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the better and more stable results can be obtained. A few random numbers can show oscillations in results and this is a difficulty for decision making. On the other hand many random numbers spend plenty of computer memory and time, but cannot increase the accuracy of simulation. In a sequence of application of Monte Carlo simulation, we should select many random numbers, otherwise by a few of them, we donot obtain stable results and oscillations may occur. By interpretation of the results, it is recommended to use more than 10000 random numbers in order to have non-oscillating and stable results. The computer program can handle the simulation with maximum 30000 random numbers. Figures 8 and 9 display the effect of numbers of random numbers.

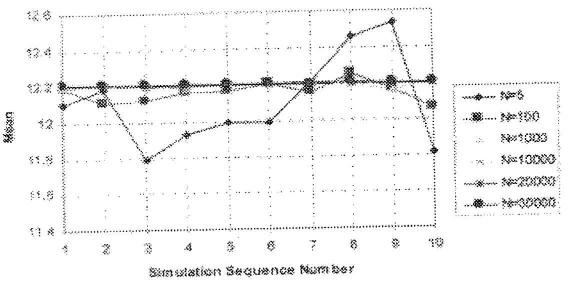

Figure (8) Effect of number of random numbers (N) on the mean of concrete carbonation front depth

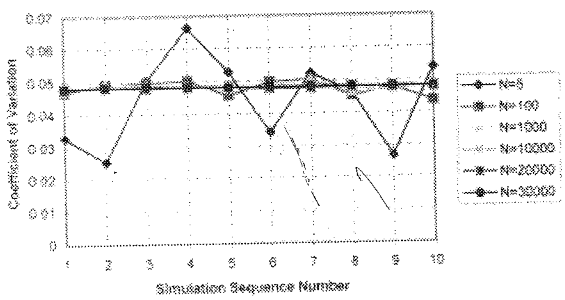

Figure (9) Effect of number of random numbers (N) on the coefficient of variation of concrete carbonation front depth

9-Conclusions

From the research work carried out on deterministic and stochastic models of carbonation depth in concrete the following conclusions can be drawn:

1-Necessity of durability design and prediction of service life of structural concrete is obvious. The proposed models in this paper are easy-to-use and can be applied in durability design procedures, especially for Persian Gulf region.

2-Engineering parameters of w/(c+csf), csf/(c+csf) and RH% are included in the models in order to relate the concrete carbonation depth with time. The use of low w/(c+csf) in concrete mixes is the most efficient way of reducing the depth of concrete carbonation.

3-Simulations of concrete complex deteriorations, such as concrete carbonation, are appropriate methods for uncertainty, risk and sensitivity analysis. An important application of probability-based simulation method is the determination of safe margins of output parameters. In other words one can find the most reliable factor of safety by these methods. The main advantage of Monte Carlo simulation method in comparison to deterministic one is its capability of showing output as a statistical parameter. Thus it is possible to conduct some risk analysis and make better decisions for Persian Gulf Region.

10-Acknowledgments

Tests of this work were conducted at the Concrete and Construction Lab of Amirkabir University of Technology.

due to the low and high relative humidities. Parabolic contribution of RH% has been introduced to overcome this imprecision of the other models. It shows that at 55% relative humidity, concrete carbonation depth is maximum.

The third parameter, csf/(c+csf), results in a partial increase of concrete carbonation coefficient and this is shown as a linear term. Similar to the results obtained in this study, there are a few reports indicating that condensed silica fume has no significant effect on the depth of carbonation of concrete [11, 12, 13].

The advantages of the model are its simplicity and inclusion of condensed silica fume. Considering these advantages the proposed model can be used in durability design procedures. Also the ability of considering low and high relative humidities are other advantages that were not found in previous models. Figures 5, 6 and 7 show some of the results obtained in the deterministic method.

b-Stochastic modelling-Monte Carlo simulation

In order to avoid extensive tests which are time consuming and costly, it is possible to apply computerized simulation. This tool has the ability of exploring the effects of all parameters on the carbonation depth as a random output.

In the present work the great advantage of this simulation is its calibration by results of several short and long-term tests. Most of the theoretical simulations have not been calibrated and this has resulted in unreliable and inaccurate models.

The advantage of the Monte Carlo simulation method is its efficiency for sensitivity analysis. This type of analysis is essential, but it is impractical to be implemented in laboratories. Using the Monte Carlo simulation, one can consider the parameter interactions and investigate the problem with the probability rules.

