Simulation and Visualization of Carbonation of Concrete based upon New Advanced Numerical Methods Considering Sustainability of Reinforced Concrete Buildings

Toshio Fukushima[1]

[1] Fukushima Institute 2 for Building Environment and Materials (FI2BEM),
2-chome, 9-18, Otto-Minami, Tsuchiura-shi, Ibaraki-ken, 300-0845 Japan
Email: fukushima-t-1564@ae.auone-net.jp ; fukutosi@hotmail.com

Abstract. Neutralization (Carbonation) of concrete has great influences on the durability of reinforced concrete structures in ordinary atmospheric environment. The progress of carbonation makes the basis of setting service life, maintenance/ modernization, and restoration/regeneration of these structures, with the corrosion of internal reinforcing bars. In considering the sustainability of reinforced concrete buildings and construction, we must understand fully the progress of carbonation from the viewpoint of sustainable development goals (SDGs), going back to the starting point. In this paper, the simulation and visualization of carbonation of concrete are reported. Based upon mathematical formulation of unsteady state simultaneous diffusion of carbon dioxide in such reinforced concrete shell structures as semi- cylindrical and semi-spherical shapes both from outside and inside spaces, computer visualization is carried out on the time-dependent change of concentration of carbon dioxide by advanced numerical analysis making best use of the newest version of mathematical software. By these procedures we can understand the situations of the progress of carbonation corresponding to the various aspects of environmental conditions.

Keywords: sustainability, carbonation, shell structures, simultaneous diffusion, numerical analysis

1. Introduction

Recently, sustainable development goals (SDGs) are cried for all over the world, involving the United Nations (UN), in order to pursuit for brilliant and hopeful future, by coexistence among nature and environment and human beings, because the global environmental problems such as global warming, depletion of natural resources, and mass generation of waste materials etc. have been threatening the sustainable earth itself. In building field, environment-conscious sustainable buildings and construction are needed by the fusion among science, technologies, and art in the future, to correspond to SDGs involving the climate change [1]. In order to realize sustainable reinforced concrete structures, we consider the balance among the environment, economy, and structural safety/long service life. Neutralization (Carbonation) of concrete has great influences on the durability of reinforced concrete structures in ordinary atmospheric surroundings. With the corrosion of reinforcing steel, the progress of carbonation makes the basis of setting service life [2]-[3], maintenance/modernization, and restoration/regeneration of these structures. In considering the sustainability of buildings and construction, we must fully understand the mechanisms of carbonation from the viewpoint of environmental change in external and internal building spaces, going back to the starting point. Looking at the outdoor environment, the concentration of atmospheric CO_2 has been increasing year by year since around 1950 with seasonal fluctuations, and as of 2022, it has already been reported to exceed 410 ppm [4]. Fukushima T. have already reported about the predictive methods of carbonation of concrete considering this trend [5]. In the future, effective reduction, and absorption measures for CO_2 emissions, such as carbon neutrality, will advance, and a certain degree of effect is expected (paradoxical moves to actively use concrete neutralization to absorb CO_2 in the atmosphere seem to be active [6]. However, the concentration of atmosphere CO_2 itself is expected to continue to be on a high trend for the time being. Looking at the indoor environment, in a closed room with insufficient ventilation, when it is compatible with new COVID-19 virus infection, it is necessary to be careful about both air conditioning and ventilation, the indoor CO_2 concentration tends to increase considerably from normal value of 300ppm. For health safety, it is recommended to keep it to 1,000 ppm or less [7]. In order to consider sustainable buildings and cities, and societies, paying special attention to resources circulation and environmental harmony, we should take these trends concerning atmospheric CO_2 into account. On the other hand, in real situations there are various shapes. Fukushima T., has established the procedure to predict the progress of carbonation in cylindrical shape [8]. This report deals with the simulation and visualization of the progress of carbonation of concrete in semi-cylindrical and semi-spherical shell by the simultaneous diffusion of carbon dioxide both from outwards and inwards, considering this change of the situations of atmospheric environment by new advanced numerical analysis using the newest mathematical software [9].

2. Research Methods

2.1 Mathematical Formulation of Simultaneous Diffusion of Carbon Dioxide in Reinforced Concrete Shell

Mathematical modelling was done for simultaneous diffusion of CO_2 in semi-cylindrical and semi-spherical reinforced concrete shells. Fundamental partial second-order diffusion is formulated as fundamental equations with the initial and boundary conditions:

2.2 Numerical Analysis

For numerical solution, program of NDSolve of mathematical software [9] is used. As the effective diffusion coefficient, the value of 3.1536[mm^2/year $^{-1}$]is used, which corresponds to the one of ordinary Portland cement concrete with 45% water-cement ratio. But, for the convenience of visualization, a hundredfold value is set. As the value of pseudo-first order carbonation rate constant, 0.01[year^{-1}] is used. Numerical method in cases of cylindrical simultaneous diffusion with pseudo-first order carbonation reaction is shown as follows:

NDSolve [D [*u* [*r*, *t*] *r*, *r*] +*D*[*u*[*r*, *t*], *r*]/3.536==D [u [r, t], t]/3.536,
u[r,0] = =300Exp[-1000000000(r-4960) (5000-r)], u [4960, t] = =1000,
u [5000, t] = =300}, u [r, t], {r,0.0001, 5000}, {t,0,90}]]
(1)

3. Research Results

Figures 1a),1b), 2a), 2b) show the results of simulation and visualization.

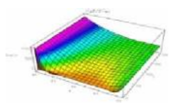

Fig.1a). 3DPlot of the Progress of Carbonation in in Semi-cylindrical Shell

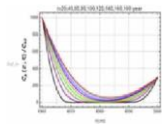

Fig.1b). Plot of the Progress of Carbonation in Semi-cylindrical Shell

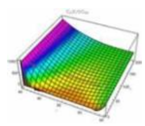

Fig.2a). 3DPlot of the Progress of Carbonation in Semi-spherical Shell

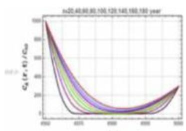

Fig.2b). Plot of the Progress of Carbonation in Semi-spherical shell

4. Summary and Conclusion

Paying special attention to the change of concentration of external and internal atmospheric carbon dioxide, simulation and visualization were done by making best use of the newest numerical analysis. The progress of carbonation of concrete by simultaneous diffusion of carbon dioxide both from inwards and outwards in semi-cylindrical and semi-spherical reinforced concrete shells were shown as time-dependent visual images. These procedures of simulation and visualization are useful to well understand the carbonation of concrete in various aspects.

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