# MODEL BASED DESIGN OF SELF-HEALING EXPANDABLE COATINGS UNDER DIFFERENT ENVIRONMENTAL CONDITIONS

E. Javierre<sup>1</sup>, V. Camañes<sup>2</sup>, S.J. García<sup>3</sup>, S. van der Zwaag<sup>3</sup> and J.M. García-Aznar<sup>2</sup>

<sup>1</sup> Centro Universitario de la Defensa, Academia General Miitar, Ctra. Huesca s/n, 50090 Zaragoza, Spain – e-mail: etelvina.javierre@unizar.es

<sup>2</sup> Departamento de Ingeniería Mecánica, Universidad de Zaragoza, C/ María de Luna s/n, 50018 Zaragoza, Spain – e-mail: Victor.camanes@gmail.com, jmgaraz@unizar.es

<sup>3</sup> Delft Center for Materials, TU Delft, Kluyverweg 1, 2629 HS Delft, The Netherlands – e-mail: s.j.garciaespallargas@tudelft.nl, s.vanderzwaag@tudelft.nl

Keywords: barrier protection, gap filling, coating, modelling, prediction

### ABSTRACT

A long-lasting barrier protection at damaged sites of coated system can be achieved by means of an active response of the primer. This may be attained through the release of reactive liquids from dispersed containers, the increase of the local mobility of the polymeric network, or the expansion of (dispersed elements in) the primer [1]. Such self-healing mechanisms provide an excellent strategy towards repeated and sustained self-repair properties and, additionally, are not incompatible with the inclusion of passive elements within the primer to produce a corrosion inhibition response.

This work focuses on the modelling and simulation of expandable coatings resembling systems that contain thin clay-based interlayers [2]. However, a similar methodology could be applied to treat the hydraulic growth of inorganic grains in PPS coatings [3]. The expansion of a theoretical porous plastic primer is triggered by the ingress of environmental moisture. The volumetric growth of the primer into the crack is investigated under different humidity, temperature and atmospheric pressure conditions resembling different geographical locations (coastline vs. inland, changes in altitude and latitude, etc). Furthermore, the reversibility of the expansion process is investigated through hysteresis cycles resembling the change of the environmental conditions over a time lapse of several hours up to days.

The self-sealing capacity of the coating is estimated from the maximum crack width that can be filled. A full characterization of self-sealing efficiency is given in terms of key design parameters such as porosity, permeability, sorption behaviour, swelling range, shear modulus, layers widths and adhesion properties.

### 1. INTRODUCTION

Computational modelling and numerical simulation are powerful tools to aid and assist the design and optimization of self-healing materials. They can be used to evaluate design hypotheses prior to experimental setup and to perform throughout parameter analysis [4,5].

The goal of this work is to address the expansion process in a self-sealing clay-based coating [2,3]. By means of an analysis of fluid-flow in porous media we compute the

time-history deformation of the coating when it is exposed to different environmental conditions.

## 2. MATERIALS AND METHODS

We model the evolution of a coating consisting of a  $7\mu$ m thick poly-siloxane topcoat and a  $15\mu$ m thick montmorillonite primer [2]. The topcoat has water-repellent properties to prevent the ingress of moisture into the primer when the coating system is intact, whereas the montmorillonite primer expands by moisture ingress where damages in the topcoat occur. We will track the deformation of a damaged coating when it is exposed to fixed environmental conditions (temperature and relative humidity). In order to reduce the computational cost, we will consider a general crosssection of the damaged coating under plane strain hypotheses. Figure 1 shows the geometry of the damaged coating and the idealized computational domain with the boundary conditions.



Figure 1: Damaged coating (taken from [2]) and computational domain.

The topcoat is modelled as a hyperelastic material. The montmorillonite primer is modelled as a permeable porous elastic material. Moisture sorption proceeds by capillary action through the exposed surfaces of the damaged coating (i.e. the left boundary of the primer and the left-bottom part of the primer where adhesion with the substrate is lost due to damage). Suction-saturation and permeability-saturation curves are defined accordingly to experimental results [6]. Moisture vapour pressure is obtained for different temperatures and relative humidity through psychrometric diagrams [7].

