Life Prediction of Existing Concrete Structures in Acid Rain Environment

Ying Huang

[1]Department of Architecture and Civil Engineering, Jiangxi Science & Technology Normal University, Nanchang, 330013, China

[a]email: huangying7871@163.com

Abstract. In the paper based on diffusion theory the acid rain erosion-carbonization model was established. The model parameters were analyzed and the model was solved by MATLAB software. At same time the failure criteria of existing concrete structure in acid rain area was developed and the life prediction method was proposed. Finally, combined with the acid rain feature in Nanchang the multi-storey teaching building life was predicted to prove the validity of the model. The calculation showed the acid rain damage to the building in Nanchang is more serious. It should be taken seriously enough.
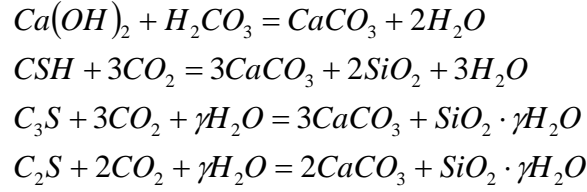
Introduction

Acid rain is the rain, snow, frost, mist or other forms of atmospheric precipitation whose PH value is less than 5.6[1]. The erosion of acid rain on the concrete structure has two ways. On the one hand, acid rain directly corroded the concrete structures. On the other hand, acid rain can make the concrete structures neutralization, which caused steel corrosion and reduce the service behavior. The major energy in China is coal. With the rapid development of economy, the coal consumption is increasing. And SO2 emissions continue to grow, which make China become the third largest acid rain area after Europe and North America. Under the effect of the multiple factors-acid rain, carbonization and load-the service behavior of concrete structures in acid rain area continue to deteriorate. But the damage on the concrete structures caused by multiple factors is not a simple superposition of a single factor. So it is necessary to carry out the research work on the working state and life prediction of concrete structures in acid rain area under the action of multiple factors.

The scholars[2-5] at home and abroad carried out a series of experimental and theoretical research works on acid rain erosion mechanism. Reference [6, 7] is about concrete carbonation regularity under stress condition. The neutralization mechanism and regularity of concrete structures under the coupling action of stress, carbonation and acid was qualitatively analyzed in reference [8]. However, research on service performance of concrete structures in acid rain area considering carbonation is few, the research needs to be deepened. The research on the working state assessment and life prediction of existing concrete structures in acid rain is rare. In the paper based on diffusion theory the acid rain erosion-carbonization model was established. The model parameters were analyzed and the model was solved by MATLAB software. At same time the failure criteria of existing concrete structure in acid rain area was developed and the life prediction method was proposed. Finally, combined with the acid rain feature in Nanchang the multi-storey teaching building life was predicted to prove the validity of the model. The calculation showed the acid rain damage to the building in Nanchang is more serious. It should be taken seriously enough.

Concrete neutralization mechanism and model

Carbonization is the physical and chemical process that the cement hydration in concrete reacted with CO_2 and decomposed carbonate compounds and other substances. The main chemical equation of concrete carbonation are as follows:

$$Ca(OH)_2 + H_2CO_3 = CaCO_3 + 2H_2O$$
$$CSH + 3CO_2 = 3CaCO_3 + 2SiO_2 + 3H_2O$$
$$C_3S + 3CO_2 + \gamma H_2O = 3CaCO_3 + SiO_2 \cdot \gamma H_2O$$
$$C_2S + 2CO_2 + \gamma H_2O = 2CaCO_3 + SiO_2 \cdot \gamma H_2O$$

