Abstract #1318, 223rd ECS Meeting, © 2013 The Electrochemical Society

Multiscale Computational Design of Aerospace Coatings Containing Corrosion Inhibitors

I.S.Cole[1], E. Sapper[2], J. Osborne[2], C. Chu[1], P. Corrigan[1], M. Venkatraman[1], F. Chen[1], M.Morks[1]
[1]CSIRO
[1]Private Bag 33, Clayton South, Victoria 3169
[2]BOEING RESEARCH & TECHNOLOGY
[2]PO Box 3707, Seattle, WA, USA, 98124

This paper reports on a new collaborative project between BOEING and CSIRO. The project aims to develop a platform that links models from the molecular scale to the engineered object scale that airplane structures reside in. The project has 2 critical components:

1. Development of a platform that permits models to be linked.
2. Selection and or development of models across the relevant platform length scales.

The platform stores all the permitted models at each scale in a GUI-driven executable. There can be more than one model for a given function at a given scale. The user can select the particular models to use for a given function, as well as how each model links to other models at the same length scale or at upper or lower length scales. The platform permits the user to define which outputs from one model correspond to inputs of the subsequent model. The platform checks that the system of all the models will function together before computing the desired solution set.

The models being developed for inclusion in the multiscale platform include:

a) Molecular scale models to define corrosion inhibitor and surface interactions.
b) Molecular dynamics and continuum-scale models of inhibitor and species diffusion through a polymer.
c) Model of inhibitor and other ion movement from a paint film to a crack or defect in a paint film.
d) Model of pit initiation on structural aluminium in a saline solution with and without an inhibitor.
e) Model of pit propagation in saline solution in the presence of an inhibitor.
f) Model of the electrochemistry and aqueous phase chemistry occurring on a surface in the presence of pit initiation and propagation.
g) Scenario Builder to define location and activity of an aircraft.
h) Microclimate model of structural areas and occurrence of wetting at surfaces within an aircraft.
i) Model defining the microclimate and occurrence of wetting on structural surfaces at the exterior of an aircraft.
j) Damage accumulator that keeps track of the progression of damage at the points of interest within an aircraft.

At present the model will focus on pitting in association with defects in paint films. In the future it will be broadened to include other modes of damage. Of the models outlined some have been developed in previous studies (g, h, i, j) while others are currently under development (b, c, d), while still others (a and e) are yet to be created. The case of molecular scale models as they connect to macroscale models is of particular interest. A number of challenges are present in the development of molecular models that reflect the real in-service conditions that occur when a structural metal or alloy is covered with an inhibited saline surface, a common test environment that serves as an in-service proxy for corrosion inhibition. The simplest models of corrosion inhibition by small organic molecules consider the electronic configuration, dipoles, and HOMO and LUMO energy levels of the molecule, all calculated in a vacuum. However, more realistic models must include the effect of the solvent, steps and defects in the surface, the structure of intermetallics and intermetallic/matrix interfaces, and the effect of dynamic surface potentials. What is of most interest is actually not the binding of an inhibitor to a metal or alloy surface, but rather how such binding effects anodic and cathodic activity on that surface.

At the larger end of the length scale a model has been developed that considers the microclimate that occurs on an aircraft both in flight and on ground. The model considers the temperature and relative surface humidity on the aircraft skin, marine aerosol generation and transport, and pollution deposition (both in flight and on ground). Atmospheric rain-washing of the aircraft and the development of wetting on the aircraft skin is also considered. The deposition of marine aerosols in flight is of critical importance, and varies greatly depending on aerosol diameter, as illustrated in figure 1 below. Fine aerosols remain in the air stream and do not impact on the surface while large aerosols either deposit and stick on the surface or are blown off the aircraft skin. Thus, depending on the aircraft speed, large marine aerosols or cloud condensation nuclei may deposit on aircraft during flight and promote corrosion.

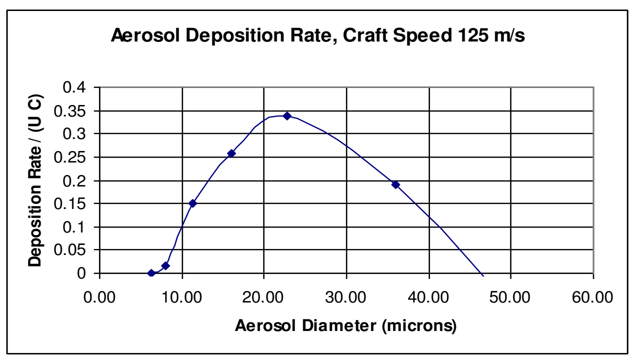

Figure 1. Marine aerosol deposition rate on a moving aircraft, as a function of average aerosol droplet diameter.

The complete multiscale model developed and presented here can link a wide range of individual models together, each residing in different length and time scale regimes. It will have significant impact in the design of protection systems for future aircraft, as well as the greater understanding of corrosion mechanisms, proponents, and mitigating factors. In particular, the model provides a means of assessing the impact of fine scale mechanisms such as species transport and adsorption, as well as component surface morphology, on the predicted service lifetime of a large-scale coated surface that experiences many ranges of atmospheric exposures in its daily use.