PARTICLE LEACHING FROM POLYMERIC COATINGS
A Combined Experimental and Simulation Study

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Introduction

Active corrosion protection by organic coatings in Aerospace

Corrosion in modern world

• Corrosion cost: 2.5 trillion US$ - 4% percent of the global Gross Domestic Product (GDP)
• 20-35% of this loss could have been saved by implementing better corrosion preventing practices. German, T. & Section, N. Corrosion news. 140 146 (2018).

In the aerospace industry corrosion impacts

• Cost
• Aircraft availability
• Safety
• Social

Organic coatings provide corrosion protection

Key steps for corrosion inhibition via leaching

1. Water uptake
2. Dissolution of active pigment
3. Transport and delivery of active species through the polymeric matrix to the defect area
4. Fast, effective, and irreversible passivation

Introduction
Active corrosion protection by organic coatings in Aerospace

Challenge
Develop coatings that are:
- Environmentally friendly
- Sustainable
- Efficient
- Cost effective

Approach
- Replacing toxic chemicals (chromates)
- Use renewable materials
- Understand and optimise performance
- Minimise use of expensive materials

UNDERSTAND LEACHING OF INHIBITORS FROM ORGANIC COATINGS
UNDERSTAND THE RELATIONSHIP BETWEEN LEACHING AND PERFORMANCE
Introduction
Lithium leaching technology protection concept

Provide fast, effective, and irreversible corrosion inhibition

1. Leaching of lithium ions
2. Lithium ion transport to defect area
3. Formation of a protective layer on the aluminium substrate

Fitting with physical model
- Oxide layer provides corrosion protective properties

The effect of the PVC
Systems of study and microstructure analysis

Epoxy model system with PVCs between 7.5 – 37.5%
Pigment ratios constant
The effect of the PVC

Lithium leaching and corrosion protection properties

Epoxy model system with PVCs between 7.5 – 37.5%
Pigment ratios constant

- Lithium leaching rate from the matrix
- Oxide layer resistance
- Polarization resistance

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The effect of the PVC

Higher pigment volume concentration result in higher leaching rates and faster exhaustion of the system
- Larger network of interconnected pigment clusters

Increase of pigment volume concentration decrease the barrier properties of the coating
- Formation of defects through the polymeric matrix which enhance water permeation

Slower dissolution rate leads to higher $R_{\text{oxid}}$ and $R_{\text{pol}}$ – Better active corrosion protection

Can we control the rate of release?
Can we control the amount released?

Develop a model that describes the leaching of inhibitors with sufficient accuracy to explore the formulation space and inform what are the desirable features or properties of the coating and inhibitor.
Release of corrosion inhibitors

*Cellular Automata Model is a good compromise to model the release of inhibitors:*

- Can capture different physical phenomena
- Can be related to real physical properties of the system
- Computationally efficient
Approach

Microstructure generation

Release simulation
Microstructure generation

- Pigment volume concentration
- Particle size distribution
Release simulation

Dissolution

- Polymer
- Solid inhibitor
- Dissolved inhibitor
- Water
Release simulation

Dissolution

Diffusion

Polymer
Solid inhibitor
Dissolved inhibitor
Water
Random distribution of inhibitor particles results in unique connectivity profiles. Averages are needed over multiple configurations to represent real systems.
Effect of PVC

Number of cells released vs. Time / days for different PVC concentrations:
- PVC = 30%
- PVC = 22.5%
- PVC = 15%
- PVC = 7.5%
Effect of solubility

Solubility

\[ S = 0.13 \text{ g/cm}^3 \]

\[ S = 0.013 \text{ g/cm}^3 \]

\[ S = 0.0013 \text{ g/cm}^3 \]
Effect of particle distribution

Spatial heterogeneity can affect the connectivity between inhibitor particles.
Effect of particle distribution
Comparison with experimental data

- PVC = 7.5%
- PVC = 15%
- PVC = 22.5%
- PVC = 30%

Concentration / g cm\(^{-3}\)

Time / days

Simulated data

Experimental data
Conclusions

• The release of corrosion inhibitors from primer coatings can be modelled using the CA approach

• Models can show the influence of microstructure and pigment properties on the release, enabling control on the factors that affect the process

• Simulations can provide important insight on the structure-property relationship in complex coatings to enable optimal formulation design
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Cellular Automata model

Discrete approach

Transition rules

Locality