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ScienceDirect
Computers and Structures 84 (2006) 2351–2362
Computers & Structures
www.elsevier.com/locate/compstruc

# Modeling adiabatic temperature rise during concrete hydration: A data mining approach

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Received 23 August 2005; accepted 1 August 2006
Available online 23 October 2006

**Abstract**

This paper presents a data mining approach for modeling the adiabatic temperature rise during concrete hydration. The model was developed based on experimental data obtained in the last thirty years for several mass concrete constructions in Brazil, including some of the hugest hydroelectric power plants in operation in the world. The input of the model is a variable data set corresponding to the binder physical and chemical properties and concrete mixture proportions. The output is a set of three parameters that determine a function which is capable to describe the adiabatic temperature rise during concrete hydration. The comparison between experimental data and modeling results shows the accuracy of the proposed approach and that data mining is a potential tool to predict thermal stresses in the design of massive concrete structures.


*Keywords:* Data mining; Neuro-fuzzy modeling; Fuzzy clustering; Genetic algorithms; Concrete hydration; Dam structures

## 1. Introduction

Data mining techniques emerged in the last decade of the past century from Information Technology and Data Base Systems community in order to deal with the growing amount of data available in commercial applications, which needs for powerful data analysis tools. This approach integrates statistical, machine learning and data base systems management technology to discover hidden or non-trivial information in large or often huge data bases.

Usually, data mining is referred as one of the several steps in a more general methodology known as Knowledge Discovery in Databases (KDD) [1]. Knowledge discovery starts with the problem definition, whose solution corresponds to the data mining task. The subsequent process consists of an interactive sequence of the following steps: (1) data acquisition; (2) selection and transformation of data; (3) model identification; and (4) model evaluation and knowledge representation. The data acquisition step concerns the extraction of the data for the analysis by integrating several spreadsheets or extracting potential useful data from operational data bases. Selection and transformation of data includes data "cleaning" by removing noise, outliers and inconsistent data; selection of relevant data for the analysis task and data transformation where the selected data is made suitable for the data mining algorithms. The selection and transformation step is generally time consuming and has a great impact on the final result. The model identification step is the kernel of the overall process and consists of the application of the appropriate data mining algorithms to the transformed data according to the analysis task. There are several pre-specified analysis including association analysis, classification, clustering and

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doi:10.1016/j.compstruc.2006.08.049

prediction. Model evaluation and knowledge representation is the final step, when the results of the data mining algorithms are evaluated and presented to practical users. Frequently, the overall process is repeated until a desirable result is reached.

In the last few years data mining techniques, such as statistics, neural networks and genetic algorithms, have been widely used in many engineering applications including the behavior of concrete materials and structures [2–7]. In this paper, we deal with massive concrete structures such as dams, industrial foundations and other structures where the knowledge of the thermal loads during construction is determinant for the designers [8].

An accurate prediction of the thermal fields and of the cracking risk can be performed using thermo-chemo-mechanical models implemented in finite element codes [4,9]. One of the main inputs in the analysis is the adiabatic temperature rise curve of concrete during hydration. Based on this curve, it is possible to derive intrinsic properties such as the normalized affinity that characterizes the hydration evolution within the framework of a thermo-activated model [10]. Therefore, it is worth to predict the adiabatic temperature rise and several models have been proposed in the last years. The comprehensive multiphase model proposed by Maekawa et al. [12] considers that several hydration reactions take place at the same time. The input variables are the contents of the mineral phases of the cement, slag and fly ash, whose hydration reactions are modeled separately, and then are combined to represent the overall hydration of the cementitious material. In the NIST model [13,14], the volume fractions, surface area fractions and other parameters concerning the mineral phases are determined from SEM/X-ray image. Based on this data, a 3D particle image of the starting microstructure is generated and the hydration model progresses. In the Van Breugel and co-workers model [15,16], the degree of hydration is simulated as a function of the particle size distribution, chemical composition of the cement, water/cement (w/c) ratio and reaction temperature. More recently, Schindler and Folliard [17] developed a multivariate regression analysis based on data obtained from semi-adiabatic tests.