It must be noted that the number of random numbers for simulation is very important.As a rule of thumb, the more random numbers,

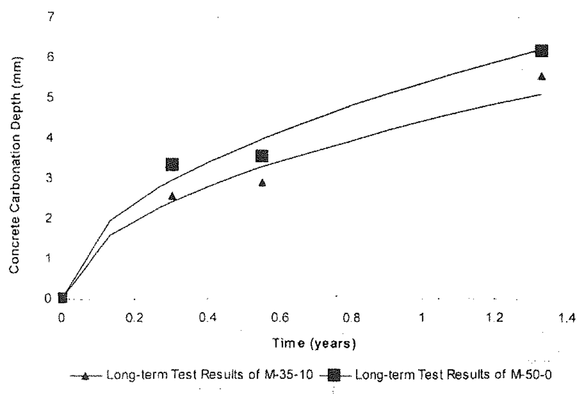

Figure (5) Comparison of model and long-term test results of two typical concrete mixes at RH% = 66% in hot-marine environment.

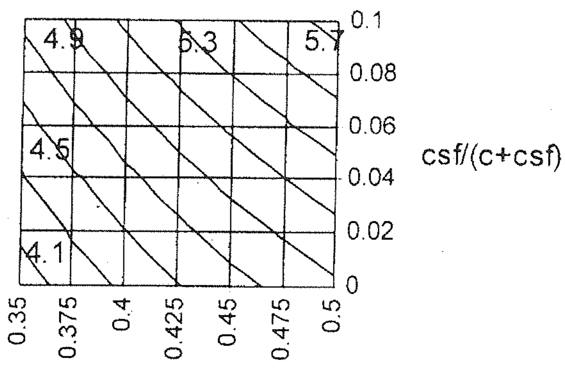

Figure (6) Concrete carbonation coefficient function with variable w/(c+csf) = 0.42 and csf/(c+csf) = 0.07.

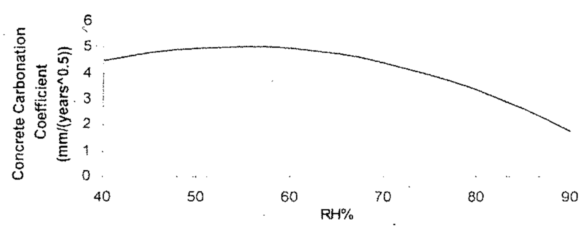

Figure (7) Concrete carbonation coefficient function with variable relative humidity for a typical mix with w/(c+csf) = 0.42 and csf/(c+csf) = 0.07.

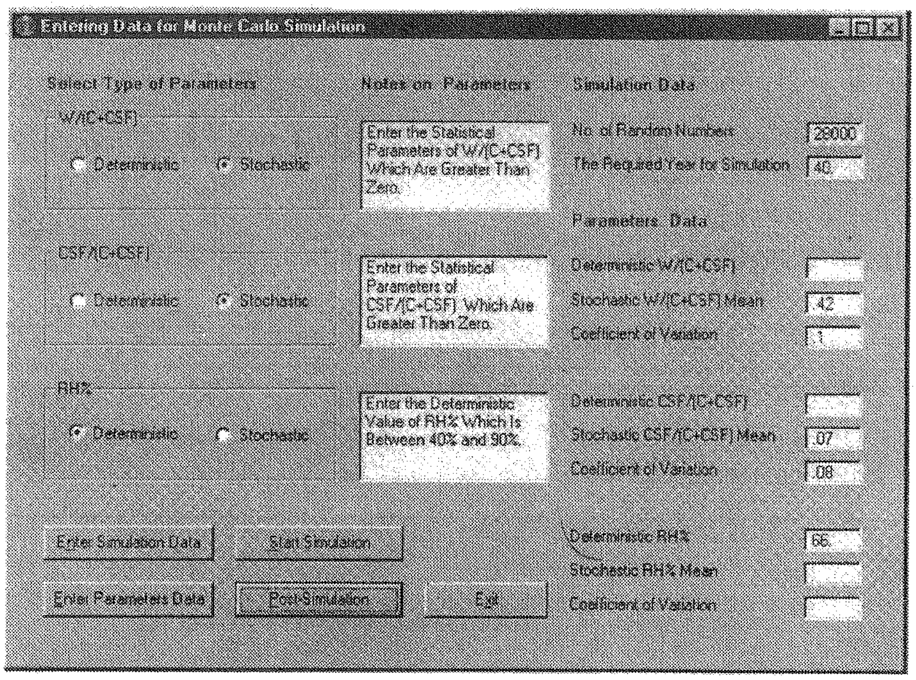

Figure (3) Input data window.