Topcoat		Primer						
Shear modulus	50 MPa	Shear modulus	250 MPa	Permeability	10⁻ <sup>10</sup> m/s			
Bulk modulus	1225 MPa	Swell range	0-300%	Porosity	0.4			

Table 1: Material properties of the coating

### 3. RESULTS AND DISCUSSION

The self-sealing capacity of the coating is estimated from the maximum crack width that can be filled. The exposed coating expands gradually as moisture is adsorbed, and the free part of the coating bends slightly due to the restraining effect of the topcoat (see Figure 2), in agreement with experimental observations and previous numerical results [2,4].



Figure 2: Initial and deformed coating after 10 min exposed to 30°C and 30% of relative humidity (close view of damaged area).

In order to study the performance of the coating at various geographical locations, we vary the environmental temperature and relative humidity. Vapour pressure, obtained from psychrometric charts, increases with both temperature and relative humidity (see Table 2).

Table 2: Vapour pressur	e (kPa	) for different tem	peratures and relative humidity	/.
-------------------------	--------	---------------------	---------------------------------	----

Temperature	Relative Humidity (%)					
(°C)	10	30	50			
15	0.17	0.49	0.83			
30	0.4	1.27	2.10			

Taking as reference the response of the coating after 10 min of exposure to 15°C and 10% RH (i.e., the temperature and relative humidity that give the lowest vapour pressure), results show that the sealing capacity of the coating increases linearly with vapour pressure (see Figure 3). In terms of the environmental conditions, this means that the largest increment in the self-sealing capacity of the coating is obtained when both temperature and relative humidity are increased simultaneously.



Figure 3: Increment in maximal crack-width sealed after 10 min of exposure to environmental conditions as function of the increment in vapour pressure. Results normalized with respect to the reference case.

### 4. CONCLUSIONS

The dependence of self-sealing capability of an expandable coating on the environmental conditions has been addressed. Results show that better performance is obtained under temperatures and relative humidity that yield a larger moisture vapour pressure.

However, thorough analyses of the material properties (both topcoat and primer) needs to be conducted in order obtain a full characterization of the self-sealing response of these types of coatings. A full set of results will be given in the presentation.

### ACKNOWLEGDEMENTS

Financial support from the Spanish Ministry of Economy and Competitiveness for this study (Project No. DPI2012-32880) is gratefully acknowledged.

### REFERENCES

[1] S.J. García, H.R. Fischer, S. van der Zwaag, A critical appraisal of the potential of self healing polymeric coatings. Progress in Organic Coatings, 2011, 72, pp. 211-221.

[2] F. Miccichè, H. Fischer, R. Varley, S. van der Zwaag, Moisture induced crack filling in barrier coatings containing montmorillonite as the expandable phase. Surface & Coatings Technology, 2008, 202, pp. 3346-3353.

[3] T. Sugama, K. Gawlik, Self-repairing poly(phenylenesulfide) coatings in hydrothermal environments at 200°C. Mater. Letter. 57 (2003) 4282.

[4] R. Rey, E. Javierre, S.J. García, S. van der Zwaag, J.M. García-Aznar, Numerical study of the scratch-closing behavior of coatings containing an expansive layer. Surface & Coatings Technology, 2012, 206, pp. 2220-2225.

[5] E. Javierre, S.J. García, J.M.C. Mol, F.J. Vermolen, C. Vuik, S. van der Zwaag, Tailoring the release of encapsulated corrosion inhibitors from damaged coatings: Controlled release kinetics by overlapping diffusion fronts. Progress in Organic Coatings, 2012, 75, pp. 20-27.

[6] J.O. Lee, W.J. Cho and S. Kwon, Suction and water uptake in unsaturated compacted bentonite. Annals of Nuclear Energy, 2011, 38, pp. 520-526.

[7] Hands Down Software, www.handsdownsoftware.com