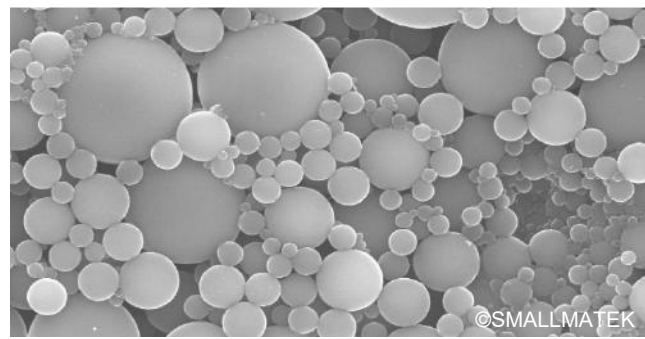


VIPCOAT



Why we need an Active Protective Coatings Ontology? How to construct?



Natalia Konchakova (Hereon), Peter Klein (Fraunhofer ITWM), Heinz A. Preisig (NTNU)



VIPCOAT project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 952903

CONTENT

- Introduction of VIPCOAT project
- Modeling workflows
- Inhibitor delivery case
- Model topology
- Active protective coating ontology
- Open Innovation Framework



Virtual Open Innovation Platform for Active Protective Coatings Guided by Modelling and Optimization

- Topic: DT-NMBP-11-2020 [Open Innovation Platform for Materials Modelling](#)
- Research & Innovation Action
- Grant Agreement [952903](#)

Coordinator:

Helmholtz-Zentrum Hereon

Dr. Natalia Konchakova

Contact: natalia.konchakova@hereon.de

- Start: **May 2021**
- End: April 2025
- Overall budget € **5 519 625**

VIPCOAT

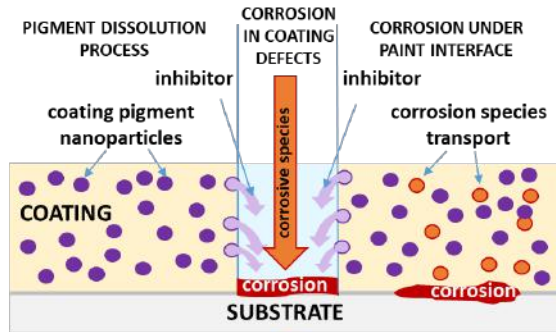
Aims and Objectives



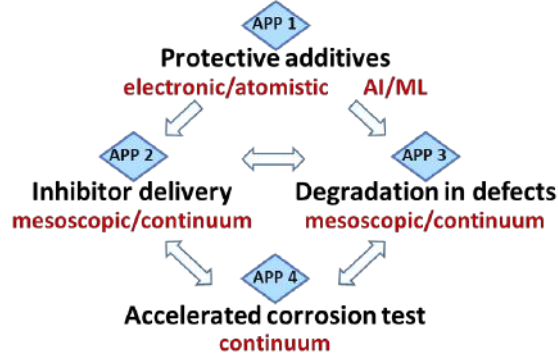
VIPCOAT: <https://ms.hereon.de/vipcoat/index.php.en>

SCIENTIFIC CHALLENGES

Active protective coating



- Effective and efficient corrosion inhibitors
- Optimal coatings microstructure and inhibitors leaching
- Materials behaviour in static and dynamic conditions (wet and dry)
- Accelerated cyclic corrosion test

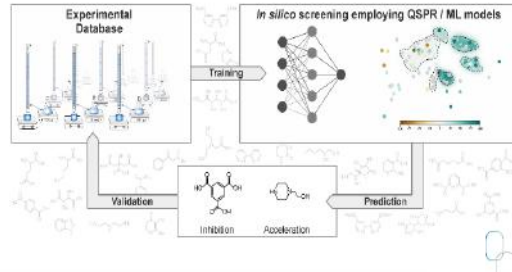


MODELLING SUPPORTED DESIGN

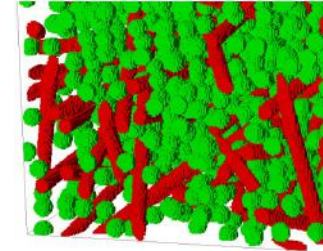
Data-driven and physics-based / multi-physics