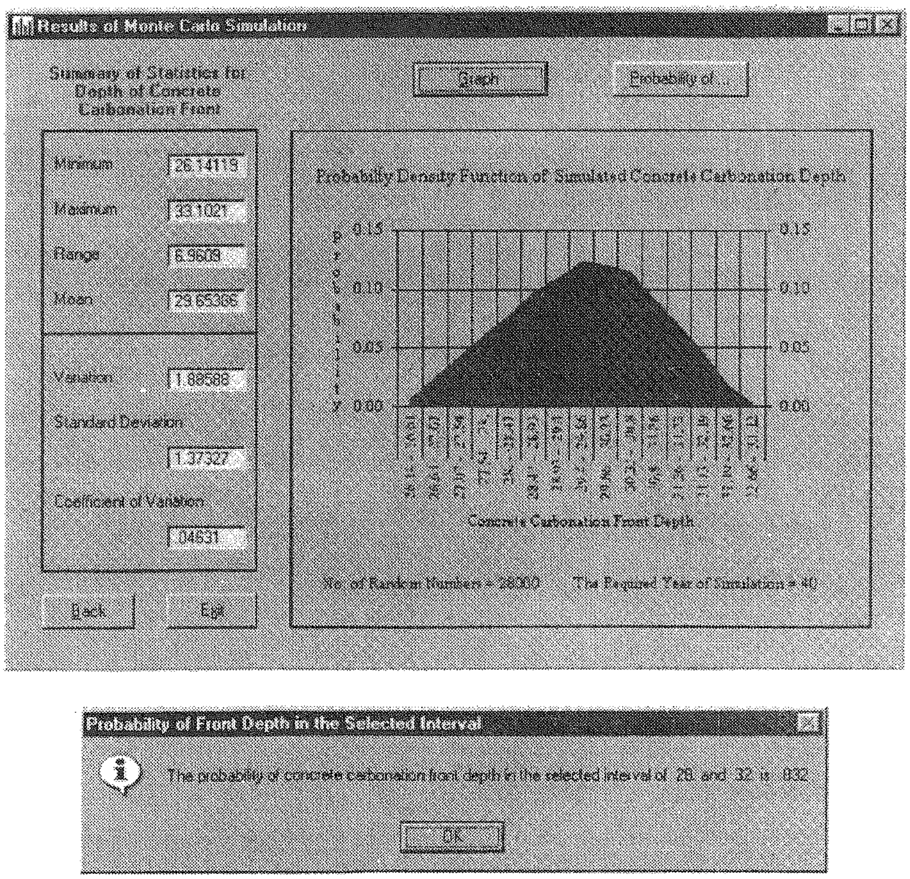

Figure (4) Output data windows.

is not applicable with deterministic models, and
3-easier sensitivity analysis.

Monte Carlo analysis is a powerful tool that can be applied for statistical analysis of the uncertainty in engineering problems. It looks like a test method that can be run by computer, instead of implementation in the laboratory. Monte Carlo simulation method is based on random numbers generation and substitution of them in the behavioral Eq. (3); [8,9].

b-3-Monte Carlo simulation by computer program for concrete carbonation depth

For simple and routine application of Monte Carlo analysis method in concerte carbonation front depth predictions, a computer program was prepared. Main principles of Monte Carlo simulation methods that are used in the program are:

1-generation of N random numbers from a uniform distribution function,

2-transformation of previous random numbers with consideration of a given or assumed probability distribution function,

3-substitution of new random numbers in the behavioral Eq. (3), and

4-statistical evaluation of results including calculation of statistical parameters and plot of concrete carbonation front depth histogram.

These steps are required for one random variable, but the capability of Monte Carlo method allows the inclusion of more random parameters as inputs. Therefore the algorithm of Monte Carlo simulation method has been extended for three random input parameters of w/(c+csf), csf/(c+csf) and RH%.

On input window of computer program, user is able to select either deterministic or stochastic parameters. Entering parameters of simulation includes the number of random numbers and the required year under investigation. Then the corresponding values of chosen parameters must be entered (see Figure 3).

Simulation can be started after data input process is completed. Results can be seen in output window, which consists of statistical summary of concrete carbonation front depth and its histogram. Also it is possible to obtain the probability of concrete carbonation front depth in specified intervals (see Figurte 4).

It must be noted that the normal distribution has been chosen for input data. The reasons of this selection are:

1-Normal distribution is widely used for many physical measurements. In fact most of the phenomena in the nature are demonstrated by normal distribution.

