A Cellular Automata model for the release of corrosion inhibitors from primer coatings

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Formulating Functional Films and Coatings III
19 - 08 - 2020

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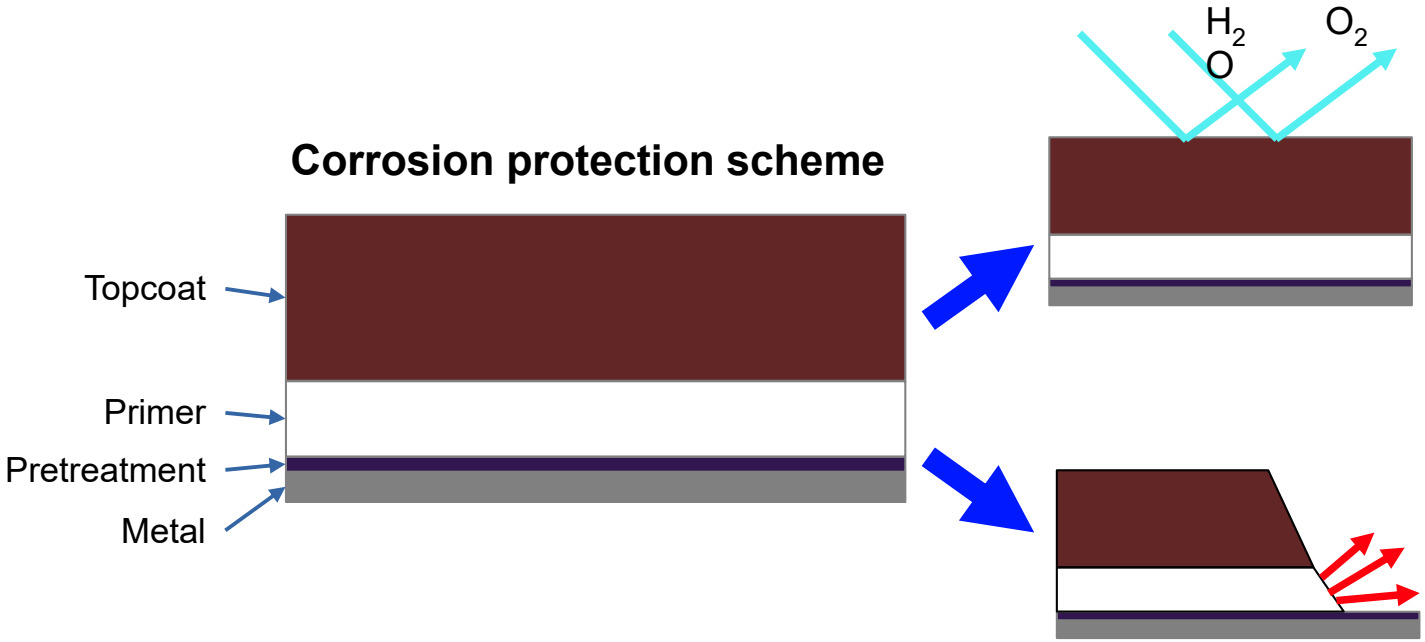
Coatings for corrosion protection



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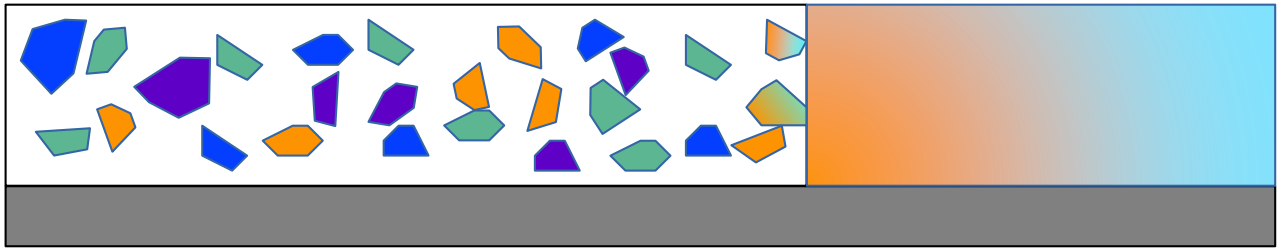
Inhibitors release from primers



Corrosion inhibitors leach out when the primer is exposed to water and protect the metal

Primer formulation
Binder + inhibitor + fillers

→

Affects the leaching behaviour
(hence protection ability)

→

How?

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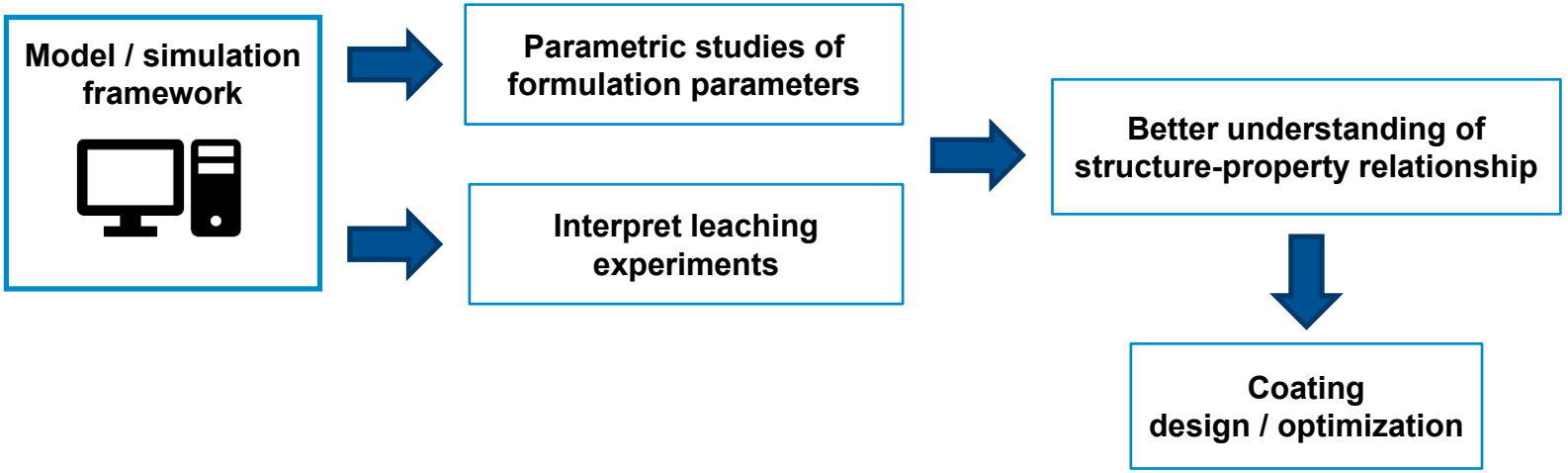
Research aim

