

Bayesian Inference for Prediction of Carbonation Depth of Concrete Using MCMC

S. TASAKA*, M. SHINOZUKA**, S. RAY CHAUDHURI***, U. J. NA****

ABSTRACT

Bayesian inference of model parameters for the time dependent carbonation depth $C = C(t)$ of concrete is presented. The statistical model is assumed to have a form of $C = \alpha t^\beta + \varepsilon$ where α implies the carbonation coefficient and ε stands for the modeling error which is assumed to have a normal distribution with zero mean and unknown variance. By the use of existing data for the natural outdoor exposed concrete, the posterior distributions of the parameters are obtained by the Markov Chain Monte Carlo (MCMC) method, the implementation of which is made using WinBUGS. The corresponding linear statistical model equation is also considered, where the effect of small variance of the error on the number of samples in MCMC is illustrated. The compatibility of probability distributions of the carbonation coefficient for different values of β is examined. It is shown that the carbonation coefficient derived from the carbonation depth for each t has a lognormal distribution if $\beta = 0.5$ (the square-root-t law), whereas, for $\beta = 0.33$, a normal distribution is a better approximation.

KEY WORDS: carbonation depth, concrete, Bayesian inference, MCMC, WinBUGS

1. Introduction

Carbonation of concrete is one of the major factors causing the deterioration of reinforced concrete structures. The corrosion of steel reinforcement will occur due to carbonation, resulting in cracking and peeling of the cover concrete. This eventually affects the lifetime of reinforced concrete structures. Accurate service life prediction is, hence, necessary for the purpose of both avoiding unexpected high repair costs and reducing the life cycle cost.

Carbonation of non-cracked concrete proceeds from the surface to the inside, and the distance between the surface and carbonation front is defined as the carbonation depth. The carbonation depth is a time dependent process, the rate of which may depend on

several properties of concrete, e.g., the water cement ratio, air content, and admixtures. The modeling of the temporal variation of the carbonation depth has extensively been studied on the basis of the square-root-t law^{1,2,3}; that is, the carbonation depth is proportional to \sqrt{t} with the time independent coefficient termed as the carbonation coefficient. Recent studies^{4,5,6} have shown that the power of t is not necessarily equal to 0.5. This is because through the carbonation process the pore volume reduction takes place and as a result the diffusivity or the carbonation coefficient changes in time, in contrast to Fick's law of diffusion. This reduction in the carbonation rate and its influence on the time dependent carbonation depth may be taken into account by putting the power of t to be less than 0.5, while keeping the carbonation coefficient as a constant.

On the other hand, the time dependent carbonation depth generally involves randomness and uncertainty due to modeling errors and the variability of the material properties of concrete. Therefore, statistical and probabilistic approaches are necessary and efficient for practical purposes⁷.

* Department of Architecture

** Department of Civil and Environmental Engineering, University of California, Irvine, CA, USA

*** Department of Civil Engineering, Indian Institute of Technology, Kanpur, UP 208016, India

**** Busan port construction office, Ministry of Land, Transport and Maritime affairs, Dong-Gu, Busan, 601-726, Korea

This article presents Bayesian statistical inference for model parameters of the carbonation depth. The Bayesian approach has the capability of treating uncertainties involved in the estimation of parameters. In other words, the parameter estimation comes up with the posterior distribution for given random samples of relevant model variables. For presenting illustrative examples, random samples are taken from existing data for the outdoor exposed concrete⁴⁾. On the basis of Bayes' theorem, the posterior distribution is obtained by the Markov Chain Monte Carlo (MCMC) method⁸⁾, the implementation of which is achieved by the open source software, WinBUGS⁹⁾.

Note that the Bayesian regression analysis for a linearized statistical model equation is also presented. The effect of the small variance of the modeling error in the linear model upon the number of samples for convergence of chains is also demonstrated in this study.

Finally, the goodness of fit of probability distributions for the carbonation coefficient is examined. Sample data derived from the measured values of the carbonation depth divided by t^β are utilized for this purpose. It is shown that the carbonation coefficient has a lognormal distribution if $\beta = 0.5$ (the square-root-t law), whereas the normal distribution becomes more appropriate when $\beta = 0.33$ which is the result of the Bayesian estimate.

2. Statistical Model of Carbonation Depth

The equation of statistical prediction model for the carbonation depth $C = C(t)$ is assumed to have the following form:

$$C = \alpha t^\beta + \varepsilon \quad (1)$$

where α and β are model parameters, and ε implies the modeling error having the zero mean normal probability distribution denoted by

$$\varepsilon \sim N(0, \sigma^2) \quad (2)$$

in which σ^2 is the unknown variance. This implies that C is normally distributed with mean αt^β and variance σ^2 .

