Applications of Computers and Information Technology

by

James R. Clifton and Geoffrey Frohnsdorff
Building and Fire Research Laboratory
National Institute of Standards and Technology
Gaithersburg, MD 20899 USA

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1.0 INTRODUCTION

The science and technology of concrete are undergoing revolutionary change due to developments in computer and information technologies that are enabling concrete researchers, engineers, and practitioners to develop, store and retrieve, integrate, and disseminate knowledge on all aspects of concrete including formulation, processing, testing, and inspection, prediction of performance, repair, and recycling. The rapid growth of computer-based systems such as simulation models, databases, and artificial intelligence decision-support systems, is evidence of the impact of computer and information technologies on concrete science and technology. The purpose of this chapter is to draw attention to recent developments in computers and information technology that are having enormous influences on the direction of the material science and technology of concrete. Development in the material science of concrete in conjunction with computer and information technology will undoubtedly contribute to great improvements in the performance of concrete in the 21st century. A major advance in concrete science and technology has already resulted from the development, application, and integration of computer-based simulation

*Deceased January 1999.

models, databases, and artificial intelligence decision-support systems. In reviewing the application of computers and information technologies to the material science of concrete a brief review of their general application to material science and engineering is presented first. Then, developments in computerized knowledge bases for concrete are reviewed and their integration to form computer-integrated knowledge systems discussed.

1.1 Computer Applications in Material Science and Engineering

Since the development of the ENIAC (Electronic Numerical Integrator and Computer), the first fully electronic computer, in 1946,[1] computers have become ubiquitous in the scientific and engineering fields. At first they were primarily used for rapid, but straightforward, numerical calculations with early applications being in the design of atomic weapons at Los Alamos and improving methods of cryptography during World War II. Then, in the 1950s, their applications were extended to data storage and retrieval beginning with the design of the EDVAC (Electronic Discrete Variable Automatic Computer) built at the University of Pennsylvania for the U.S. Army Ballistic Research Laboratory.[1] Early, and still important, applications to engineering were in "number crunching" including structural analysis using finite element modeling, computer-aided design (CAD), and relational modeling involving the fitting of data. In the early 1970s, pioneering work by Feigenbaum[2] in the development of the chemical identification expert system, Dendral, was an early introduction to the concept of AI (Artificial Intelligence) and was instrumental in demonstrating the use of computerized scientific and engineering knowledge in the solving of complex problems. A further revolution is now taking place in the computerized dissemination of data, information, and knowledge, by the development of the Internet, fostered in the U.S. Congress by the High Performance Computing Act of 1991[3] which was soon extended to define the National Information Infrastructure. Innovations in computer and communication technologies coupled with this legislative initiative have stimulated the worldwide explosive growth of the Internet.

These advances in computers and communications have enormous implications in concrete science and technology in such areas as *(i)* prediction of concrete performance through fundamental computational models resulting in more reliable service life designs of concrete; *(ii)* collaboration in research and in problem-solving efforts in the concrete field, through sharing of data, information, and knowledge among geographically-dispersed colleagues, research organizations, manufacturing companies, and contractors; *(iii)* development of computer-integrated knowledge systems which have the potential for representing virtually all scientific and engineering knowledge of concrete and making the knowledge readily available to those needing it. Although, at present, most knowledge of concrete is still stored in printed form and in the brains of concrete technologists, its electronic representation is growing rapidly, e.g., the ACI Manual of Concrete Practice[4] is available on CD-ROM disks and simulation models of the microstructure of cements and the transport properties of concrete can now be downloaded from the Internet.[5] Civil engineering World Wide Web sites dealing with concrete are also located on the Internet.[6]

One of the most exciting recent developments in the application of computers to the design of materials is the simulation modeling which is being extensively used by chemists in the development of new complex molecules for medical purposes.[7] In the future, we anticipate that significant advances in knowledge of concrete and other cement-based materials will result from simulation modeling.

2.0 COMPUTER MODELS

Material science involves the development and application of knowledge concerning relationships among microstructure, processing, and properties of materials. Modeling has become an integral component of material science and now drives many advances in the fundamental knowledge of materials, including cement-based materials. A model of a material can be defined as "a theoretical construct, which is made using valid scientific principles expressed in mathematical language, that can be used to make quantitative predictions about a material's structure or properties."[8] In another definition, models are considered to be theoretical and mathematical representations that predict experimental observations.[9]

2.1 Types of Models

Several types of models can be identified, including physical, conceptual, logical, statistical, constitutive, and simulation models.[10] A miniature version of a concrete dam or building can be labeled as a *physical model*. It constitutes a material representation of an object with real-world features. *Logical models* deal with axioms and rules of deductive inference that permit the creation of logically-correct statements by applying the rules of formal logic. Regarding applications of computers to concrete, we are interested in statistical, constitutive, and simulation models. *Statistical models* are often derived by data fitting using regression relations; however, some models, such as those developed by Parrot[12] and Powers,[11] while involving data fitting, also incorporate knowledge of physical reality. *Constitutive models* deal with observed patterns in properties[9] with mathematical relations being derived to represent the observed patterns; however, the basis for the model cannot be determined directly and cause and effect are linked by assumed mechanisms. A *simulation model* includes some sort of stored or analytical representation of a system, which is operated by prescribed algorithms that give numerical information on desired physical or other properties.[8] In the case of cement-based materials, simulation models deal directly with microstructure at the level of individual cement particles and their hydration products and the resulting microstructure. They may also cover a wide range of scales, from nanometers to meters. Such multi-scale models may be used to simulate the microstructure development in a hydrating cement paste or to predict properties of concrete in a structure. An example is a model for predicting chloride ion diffusivity of portland cement concrete.[13][14] In the future, the authors believe that simulation modeling will be an essential tool in all branches of science and engineering and it will make practical the material design of concretes optimized for their applications.

