# MODELLING SUSTAINABLE ACTIVE PROTECTIVE COATINGS

## Discussion Notes and Summary of VIPCOAT Round Table at EUROCORR 2022

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## Preamble

The VIPCOAT[1] project is funded under the Horizon 2020 call DT-NMBP-11-2020, which asked for proposals on *Open Innovation Platform for Materials Modelling* (OIP) as Research and Innovation Actions. VIPCOAT aims to deliver such a platform which guides industrial end-users in making optimal decisions based on predictive modelling. The VIPCOAT OIP is designed to engage multiple (quadruple helix) stakeholders in a collaborative environment through a guided innovation process. The proposed platform, although being designed for a multitude of industrial applications, uses active corrosion protection coatings as the specific business case for guiding the innovation platform implementation and development. The concept is specifically applied to the aeronautic sector, as one of the most challenging cases in terms of materials protection. The VIPCOAT platform is designed to be adaptable for the development of sustainable active protective coatings for other industrial applications, like automotive and maritime industries, infrastructure for energy production, medical devices, architectural and civil engineering application.

To discuss the actual requests from European industry and important scientific topics in novel approaches in surface protection of metallic structures, the VIPCOAT consortium organized a joint session and, together with the European Federation of Corrosion (EFC), a Round Table on "Modelling Sustainable Active Protective Coatings" at EUROCORR congress 2022 in Berlin on August 30, 2022.This paper summarizes the ideas on the topics, open questions and industrial relevant aspects as discussed during the Round Table session.

## Scientific focus and technological challenges considered at the joint session

Protection of metallic structures against corrosion and efficient natural recourses management requires coating systems that provide a barrier to aggressive service conditions, but also contain active elements which protect the structure in the case of coating degradation or damage. The efficient design and development of future environmentally friendly and sustainable corrosion protection systems requires new approaches to reduce development cycles and to save resources and development costs. This is especially relevant for new environmentally-friendly active protective coatings as a result of their complexity. Moreover, the absence of reliable accelerated test specifications often leads to over-engineering of protective coating system compromising economic and ecologic aspects. These issues could be solved more effectively by using both data-based and physics-based modelling approaches aiming at supporting decision making on optimal composition and structure of coating systems, as well as predicting their behaviour in various service environments and optimizing in circular economy approaches. New innovative modelling tools to predict corrosion protection are needed to support asset management and novel material designs. In addition, relevant and accurate data need to be identified for the development and validation of the models.

The Joint session of VIPCOAT project and four EFC Working Parties – "Corrosion Control in Aerospace", "Physico-chemical methods for Corrosion Testing", "Coatings", and "Surface Science, Corrosion Mechanisms and Modelling", had the aim to bring together scientists and engineers from academia and industry to share the latest results and innovations related to the development of computational models for active corrosion protection technologies.

[1] https://cordis.europa.eu/project/id/952903, https://ms.hereon.de/vipcoat/

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The session provided a forum for exchange of knowledge and ideas between academia, coating developers, and end users on the following topics:

- Machine Learning (ML)/ Artificial intelligence and physics-based approaches for predictive modelling of coatings performance in static and dynamic conditions including inhibitor efficiency, leaching kinetics, degradation in coating defects and prediction of in-service behaviour;
- Optimization techniques and metadata for industry-relevant corrosion-protective coatings;
- Experimental techniques to obtain required data as basis for model validation.
- Business decision support systems and open innovation platforms for new coating co-creation and development.

More than 100 industrial and academic experts participated in the event and the 45 Minutes Round Table discussion followed directly after the conference session.

## Discussion Notes of VIPCOAT Round Table

Below we summarize the topics, open questions and important issues discussed during the VIPCOAT Round Table hour at EUROCORR 22:

- Communication between experts working on modelling at different scales is an important issue. People working on models at atomic scale would be happy to have a possibility to discuss approaches and typical issues applicable to meso-scale or continuum simulations. Especially this communication gap in modelling multi-physics phenomena like corrosion and corrosion protection needs to be bridged.

- Effective communication between modellers and experimentalists is essential to understand the mutual needs and requirements on necessary data and their exchange. Moreover, expert discussions on criteria for reliable and relevant experiments used for model validation is needed.

- To create industrial relevant models, scientists need to understand industrial needs and final product requirements (initial data and output). Communication between modellers and end-users is important, preferably involving all parties **along the value / production chain.** In some cases it is important to invite all parties: From raw materials supplies to end-users and from modellers to the end-product manufacturers, to the discussion and (strategical) decision making.

- Industrial requirements and needs should be considered as the main guidelines for new models development: which models and approaches should be developed prioritized by taking into account the **needs of society** and industrial end-users.

- Modellers and experimentalists should support industry starting from the actual state of the art in the area of relevant challenges/ issues, pick the industry up where they are and help them to find an optimal solution using modelling and characterization methods.