Develop a model of the release of inhibitors to investigate the relationship between coating formulation and leaching behaviour



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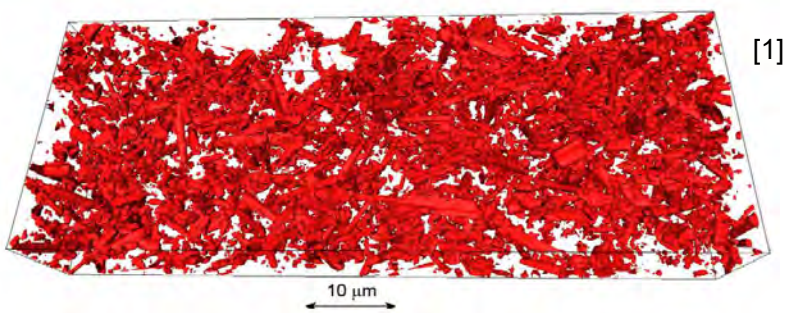
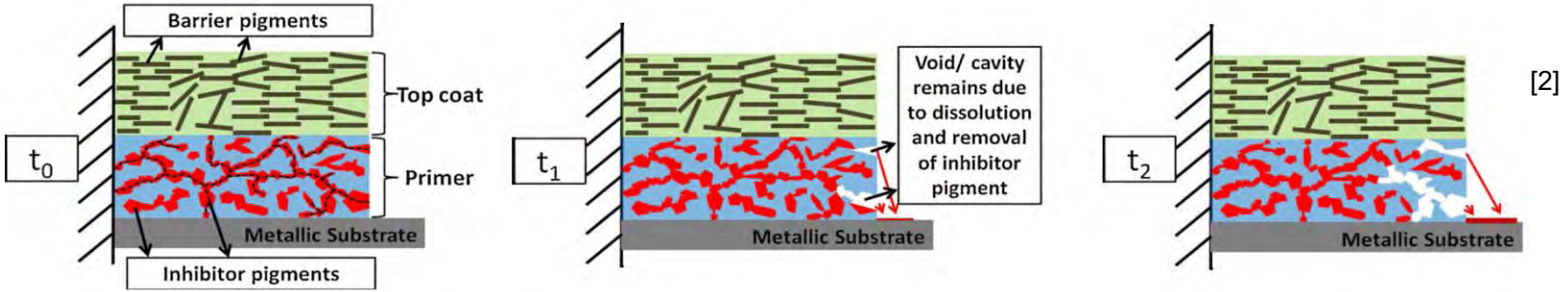
Experimental evidence

- Pigment particles form clusters
- Clusters dissolution leaves interconnected cavities
- Pigment volume concentration and particle size distribution determine the microstructure
- Inhibitor properties (e.g. solubility) affect the release rate



[1]



[2]

[1] Trueman et al., *Corr. Science.*, 75 (2013) 376-385
[2] Emad et al., *Prog. Org. Coat.*, 134 (2019) 360-372

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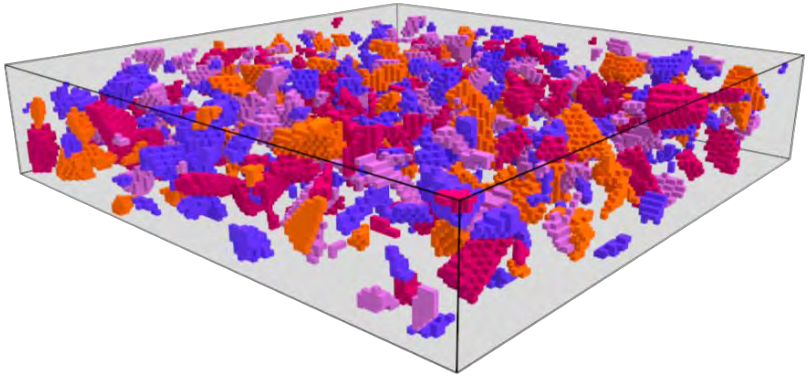
Model implementation

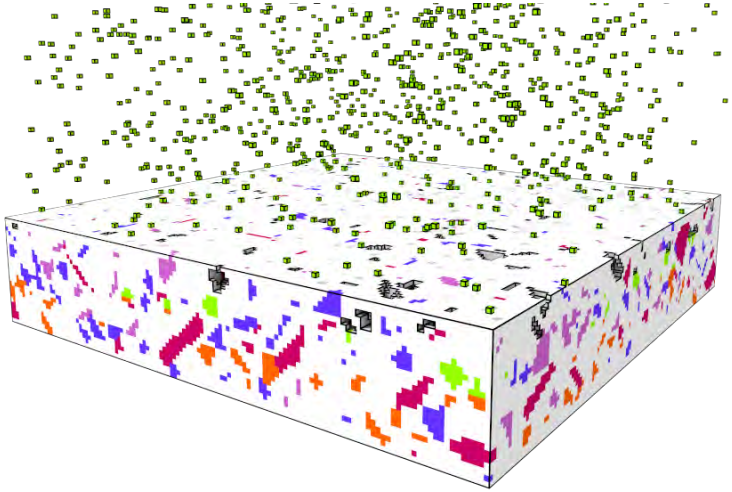
MANCHESTER 1824
The University of Manchester

AkzoNobel

Step 1 – Microstructure generation



Step 2 – Release simulation



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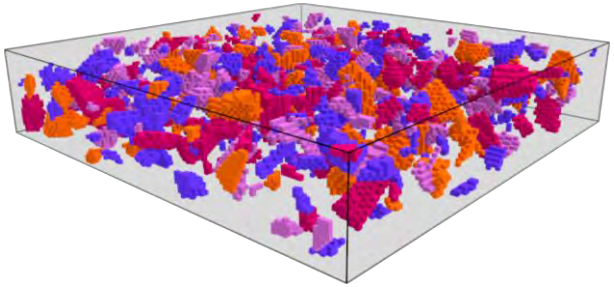
SUSTICOAT

