DoH_∞ also depends on the cement *Blaine* fineness. However, DoH_∞ is assumed as a function of w/c only for simplicity.

E_a [$J.mol^{-1}$] and Q_{pot} [$J.g^{-1}$] (potential heat) are estimated by

$$E_a = 22100 \cdot C_3A^{0.30} \cdot C_4AF^{0.25} \cdot Blaine^{0.35} \quad (8)$$

$$Q_{pot} = 500 \cdot C_3S + 260 \cdot C_2S + 866 \cdot C_3A + 420 \cdot C_4AF \quad (9)$$

Eq. (8) was determined based on [7], and Eq. (9) corresponds to the sum of the heat of hydration of individual compounds. Although Q_{pot} is not used in the calculations, it is included in the application to provide means to compute the adiabatic temperature rise in concrete.

Prior to running the simulation, the step size must be determined. In case the simulation involves long term analysis (i.e. *End time > 100 days*), it is recommended to use *step size = 0.0* so the application will adjust automatically the step size. The parameters from the GUI can be saved to a .txt file (*Save Project* button or *Save as* and *Save* in the menu). Besides, the menu option *Open Project* or the button *Load Project* can be used to import a .txt project file.

Once the calculation is in progress (*Start* button), changing values in the GUI will have no effect on the results. Simulation results can be save to a .txt file or plotted (*Save* and *Plot* buttons under *Simulation Results* field). The legends in both graphs are draggable so the user can adjust it, and the data (Doh , t , and T_c) can be tracked by clicking on the left mouse button.

The CEMHapp allows for importing and plotting experimental data from a .txt file (*Import* and *Plot* buttons). Such data can be compared to simulation results by clicking on *Plot All* button. The plots can be save in .pdf using the *Save plot* button, and individual plots can be saved by clicking on the desired graph with the right mouse button. Examples of project, simulation results, experimental data, and plot files are available in the CEMHapp package.

4 Application

The cement properties (Table 1) considered in this application were obtained from [6, 7]. The experimental data available in ExpData.txt file were also taken from these publications. The model's parameters estimated by the CEMHapp are detailed in Table 1. DoH_{∞} was set at 0.90 to fit the simulation to experimental results. The estimated E_a was replaced with the value presented in [7].

Table 1: Cement properties [6, 7] and estimated parameters.

Cement properties		Estimated parameters	
C_3S , [-]	0.514	β_1 , [h^{-1}]	0.719
C_2S , [-]	0.226	β_2 , [-]	0.018
C_3A , [-]	0.111	η , [-]	6.821
C_4AF , [-]	0.079	DoH_{∞} , [-]	0.90
$Blaine$, [m^2/kg]	372.0	E_a , [$J.mol^{-1}$]	45721
w/c , [-]	0.50	Q_{pot} , [$J.g^{-1}$]	445.07

The End time and step size were set at 10 and 0.10 *days*. The graphs from CEMHapp are shown in Fig. 2a-d. The simulation results and parameters used in the analysis are available in SimResults.txt and ProjectFile.txt files, respectively.

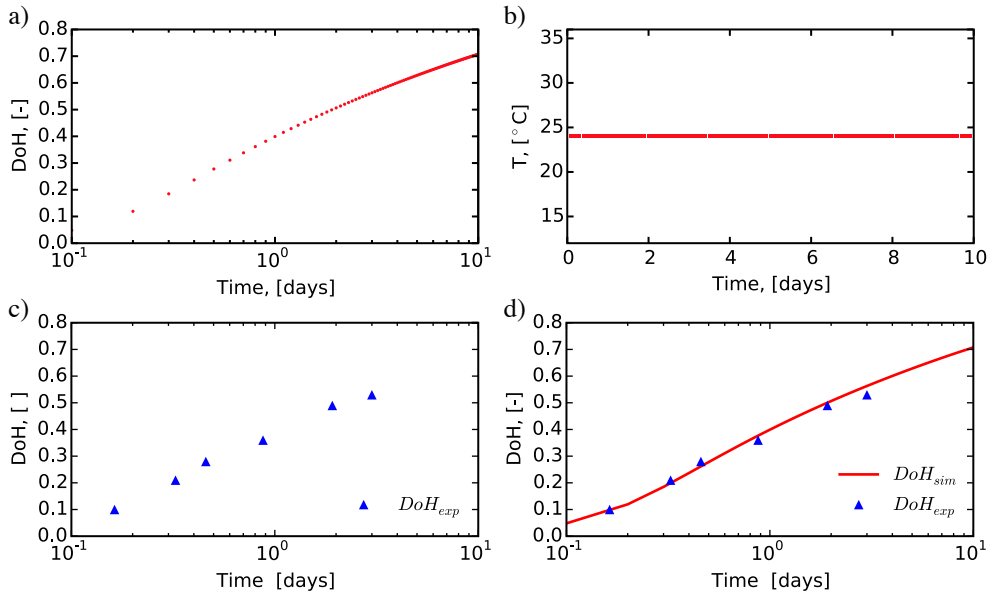


Figure 2: Output from CEMHapp: a) simulated DoH curve, b) Temperature profile, c) experimental data from [6, 7], and d) simulated and experimental results.

Acknowledgements

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