For the given sets of data (C_i, t_i) where $C_i = C(t_i)$, the estimation of the model parameters α , β and σ^2

can be made by nonlinear regression analysis methods. On the other hand, Eq.(1) may be rewritten as

$$\ln C = \ln \alpha + \beta \ln t + \varepsilon' \quad (3)$$

where

$$\varepsilon' \sim N(0, \sigma'^2) \quad (4)$$

Thus, $\ln C$ has a normal distribution with mean $\ln \alpha + \beta \ln t$ and variance σ'^2 .

In this paper the Bayesian approach is applied to Eqs.(1) and (3). The prior distribution may be subjective, so as to reflect expert opinions, and/or non-informative in a sense that there is little or no prior knowledge about the parameters.

3. Bayesian Inference

Let $X_i, i = 1 \sim n$, be random samples of the population X , the parameter of which is denoted by $\theta = (\theta_1, \theta_2, \dots, \theta_m)$, where n and m imply the number of random samples and parameters of X , respectively. Let $p(x|\theta)$ be the conditional probability density function of X , given θ , which can be considered as the likelihood function of θ , given x . Let $p(\theta)$ be the prior distribution of θ . Then, the posterior distribution of θ , $p(\theta|x)$, is obtained by Bayes' theorem as follows¹⁰⁾:

$$p(\theta|x) = \frac{p(x|\theta)p(\theta)}{\int p(x|\theta)p(\theta)d\theta} \quad (5)$$

where the denominator implies the normalizing constant. In this study $X_i = (C_i, t_i)$ with a deterministic t_i and $\theta = (\alpha, \beta, \sigma^2)$. The likelihood function thus becomes a function of n independent and identically distributed samples as follows:

$$p(x|\theta) = \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(C_i - \bar{C}_i)^2}{2\sigma^2}\right] \quad (6)$$

where \bar{C}_i is the mean value of C_i which is equal to αt_i^β .

For the prior distribution we assume that α and β have a zero mean normal distribution and σ^2 an inverse gamma distribution; that is,

$$\alpha, \beta \sim N(0, \sigma_0^2), \quad \sigma^2 \sim IG(\nu_0, \lambda_0) \quad (7)$$

$$\nu_0 = \lambda_0 = 0.001.$$

in which σ_0^2 , ν_0 (shape parameter) and λ_0 (scale parameter) are hyper parameters. Note that the inverse gamma probability density function is given in the form:

$$f(x|\nu_0, \lambda_0) = \frac{\lambda_0^{\nu_0}}{\Gamma(\nu_0)} \left(\frac{1}{x}\right)^{\nu_0+1} \exp\left(-\frac{\lambda_0}{x}\right), x > 0 \quad (8)$$

To represent the non-informative prior distribution, a large value for σ_0^2 and small values for ν_0 and λ_0 are assumed¹¹⁾. Figure 1 shows an illustration of the inverse gamma probability density function with $\nu_0 = \lambda_0 = 0.001$.

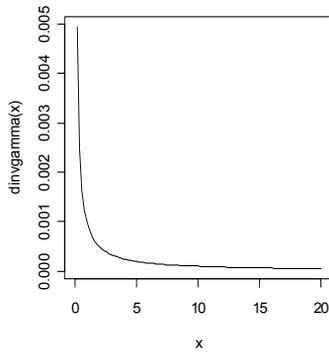


Fig.1 The inverse gamma distribution (σ^2) with $\nu_0 = \lambda_0 = 0.001$

The MCMC method enables us to draw samples from the posterior distribution $p(\theta|x)$. A major advantage in MCMC is that there is no need to compute the normalizing constant in Eq.(5) which usually involves multidimensional numerical integration.

4. Prediction of Carbonation Depth

Test data of carbonation for outdoor exposed ordinary and flowing concrete at 2, 4.5, 15 and 25 years are used⁴⁾. Numerical values of the carbonation depth obtained from the figures of the referred measurements are given in Table 1. The numeral shown in the specimen identification implies the value of slump in cm. A total of 20 pairwise data (C_i, t_i) are used for the parameter estimation.