2.2 Mathematical Language of Models

The mathematical language of a model may take several forms, such as a set of deterministic empirical equations that have been fitted to experimental data, or a set of physically-appropriate differential equations whose coefficients have been determined from experimental data, or a set of differential equations or computer algorithms that do not depend on any special experimental input, only a comprehensive knowledge of physics and chemistry. Examples of models based on different mathematical languages are described by Garboczi and Bentz,[8] and Jennings, et al.[9]

2.3 Material Science Models of Cement-Based Materials

During the past three decades many computational models based on material science have been developed for cement-based materials. Prior to the advent of computer simulation most models of cement-based materials were of the constitutive type. In the future, simulation modeling will likely predominate. Too many models have been developed to give more than a brief review which is the intent of this section. The models are somewhat arbitrarily grouped into cement hydration models, microstructure models, and simulation models.

Cement Hydration Models. An early review of mathematical models of cement hydration was prepared by Pommersheim and Clifton.[15] They found, at the time of their review in 1979, that most models of cement systems addressed one or the other of tricalcium silicate and dicalcium silicate. The models were composed of rate equations, constitutive relations, and conservation equations. Probably the first comprehensive model for the hydration of tricalcium silicate was developed by Kondo and Ueda in the 1960s.[16] Frohnsdorff, et al.,[17] also developed an early (1968) general mathematical model which was applied to the hydration of tricalcium silicate (C_3S). The kinetics of tricalcium silicate hydration was modelled by Pommersheim and Clifton.[18][19] In their model, a hydrating C_3S particle had three product layers: inner, middle, and outer (Fig. 1), with the middle layer (or barrier layer) forming almost instantaneously and then gradually disappearing. The rate of hydration was controlled by diffusion through these product layers. This approach was further advanced by van Breugel in the HYMOSTRUC model, which incorporated particle size distribution, concentration gradients, heats of hydration, rates of diffusion, temperature, and relative humidity.[20] While not a model, the research by Nonat[21] on factors affecting the hydration of C_3S, is mentioned as it provides data needed for model development. Data was presented on kinetics of hydration of tricalcium silicate, the thermodynamics, morphological and structural characteristics of calcium silicate hydrate (C-S-H), and particle interactions during setting. It was found that the concentration of lime in the pore solution was the most important parameter affecting the hydration kinetics and the morphological and structural features of the C-S-H formed.

A major effort aimed at developing a conceptual basis for the mathematical modeling of the hydration of portland cement was performed by RILEM Technical Committee 68-MMH on Mathematical Modeling of Cement Hydration, resulting in several reports in the 1980s. A task group chaired by Taylor[22] summarized conceptual models for the hydration of tricalcium silicate (at room temperature and a water/cement ratio of 0.5 by mass), with the objective of providing an introduction to the more difficult problem of developing scientifically sound mathematical models for portland cement hydration. Their conceptual model considered phase equilibria, morphology and nature of the reaction products, and pore solution composition. Also, they discussed the mechanisms thought to control hydration during the three major phases of C_3S hydration: the induction, acceleratory, and deceleratory periods. In a companion study, a task group chaired by Young[23] examined the conceptual basis for the hydration of dicalcium silicate (C_2S). They concluded that C_2S hydrates slower than C_3S because, unlike C_3S, the anhydrous silicate lattice in C_2S contains no oxide ions. As part of the same general study, a task group chaired by Brown[24] examined the hydration of tricalcium aluminate (C_3A) and tetracalcium aluminoferrite. They reported that the reactions of C_3A with water and calcium sulfate produced ettringite and monosulfate, depending on the relative proportions of the reactants, and metastable calcium aluminate hydrates which converted into the cubic hydrate, C_3AH_6.

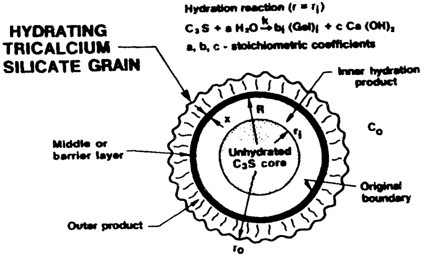


Figure 1. Schematic of hydrating C_3S grain.[18]

Few models of the hydration of typical portland cements have been reported. One of the most significant early studies was that by Brunauer, et al.,[25] who investigated the hydration of portland cement pastes at low porosities (w/c ratios of 0.2 and 0.3, by mass) and mathematically analyzed the data. In developing their model, they assumed that the hydration rate was directly proportional to the product of the rate constant, a function depending on the w/c ratio and the amount of unhydrated cement, and inversely proportional to the mass of hydration products raised to a positive power. Model constants were obtained using a differential method of data analysis. The model predicted that the hydration rate decreased as the hydration product volume increased and as the w/c ratio decreased. Probably the most advanced model of the hydration of a portland cement yet developed is that by Bentz.[26] It is a three-dimensional computer model for the simulation of portland cement hydration and microstructure development. This model will be further described in the section on simulation modeling.

Microstructural Models. The microstructure of cement-based materials is controlled by their constituents, the mixture proportions, processing (e.g., mixing, consolidation, and curing), and degree of hydration. The properties of the hardened cement-based materials are dependent on their microstructure; the capillary pore structure, which includes the transition zone between the cement paste and aggregates, usually governs the transport properties of concrete, while larger voids reduce the strength of concrete. Therefore, microstructure characterization and modeling have come to make a major contribution to understanding the performance of cement-based materials. The progress of microstructure modeling has been comprehensively reviewed in two parts by Jennings, et al.[9][27] Part 1 deals with historical developments and provides a general overview, while Part 2 addresses recent developments. In Part 1, models of the microstructure of cement-based materials and of shrinkage and creep are described, while Part 2 describes models linking microstructure with flow properties, moisture capacity, and shrinkage and creep. Garboczi and Bentz reported on the state-of-the-art of fundamental computer simulation models for cement-based materials[8] and with Martys, reviewed[28] relationships between transport properties and the microstructure of cement-based materials. Van Breugel[29] used simulation models to link microstructural development with hydration kinetics of cement-based materials.