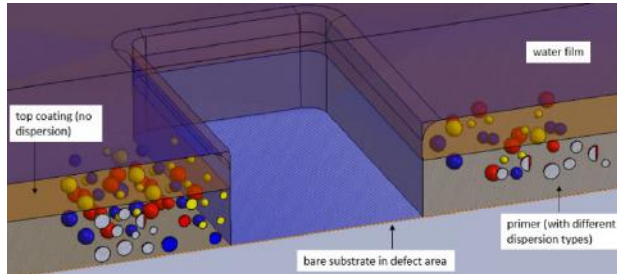
Protective Additives



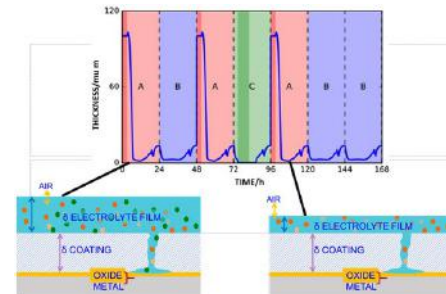
Inhibitor Delivery



Materials Degradation



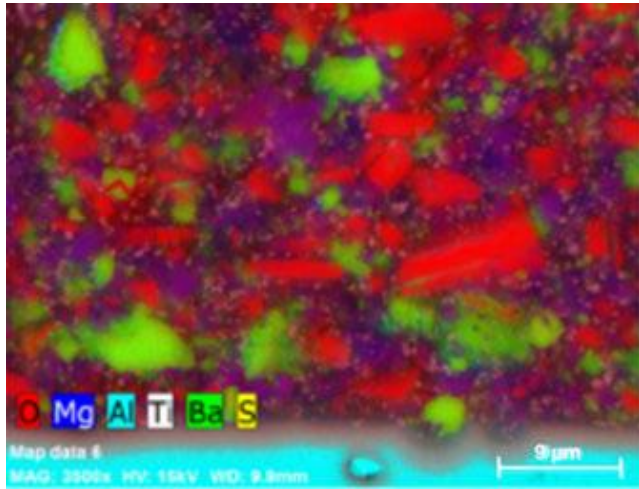
Degradation under Dynamic Conditions



- C. Feiler, D. Mei, B. Vaghefinazari, T. Würger, R. H. Meißner, B. J. C. Luthringer-Feyerabend, D. A. Winkler, M. L. Zheludkevich, S. V. Lamaka, *Corros. Sci.* 2020
- D. Würger, D. Mei, B. Vaghefinazari, D. A. Winkler, S. V. Lamaka, M. L. Zheludkevich, R. H. Meißner, C. Feiler, *npj Mater. Degrad.* 5, 2, 2021.
- J. Höller, J. Niedermeyer, C. Redenbach, N. Ecke, A.K. Schlarb, H. Andrä, P. Klein, *Heat Mass Transfer* 56, 2847–2857, 2020.
- N. Van den Steen, H. Simillion, O. Dolgikh, H. Terryn, J. Deconinck, *Electrochimica Acta*, 187, 714-723, 2016.
- [OntoTrans First Open Workshop, March 15-16, 2022, online](#)

MATERIALS DESIGN

Example: Inhibitor Delivery



- Model delivery of inhibitors from coatings to defects
- Inhibitor release: different solubility, active nano-containers
- Geometry models: use synchrotron images to calibrate stochastic geometry generators
- Use images in diffusion-convection simulation → predict leaching performance