Automaton states and rules

	Cell states
Inert	Polymer
Soluble	Solid inhibitor
Mobile	Dissolved inhibitor
Insoluble	Filler 1
	Filler 2
	…
	Filler N
	Liquid
	Pore

Transition rules
Dissolution
Diffusion



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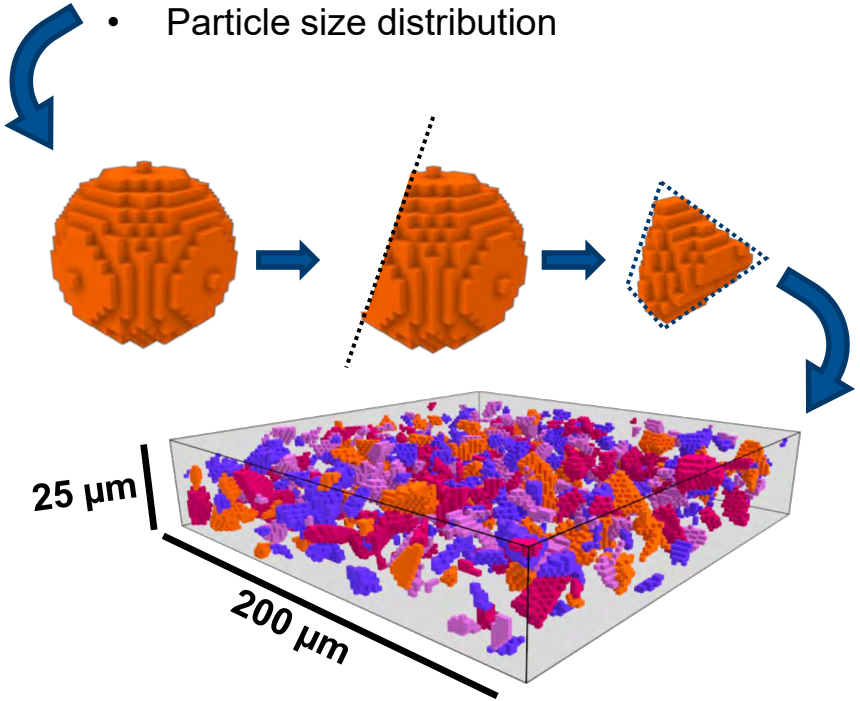
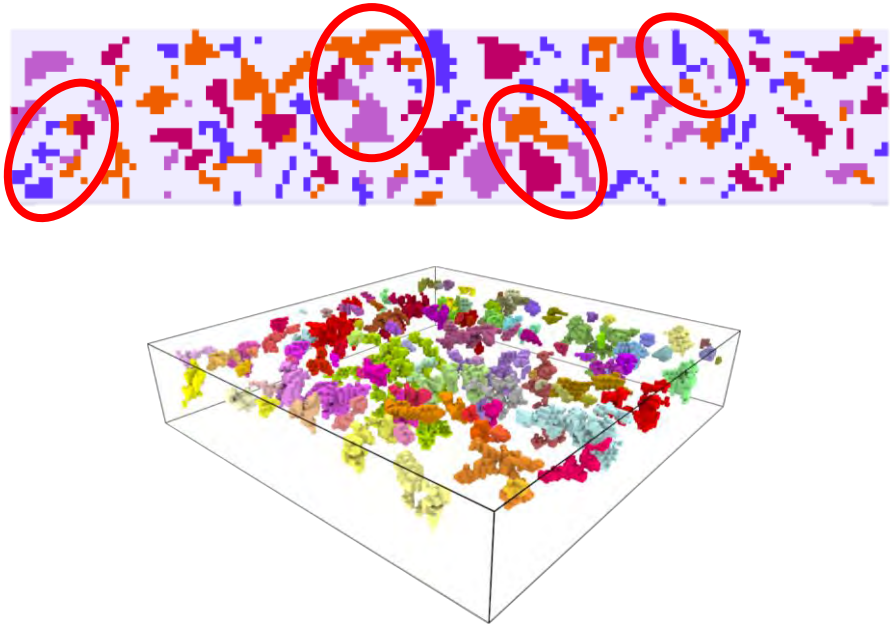
Microstructure generation

- Pigment volume concentration
- Particle size distribution



Clusters formation



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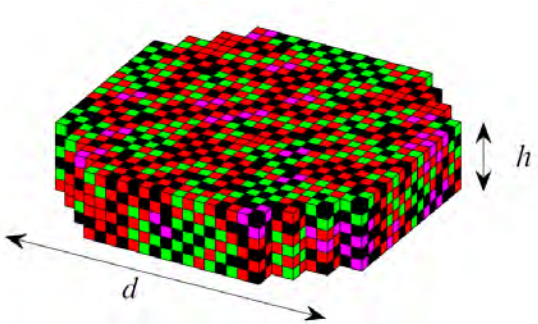
Simulation approach: Cellular Automata model