2-In wide ranges of parameters, normal distribution can approximate other distributions like binomial and hypergeometric ones, and

3-The most important property of normal distribution in statistics is relatively easy inferences about the population means, which are based on sampling and sample spaces. Normal distribution can be used in calculation of probabilities for sample mean levels, too [10].

8-Discussion

a-Deterministic modelling

This model which involves three parameters of w/(c+csf), csf/(c+csf) and RH% can be applied in durability design for prediction of concrete carbonation depth, x, at time, t.

It can be seen that with increasing w /(c+csf), concrete carbonation coefficient increases linearly. This was observed in many other models proposed by various researchers.

Most of the existing models are not able to exhibit the decrease of carbonation depth of phenomena for reliability analysis and/or risk acceptance of decisions have been considered. These considerations enter some complexity into codes and needs introduction of statistical or stochastic models. Consideration of the models enables the designer to examine the process and make appropriate decisions with some accepted risks. Therefore it would be possible to apply uncertainty analysis in the design procedures.

The objective of present study is the determination of concrete carbonation depth due to some uncertainties, which exist in the input parameters of the model.

It is observed that all input parameters in Eq. (3) have been considered as deterministic. Therefore the output is determinstic. But what about the random or stochastic input parameters? Obviously the output should be a random or stochastic value, too. This means that it is not possible to use Eq. (3) for uncertainty analysis.

If any input parameter is random, the response of the system as output result can be affected and consequently shows a stochastic behavior of the system.

There are a few methods that can exhibit uncertain responses. Useful probabilistic expressions of specific levels or confidence intervals can be obtained by these methods.

Two methods, which are commonly applied, are:

1-Linear statistical analysis

2-Monte Carlo analysis

It can be seen that Eq. (3) is nonlinear at least with respect to relative humidity, therefore the first method due to its linear nature cannot show precise responses. In the present investigation second method, i.e., Monte Carlo simulation method, is selected for conducting the uncertainty analysis.

b-1-Stochastic concrete carbonation depth modelling by means of Monte Carlo simulation method

Carbonation of concrete is a complex phenomenon, which is difficult to be modelled. The present models are not analytically precise and simple. The interaction of parameters affecting carbonation may increase the complexity. It is therefore necessary to carry out a number of tests to determine the relationships among various parameters. These types of models are based on experimental results. However in most cases the number of tests should be limited. In such circumstances it is preferred to use a simulation method [8].

It is worth to use real or calibrated data in the simulation technique. This enhances its accuracy, feasibility and applicability.

b-2-Basic concepts of the Monte Carlo simulation method

It is not always possible to include all parameters in the adoption of a model. Eq. (3) is an example of a model with limited parameters as input data. Ordinary models restrict the user to deterministic analysis.

However these models can be used in simulation of complex behaviors. These methods are called Monte Carlo simulations.

Processes, which are not deterministic, can be categorized as probabilistic. Monte Carlo simulation is a probabilistic model. Since the concrete carbonation front depth is probabilistic, it is possible to use Monte Carlo simulation in stochastic evaluation of the random depth.

Some Monte Carlo simulation advantages for stochastic modeling of concrete carbonation front depth are:

1-relative simplicity for approximation of complex stochastic system in behavioral nonlinear Eq. (3),

2-performance prediction in a wide range of parameters and ambient conditions, which