The statistical prediction model for the carbonation depth shown in Eq.(1) is assumed. Three parameters α , β and σ^2 are supposed to have the non-informative prior distribution given by Eq.(7) with $\sigma_0^2=10,000$ and

Table 1 Carbonation depth with respect to time

Duration years	Specimen (mm)					
	C-12	C-15	C-18	C-21	F8	F12
2	6.4	3.4	4.8	4.2	6.1	5.3
4.5	7	6.6	6.4	6.4	6.2	6.3
15	8.1	9.1	10.2	9.4	11.5	8.8
25	—	—	—	10	—	13.9

C: Ordinary concrete, F:Flowing concrete

Figure 2 presents the history of samples of each parameter in which the total number of samples, N , is 100,000 and the burn-in period (discarded samples at the beginning of the MCMC run), N_b , is 10,000. It can be observed that sufficient mixing is achieved, implying that the samples are in the steady state. In other words, the samples used for obtaining Bayesian estimates are from convergent Markov chains. Note that mixing is not yet fully achieved when $N = 10,000$ (cf. Fig.6).

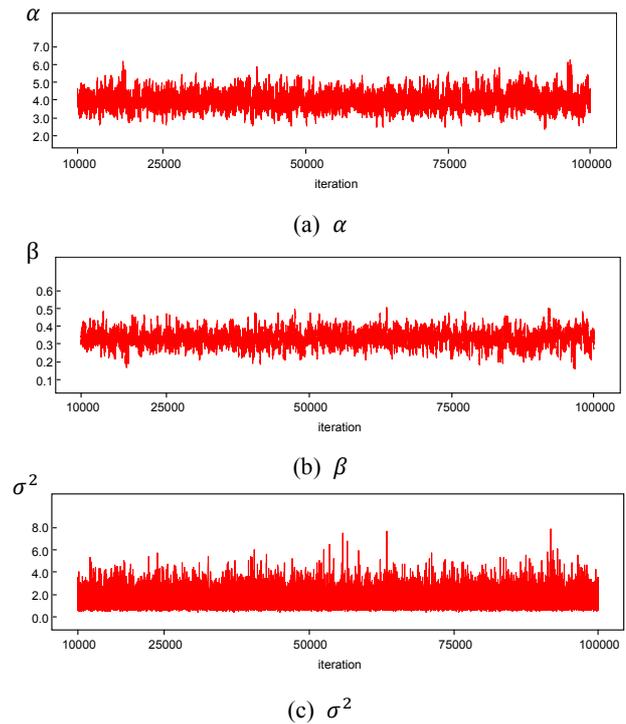


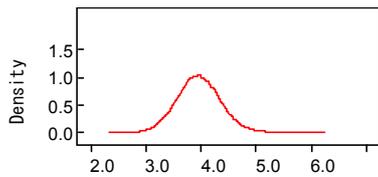
Fig.2 Sample histories of parameters with $N = 100,000$ and $N_b=10,000$

The posterior distribution of the samples of each parameter is given in Fig.3 and statistics of those parameters are presented in Table 2. It can be observed from the mean and median values that α and β are nearly normal. Values of the coefficient of variation of α and β are 9.8% and 12.3%, respectively, and those

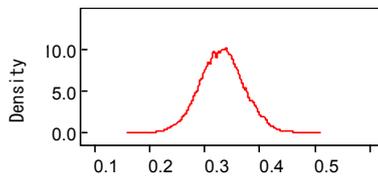
are smaller than that of σ^2 (37.9%). If the posterior distribution of σ^2 is approximated by the inverse gamma distribution, then the shape and scale parameters, ν and λ respectively, may be obtained by statistics given in Table 2 as follows.

$$\nu = \left(\frac{\text{mean}}{SD}\right)^2 + 2 = 8.978$$

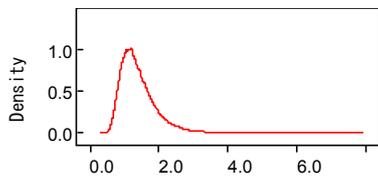
$$\lambda = \text{mean} \cdot (\nu - 1) = 11.169$$



(a) α



(b) β



(c) σ^2

Fig.3 The posterior distribution of each parameter

The resulting probability distribution is shown in Fig. 4. A good agreement is observed when compared with that in Fig.3.

From Table 2 we can see that the mean values of the carbonation coefficient, α , and the power of t , β , are 3.96 and 0.33, respectively. These Bayesian estimates are fully consistent with the deterministic regression analysis results as given in Ref.4, the values of which are 3.897 and 0.34.

