



A mathematical model to predict adiabatic temperatures from isothermal heat evolutions with validation for cementitious materials



Qinwu Xu ^{a,*}, Kejin Wang ^{b,*}, Cesar Medina ^c, Björn Engquist ^a

^a Institute for Computational Engineering and Sciences, The University of Texas at Austin, TX 78721, USA

^b Civil, Environmental and Construction Engineering, Iowa State University, Ames, IA 50011, USA

^c The Transtec Group, Inc., Austin, TX 78731, USA

ARTICLE INFO

Article history:

Received 31 December 2014

Received in revised form 7 May 2015

Accepted 8 May 2015

Keywords:

Calorimetry

Thermodynamics

Heat transfer

Temperature

ABSTRACT

Predicting transient temperature developments of adiabatic calorimetry using experimental data of heat evolution of isothermal calorimetry can save engineering costs and improve efficiency. We proposed a multilayer physical model and mathematical solution to carry this task based on the laws of mass action and thermodynamics. We proved that the model is adequate and reported simulation results for cementitious materials.

© 2015 Elsevier Ltd. All rights reserved.

1. Introduction

Calorimetry is a process that measures heats of a body due to chemical reaction, physical changes or phase transitions under certain constraints. Generally two calorimetry processes are used: (1) Isothermal calorimetry under isochoric condition, during which the “volume” (i.e. temperature) of the closed system remains constant; (2) adiabatic calorimetry, in which the system is insulated without heat energy exchange with the outside environments. However, no full adiabatic calorimeter can be warranted as there are always some heat exchanges between the body and calorimeter container, and mathematical calibration is always used to attain the full adiabatic condition. Therefore, the semi-adiabatic calorimetry device is also in which heat loss and gain of the system is permitted.

Calorimetry has also been adopted as an important laboratory technique for cementitious materials to measure its hydration heat and evaluate material properties [1]. Cement hydration is a chemical combination of cement and water in which dissolution of cement grains induces ionic concentration in “water”, and then compounds form from this solution and precipitate out as solids after reaching a saturation concentration [2]. The chemical reactions of calcium and silicon components of cements with H₂O form

crystals such as C-S-H and CH (from C₃S and C₂S reactions) and Aft and AFm (from C₃A, and C₄AF reactions) [3,4]. These reactions generate hydration energy (i.e., heats) upon the attachments of water molecules to ions [3,4]. Calorimetry can measure the heat evolution and hydration properties that play crucial roles in the early-age concrete performance, such as strength developments and cracking propagation [5,6]. Isothermal test measures heat evolution rate of cement mortar, and semi- and adiabatic tests measure temperature developments of mortar or concrete mixture. Both isothermal and adiabatic measured reaction curves can be used to determine hydration parameters and to predict temperature and strength developments of constructed facilities [7]. Previous study has shown that isothermal calorimetry can be used to determine cement hydration parameters more effectively [8] while the adiabatic tests may attain higher accuracy in predicting temperature developments of concrete pavements [9]. Calorimetry equipment and tests are often costly, while the true adiabatic condition is difficult to reach. Therefore, it is very useful to develop a model that can convert the heat evolution of the isothermal tests to temperature developments of adiabatic calorimetry. Wadsö [8] proposed a relatively simple model to compare isothermal and adiabatic calorimetry, and he concluded that semi-adiabatic calorimetry was not a good method to assess seven-day heats (isothermal) as there were many not so well known parameters needed for the necessary evaluation of the results. Unfortunately, very limited studies have been conducted

* Corresponding author. Tel.: +1 515 294 2152.

E-mail addresses: qinwu.xu@utexas.edu (Q. Xu), kejinw@iastate.edu (K. Wang), cesar@thetranstecgroup.com (C. Medina), engquist@ices.utexas.edu (B. Engquist).

Nomenclature

C	heat capacity (J/kg °C)	Q	generated heat (J/g)
k	thermal conductivity (W/m °C)	θ	degree of heat generation
h	heat transfer coefficient (W/m ² °C)	P	heat generation rate (mW/g)
ρ	material density (kg/m ³)	T	Temperature (°C)
α	thermal diffusivity (m ² /s)		
Q_T	total heat of hydration (J/g)		

to propose more effective models with further physical interpretation.

The motivation of this study is to develop such a physical model and mathematical solution to predict temperature developments by using experimental data of isothermal tests according to the laws of mass action and thermodynamics. We validated the model for cementitious materials and reported simulation results.