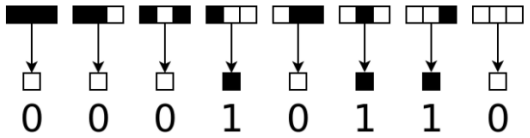
The University of Manchester

AkzoNobel

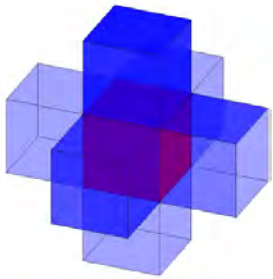
Discrete approach



Transition rules



Locality



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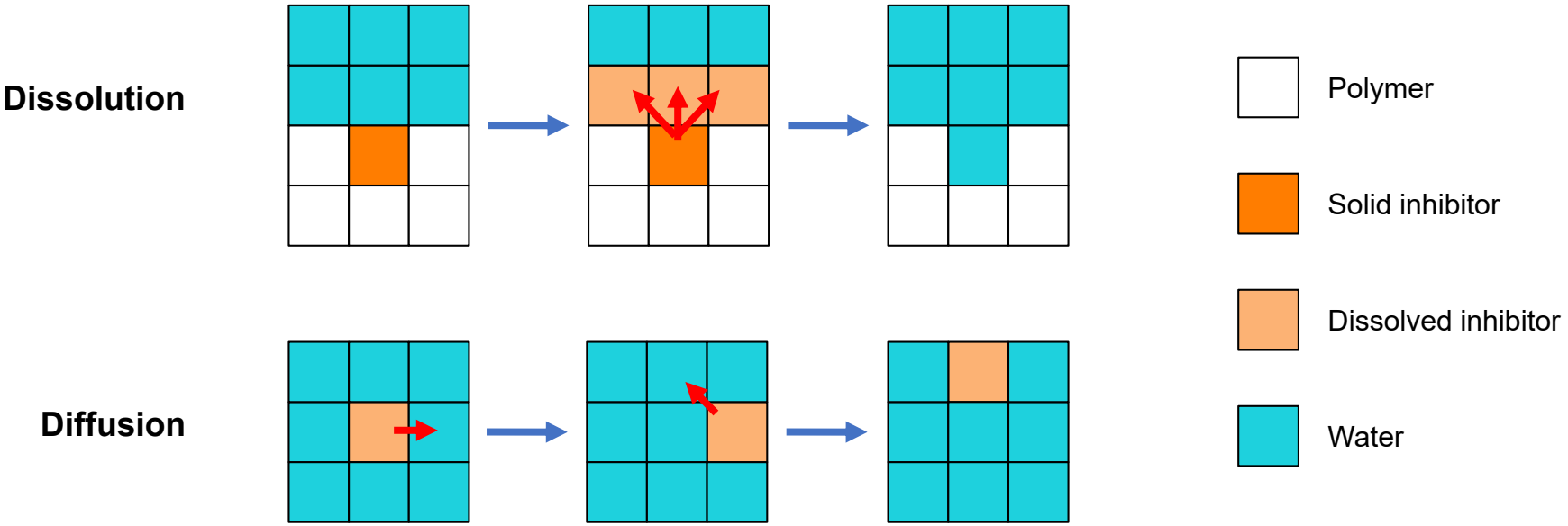
SUSTICOAT

Release simulation



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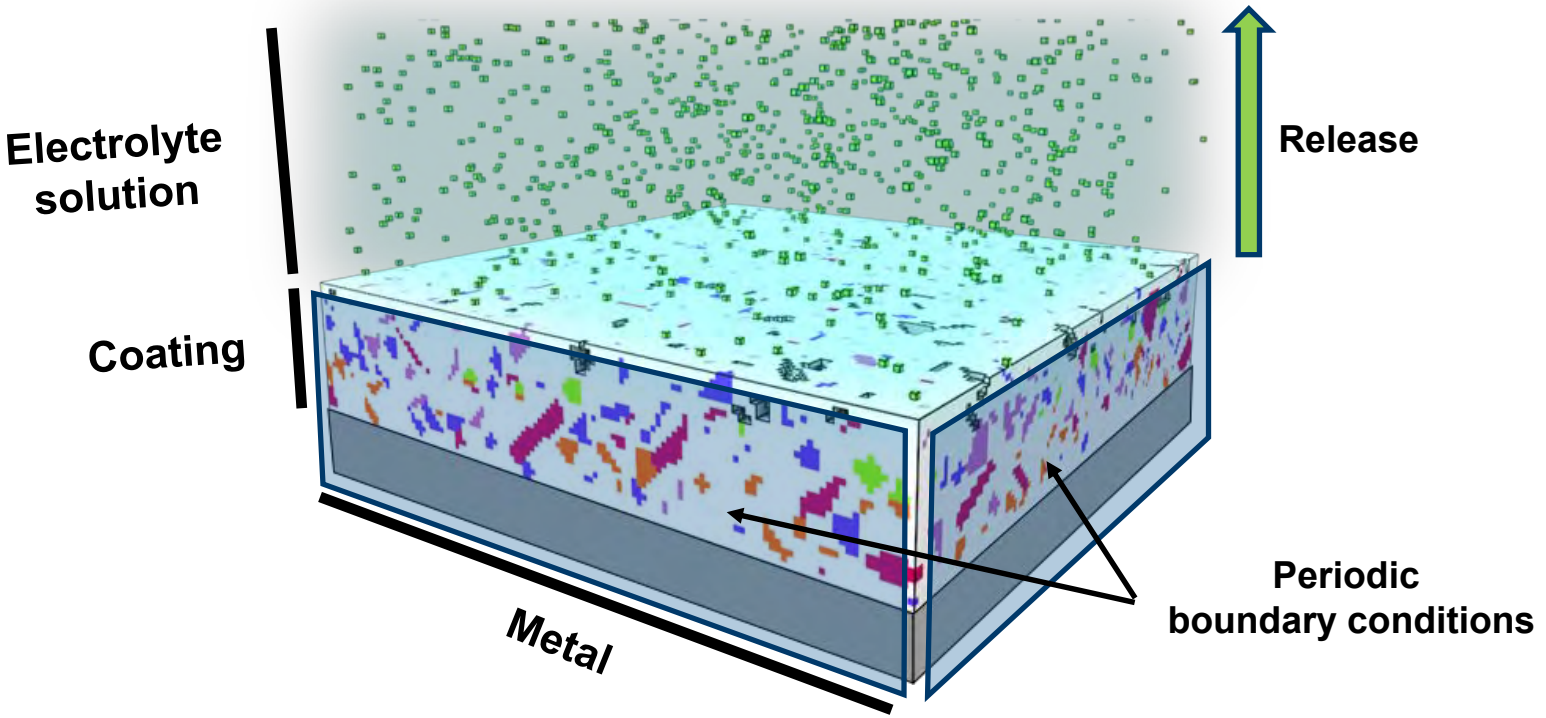
Simulation setup