Table 2 Statistics of each parameter

	α	β	σ^2
mean	3.96	0.33	1.40
median	3.95	0.33	1.29
SD	0.39	0.041	0.53

SD:Standard Deviation

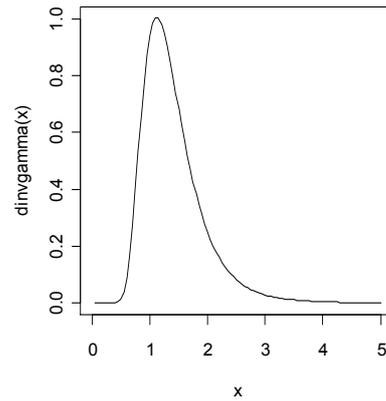


Fig.4 The inverse gamma distribution (σ^2)

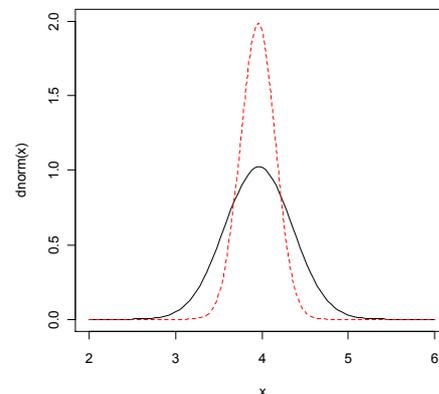
5. Illustration of Additional Bayesian Updating

Assuming that the posterior distribution of the model parameters has been expressed by known probability distribution functions, then Bayesian updating can be

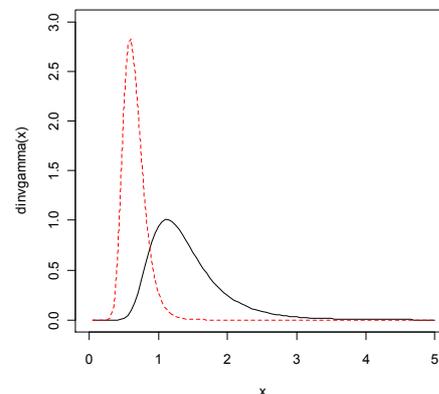
Table 3 Statistics of each parameter (Additionally updated)

	α	β	σ^2
mean	3.95	0.33	0.65
median	3.95	0.33	0.63
SD	0.20	0.021	0.16

SD:Standard Deviation



(a) α



(b) σ^2

Fig.5 Comparison between prior and posterior distributions

made by using the prior distribution replaced by the obtained posterior one, and applying Bayes' theorem again to update the posterior distribution.

Table 3 shows statistics of each parameter of the updated posterior distribution obtained again by the use of WinBUGS. Note that, for the purpose of illustration, the same 20 pairwise data given in Table 1 are employed in the updating. It can be observed that the mean values of α and β are almost the same as those in Table 2, but the standard deviations are reduced to almost one-half. This means that the uncertainty existing in the parameter estimation is decreased to a certain extent through the Bayesian updating.

Figure 5 presents the comparison between the prior and posterior distributions of α and σ^2 , where the dotted line denotes the posterior distribution. It is seen that not only the standard deviation, but also the mean value of σ^2 , has been decreased.

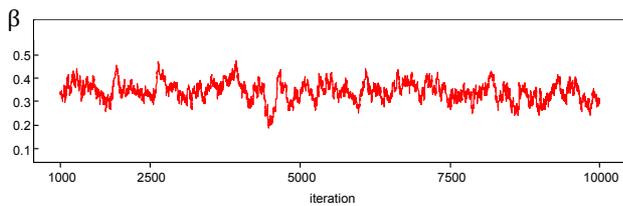
6. Bayesian Linear Regression Analysis

Another possible Bayesian approach is to make use of the statistical model Eq.(3) instead of Eq.(1). The pairwise data (C_i, t_i) are now changed into $(\ln C_i, \ln t_i)$.

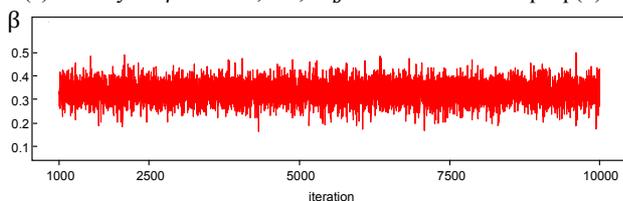
Table 4 Statistics of each parameter

	$\ln \alpha$	α	β	σ^{-2}
mean	1.36	3.91	0.33	0.026
median	1.36	3.90	0.33	0.025
SD	0.080	0.31	0.039	0.010

SD:Standard Deviation



(a) History of β : $N=10,000, N_b=1000$ for model eq.(1)



(b) History of β : $N=10,000, N_b=1000$ for model eq.(3)

Fig.6 Effect of small variance on convergence

The result of the Bayesian regression analysis is given in Table 4. Statistics of α are derived from $\ln \alpha$

under the assumption that α is lognormal. However, since the variance of $\ln \alpha$ is rather small, α can be considered nearly normal. We can see that α and β are in good agreement with those given in Table 2, whereas the uncertainty of modeling error, σ'^2 , is much smaller than that of σ^2 . The effect of this small variance in the modeling error upon the MCMC analysis is demonstrated by examining the number of samples which are necessary for convergence of chains. Figure 6 presents sample histories of the posterior distribution of β , and reveals that 10,000 samples are insufficient for convergence of chains for Eq.(1), but sufficient for Eq.(3).

