# 합성 콘크리트 공극 솔루션에서 철근에 히드라존 기반 헤테로고리 화합물의 흡착에 대한 실험 및 계산 통찰력

## Experimental and computational insights into the adsorption of a hydrazone-based heterocyclic compound on steel rebar in synthetic concrete pore solution

하산 르가즈[1] · 카르틱 수비아[2] · 이한승[3*]
Lgaz, Hassane[1] · Karthick Subbiah[2] · Lee, Han-Seung[3*]

**Abstract** : The corrosion inhibitive effect of a new hydrazone-based heterocyclic compound for steel in simulated concrete pore solution with 3.5 wt.% sodium chloride was investigated by experimental and computational techniques. Electrochemical studies, up to 30 days of immersion, and surface analysis (X-ray photoelectron spectroscopy (XPS), atomic force microscopy (AFM), and scanning electron microscope (SEM)) were performed to assess the corrosion protection abilities of investigated compound for steel rebar. Results showed that adding the organic compound to the chloride contaminated concrete pore solution decreased the corrosion rate of the steel rebar thanks to the effective adsorption of inhibitor molecules. After 30 days of immersion of steel rebar in inhibited chloride contaminated synthetic concrete pore solution, the inhibition efficiency exceeded 80% at low concentration of 1 mmol/L. Computational studies by Density Functional based Tight Binding (DFTB) method revealed the formation of covalent bonds between the hydrazone molecule and the iron surface.

**키워드** : 철근, 부식, 부식억제, 콘크리트 기공용액
**Keywords** : steel rebar, corrosion, corrosion inhibition, concrete pore solution

## 1. Introduction

Corrosion of steel rebar is one of the main causes of the failure of reinforced concrete structures. The steel rebar provides appropriate corrosion resistance in the concrete environments (pH range of 12−13.5), owing to the growth of a protective passive (oxide) layer. However, this protective layer is insufficient because the concrete has pores and cracks.

In an effort to develop new corrosion inhibitors with outstanding structural, electronic, eco-friendly, and functional characteristics, our research team has given a lot of attention to the functionalization of nonsteroidal anti-inflammatory drugs (NSAIDs) [2].

We report herein the application of a new hydrazone derived from 5-methoxy-2-methyl-3-indoleacetic acid (MMIAA) for steel rebar protection in concrete environments. Besides, computational studies were conducted to investigate the nature of interactions between the hydrazone molecule and the steel rebar surface.

## 2. Materials and Method

The steel rebar was employed in the present work. The used corrosion inhibitor was synthesized according to the procedure reported in [3]. The SCPS solutions consist of 3.36 g/L of KOH, 8.33 g/L NaOH prepared per liter of saturated Ca(OH)2 solutions, with 35 g NaCl/L for contaminated solutions.

Experiments have been carried out using electrochemical and characterization techniques such as XPS, AFM, XRD, and SEM/EDS. Inhibitor molecule's adsorption over the Fe(110) surface was carried out within the density functional based tight-binding (DFTB) framework using the DFTB+ software.

1) 창의융합교육원, 연구 교수, 화학 박사
2) 한양대학교, 박사 후 연구원
3) 양대학교 ERICA 건축학부 교수, 교신저자(ercleehs@hanyang.ac.kr)

## 3. Results and Discussion

The EIS results of steel rebar immersed in SCPS with 3.5% NaCl containing various concentrations of hydrazone at various exposure periods are shown in Fig. 1a-f. It can be seen from Fig. 1a that the Nyquist plots semicircle diameters of the hydrazone at concentrations of 0.25, 0.5, 0.75, and 1.00 mmol.$L^{-1}$ was larger than the blank system (0 mmol.$L^{-1}$). The capacitance loop diameter grew as the inhibitor concentration increased, which indicates the formation and growth of inhibitor molecules on the steel rebar surface.

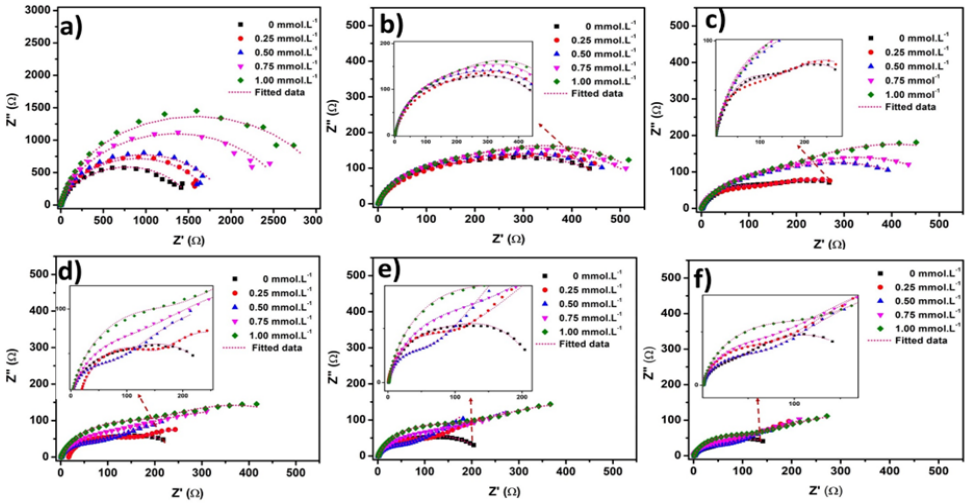


**Figure 1.** Nyquist plots for the steel rebar in the SCPS with 3.5% NaCl containing different concentration of inhibitor.

Potentiodynamic polarization studies reveal that the corrosion current density ($I_{corr}$) of steel rebar in SCPS with 3.5% NaCl containing inhibitor is notably lower than the uninhibited system and increasing inhibitor concentration decreases the $I_{corr}$ values. SEM was used to examine the surface morphological image of the steel rebar after 30 d in the SCPS with 3.5% NaCl containing different concentrations of the inhibitor. DFTB calculations confirm that, upon adsorption, molecules tend to chemically adsorb on the Fe(110) surface.

## 4. Conclusion

In this study, EIS studies revealed the enhancement of the inhibition effect by increasing the concentration of tested hydrazone up to 1 mmol/L; the charge transfer resistance values of steel rebar were higher than that of all other systems.

## Acknowledgement

이 성과는 2018년도 정부(과학기술정보통신부)의 재원으로 한국연구재단의 지원을 받아 수행된 연구임(No. NRF-2018R1A5A1025137).

## References

1. Bolzoni F, Brenna A, Ormellese M. Recent advances in the use of inhibitors to prevent chloride-induced corrosion in reinforced concrete. Cement and Concrete Research. 2022. p. 106719.
2. Lgaz H, Lee H. Facile preparation of new hydrazone compounds and their application for long-term corrosion inhibition of N80 steel in 15% HCl: An experimental study combined with DFTB calculations, Journal of Molecular Liquids. 2022. p. 117952.