The reviews by Jennings, et al., were contributions to the proceedings of a NATO Advanced Research Workshop on the Modeling of Microstructure and Its Potential for Studying Transport Properties and Durability, held in 1994.[30] The contents of the proceedings are:

Part I: Modeling Pore Structure

- Scale and resolution of models
- Spatial distributions
- Data bases and expert systems

Part II: Transport Mechanisms and Durability

- Transport mechanisms
- Major parameters affecting transport properties
- Corrosion mechanisms and parameters

Simulation Models. The first application of simulation modeling to cement-based materials appears to be that described in 1985 by Roelfstra, Sadouki, and Wittman.[31][32] They used a two-dimensional (2-D) finite element modeling approach to simulate the elastic properties of concrete. The cement paste microstructure was treated as a continuum, but they used simulation techniques to generate realistic 2-D shapes of certain classes of aggregates. Random elastic moduli information was stored in finite elements from which they were able to make 2-D computations of elastic moduli, diffusion coefficients, and thermal expansion coefficients of the concrete. The next major development was the computer simulation model of Jennings and Johnson in 1986[33] which was later revised and improved by Struble, et al.[34] This model simulated the development of the microstructure in 3-D of a tricalcium silicate paste, starting with a numerical representation of the initial cement particle/water mixture and then, in successive iterations, operating on this stored information and calculating the progress of the changes in small increments using an algorithm for consuming the tricalcium silicate and generating hydration products. The tricalcium silicate particles were modeled as spheres with a size distribution typical of portland cement.

A continuum model developed to produce computer representations of cement microstructures is based on the mosaic method.[35] In this approach, a 2-D space is divided by a set of intersecting lines and the resulting polygonal shapes taken to represent unhydrated and hydrated cement particles and hydration products (an analogous approach was used in 3-D). Although multiple discrete phases can be modeled using this method, simultaneously modeling multiple continuous or percolated phases, such as C-S-H gel, capillary porosity, and calcium hydroxide (CH), presents a computational challenge.

An alternative approach to continuum-based models has been the development of "digital-image-based models."[28] In these models, each particle of cement or hydration product is represented as a collection of elements (pixels). Hydration can then be simulated by operating on the entire collection of pixels using a set of cellular-automaton-like rules. This allows for the direct representation of multi-size, multi-phase, non-spherical, cement particles. The model has evolved from one based simply on the hydration of C_3S to one that considers all of the major phases present in portland cement.[26] In addition, due to the underlying pixel representation of the microstructure, mapping the microstructure onto a finite difference or finite element grid becomes trivial. Thus, properties such as percolation, diffusivity, complex impedance, and setting behavior, are easily computed. To adequately model the hydration behavior of a cement by this approach, it is necessary to accurately characterize the starting material, the cement powder. Using a combination of scanning electron microscopy (SEM) and x-ray powder diffraction, along with imaging processing techniques, Bentz and Stutzman[36] have developed a method for obtaining 2-D images of unhydrated cements, which are converted into realistic 3-D representations for use in simulations of cement hydration.

The processes involved in the simulation model of cement hydration and the application of the model in predicting the properties of the hydrated cement paste were described by Bentz.[26] The reactions given in Fig. 2 are implemented as a series of cellular automaton-like rules which operate on the original 3-D representation of cement particles in water. Simple rules are provided for the dissolution of solid material, the diffusion of the generated diffusing species, and the reactions of diffusing species with each other and with solid phases. These rules are summarized in the state transition diagram in Fig. 3. The simulated microstructure is scanned, the rules applied to pixels exposed on the particles surfaces and, when all the possible events have occurred for these pixels, defined as one cycle (or scan), another cycle is implemented. The cycles are repeated until the reactions are complete or the desired degree of hydration has been achieved. Then, the properties of the "virtual" cement may be calculated and compared to experimental data. An example of the level of agreement between a measured cement property and the results from the model is given in Fig. 4 for chemical shrinkage. Similarly, good agreements have been obtained for degree of hydration and heat of hydration. By incorporating a maturity relationship, the model gave reasonable predictions of the compressive strengths of mortar specimens.

By a multi-scale approach, many of the material properties of concrete can be predicted starting with the hydration of C_3S to form C-S-H gel and CH at the nanometer level. Then, using the nanometer-scale model to form a continuum structure, the cement paste structure is modeled on the micrometer scale. The microstructure of the cement paste is then used to calculate appropriate properties of a continuum in which the aggregates are embedded to form a mortar/concrete model on the meter scale. This approach has been demonstrated for predicting the chloride ion diffusivity of portland cement mortar and concrete.[13][14]

On the nanometer scale, the connectivity of the gel pores is considered to control diffusivity, while the percolation of capillary pores is treated at the micrometer scale. Then the contributions of gel pores and capillary pores, including those from the transition zone between the cement paste and aggregates, are combined in calculating the diffusivity of mortars and concretes.

The above simulation modeling of cement-based materials is included in a 1200 page "electronic monograph" prepared by Garboczi, Bentz, and Snyder based on the simulation modeling of cement-based materials carried out at NIST (available on the Internet at http://ciks.cbt.nist.gov/garboczi). This monograph provides comprehensive insights into many aspects of the computational material science of concrete.

Silicate Reactions

$$\begin{array}{ccccccc} C_3S & + & 5.3H & \rightarrow & C_{1.7}SH_4 & + & 1.3CH \\ 1 & & 1.34 & & 1.521 & & 0.61 \end{array}$$

$$\begin{array}{ccccccc} C_2S & + & 4.3H & \rightarrow & C_{1.7}SH_4 & + & 0.3CH \\ 1 & & 1.49 & & 2.077 & & 0.191 \end{array}$$

Aluminate and Ferrite Reactions

$$\begin{array}{ccccc} C_3A & + & 6H & \rightarrow & C_3AH_6 \\ 1 & & 1.21 & & 1.69 \end{array}$$

$$\begin{array}{ccccccc} C_3A & + & 3C\bar{S}H_2 & + & 26H & \rightarrow & C_6A\bar{S}_3H_{32} \\ 0.4 & & 1 & & 2.1 & & 3.3 \end{array}$$

$$\begin{array}{ccccccc} 2C_3A & + & C_6A\bar{S}_3H_{32} & + & 4H & \rightarrow & 3C_4A\bar{S}H_{12} \\ 0.2424 & & 1 & & 0.098 & & 1.278 \end{array}$$

$$\begin{array}{ccccccccccc} C_4AF & + & 3C\bar{S}H_2 & + & 30H & \rightarrow & C_6A\bar{S}_3H_{32} & + & CH & + & FH_3 \\ 0.575 & & 1 & & 2.426 & & 3.3 & & 0.15 & & 0.31 \end{array}$$

$$\begin{array}{ccccccccccc} 2C_4AF & + & C_6A\bar{S}_3H_{32} & + & 12H & \rightarrow & 3C_4A\bar{S}H_{12} & + & 2CH & + & 2FH_3 \\ 0.348 & & 1 & & 0.294 & & 1.278 & & 0.09 & & 0.19 \end{array}$$

$$\begin{array}{ccccccccc} C_4AF & + & 10H & \rightarrow & C_3AH_6 & + & CH & + & FH_3 \\ 1 & & 1.41 & & 1.17 & & 0.26 & & 0.545 \end{array}$$