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- An OIP could be an excellent tool to provide modelling and decision support along a production chain. The questions are:
    - How to collect the right data for simulation?
    - How can the quality of the data be ensured for data consumers?

- Molecular Dynamics (MD) simulation, Machine Learning (ML) models or physics-based models: Which priority should be given for each model approach now? The question could not be answered towards a conclusion during the Round Table discussion. A case by case approach seems to be the only possible route today.

- Standardization of tests is important. Today, many data are collected by different institutions without using an agreed standard or at best by using their own internal standards. Only a limited number of users can profit from these data. Uselessness and incompatibility of a wide variety of data is an issue. Standardization and development of tests compatible to the envisioned digital transformation are needed.

- Data sharing is an open issue. In particular, the most important aspects are:
    - Could we use an OIP for the data sharing?
    - How can data security issues be solved?
    - Which IT issues should be considered?

- Quality of models and different models integration into a platform: corrosion testing and modelling for aerospace and automotive industries have different requirements and thresholds. Experienced researchers and industrial experts should be involved to the project implementation to avoid shortcomings in testing, characterization and modelling tasks. Moreover, the integration of research efforts in the platform and an assurance of interoperability of data and software/modelling tools are additional challenges to be handled by OIPs.

- Open source models and commercial modelling tools provide different support for end-users. The issue is to identify who takes responsibility for the quality of the modelling results (?)

- Do the models include coating degradation due to the influence of day-light I UV?
  If yes, which approaches are efficient, and how to validate the model?

- Licensing schema for VIPCOAT Apps:
  How will it work, for which users and for which cases? These issues should be decided later by providing an overall business model for the VIPCOAT OIP.

- Model creation and validation issues :
    - Do we have correct, reliable, repeatable and relevant data for the initialization of models?

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- Do we have enough correct validation data for our modelling to be able to assess the reliability of simulation results?
- Where can we find, reliable and relevant input and validation data?
- How to conduct sensible validation experiments? Who is able to carry such experiments and deliver the needed data?
- How to find credible partners for both, modelling and validation?

- VIPCOAT OIP is a complex product. The approach now is to start from simple cases to demonstrate that all VIPCOAT components work (together) efficiently and correctly. After that, VIPCOAT developments should focus on the next level of complexity.

- Industrial participants are very sceptical with the "Open" aspects of the platforms. The main issues are security and the need to disclose data outside of their organization. Concepts of secure data transfer and storage need to be implemented (which is technically possible) and industry needs to be convinced
  - *Remark 1:* Open Innovation Platform – openness definition: descriptions of model formulations of coatings and publicly available data will be made available for a demonstration of the open part of the platform. However, Open Innovation does not mean that results of new projects will be open to all users. The access to the OIP should be negotiated and agreed with all partners of an innovation process/ project.
  - *Remark 2*: Open does not mean "free".

- Accelerated corrosion testing:
  Industry (aerospace, automotive and others) has extremely high demands to have access to good models suitable for accelerated corrosion testing supporting Research & Development and for the quality control. Corrosion experts would be happy if they would have modelling tools available to predict materials behaviour under cyclic load conditions. Modelling support for accelerated corrosion testing is needed and required.

## Summary

The fruitful discussion during the Round Table has demonstrated a high interest of the surface science community in open discussions regarding scientific and industrial relevant topics and challenges around modelling supported design, materials performance prediction and surface protection based on computational analysis.

The most important topics are accelerated corrosion testing, new coating development and optimisation aspects. Modelling and optimization tools are needed to constantly innovate on these issues and to support industrial decision making. Moreover, the main aim of an innovation platform OIP is to stimulate innovation by connecting different stakeholders leading to an acceleration of development processes. The VIPCOAT OIP could be a relevant solution in this field for industry and academia to support co-creation and co-development of new products.

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The Round Table discussion disclosed a lot of open questions and needs raised by the EFC community, which should be considered by modellers, experimentalists and end-users in a collaborative fashion.

A clear request for organizing a similar event at the next EUROCORR had been expressed by the community. The main reflection from the participants on the format of the event was related to the limited duration of the Round Table. It was highly recommended to organize a second Round Table during the next EUROCORR and to use an extended time window. This opinion had been reported to the international organization committee and to the local organizers of EUROCORR 2023. As a result, a corresponding event – VIPCOAT joint session[2] and the Round Table "Multi-scale modelling for design of protective coatings"- will be organized at EUROCORR 2023. The duration of the VIPCOAT session and the Round Table is aimed to be extended to one day, including at least 90 minutes dedicated to the Round Table discussion.

[2] eurocorr-2023-joint-session-wp22-wp8-wp14-wp6-wp25.pdf (clvaw-cdnwnd.com)

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