Corrosion inhibition performance of the Nystatin Drug toward the Mild Steel in Acidic Media – An Experimental and Theoretical Study

Valbonë Mehmeti
Fetah Podvorica
University of Prishtina "Hasan Prishtina", Prishtinë, Kosovë
valbona.mehmeti@uni-pr.edu

The corrosion behaviour of mild steel in 0.5 M aqueous hydrochloric acid medium in the presence and absence of nystatin drugs was investigated using potentiodynamic polarization measurements, quantum chemical calculations, and molecular dynamic simulations [1].
Potentiodynamic measurements indicate that as a result of its adsorption on the mild steel surface, this molecule operates as a mix inhibitor. The objective of this study was to use theoretical calculations to acquire a better understanding of how inhibition works.

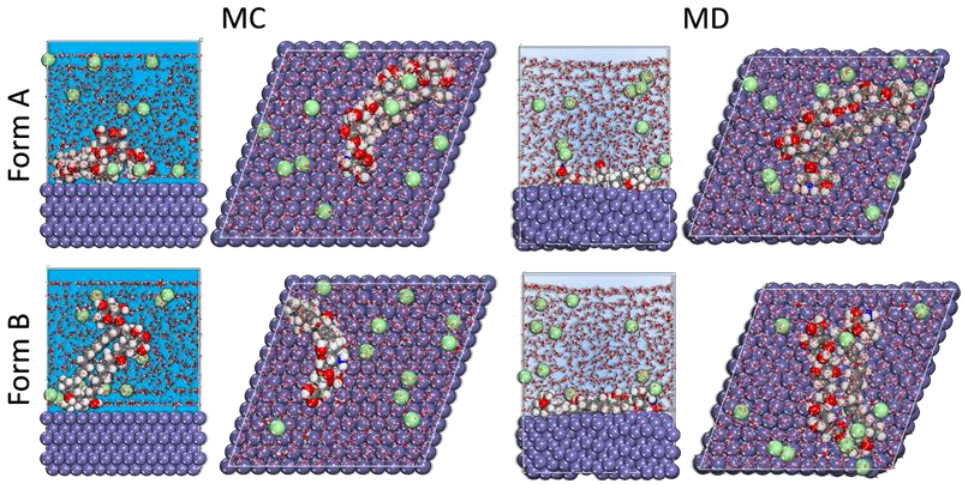

Figure 1: A. MC and B.MD obtained from the adsorption configurations of the Nystatin inhibitor in the simulated corrosion media on the Fe surface.

The adsorption behaviour of the examined compound on the Fe (1 1 0) surface was evaluated using Monte Carlo simulation. Furthermore, the molecule was studied using Density Functional Theory (DFT), to determine the relationship between the molecular structure and its corrosion inhibition behaviour. Adsorption energies between Nystatin and mild steel were calculated more precisely using Molecular Dynamics under Periodic Boundary Conditions (PBC). The predicted theoretical parameters were found to be in agreement with the experimental data, which was a considerable help in understanding the corrosion inhibition mechanism displayed by this inhibitor.

References

[1] Valbonë Mehmeti, Corrosion Science and Technology, 1, 21-31, (2022)