Figure 2. Cement model reactions (numbers below reactions indicate volume stoichiometry).[26]

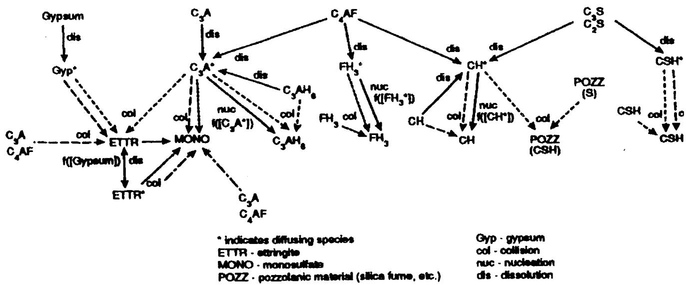


Figure 3. State transition diagram for three-dimensional cement hydration model.[26] Arrows denote reaction to form hydration product; F[X] denotes that nucleation or dissolution probability is a function of the concentration of X.

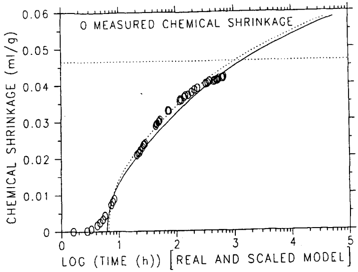


Figure 4. Measured and model chemical shrinkage vs. time for CCRL Portland cement 115 with w/c of 0.40.[26]

3.0 DATABASE SYSTEMS

A database system is defined by Date[37] as a computerized record-keeping system, while a database is a collection of computerized data files with persistent data. A database system contains a description of its structure in the form of a data dictionary and data schema, where the data dictionary[38][39] is a guide to the information in a database and the database schema provides a perspective—a way of seeing—the information in the database. In other words, a database system is a self-describing collection of files containing within itself a description of its structure.

3.1 Applications of Databases in Concrete Technology

The process of developing scientific and engineering databases in science and engineering and their application has been described by Rumble and Smith.[38] Some examples of data to be represented in concrete databases are:

- Composition and physical properties of concrete-making materials

- Properties of concrete such as transport properties, mechanical properties, fire performance, and durability vs. mixture design
- Rheological properties and consolidation characteristics of concrete mixtures
- Performance data from research, laboratory and field studies
- Pictures of distresses in concrete materials and structures
- Representational images such as graphs of relationships and the results of models
- Standards and guidelines
- Bibliographic information

Design and development of databases which are intended to be of lasting value can require considerable effort, be expensive, and require specialized skills.[40] Nevertheless, database development should be an inherent part of any significant project related to research, design, performance testing and prediction, and evaluation of the field performance of concrete. The justification for investing in creating databases for scientific and engineering data necessitates comment. From a business standpoint, several benefits are apparent[37] which are also applicable to scientific and engineering databases; they include reduction of voluminous paper files, persistence and rapid retrieval of data, organization of data to facilitate analysis, and availability of up-to-date data. From a societal point-of-view, scientific and engineering databases can prevent "reinventing the wheel" research and also, by data-sharing, provide data to other researchers for input to models and for model validation. The integration of large amounts of data in a single database, known as "data banking,"[37] makes it practical to gain more knowledge from the processing of the data (data mining).[41] Frohnsdorff[42] has suggested that the development and maintenance of national databases for concrete and concrete materials should be supported by both the private sector and the government.

3.2 Existing Databases for Concrete and Concrete Materials

The number of numeric databases for concrete and concrete materials is far fewer than those for other materials, such as metals and plastics.

Westbrook, Kaufman, and Cverna, recently reviewed[43] the state-of-the-art of electronic access to numeric scientific and engineering databases—of some 100 available, none of them addressed concrete. Restricting coverage to electronically-distributed (e.g., by computer disk, CD-ROM, or over the Internet) and nonproprietary databases, our search disclosed only a few dealing with concrete and concrete materials. While there must be an enormous number of printed records of data on the properties and performance of concrete, e.g., in handbooks and in the records of organizations such as Federal and State construction agencies, cement and concrete trade associations and their members, and large construction companies, few appear to be in computerized form. Examples of three numeric databases available on computer discs are *(i)* a database developed at the Oak Ridge National Laboratory for the Nuclear Regulatory Commission containing age-related material data for concrete and concrete-related materials used to construct nuclear power plants;[44] *(ii)* a database developed by North Carolina State University under the Strategic Highway Research Program[45] on the properties of high-performance concrete; and *(iii)* a research-oriented database on creep and shrinkage of concrete prepared under the auspices of a RILEM technical committee.[46] An example of a bibliographical database for technical literature is ICONDA (CIB's International CONstruction DAtabase),[46][47] which covers international literature on construction technology including concrete. It has over 25,000 citations and this listing is rapidly increasing.

An important activity pursued by both the government and private sectors has been aimed at making databases accessible through the Internet.[5] Recently, two databases for concrete have become accessible over the Internet. A database on the properties of concrete aggregates developed by the Bureau of Reclamation,[48] which can be downloaded from the Internet using FTP (File Transfer Protocol), and transferred to Microsoft Access for searching. A database based on virtually all—more than 300—portland cements manufactured in North America in 1995, prepared by Gebhardt for ASTM Committee C-1 on Cement,[49] is also accessible through the Internet.[5] In this case, the database can be searched on-line, and the search is platform-and software-independent, i.e., it is an open system. This is possible through the use of the Remote Data Access [RDA] standard, which is a standard for accessing data from distributed SQL-compliant relational databases.[50] The RDA standard provides protocols for establishing remote connections between a database client and a database server. In addition to making the concept of open, distributed databases a reality, RDA will facilitate electronic commerce in which distributed database developers can be compensated. The attributes of distributed databases are discussed in detail by Burleson[51] and Date.[37] We predict that by the Year 2000, distributed databases on concrete and concrete materials properties will be commonplace. By 1998, the data sets on compositions and ASTM test data of portland cements in the proficiency sample program of the ASTM Cement and Concrete Reference Laboratory[52] will be accessible from the Internet through RDA.