In concrete carbonation process CO_2 diffusion rate in concrete pores is the control factor[9]. And CO_2, CH, CSH and non-hydrated silicate compounds is in accordance with law of conservation of mass. Based on the diffusion theory the carbonation model was established by Greek scholars V. G. Papadakis. Generally the length size of concrete member is large than the section size, the three-dimensional problem was simplified as a two-dimensional problems of CO_2 diffusion in concrete. Assuming that the ambient temperature and humidity is relatively stable, the active ingredient in cement completely hydrated. Then the carbonization model is as follows:
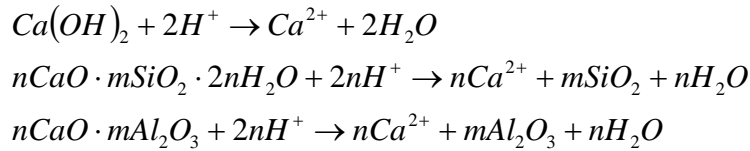
$$\frac{\partial}{\partial t}[CO_2] = D_{CO_2}\left(\frac{\partial^2[CO_2]}{\partial x^2} + \frac{\partial^2[CO_2]}{\partial y^2}\right) - (K_{CH} + 3K_{CSH})[CO_2] \tag{1}$$

$$\frac{\partial}{\partial t}[CH] = -K_{CH}[CO_2] \tag{2}$$

$$\frac{\partial}{\partial t}[CSH] = -K_{CSH}[CO_2] \tag{3}$$

Where, D_{co2} is CO_2 diffusion coefficient in concrete; $[CO_2]$, $[CH]$, $[CSH]$ respectively refer to the concentration of CO_2, CH, CSH; K_{CH}, K_{CSH} respectively refer to the carbonation reaction constant of CH, CSH(K_{CH}, $K_{CSH} = 7.8\times10^{-3}m^3\cdot(mol\cdot s)^{-1}$); x, y is respectively distance to concrete surface; t is carbonization time.

Acid rain is rich in H^+ ions. When acid rain drop down the concrete surface and into the concrete pores the neutralization reaction with H^+ ions and the cement hydration occurred, which make the PH of concrete decrease and rebar depassive. The main chemical equations of acid rain erosion are as follows:

$$Ca(OH)_2 + 2H^+ \rightarrow Ca^{2+} + 2H_2O$$
$$nCaO \cdot mSiO_2 \cdot 2nH_2O + 2nH^+ \rightarrow nCa^{2+} + mSiO_2 + nH_2O$$
$$nCaO \cdot mAl_2O_3 + 2nH^+ \rightarrow nCa^{2+} + mAl_2O_3 + nH_2O$$

In the process of acid rain H^+ ions transport in concrete by diffusion. When the active ingredient in cement completely hydrated the H^+ ions diffusion model is as follows:

$$\frac{\partial}{\partial t}[H^+] = D_{H^+}\left(\frac{\partial^2[H^+]}{\partial x^2} + \frac{\partial^2[H^+]}{\partial y^2}\right) - (K'_{CH} + 3K'_{CSH})[H^+] \tag{4}$$

$$\frac{\partial}{\partial t}[CH] = -K'_{CH}[H^+] \tag{5}$$

$$\frac{\partial}{\partial t}[CSH] = -K'_{CSH}[H^+] \tag{6}$$

Where, D_{H^+} is H^+ diffusion coefficient in concrete; K'_{CH}, K'_{CSH} respectively refer to the reaction constant of CH, CSH in acid rain solution(K'_{CH}, $K'_{CSH} = 7.8\times10^{-3}m^3\cdot(mol\cdot s)^{-1}$); $[H^+]$ is the concentration of H^+.

Solution of acid rain-carbonization model

Based on gas diffusion mechanisms in porous solid media CO_2 diffusion coefficient in concrete is related to concrete media status and CO_2 dynamic characteristics. That is, it is effected by concrete properties (strength, stress state) and environmental factors (temperature, relative humidity). The larger concrete strength is, the more concrete dense is. The smaller the porosity is, the slower gas diffusion rate is. When the concrete is in the state of compression the pore volume of concrete decreases and gases diffuse slowly. On the contrary when the concrete is in the state of

tension the pore volume of concrete increases and gases diffuse quickly. Based on thermodynamic principles the higher the temperature is, the more intense molecular motion is and the faster gas diffusion rate is. The bigger the relative humidity is, the higher pore water saturation in concrete is and the slower the gas diffusion rate is. So calculation model of CO_2 diffusion coefficient in concrete was established as follows.