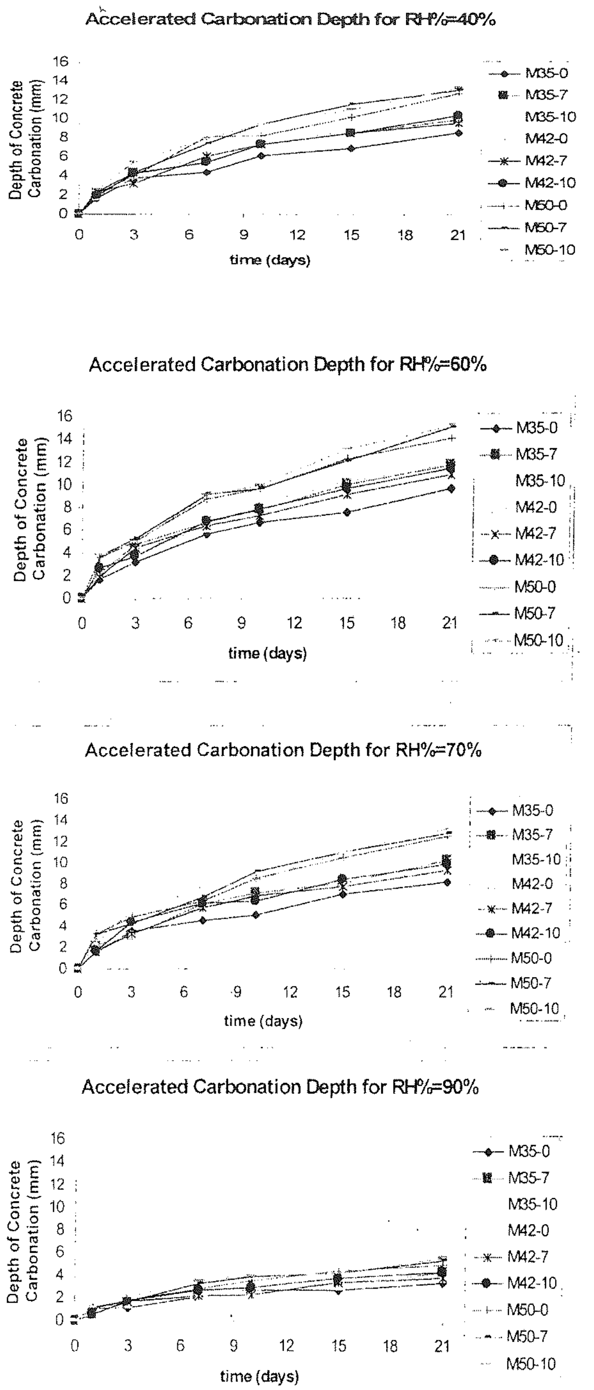

Figure (2) Accelerated test results.

In order to find the appropriate model based on the results and basic assumptions, 45 models were examined for the accelerated test conditions. Then several statistical analyses of regression, correlation and analysis of variance were carried out. This resulted in the selection of one model. This model was calibrated by incorporating the long-term test results. Finally the calibrated model of concrete carbonation depth was derived:

$$x = k.\left[\frac{w}{c+csf}.(-3.57 + 0.36RH\% - 0.00326RH\%^2) + 1.38\frac{csf}{c+csf}\right].\sqrt{t} \quad (3)$$

where:

$$k = 2.51 - 1.84\frac{w}{c+csf} + 2.18\frac{csf}{c+csf} \quad (4)$$

The following limitations should be considered in the application of the model.

$$0.35 \le \frac{w}{c+csf} \le 0.50$$

$$0.00 \le \frac{csf}{c+csf} \le 0.10$$

$$40\% \le RH\% \le 90\%$$

a-Deterministic application of the proposed model for concrete carbonation depth

As mentioned earlier, Eq. (3) is a model that is used for prediction of carbonation depth of a concrete mix at various ages knowing w / (c+csf), csf/(c+csf) and relative humidity. The determinstic attribute is selected for the type of model output. It is a fixed value. There is no need for knowing the statistical distribution of input parameters. This is a great limitation for new procedures of design codes. Observed data of concrete carbonation show that the front depth is not a fixed value and in fact is random or stochastic. Recently it has been important to know the scatter of results for margins of design processes.