3.3 Standards for Databases, Database Formats, Quality of Data

An important consideration in developing databases for concrete is the standardization of formats and the quality and reliability of the data. ASTM Committee E49 on Material and Chemical Property Data pioneered the development of material database formats and guidelines for materials.[5] The committee's goal is "to promote and develop standard classifications, guides, practices, and terminology, for building, processing, and exchanging information among computerized material and chemical property databases." Because knowledge of the quality of data values will often be critical to the use of a database, databases should incorporate quality indicators such as those prepared by ASTM E 1484[53] and given in Table 1. Building on the work of ASTM E49, ACI Committee 126, Database Formats for Concrete Materials Property Data, has developed formats to be used in reporting and storing data on the composition and properties of cements, aggregates, chemical admixtures, mineral admixtures; on the processing of concrete; and on the properties and performance of concrete. Recommended database formats for chemical admixtures have the following four data segments for recording the identity of a chemical admixture and its properties and performance in concrete.[39]

- Constituent identification
- Chemical and physical characteristics
- Manufacturer's recommendations
- Performance in concrete

The recommended data elements for identification of a chemical admixture are presented in Table 2; they are typical of those for the other data segments as well as those for other concrete materials property data sets. Chemical and physical data segments for chemical admixtures are presented in Table 3, which shows the hierarchical format of the database.

Table 1. Data Quality Standards[1]

Limited Use Data

- Data are traceable to an individual, organization, or reference
- After an independent review, an identifiable authority approved the digitized version for inclusion in the database
- Basis of data is identified
    a. Experimental measurements
    b. Derived Data
    c. Estimated Data
- Type of data is indicated
    a. Original point values
    b. Analyzed data
        1. Standard fit - specify fit and data
        2. Fit unknown

Qualified Data

- Number of measurements and data sets stated
- Nominal confidence limited estimated
- Traceable materials specification assures reproducibility
- Testing methods are specified and conform to a standard
- Data are traceable to a testing data—generating organization or individual

Highly Qualified Data

- High confidence limits determined (i.e., 0.99, 0.95, *n*)
- Perform minimum number of individual measurements
    a. From minimum number of sample lots
    b. From multiple suppliers (if appropriate)
- Data determined for each variable that significantly affects property
- Independent testing performed (other than from the producer and preferably by several leading laboratories)
- A second, independent evaluation (evaluator identified)
- Producer(s) identified

[1]From Reference 53

Table 2. Data Elements for the Identification of Chemical Admixtures for Concrete[1]

Constituent Designation Data Segment Number	Name	Type	Format
3001.xx	Constituent Class	Essential	Alphanumeric String
3002.xx	Constituent Common Name	Essential	Alphanumeric String
3003.xx	Constituent Producer Name	Essential	Alphanumeric String
3004.xx	Constituent Producer Plant Location	Essential	Alphanumeric String
3005.xx	Constituent Producer's Identification Number	Essential	Alphanumeric String
3006.xx	Constituent Standards Organization	Desirable	Alphanumeric String
3007.xx	Constituent Specification Number	Desirable	Alphanumeric String
3008.xx	Constituent Specification Version	Desirable	Alphanumeric String
3009.xx	Constituent Specification Designation	Desirable	Alphanumeric String
3010.xx	Constituent Notes	Desirable	Alphanumeric String

[1]From Reference 39.

Table 3. Chemical and Physical Data Elements forAdmixtures for Concrete[1]

Number	Name	Type	Format
3011.xx	Chemical Name	Essential	Alphanumeric String
3012.xx	Percent by Mass	Essential	Floating Point
3013	Total Solid	Essential	Floating Point
3014	Total Solid Units (customary units)	Desirable	Alphanumeric String
3015	Total Solid Units (SI units)	Essential	Alphanumeric String
3016	Customary to SI Conversion Factor	Desirable	Floating Point
3017	pH	Desirable	Floating Point
3018	Density	Desirable	Floating Point
3019	Density (customary units)	Desirable	Alphanumeric String
3020	Density (SI units)	Essential	Alphanumeric String
3021	Customary to SI Units Conversion Factor	Desirable	Floating Point
3022	Comments	Desirable	Alphanumeric String

[1]From Reference 39

3.4 Future Advances in Databases

Advances continue to be made in database technology in such areas as improved database languages, management systems with more efficient search capabilities, and overall ease of database development. It is to be expected that the advances will benefit concrete technology.

In the near future, the most important advances in database technology are likely to be in distributed open systems. Looking further ahead, Brodie[54] predicted that information systems of the future will go beyond distributed database technology to provide intelligent interoperability incorporating artificial intelligence and natural language processing. Ways in which artificial intelligence and databases can be integrated and how distributed artificial intelligence can be realized have been further discussed by Bell and Grimson.[55] They propose that the integration can be achieved in three ways:

1. Enhanced expert systems
2. Intelligent databases
3. Intersystem communications

In an enhanced expert system approach, the expert system (expert systems are defined in the following chapter) would be augmented with data management functions or interfaced to a dedicated general-purpose database management system; an intelligent database would have a deductive database management system embedded in it and in intersystem communication, both an expert system and a database would coexist and communicate with each other. In this case control might reside with either system or in an independent system. If the control resided with the expert system, it would have the capability of selecting databases germane to a specific problem from a matrix of distributed databases. In addition, it would control the retrieval, flow, and interpretation of data and knowledge, and transform them into conclusions and recommendations for presentation to the user. The importance to concrete technology is that the problem-solving ability of an integrated system controlled by an expert system would be limited only by the limits of our level of fundamental knowledge of concrete and our ability to represent that knowledge in an appropriate form; thus, it would have virtually unlimited potential for growth.