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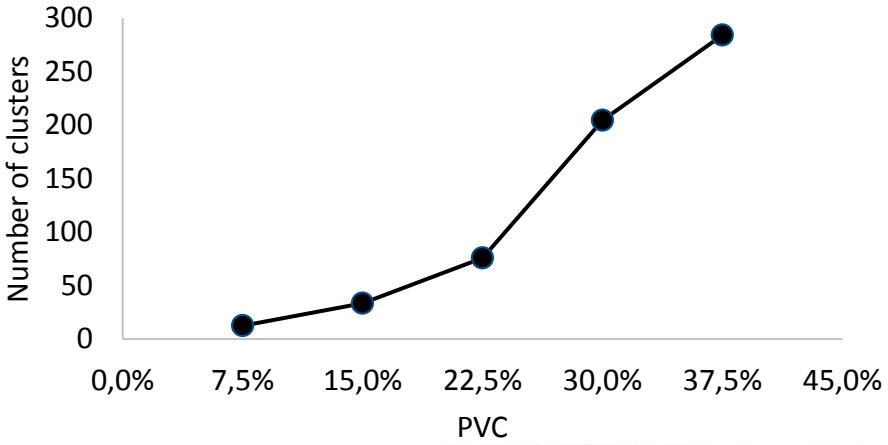
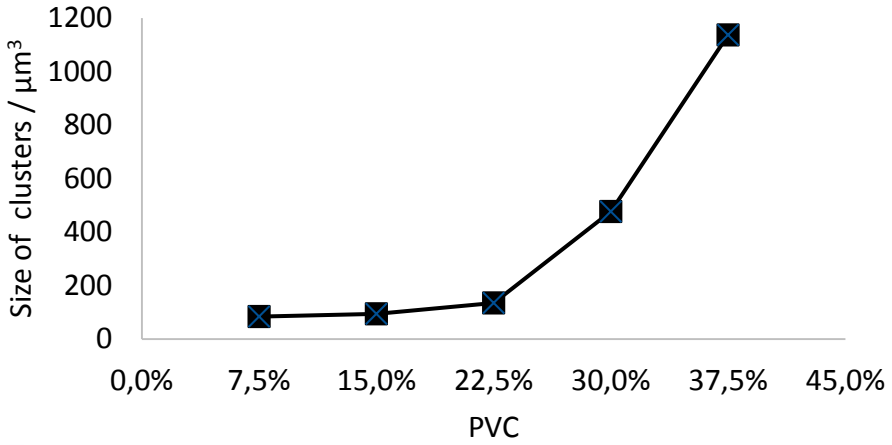
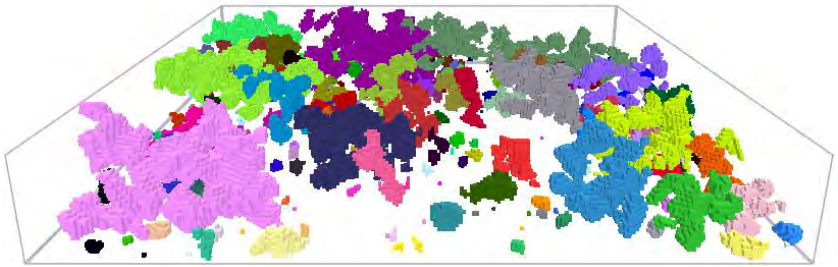
Microstructure analysis

Average number of particle clusters



Average size of particle clusters





Each colour identifies a cluster of particles

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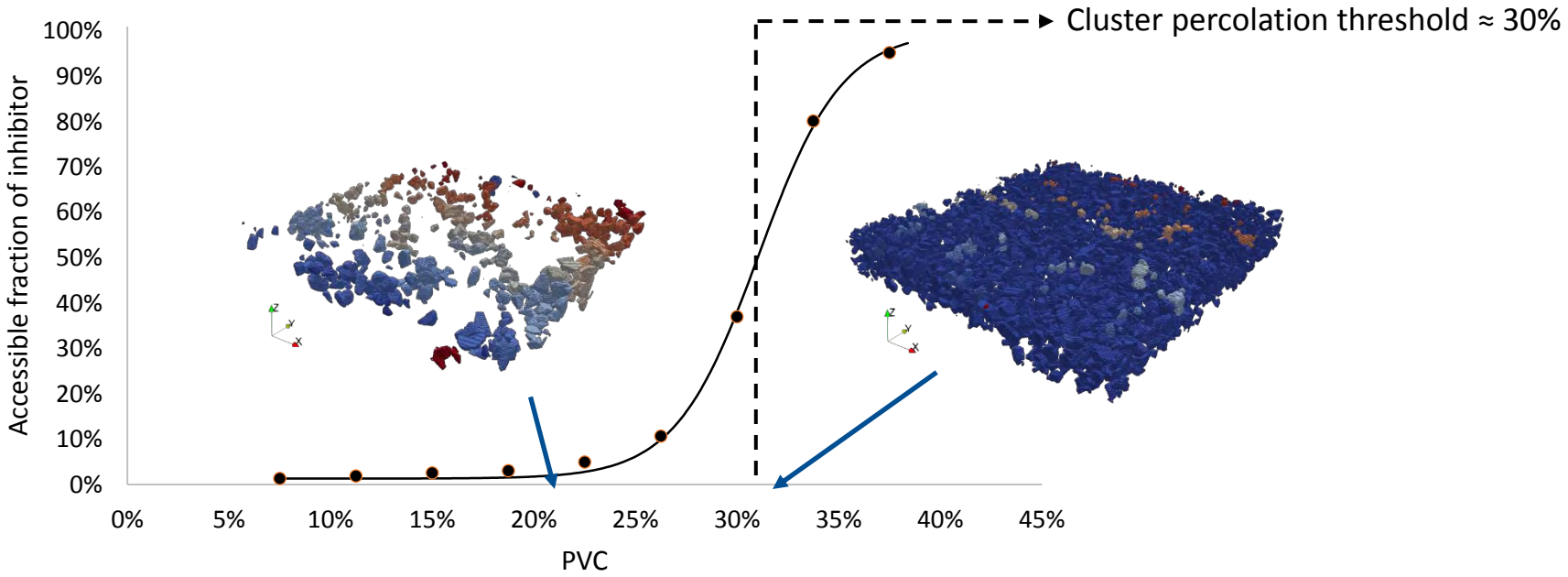
Clusters percolation

The leachable fraction of inhibitor shows a percolating behaviour as a function of the PVC