b-Stochastic application of the proposed model for concrete carbonation depth

In recent research works, stochastic nature

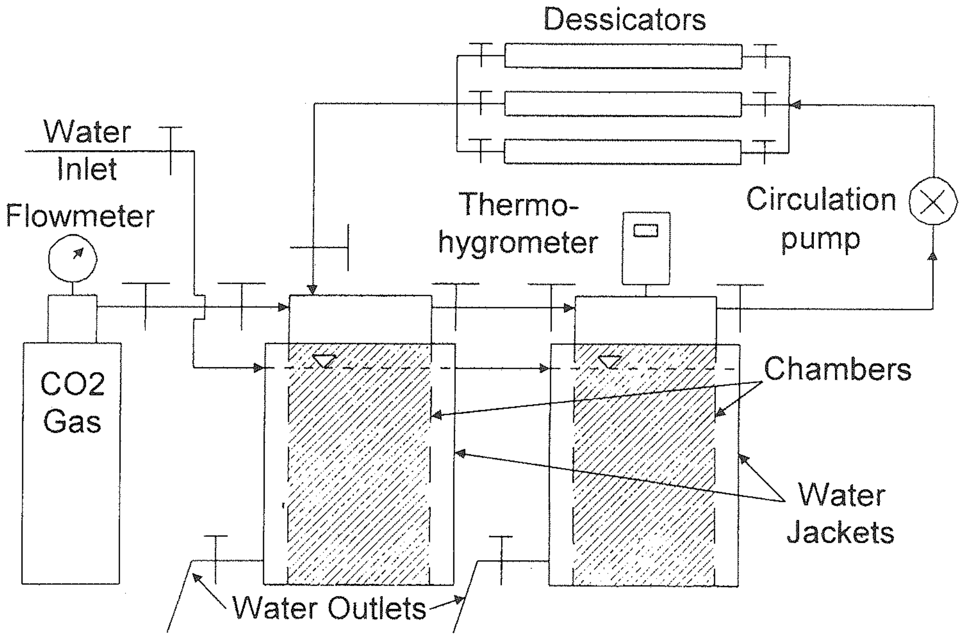

Figure (1) Schematic layout of the accelerated concrete carbonation apparatus.

Circulation of water in water jackets can control the temperature inside the chambers. Temperature and relative humidity inside the chambers were measured by a thermo-hygrometer measurement device.

Concrete specimens were prepared in cylindrical molds. They were exposed to the CO_2 gas only at two ends. Their lateral surfaces were covered by a plastic to avoid carbonation.

After 1, 3, 7, 10, 15, and 21 days specimens were removed from the chambers and their carbonation depths were measured.

d-Long-term tests

Some specimens were placed in the coastal region of Persian Gulf and protected from the rain. The depth of carbonation of these specimens was also measured at different times. The results were used for the calibration of the accelerated ones.

e-Measurement of concrete carbonation depth

In both accelerated and long-term tests, the cylindrical concrete specimens were splitted longitudinally. After removing all loose particles from the freshly broken surface, a chemical solution of ethyl alcohol and phenolphethalein was sprayed on the broken surfaces. Depth of carbonation is the distance between exposed surface of specimen to CO_2 gas and the border of color change to purple. This length must be measured at two times: firs after spraying chemical solution and then after 24 hours. The final result is the average of the two measurements.

7-Proposed model based on the test results

In the accelerated conditions, 432 concrete specimens were tested. In addition there were 90 specimens for long-term tests. It is worth mentioning that up to now some of the long term specimens have been tested and the remaining ones have been kept for further investigations. Figure 2 shows the accelerated test results.

Table (2) Fine and coarse aggregate gradations.

Sieve No.	Percent passed, by weight	
	Coarse aggregate	Fine aggregate
1/2 "	100.00	-
3/8 "	96.34	100.00
No. 4	12.52	99.40
No. 8	0.17	87.80
No. 16	-	73.50
No. 30	-	33.50
No. 50	-	11.80
No. 100	-	0.60
No. 200	-	0.30

Table (3) Concrete mix proportions and compressive strength of concrete specimens

Mix Designation	$\frac{w}{c+csf}$	$\frac{csf}{c+csf}$	Slump (cm)	F_{cu} * (MPa)
M-35-0	0.35	0.00	9	67
M-35-7	0.35	0.07	10	69
M-35-10	0.35	0.10	10	65
M-42-0	0.42	0.00	10	53
M-42-7	0.42	0.07	9	59
M-42-10	0.42	0.10	9	62
M-50-0	0.50	0.00	11	44
M-50-7	0.50	0.07	10	49
M-50-10	0.50	0.10	9	52

* 28 days Compressive strength of 10 cm concrete cubes.

It consists of two chambers for accelerating carbonation reactions. Increased concentration of CO_2 to 50% by volume in chambers can accelerate concrete carbonation reactions. After placing the specimens in the chambers, they were filled from CO_2 cylinders to adjust the CO_2 concentrtion at 50 percent. This concentrartion was preserved for all accelerated tests. It was regulated by an attached gas flowmeter to CO_2 container.

Circulation of the CO_2 and air mixture in the closed circuit produces similar condition in both chambers. When carbonation proceeds water is released from the specimens which changes the relative humidity. Relative humidity should be kept constant throughout the tests. To overcome this problem, chemical dessicators were used in three separated tubes. Air was circulated through dessicator tubes by a circulation pump.

In order to investigate the effect of relative humidity on the carbonation of concrete, tests were carried out at 40, 60, 70, and 90 percent relative humidities.

Temperature rises during the process of accelerated concrete carbonation. In order to maintain the temperature at about 27°C, two water jackets were used around the chambers.

function of the carbonation process. On the other hand in order to obtain a reliable model, a number of long-term tests should be carried out. These tests are required for calibration of the previously found function in the accelerated tests. The long-term tests were carried out in hot-marine regions of Persian Gulf. Many concrete structures in the Persian Gulf region suffer from carbonation, which leads to the early corrosion of reinforcement.

a-Materials and concrete mixes

Type 1 Portland Cement, condensed silica fume, superplasticizer, graded fine and coarse aggregates were used throughout this research program. Chemical composition and physical properties of cement and condensed silica fume are shown in Table 1. Both cement and condensed silica fume are products of Iranian factories. Table 2 shows the gradation of aggregates. Tables 1 and 2 are based on the test results conducted by the authors.