4.0 ARTIFICIAL INTELLIGENCE AND KNOWLEDGE-BASED SYSTEMS

A recognized success of the artificial intelligence (AI) field has been the development of intelligent knowledge-based systems.[56] Three types, each of which can be used to solve problems in the concrete domain are expert systems, neural networks, and case-based reasoning systems. Expert systems and neural networks are well-established problem solvers while case-based reasoning is likely to become a competing technology.

4.1 Expert Systems

Expert systems are regarded as the first success of artificial intelligence (AI) technology. Their function is to capture the knowledge and heuristic reasoning of human experts and apply it to the solution of problems which are sufficiently difficult to normally require the service of domain experts.[56] Early expert systems were authentic expert systems in that they captured the knowledge, largely in the form of heuristics, of a single domain expert, e.g., an expert in a specific domain such as causes of human illness. Today's expert systems often include heuristic and factual knowledge from several experts and from other sources such as models, guides, and standards; for this reason they are sometimes termed *knowledge-based systems*. Expert systems consist of two essential elements—knowledge bases and inference (logic) systems (Fig. 5).

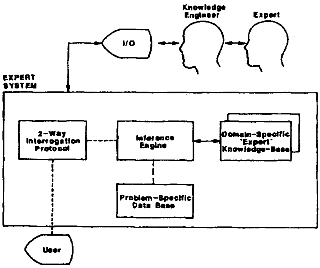


Figure 5. Architecture of an expert system.[58]

The *knowledge base* contains concepts and knowledge the system needs about relationships among the concepts. The *inference system*, often in the form of rules, simulates the way an expert makes inferences about the subject. In their simplest and most-often-used form, expert systems are analogs of expert opinion and are often termed "shallow systems." When combined with databases or mathematical models to support expert opinion they may be termed "deep systems." In general, expert systems are most effective in limited domains in which well-defined solutions exist. Also, they are best developed for domains in which the knowledge base is relatively stable, otherwise they may be obsolete before being completed. The development, principles, and applications of expert systems to concrete have been discussed by Clifton and Oltikar,[57] and Clifton and Kaetzel.[58]

4.2 Application Domains

The value of expert systems as aids to decision making has been demonstrated in a range of technical fields. Well-known examples are in medical diagnosis,[58] identification of chemical compounds,[2] and guiding the overhaul of diesel engines.[60] Expert systems are also applicable to many types of problems which occur in concrete technology, including the following categories:[5]

1. *Diagnosis*—Diagnostic systems were among the first expert systems developed. An example from the concrete field is HWYCON[61] which was developed to assist highway inspectors in identifying the causes of distress in concrete highway pavements and bridges and recommending remedial action; it has also found use in graduate courses in engineering materials.
2. *Selection*—Selection systems can form a basis for selecting the most cost-effective durable concrete for specific applications. A prototype expert system, DURCON (from DURable CONcrete)[57] was developed in the 1980s to represent the knowledge contained in the American Concrete Institute's "Guide to Durable Concrete."
3. *Scheduling/processing planning*—Scheduling systems may have application in strategic planning or simulation in construction. In this case, the expert system is likely to contain a model of the construction process.

4. *Monitoring/control system*—Expert systems that continuously monitor and in some cases control complex processes, can handle large amounts of input data and respond to routine situations. For example, an expert system could be used to monitor the structural condition of concrete structures.
5. *Computer-aided design*—Computer-aided design (CAD) systems based on expert system technology have enabled engineers and architects to develop customized models of plants, factories, and concrete structures.

The state-of-the-art of expert systems for construction materials, with the emphasis on concrete, was recently reviewed by Kaetzel and Clifton.[62] They found that the most successful applications of expert systems have been in the design of structures and structural components, distress identification and failure diagnostics, repair and rehabilitation, and project planning. In the area of concrete, fifteen expert systems were identified of which seven were operational.

In a recent workshop on standards for cement and concrete[63] it was recommended that standard practices and other standard documents should be expressed in the form of expert systems; one of the benefits would be that key provisions could be retrieved much more quickly than by reference to text and the interpretation of standards in an expert format would be more straightforward.

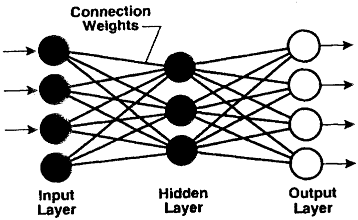
Future Trends in Expert Systems. In the 1970s and early 80s, expert systems were promoted as the solution to many of mankind's problems; eventually, the excessive optimism dissipated and many expert system development efforts were terminated. The major problem was that expectations were not being met rapidly enough. Conclusions from a recent survey were that the greatest barriers to growth in expert systems were difficulties in system integration (which relies on standards), the knowledge bottleneck (effective transfer of human knowledge into an expert system), and management inertia (the memory of artificial intelligence failures in the 1980s).[56] Automated knowledge-acquisition tools now present the potential of reducing and possibly eliminating the knowledge-acquisition barrier with domain experts being able to enter knowledge directly into an expert system without the intervention of knowledge engineers. This will simplify both the development and maintenance of expert systems. The impact of automated knowledge-acquisition on concrete knowledge will be substantial, e.g., the benefit of being able to capture and preserve the knowledge of the few true concrete experts would be immeasurable.

Expert systems will be increasingly interfaced with databases, neural networks, and various types of mathematical models, to form integrated systems. Visual information (graphical information and images of all sorts) will be an increasingly important component of expert systems (e.g., images of pavement distresses in HWYCON[61]), to aid in the decision-making process. Also, as suggested by the increasing attention by academic and corporate researchers,[64][65] expert systems will be distributed under the umbrella of distributed artificial intelligence. While traditional AI emulates some forms of human intelligence with single, unified systems, distributed artificial intelligence systems (DAIS) brings a decentralized approach to intelligence.[56] Applications that are especially suited to DAIS are those in which an important aspect of a problem is itself distributed. An example in concrete technology is the consolidation and curing of concrete pavements in which several processes affect the quality of the hardened concrete.