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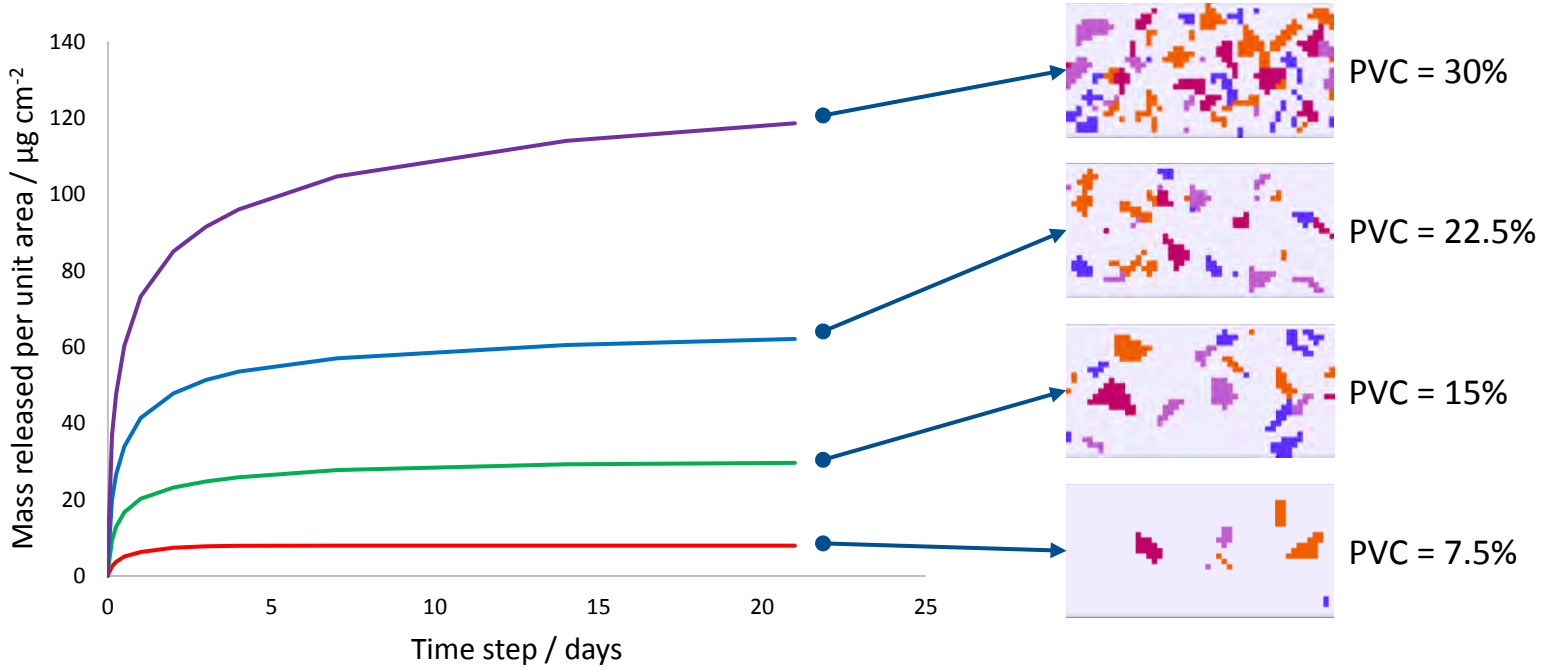
Parametric study of the effect of PVC

Increasing PVC results in increased release due to increased particle connectivity



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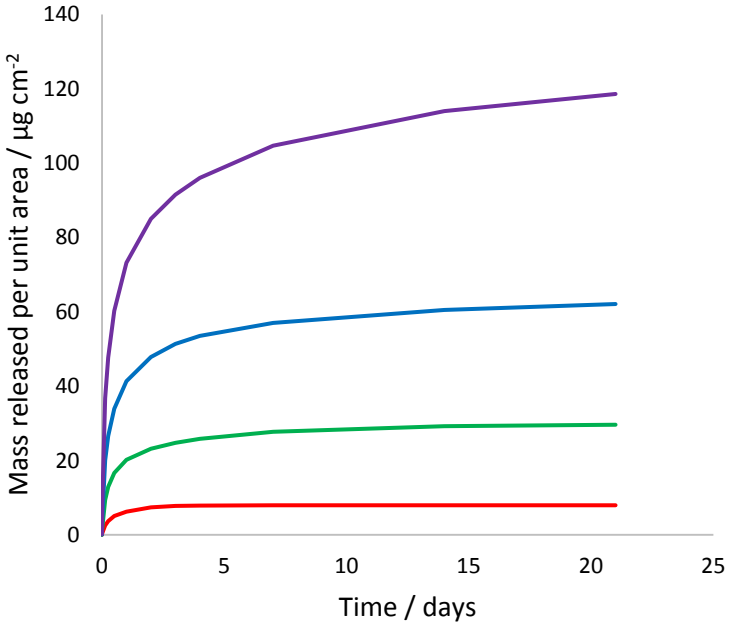
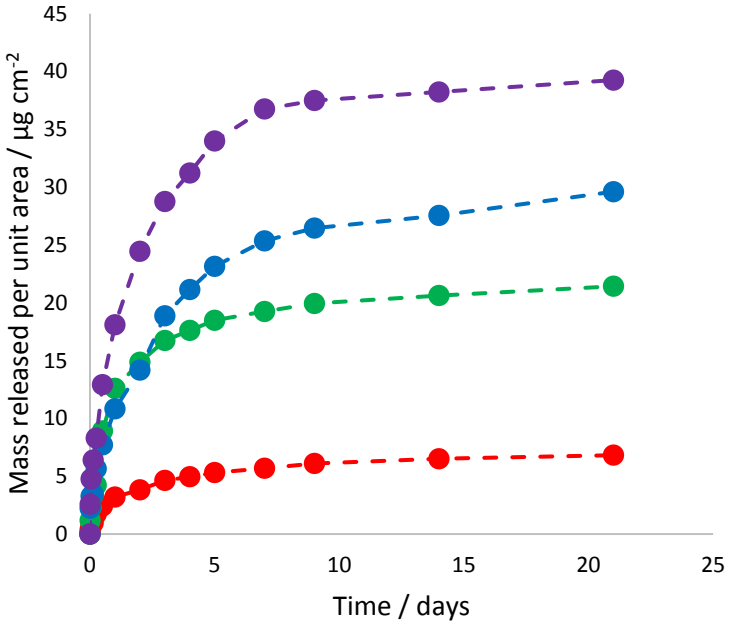
Parametric study of the effect of PVC