The main parameters of concrete mix designs are w/(c+csf) and csf/(c+csf). In all concrete mixes, the slump of fresh concrete maintained within the range of 10 ± 1 cm. Superplasticizer was used to adjust the slump of concrete mix proportions and compressive strength of concrete specimens. Table 3 show the concrete mix proportions and compressive strength of concrete specimens. In this table the mix designation is selected for the second and third column values.

b-Ambient conditions of hot-marine regions of Persian Gulf

Considering the meteorological data of Bandar-Abbass stations, which is a coastal region of Persian Gulf, the annual mean temperature and relative humidity values are:

annual mean temperature = 27°C

annual mean relative humidity = 66%

c-Accelerated tests

In order to conduct the accelerated tests, an apparatus as shown in Figure 1 was set up.

Table (1) Chemical composition and physical properties of cement and silica fume.

Chemical properties(% by weight)			Physical properties		
Chemical composition	Cement	Condensed silica fume		Cement	Condensed silica fume
SiO_2	21.46	91.70	Specific Gravity	3.125	2.20
Al_2O_3	5.55	1.00	Fineness (m^2/kg)		
Fe_2O_3	3.46	0.90	Blaine	330	-
CaO	63.95	1.68	Specific Surface	-	14000
MgO	1.86	1.80	Setting Time (min)		
Na_2O	0.26	-	Initial	135	-
K_2O	0.54	-	Final	245	-
SO_3	1.42	0.87	Compressive Strength (kg/cm^2)		
LOI	0.81	-	3 days	170	-
Insol. Res.	0.58	-	7 days	270	-
Free Lime	0.76	-	28 days	400	-
C_3S	50.96	-			
C_2S	23.10	-			
C_3A	8.85	-			
C_4AF	10.53	-			

concrete carbonation and applying the diffusion theory, it is possible to derive a partial differential equations system. This mathematical system which is based on the chemical and physical laws can be appropriate for investigation of concrete carbonation and front depth determination at a specified time.

Although this method is powerful, there is not any interest for inclusion of it in the design specifications and codes. Design engineers prefer to use a simple and comprehensive model, which includes common and important engineering parameters. To achieve this goal, some simplifications and reliable assumptions are needed.

Considering these limitations, it was decided to make a simple but applicable model. This model was based on diffusion theory and calibrated with the data obtained in the real accelerated and long-term tests. Such models are more reliable than merely theoretical or experimental ones.

For the first step of finding the model frame, the well known carbonation model which is based on Fick's laws was used [6], [7]. This model is shown by the following equation.

$$x = A\sqrt{t} \qquad (1)$$

where:
x = diffusion depth,
A = coefficient of diffusion, and
t = time.

This equation is called the "square root of time law". The results obtained in both accelerated and long term carbonation fit this equation. In order to construct a reliable model, Eq. (1) was calibrated with the application of data obtained from experimental work. The calibration affects the coefficient of diffusion value.

5-General form of the proposed model

Investigation of the existing models revealed the fact that chemical or physical parameters were mainly used. These parameters are not familiar for most of design engineers. The most common applied parameters in the design are water to cementitious materials ratio, replacement level of pozzolans, relative humidity, temperature, mix proportions, compressive strength, and so on.

In this research work due to the characteristic of concrete carbonation process, which is the combination of internal and external parameters, it was decided to find a model in the following form:

$$x = k.f\left(\frac{w}{c + csf}, \frac{csf}{c + csf}, RH\%\right).\sqrt{t} \qquad (2)$$

where:
x = concrete carbonation depth (mm),
k = calibration factor,
w/(c+csf) = water to cementitious materials ratio,
csf/(c+csf) = condensed silica fume to cementitious materials ratio,
RH% = ambient relative humidity (%), and
t = time (years).

It should be noted that the ambient temperature has a little effect on the carbonation process [5], [6]. Therefore in the proposed model, temperature was assumed as a constant parameter in calibration. As can be seen, a set of selected engineering parameters was implicitly included in the coefficient of carbonation in Eq. (1).