$$D_{CO_2} = k_{fcuk}k_{\sigma}k_T k_{RH} \tag{7}$$

Where, k_{fcuk} is the strength correlation coefficient of CO_2 diffusion coefficient, the experimental data in references [11~13] was fitted and $k_{fcuk}=(5.02-1.26\ln f_{cuk})\times10^{-8}$, $f_{cuk}\leq50MPa$; k_{σ} is the stress correlation coefficient of CO_2 diffusion coefficient, $k_{\sigma}=1.01362-0.01386\sigma_c$, $k_{\sigma}=0.99261+0.07911\sigma_t$[14], σ_t, σ_c respectively is tensile stress and compressive stress; k_T is the temperature correlation coefficient of CO_2 diffusion coefficient, $k_T=0.02K-4.86$[15]; k_{RH} is the relative humidity correlation coefficient of CO_2 diffusion coefficient, $k_{RH}=((1-RH)/(1-RH_0))^{2.2}$, $RH_0=0.7$[16].

H^+ diffusion coefficient in concrete is related to concrete water-cement ratio, stress state, temperature and humidity. Refer to the chloride ion diffusion coefficient H^+ diffusion coefficient in concrete is as follows.

$$D_{H^+} = 10^{(-12.06+2.4W/C)} \cdot k'_{\sigma} \cdot k'_T \cdot k'_{RH} \tag{8}$$

Where, W/C is concrete water-cement ratio; $k`_{\sigma}$ is the strength correlation coefficient of H+ diffusion coefficient, $k`_{\sigma}=1-1.2463\delta_c+1.9091\delta_c^2$ or $k`_{\sigma}=1-0.129\delta_t+0.8291\delta_t^2$ [19], $\sigma_t$, $\sigma_c$ respectively is the ratio of tensile stress and ultimate tensile stress, the ratio of compressive stress and ultimate compressive stress; $k`_T$ is the temperature correlation coefficient of H^+ diffusion coefficient, $k`_T =\exp(U/R(1/T_{ref} -1/T))$ [20], $U$ is activation energy in diffusion process(=35000J/mol), $R$ is gas constant(8.314472J/K mol), $T_{erf}=293K$; $k`_{RH}$ is relative humidity correlation coefficient of H^+ diffusion coefficient[16], $k`_{RH}=[1+(1-h)^4/(1-h_c)^4]^{-1}$, $h_c=0.75$.

The main mineral composition of Portland cement clinker is C_3S, C_2S, C_3A and C_4AF. And $m_{c3s}=55\%$, $m_{c2s}=20\%$, $m_{c3A}=13\%$, $m_{c4AF}=9\%$. According to cement hydration reaction equation the neutral substance concentration in fully-hydrated concrete is as follows. $[C_3S]^0=0$, $[C_2S]^0=0$, $[CSH]^0=0.5[C_3S]^0+0.5[C_2S]^0$, $[CH]^0=1.5[C_3S]^0-4[C_4AF]^0+0.5[C_2S]^0-[C_3A]^0+[CSH]^0$. When cement hydrated completely the substances reacted with CO_2 and H^+ are CH and CSH. According to concrete carbonation reaction equation CO_2 consumption per unit volume of fully-hydrated concrete can be calculated, $m_{co2}=[CH]^0+3[CSH]^0$. According to acid rain erosion reaction equation H^+ consumption per unit volume of fully-hydrated concrete can be calculated, $m_{H+}=[CH]^0$.

When the acid rain erosion and carbonization in concrete structures occur at the same time the initial conditions of acid rain erosion-carbonization model are as follows.

$[CO_2(0, x)]=0$; $[H^+(0, x)]=0$; $[CH(0, x)]= [CH]^0$; $[CSH(0, x)]= [CSH]^0$.