Simulated release



Experimental release



PVC = 7.5%

PVC = 15%

PVC = 22.5%

PVC = 30%

Similar trends, but different amount released

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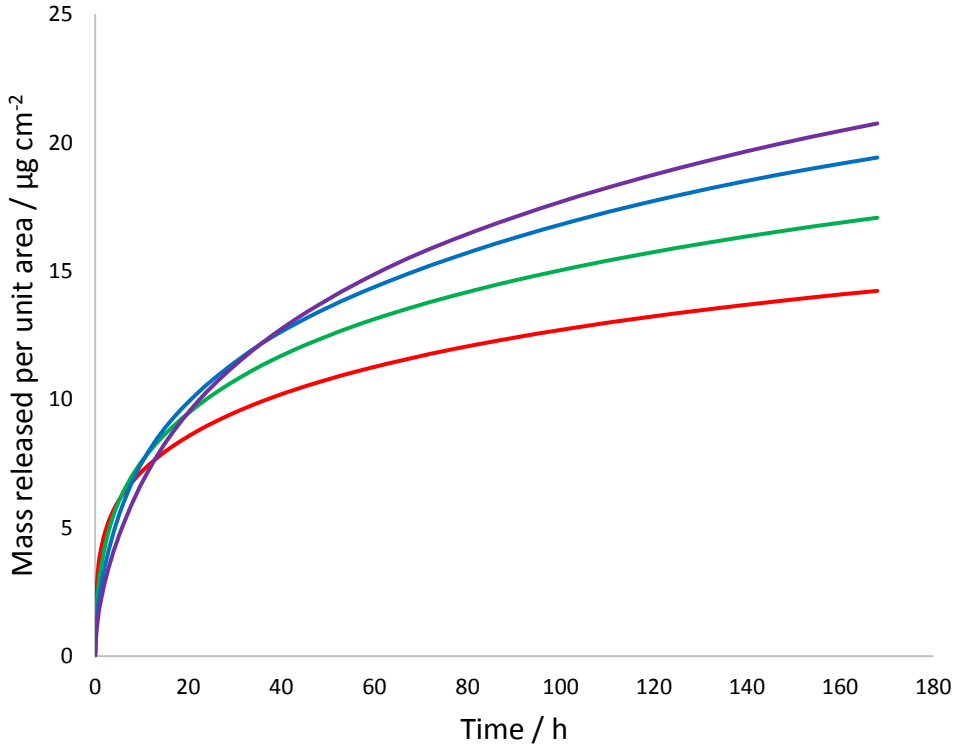
Parametric study of the effect of particle size

Short time release:
controlled by pigment volume fraction (same for all systems)

Long time release:
controlled by internal coating structure (determined by particle size)



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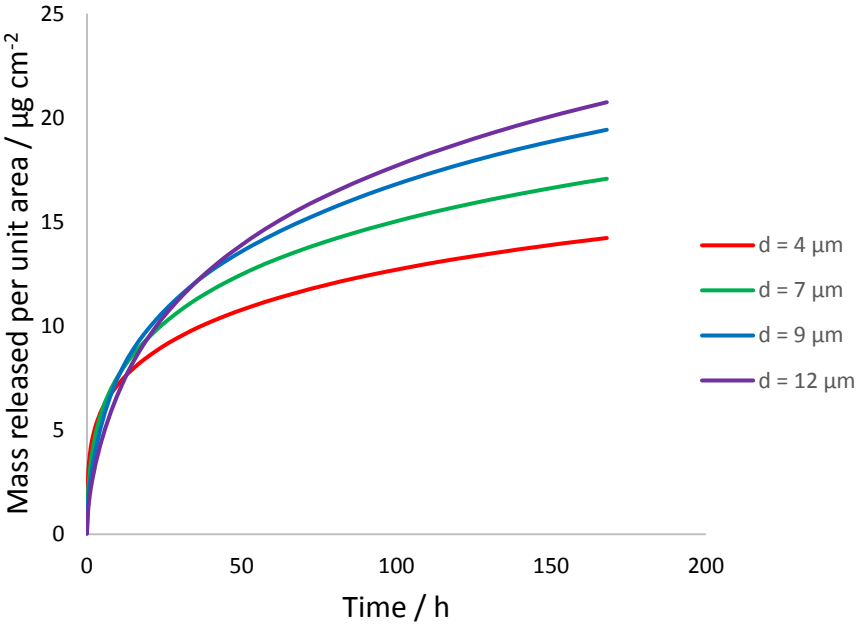
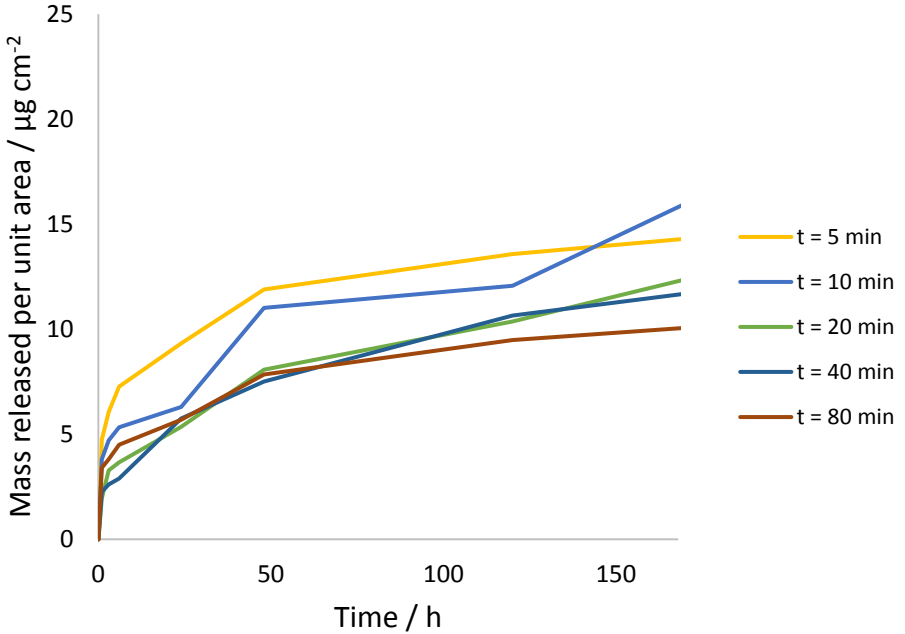
Parametric study of the effect of particle size