2. Experimental tests

We conducted isothermal tests on one cement mortar at four different temperatures (5, 20, 30 and 40 °C), and semi-adiabatic tests on concrete mixtures. Table 1 presents the chemical compositions of binder (cement plus fly ash or FA) and a Loss of ignition presents Table 2. the mixture design. As compared to cement mortar, concrete mixture contains the same mix portion of binder for the cement, FA, sands or fine aggregates, water, and additives (binder ratio of cement: FA: sand: water is 0.80: 0.2: 0.50: 0.40 in mass), but also includes coarse and intermediate aggregates. Tables in Fig. 1 list the mixture design and measured chemical components of cement and FA. Isothermal tests measured the heat generation rate per mass $P(t)$ (W/g) as shown in Fig. 1(a). The produced curves have clearly illustrated a typical heat evolution procedure: initial dissolution of solids that increase ionic concentration rapidly where spike appears, induction period with low P , acceleration to peaks which are primarily induced by C_3S hydration, and deceleration to a steady state [2]. In the semi-adiabatic tests, the cylindrical concrete specimen (150 mm × 300 mm in diameter and height) is placed in the calorimeter container -IQ drum, and temperature developments at time were measured as shown in Fig. 1(b).

3. Proposed model and analysis

In this section we proposed a physical model and mathematical solution along with its validation results on cementitious

Table 1
Oxide composition of cement and fly ash.

	Cement	Fly ash
CaO	49.34	26.20
SiO ₂	29.64	34.90
Al ₂ O ₃	8.20	20.10
Fe ₂ O ₃	3.31	5.78
Na ₂ O	0.30	1.72
K ₂ O	0.73	0.42
MgO	3.08	4.63
SO ₃	3.30	2.27
P ₂ O ₅	0.10	1.01
TiO ₂	0.51	1.64
SrO	0.12	0.42
Mn ₂ O ₃	0.07	0.05
LOI ^a	1.29	0.38

^a Loss of ignition.

Table 2
Mix design of mortar and concrete.

	Mortar	Concrete	Unit
Cement	443	262	kg/m ³
Fly ash	110	65	
Coarse agg. ^a	0	926	
Medium agg.	0	162	
Sand/fine agg.	1313	777	
Water	221	131	
AEA ^b	20	20	ml/100 kg binder
WR ^c	261	261	

^a Aggregates.

^b Air entraining agents.

^c Water reducer.

materials. The cement paste (combination of cement and water) is presented in a continuous phase as interweaved by sands (mortar) and/or aggregates (coarse and medium, for concrete) and additives. Small air voids also exist in the mixture, but would not functionally affect the chemical reaction (see Fig. 2(a)). We proposed a multilayer physical model for simulating the thermodynamic system of calorimetry as shown in Fig. 2(b). In this model each layer represents one phase of the system. In the multilayer model, the core is the cement paste as the heat source of chemical reaction, additive is the second layer which may or may not affect the chemical reaction dependent on the material, then sands (mortar) and/or aggregates (concrete), and the calorimeter container is the most exterior layer which may exchange thermal energy (at the semi-adiabatic condition) with the outside environments. The total hydration energy (or total heat) can be regarded the same for mortar and concrete given the same chemical composition of binder (cement plus FA) in this multilayer model. The thermodynamic system can be projected on a temperature-heat degree ($T - \theta$) polar coordinate system (see Fig. 2(b)). The degree of heat generation θ is proportional to the degree of cement hydration [10]. Here θ is projected to a phase angle such that $\theta \in [0, 2\pi]$, and can be expressed as follows:

$$\theta = 2\pi(Q/Q_{tot}) \quad (1)$$

where Q is accumulated heat of cement hydration (J/g), Q_{tot} is the total heat of hydration energy (J/g).

Q_{tot} can be estimated from the chemical compositions of binder as follows [11]:

$$Q_{tot} = 500P_{C_3S} + 260P_{C_2S} + 866P_{C_3A} + 420P_{C_4AF} + 624P_{SO_3} + 1186P_{FreeCa} + 850P_{MgO} \quad (2)$$

where P is the mass ratio of binder component (%).

Following this equation the Q_{tot} is calculated as 415 J/g including 404.1 J/g and 10.5 J/g contributed by cement and FA, respectively, for materials used in this study given mass ratios of each component. Given the same chemical composition of cement and mix portion for mortar and concrete, Q_{tot} (J/g) is the same and thus θ is proportional to Q . $\theta = 0$ before hydration and $\theta = 2\pi$ at the infinite time. According to the law of mass action, the chemical

Download English Version:

<https://daneshyari.com/en/article/7056557>

Download Persian Version:

<https://daneshyari.com/article/7056557>

[Daneshyari.com](https://daneshyari.com)