Session: Multi-scale modelling for design of protective coatings

Protective coatings are among the most effective ways of reducing the corrosion impact on metallic structures and increasing their service life. The design of protective coatings is still based on lengthy and labor-intensive testing and certification. Corrosion testing is time-consuming (months to years) and testing procedures may have limited correlation with the real in-service conditions. In contrast, the clear request is to develop coatings faster and to protect end user assets longer at reasonable cost. This has put the coating formulators, manufacturers and users in a challenging position. To accelerate coating development, modeling and simulation approaches can provide a valuable support and help to find the optimal solution saving time and resources.

This session, organized as **a joint effort** of EFC **WP22** (Corrosion Control in Aerospace), **WP8** (Physico-Chemical Methods for Corrosion Testing), **WP14** (Coatings), **WP25** (Atmospheric Corrosion), **WP17** (Automotive Corrosion) and **WP6** (Surface Science, Corrosion Mechanisms and Modeling), with support of VIPCOAT EU project will consider and discuss new approaches on multi scale modelling and optimization of novel active protective coatings.

The session will provide a forum for scientists working in academia and industrial R&D to exchange ideas and present new results and best practice on the following topics:

- Multiscale modeling of inhibitor behavior (atomistic-, mesoscale-, continuum modeling);
- Artificial intelligence and physics-based modeling approaches for inhibitor efficiency prediction;
- Simulation of inhibitor leaching from active protective coatings;
- Modelling of corrosion and inhibition processes in coating defects;
- Simulation of atmospheric corrosion of coated substrates including propagation of paint delamination and creepage;
- Experimental methodologies to deliver input data for the models and serve as validation means;
- Predictive modelling of in-service performance of coated metals;
- Digitalised accelerated corrosion testing;
- Modeling requested data acquisition, management and (digital) sharing;
- Open innovation and simulation platforms for protective coating development;
- Decision support systems and Open Innovation Platforms for new inhibitors and protective coating development;
- Industry needs, challenges and requests in view of new coating development, further tests and modelling tools implementation.

Expected Joint Session duration: 1-1,5 day

Format: up to 3 half-day slots, which will include one Keynote lecture (double time slot) per half day. <u>VIPCOAT</u> OIP¹ demonstration and round table discussion will be held at the end of the session.

We are looking forward to your contribution and participation in EUROCORR 2024 on September 1 - 5 2024, in Paris, France. Please submit your abstracts online via www.eurocorr.org.

Expected audience: 100–150 attendees

¹<u>https://cordis.europa.eu/project/id/952903</u>, <u>https://ms.hereon.de/vipcoat/</u>, VIPCOAT - Virtual Open Innovation Platform for Active Protective Coatings Guided by Modelling and Optimization, H2020 project, Grant Agreement No 952903