When the acid rain erosion and carbonization in concrete structures occur at the same time, assuming erosion of CO_2 and acid rain is one-side, the boundary conditions of acid rain erosion-carbonization model are as follows.

$$[CO_2(t, 0)]=[CO_2]^0; [CO_2(t, L)]=0;$$
$$[CH(t, 0)]=0; [CH(t, L)]= [CH]^0;$$
$$[CSH(t, 0)]=0; [CSH(t, L)]= [CH]^0;$$
$$[H^+ (t, 0)]=[H^+]^0; [H^+ (t, L)]=0;$$

Where, t is time; L is the specimen thickness.

The acid rain erosion-carbonization model can be solved by the finite different method in the two-dimensional conditions. Forward difference was adopted to time and central difference was adopted to space. The partial differential equations were solved based on MATLAB software.

Failure criteria of concrete structure

When reinforced bar began corroded the concrete structure had reached the durability limit state based on code for durability design of concrete structures (GBT50476-2008)[22]. While the passive film on reinforced surface was damaged the reinforced was in the active state. When both water and

oxygen are sufficient reinforced can be corroded. The study[17] showed that, when PH was less than or equal to 9 passive film on reinforced surface in concrete was completely destroyed and reinforced was in fully activated state. When PH was larger than or equal 11.5, the integral passive film was formed on reinforced surface. Assumed the passive film on reinforced surface was completely destroyed reinforced began to corrode. So when PH is less than or equal to 9 reinforced began to corrode and the concrete is in the neutral state. The PH calculation formula is as follow [17].

$$PH = -\lg K_w + \lg(4.32 \times 10^{-2} \times [CH]/[CH]^0) \tag{9}$$

Where, K_w is ionization constants of water, $K_w = 1 \times 10^{-14}$.

Acid rain erosion-carbonization model validation

The environmental parameters-PH value of acid rain (4.55), the annual average temperature (290.65K), the annual average relative humidity (78%), the average content of CO_2 in the air (volume percentage 0.0385%) and the average content of SO_2 ($46\mu g/m^3$) were determined according to the acid rain characteristics and air quality statistics in Nanchang from 2009 to 2013[23]. The multi-storey teaching building was built in 1994. The main structure is cast-in-situ frame structure. C20 concrete was used in roof slab, the cubic compressive strength of concrete in 28d is 22.0MPa, the water cement ratio is 0.5, the amount of cement is 400Kg, sand ratio is 34%, the concrete cover thickness is 15mm. C25 concrete was used in frame column, the cubic compressive strength of concrete in 28d is 26.7MPa, the water cement ratio is 0.45, the amount of cement is 400Kg, sand ratio is 36%, the concrete cover thickness is 25mm. Take the roof slab in bearing chair, the roof slab in mid-span, external column as the object the rain erosion- carbonization model was adopted to calculate neutralization depth every decade (see table 1).

Table 1 the neutralization depth

the neutralization depth (*mm*)		
Time (year)	the roof slab in bearing chair	the roof slab in mid-span	external column
10	10.6	7.1	4.9
20	15.0	10.1	7.0
30	18.4	12.4	8.6
40	21.3	14.3	9.9
50	23.8	16.0	11.1

Table 1 showed that the neutralization depth exceeds the concrete layer thickness in about 20 year at the bearing chair of roof slab and the neutralization depth exceeds the concrete layer thickness in about 45 year at the mid-span of roof slab. According to failure criteria of concrete structure the lifetime of multi-storey teaching building is about 20 year. So the acid rain damage to the building in Nanchang is more serious. It should be taken seriously enough.

Conclusion

(1)The acid rain erosion-carbonization model was developed based on the diffusion theory. The model parameters-CO_2 diffusion coefficient, H^+ diffusion coefficient in concrete were analyzed. The boundary conditions and initial conditions were determined. The neutralization depth calculation method of existing concrete structures in acid rain area was obtained.

(2)The lifetime calculation method of existing concrete structures in acid rain area was obtained by determining the failure criteria of concrete structure.

(3) The acid rain erosion-carbonization model in the paper was used to calculate neutralization depth of the multi-storey teaching building in Nanchang. The lifetime of the multi-storey teaching building is about 20 years. So the acid rain damage to the building in Nanchang is more serious. It should be taken seriously enough.

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