7. Probability Distribution of the Carbonation Coefficient

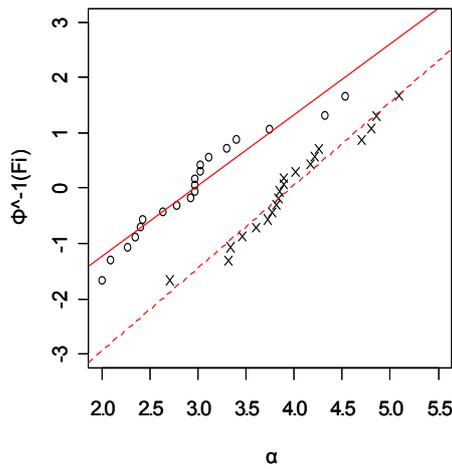
From the data of the carbonation depth, C_i , given in Table 1, data of two different carbonation coefficients, $\alpha_i^{0.5}$ and $\alpha_i^{0.33}$, are used to find the compatible probability distribution of each carbonation coefficient. Here, $\alpha_i^{0.5}$ denotes the carbonation coefficient calculated by C_i/t^β with $\beta = 0.5$ for each t , and $\alpha_i^{0.33}$ is similarly defined. Plotting these data on several probability papers enables us to find the most suitable probability distribution for the respective carbonation coefficient. In this study, consideration is limited to the case of normal and lognormal distributions only.

Figure 7 shows the result of linear least squares fitting for the plotting on normal and lognormal probability papers, in which the ordinate represents the value of $\Phi^{-1}(F_i)$ with $\Phi(\cdot)$, the standard normal probability distribution function, and

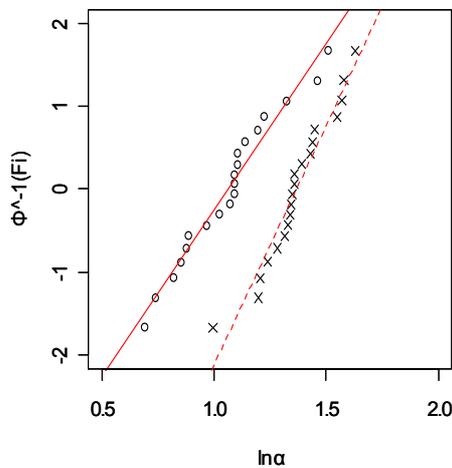
$$F_i = \frac{i}{n + 1}, i = 1 \sim n \tag{9}$$

where n means the number of data.

Table 5 gives the result of R^2 , which provides information on the goodness of fit, for each probability distribution. We can see that the lognormal distribution is more suitable when $\beta = 0.5$, but the normal distribution seems to be more appropriate when $\beta = 0.33$.



(a) Normal probability paper



(b) Lognormal probability paper

Fig.7 Least squares fitting of probability distributions;
 ○($\beta = 0.5$) and ×($\beta = 0.33$)

Table 5 Results of the goodness of fit

Distribution	β	R^2
Normal	0.5	0.9243
	0.33	0.9554
Lognormal	0.5	0.9650
	0.33	0.9462

8. Conclusions

Carbonation of concrete is one of the major factors causing the deterioration of reinforced concrete structures and thus reducing their service life prediction. In this study an attempt is made to utilize the Bayesian inference model for updating the model parameters of carbonation depth prediction. The following observations are made:

(1) The Bayesian method was applied to the prediction of the carbonation depth of concrete, and WinBUGS was found to be efficient for the implementation of the

MCMC algorithm.

(2) For a given set of data of the carbonation depth the Bayesian approach can be easily applied to get the posterior distribution of model parameters, and further additional updating can be made even if only a small number of data is available. This will be useful for making decisions and improving risk management of structures with limited information.

(3) The goodness of fit of probability distributions for the carbonation coefficient may depend on the rate of carbonation. For the given parameter space, the lognormal and normal distributions are appropriate for cases where $\beta = 0.5$ and 0.33 , respectively.

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