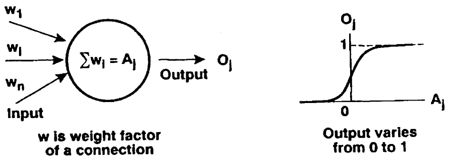
4.3 Neural Networks

As the name implies, neural networks were developed as an attempt to model the functioning of neurons in the human brain;[66] however, since, at best, they are simplistic models of human intelligence, other names have been introduced for neural networks; they include adaptive systems, parallel distributed processing models, and self-organizing systems.

Description of Neural Networks. A brief description of neural networks is given here; detailed information may be obtained from such books as Ref. 66 and 67. Neural networks use networks of simple but highly-connected "neurons" which process input data to give the desired outputs. The connected elements can consist of one or more layers. A 3-layer network is presented in Fig. 6. Similar to regression equations, the connections between the elements have adjustable weights. Several approaches have been developed for adjusting the weighted connections by training with actual data. Neural networks are able to work with incomplete or unreliable sets of data. They excel at relatively low-level, data-rich tasks such as image processing.[56] With expert system technology's focus on high-level reasoning, a natural synergy should exist between neural-net (NN) and expert systems (ES). Coupled ES-NN systems could use a neural net for initial filtering and processing of data, followed by use of an expert system for specific reasoning functions.[56] For example, while neural networks appear to have great potential for empirically determining the effects of different variables on the performance of concrete they do not provide information on the reasons for the observed effects. In a coupled ES-NN system the expert system part could assist in determining reasons for the observed effects. Coupled ES-NN systems have been applied by the Bechtel AI Institute to inspect for defects in manufactured items and to give recommendations on corrective actions.[56]



(a)



(b)

Figure 6. Artificial neural network.[5] *(a)* A 3-layer neural network with connections. *(b)* Connection weights, W_n, and output, O_j.

Application of Neural Networks. Some applications of neural networks to concrete and related materials have included prediction of thickening times of oil-well cements,[68] prediction of shear strength of concrete beams,[69] evaluation of the condition of deteriorating concrete structures,[70] interpretation of impact-echo test results,[71] and prediction of the depth of carbonation of concrete.[72] An example of the possible application of neural networks is the design of concrete mixtures. This is because, at present, much of the vast body of data on mixture design is incomplete and fuzzy—just the type of data for which neural networks are best suited.

4.4 Case-Based Reasoning

Case-based reasoning is based on the paradigm of human thought in cognitive psychology that contends that human experts derive their knowledge from solving numerous cases in their problem domain. Although humans may generalize patterns of cases into rules, the principle unit of knowledge is "the case."[73] Thus, the reasoning is by analogy or association with the solutions for previous similar cases. Case-based reasoning can be particularly useful in areas where traditional rule-based reasoning is relatively weak, such as knowledge acquisition, machine learning, and reasoning with incomplete information. At present, prototype computer programs are being tested for their effectiveness in problem-solving tasks using the case-based reasoning approach. Manual systems have been successfully used in medicine, law, and in design and failure analysis. Such systems have dealt with conceptual design of office buildings and building failure analysis.[74] A possible application of case-based reasoning to concrete problems is the identification of causes of concrete deterioration where the records are incomplete and traditional methods of analysis are inconclusive.

5.0 COMPUTER-INTEGRATED KNOWLEDGE SYSTEMS (CIKS) FOR CONCRETE

5.1 Features and Development of a CIKS

A computer-integrated knowledge system (CIKS) is a computerized intelligent system of integrated knowledge bases providing the knowledge needed for solving complex problems.[75] The term *knowledge base* denotes any entity that contains knowledge, including models, databases, images, handbooks, guides, and standards and codes. Integration means that knowledge and data flow seamlessly (automatically) across interfaces, i.e., from one knowledge base to another.[5] A CIKS can be developed to solve problems which may require the use of databases or a wide spectrum of knowledge ranging from the experience of experts in the form of heuristics to fundamental knowledge and factual data that is contained in either locally or globally distributed databases.

The development of a CIKS involves the following major steps:[5] *(i)* defining the purpose of the system and the intended users; *(ii)* identifying and developing the appropriate architecture for the system; *(iii)* developing an information model; *(iv)* developing a prototype system; and *(v)* establishing methods for determining the reliability of, and for maintaining, the CIKS. The reliability of a CIKS will depend on the quality of the knowledge it contains.

5.2 Application of CIKS to Concrete Technology

Two examples of different applications of CIKS technology to construction materials and systems are presented, followed by a description of a prototype system for reinforced concrete.

Service Life Design. The conceptual CIKS shown in Fig. 7 incorporates an expert system along with models and databases. It maps a methodology for designing a concrete mixture design to obtain a specific service life.[5] First, an expert system and mathematical models are used to define the necessary material properties required by the concrete to give the desired service life. Then, distributed databases are searched to determine if existing mixture designs can be found which will give the necessary material properties at an acceptable cost. If such a mixture design is found it is specified; if not, a new mixture must be formulated. Several methods can be used, possibly in combination, to formulate a new mixture that is more likely to give the required properties. The new mixture can be tested, either by models or standard test methods, or a combination. If the new mixture gives the required properties, it is specified; if not the process is repeated. Note that data on each new mixture designed are "banked" into the database for further reference by those who have access to the system. An operational, prototype CIKS that can provide an estimate of the service life of reinforced concrete in which the most probable mode of degradation is chloride-induced corrosion is described in a following section.

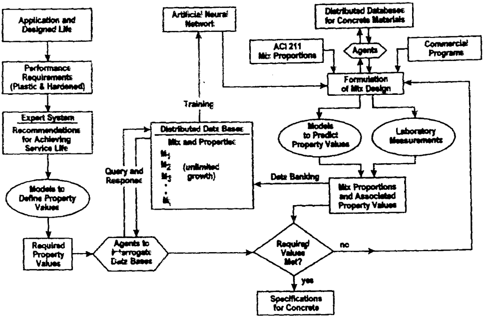


Figure 7. Conceptual CIKS for designing mixtures for HPC, based on service life requirements.[5]

Electronic Handbooks. In a recent workshop on CIKS for high-performance construction materials and systems (HPCMS),[75] a prevailing opinion was that, in the near future, a likely application of CIKS to HPCMS will be the dissemination of databases on the types, properties, and sources of commercially-available construction materials. Such databases, which could be considered to be electronic handbooks, would be of great value to designers and material specifiers. The integrating of databases with models giving reliable predictions of performance and life-cycle costs[81] should help to make apparent the technical and economical benefits of high-performance concrete and other high-performance construction materials. The integrated system should be more effective than stand-alone databases in stimulating the use of high-performance construction materials.