In this paper, a prediction model for the adiabatic temperature rise of concrete hydration is developed within a data mining perspective. The input of the model is a variable data set that corresponds to physical and chemical properties of the binders, and concrete mixture proportions. The output is a set of three constants that determine a function which is capable to describe the adiabatic temperature rising of concrete.

The model is based on the data set of mass concrete adiabatic tests carried out in the last thirty years by *Furnas Centrais Elétricas S.A.* (Brazil) [18]. The tests concerns the most important mass concrete constructions in Brazil, such as Itaipu dam (11,000,000 $m^3$ of concrete, with a production capacity of 12,600 MW, the hugest hydropower plant in operation in the world), Tucurui dam (6,000,000 $m^3$ of concrete, 8000 MW of production capacity), Xingó dam (1,300,000 $m^3$ of concrete, 3000 MW of production capacity), and several other mass concrete used for the construction of hydroelectric and nuclear power plants.

## 2. The hydration reaction of cementitious materials

Typical cement chemistry notation will be used throughout this paper: C = CaO, S = $SiO_2$, F = $Fe_2O_3$, A = $Al_2O_3$, N = $Na_2O$, K = $K_2O$, $\overline{S}$ = $SO_3$ and H = $H_2O$; C–S–H represents calcium silicate hydrate, where the symbol '–' indicates no exact stoichiometric proportions; CH represents calcium hydroxide, or $Ca(OH)_2$; AFt is the abbreviation of ettringite $Ca_6A_{12}(SO_4)_3(OH)_{12}\cdot 26H_2O$, and AFm is the abbreviation of monosulfate, $Ca_4Al_2O_6(SO_4)\cdot 14H_2O$.

In fact, what is called cement hydration reaction (*cement + water → hydrates + calcium hydroxide + heat*) is the combination of hydration reactions that takes place when concrete is becoming mature. For Portland cement hydration, the main reactions are based on the mineral compounds of the clinker. They can be written in a simplified form as:

$$C_3S + H \rightarrow C\text{–}S\text{–}H + CH + \text{heat} \quad (1)$$

$$C_2S + H \rightarrow C\text{–}S\text{–}H + CH + \text{heat} \quad (2)$$

$$C_3A + C\overline{S}H_2 + H \rightarrow AFt + \text{heat} \quad (3)$$

$$C_4AF + C\overline{S}H_2 + H \rightarrow AFt + CH + FH_3 + \text{heat} \quad (4)$$

$$\begin{matrix} C_3A \\ C_4AF \end{matrix} + AFt + H \rightarrow AFm + CH + FH_3 \quad (5)$$

All these reactions have its own kinetics [11], and the reagents, i.e., the clinker minerals, have different heats of hydration at complete reaction ($Q_\infty$), which are, approximately, in kJ/kg: $Q_\infty^{C_3S} = 505$; $Q_\infty^{C_2S} = 260$; $Q_\infty^{C_3A} = 870$ and $Q_\infty^{C_4AF} = 420$ [12].

The hydration of cement, mortar and concrete can be identified by the adiabatic temperature rise measured in an adiabatic calorimeter, but in this case it corresponds to the combined exothermicity of all the reactions in course. This adiabatic temperature rise will depend on several parameters that characterize the cementitious materials, such as cement chemical composition and fineness, content and type of mineral additions, and mixture proportions.

Mineral additions strongly influence the hydration of cementitious materials. If pozzolans are added to cement, they react with calcium hydroxide forming more C–S–H in an exothermic reaction. If the pozzolan is composed mainly by silica oxide, the following reaction equation can be written:

$$S + CH + H \rightarrow C\text{–}S\text{–}H + \text{heat} \quad (6)$$

The pozzolanic reaction tends to proceed more slowly than the reaction of the clinker compounds. Nevertheless, even though the pozzolanic addition tends generally to