6-Accelerated and long-term tests

A special program for necessary experiments was prepared. Due to the slow rate of concrete carbonation process, it was decided to accelerate some of the tests. This type of test shows the general behavioral their criteria and recommendations. The above definition needs to introduce a function of performance, which is time-dependent. These types of deterioration modelling and introducing new and capable models are the main topics in the durability research programs.

In the present investigation, carbonation of concrete under accelerated and long term conditions are studied. Carbonation is a time-dependent phenomenon and initiates the corrosion of steel reinforcements. Attempt was made to model the depth of carbonation by means of deterministic and stochastic methods.

2- Concrete carbonation phenomenon

One of the common deteriorations of reinforced concrete structures is corrosion of steel bars. The main causes of corrosion of steel bars are carbonation and/or ingress of chloride ion in the porous media of concrete.

Concrete has a high pH (more than 12. 6) and this produces a protection against corrosion of embedded steel reinforcements. A thin film of protective oxide covers the steel reinforcements and consequently corrosion cannot continue or becomes slow. Time of corrosion initiation is the time of destruction of this protective layer on the reinforcements. At this stage the pH of concrete is dropped below about 9.0. Proper concerte mix design and selection of sufficient cover depth can obtain protection of steel bars against carbonation. If the above mentioned prevention methods are considered in the design procedure, the carbonation phenomenon will not be an important parameter for the achievement of the required service life of the concrete structures. In order to achieve this goal, it is necessary to introduce appropriate and capable models for the prediction of the depth of carbonation of concrete.

3-Physicochemical processes of concrete carbonation

The physicochemical processes involved in concrete carbonation are:

1-The chemical reactions from which carbonatable materials are produced.

2-The diffusion of atmosphere CO_2 in the gaseous phase of the concrete pores.

3-The dissolution of solid $Ca(OH)_2$ in the pore water and the dissolution of dissolved $Ca(OH)_2$ in the aqueous phase of the pores.

4-The dissolution of CO_2 in the pore water and its reaction with dissolved $Ca(OH)_2$.

5-The reaction of CO_2 with the other solid carbonatable constituents of hardened cement paste.

6-The reduction of pore volume due to solid products of hydration and carbonation.

7-The condensation of water vapor on the walls of concrete pores, in equilibrium to the ambient temperature and relative humidity conditions.

In some researches these steps have been considered and a set of differential equations have been derived for investigating the problem, but these types of methods cannot be practical and easy to use [5]. Appropriate and reliable models for the inclusion in the specifications must be simple, accurate and practical.

It is worth mentioning that the appropriate models are those with the theoretical bases and calibrated by means of experimental results. This was applied and followed throughout this investigation.

4-Theoretical concept of the proposed model, Diffusion theory

Considering the multistage process of

Deterministic Modelling and Stochastic Monte Carlo Simulation of Relatively High-Strength Concrete Carbonation Depth for Hot-Marine Regions of Persian Gulf

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Abstract

Today durability and consideration of maintenance and repair methods of concrete structures have become necessary in the design procedures. These are not only important in the design stages, but also necessary for management. Carbonation of concrete is the major factor for initiation of steel reinforcement corrosion. This type of deterioration exists in the southern regions of Iran, especially in the hot-marine environment of Persian Gulf.

In this paper, a deterministic model of concrete carbonation, based on the experimental data, was proposed. Then by using the Monte Carlo simulation technique, a stochastic model for the depth of carbonation of concrete was developed. The advantage of the presented models is the contribution of condensed silica fume as a relatively new pozzolan, which was not found in the past investigations.

Key Words

Deterministic modelling, Monte Carlo simulation, Concrete carbonation, Condensed silica fume, Hot-marine environment, Persian Gulf.

1-Introduction

Since the last decade researchers have given a great attention to attain some knowledge on the mechanisms and modelling of reinforced concrete deteriorations. This is due to the new ideas and development in the design process. Recently the durability design and service life prediction of structures has become the main issue in the design procedures [1,2].

Durability design is mainly used for the completion of the design concrete structures. New horizons of its usage in maintenance, improvement and repair methods are now opened. Provision of technical codes and reliable and advanced specification are the first steps in the durability design of structures.

It must be noted that, there are two basic applications for the service life prediction in durability design methods:

1-Quantitative design of new structures

2-Prediction of residual service life and performance of available structures in order to control and manage the required methods of maintenance, improvement and repair [3,4].

Durability can be defined as: capability of a building, assembly, component, structure, product or material to maintain minimum performance over at least a specified time under the influence of degradation factors [2]. This definition infers that the time has a great influence on the performance of materials. Unfortunately most of the existing specifications have not considered time in