A Prototype CIKS for Concrete. A prototype CIKS for predicting the service life of chloride-exposed steel-reinforced concrete has recently been developed[76] (also, available on the Internet at *http://ciks.cbt.nist.gov/~bentz/welcome.html*). The system consists of a series of hypertext markup language (HTML) pages and forms which can be accessed over the World Wide Web. It includes numeric and literature databases, ACI guidelines for proportioning concrete mixtures for ordinary and high-strength concretes, simulation and service life models, and guidance on analyzing experimental results.. Forms for use in submitting input to the computer program are for:

1. Mixture proportioning of ordinary and high-strength concrete.
2. Estimating the chloride ion diffusion coefficient of a concrete as a function of mixture proportions.
3. Simulating the chloride concentration profile in a concrete exposed to an external source of chloride ions.
4. Predicting the service life of reinforced concrete exposed to an external source of chloride ions.

The steps in designing a concrete and predicting its service life are as follows: The main menu viewed upon accessing the system is shown in Fig. 8. The first step in obtaining a concrete with a desired service life is selecting the concrete materials and the mixture proportions. The current ACI guidelines for ordinary concrete[77] and for high-strength concrete[78] are computerized and they form the basis for designing the concrete mix proportions. The user fills in the form shown in Fig. 9 for proportioning an ordinary-strength concrete; then, a trial mixture design is proposed to the user along with the predicted chloride ion diffusivity *(D)*. The prediction of chloride ion diffusivity is based on a model developed at NIST.[13][14] The next step is to predict the service life of the reinforced concrete based on the assumption that the service life is the same as the initiation period (the time for the corrosion-threshold concentration of chloride ions to accumulate at the depth of reinforcement). The time for the threshold of chloride ions to reach the reinforcement is modeled using Fick's second law of diffusion.[79] In addition to knowing the value of *D*, the depth of concrete cover over the reinforcement, the concentration of chloride ions at the concrete surface must be known or assumed. Using the values given in "Example 1, Bridge Deck," from the report by Weyers and Cady,[80] the service life predictions for an ordinary concrete and a higher strength concrete are given in Table 4.

1) Ordinary strength concrete mixture proportioning (ACI 211.1-91)
2) High strength concrete mixture proportioning (with/without a water reducer) (ACI 211.4R-93 Guide)
3) Predict the chloride ion diffusivity of a concrete based on mixture parameters
4) Predict the service life of a reinforced concrete structure exposed to chloride
5) Predict the chloride ion penetration profile of a concrete after a specific time
6) Advice on analyzing chloride ion penetration profile data
7) View the literature database on chloride ion diffusivity in concrete

Figure 8. Main Menu of model CIKS for concrete.[76]

Ordinary Strength Concrete Mixture Proportioning
Based on ACI 211.1-91 Standard Practice

Compressive Strength **3500** psi (Permitted range of 2000-6000 psi)
Max. Agg. Size **1.5** in. Guidance
Dry Rodded Unit Weight of Agg. 100 lbs per cubic ft.
You may specify slump by changing value below and
turning "Specific Slump" to **On** or
you may have slump selected based on construction type
selected further down (by leaving "Specify Slump" at it **Off** value).
Slump **2.0** in.
Specify Slump On
Fineness modulus of fine ***aggregate 2.8***

Figure 9. Data entry form for the model CIKS for concrete.[(7] Showing example inputs in bold characters; SI units can be selected if desired.

Table 4. Mixture Proportions and Properties for Concrete Calculated Using the Prototype CIKS for Concrete[76]

Compressive Strength	24.1 MPa (3500 psi)	48.2 MPa (7000 psi)
w/c	0.62	0.31
Air Content	1.0%	1.5%
Cement	272 kg/m^3	597 kg/m^3
Water	167 kg/m^3	185 kg/m^3
Fine Aggregate	874 kg/m^3	470kg/m^3
Coarse Aggregate	1172 kg/m^3	1201 kg/m^3
$d \times 10^{-12}$ m^2/s	7.0	0.9
Estimated Service Life	3.8 years	29.2 years

6.0 SUMMARY

The purpose of this chapter is to draw attention to recent advances in computers and information technology that are contributing to major advances in the material science and technology of concrete. For example, these advances in computer technology have enormous implications in concrete science and technology in such areas as prediction of concrete performance, including service lives; sharing of data, information, and knowledge among geographically-dispersed concrete researchers and practitioners; and development of knowledge-based systems such as computer models and artificial intelligence decision-support systems. Also, integrating these knowledge-based systems can form systems (computer-integrated knowledge systems) that have the potential for representing virtually all scientific and engineering knowledge of concrete and making the knowledge readily available to those needing it.

In this chapter the development and application of knowledge-based systems were reviewed in the sequence: computer models; databases; artificial intelligence knowledge-based systems; and concluding with computer-integrated systems. The history of mathematical modeling of cement-based materials was reviewed from a material science perspective with an emphasis on simulation modeling as the authors believe that it will soon become the basis for the material design of concrete optimized for its application. Only a few databases were found which addressed concrete and its constituents. The development of distributed databases which are platform-independent is now possible by the use of a Remote Data Access

(RDA) standard, which is a standard for accessing data from distributed SQL-compliant relational databases. In the future it is likely that distributed databases will be linked with expert systems, with the expert system controlling the search and retrieval of data. Three types of artificial intelligence (AI) knowledge-based systems, each of which can be used to solve problems in the concrete field, were reviewed: expert systems; neural networks; and case-based reasoning systems. Expert systems and neural networks are well-established problem solvers, while case-based reasoning will likely become a competing technology. Two examples of different applications of CIKS technology to construction materials and systems were presented, followed by a demonstration of a prototype system for predicting the service life of reinforced concrete exposed to an external source of chloride ions.

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