Simulated release



Experimental release



Similar trend, similar amount released

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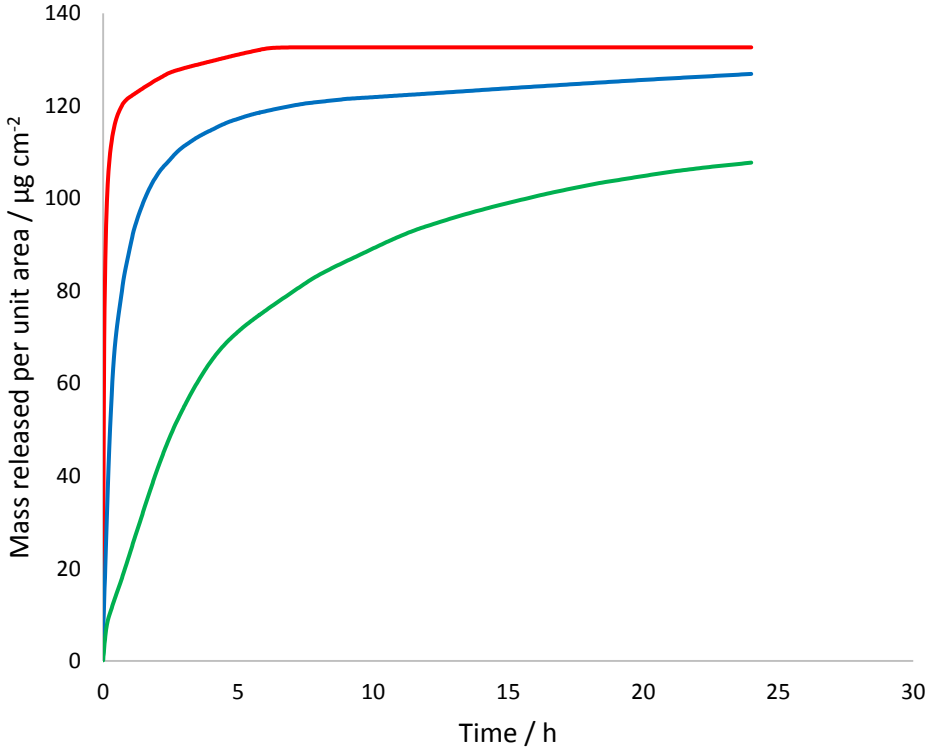
Parametric study of the effect of inhibitor solubility

Low solubility leads to slow initial release (critical for protection)

High solubility leads to fast depletion



PVC = 30%

Solubility

S = 0.13 g/cm³

S = 0.013 g/cm³

S = 0.0013 g/cm³

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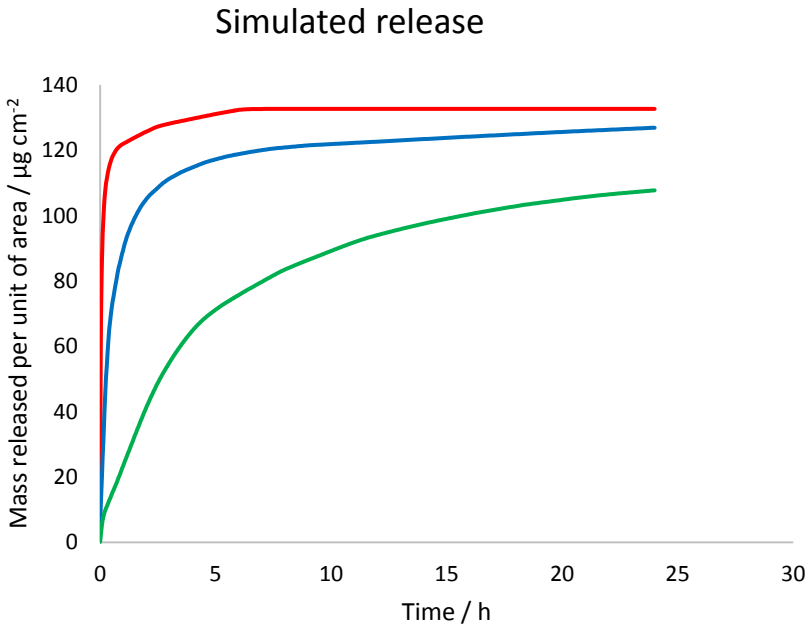
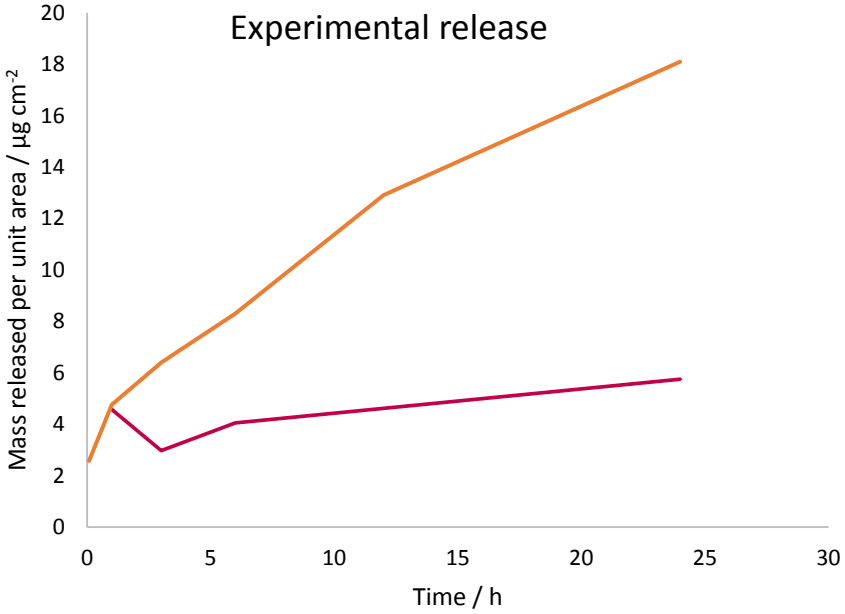
Parametric study of the effect of inhibitor solubility





S = 0.13 g/cm^3 S = 0.013 g/cm^3 S = 0.0013 g/cm^3

Lithium carbonate S = 0.0133 g/cm^3

Lithium phosphate S = 0.0004 g/cm^3

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Conclusions

- The model qualitatively reproduces the experimental correlations between leaching behaviour and formulation parameters (e.g. PVC, size, solubility), allowing parametric investigations of the effect of the formulation
- Quantitative comparison with experimental data is limited, suggesting that other factors not included in the model may play a role in the release process
- Better understanding of the phenomena is needed to direct the modelling work and identify what is missing in the model
- Quantitative characterization of coating microstructure is needed to validate the virtual coating model

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Acknowledgement

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