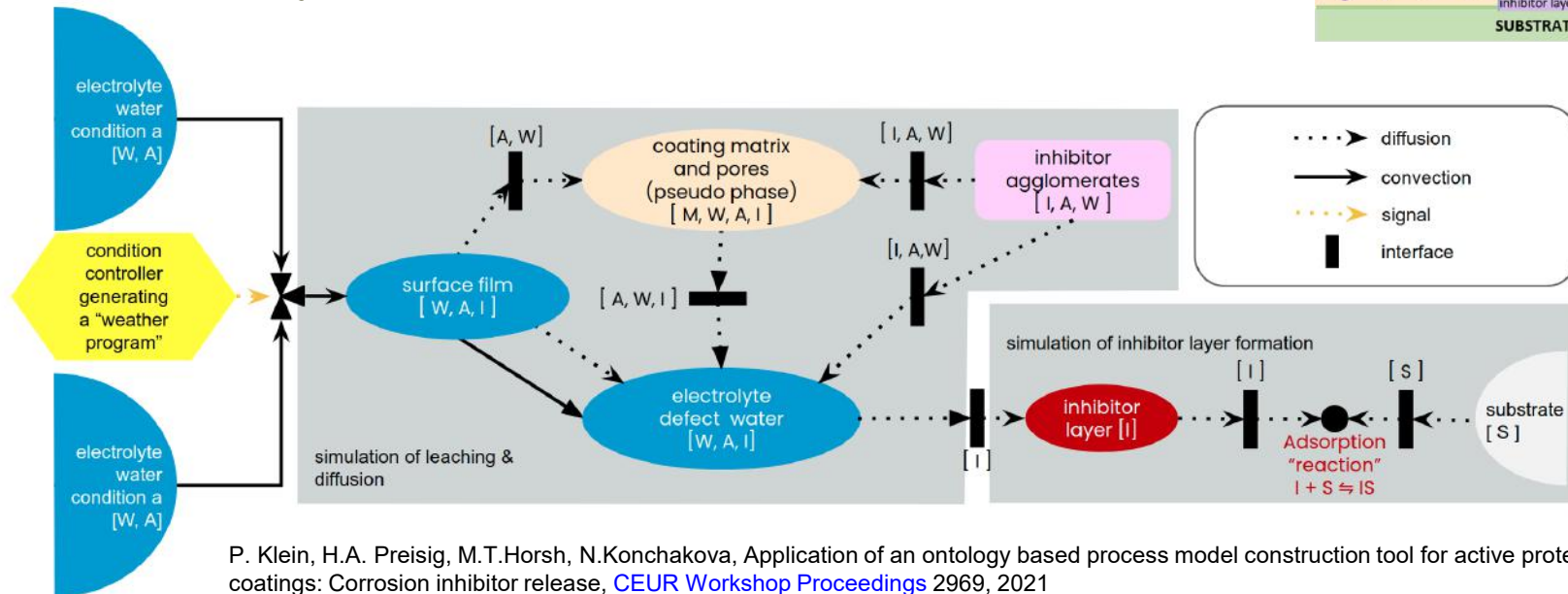
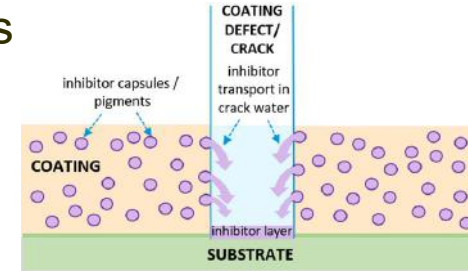
J. Höller, J. Niedermeyer, C. Redenbach, N. Ecke, A.K. Schlarb, H. Andrä, P. Klein, *Heat Mass Transfer* 56, 2020.
J.S.Laird, P.Visser, S. Ranade, A.E. Hughes, H. Terry, J.M.C. Mol, *Progress in Organic Coatings*, 134, 2019.

MODEL TOPOLOGY

Example: Inhibitor Delivery



- Refined MODA workflow - directional graph of MODA entities
Embedding: reservoirs – intensive quantities → BC
- Processes: dynamic & even-dynamic 0-3D systems separated by interfaces



DOMAIN SPECIFIC ONTOLOGY

Active protective coating



On the way to an ontology creation

- Ontology as construction regulation → structurally consistent variable/ equation systems
- Define the scope of ontology
- Terminology identification with the experts in the field
- Knowledge graph for digital processes / logical consistency
- **Process Modelling Suite** as tool



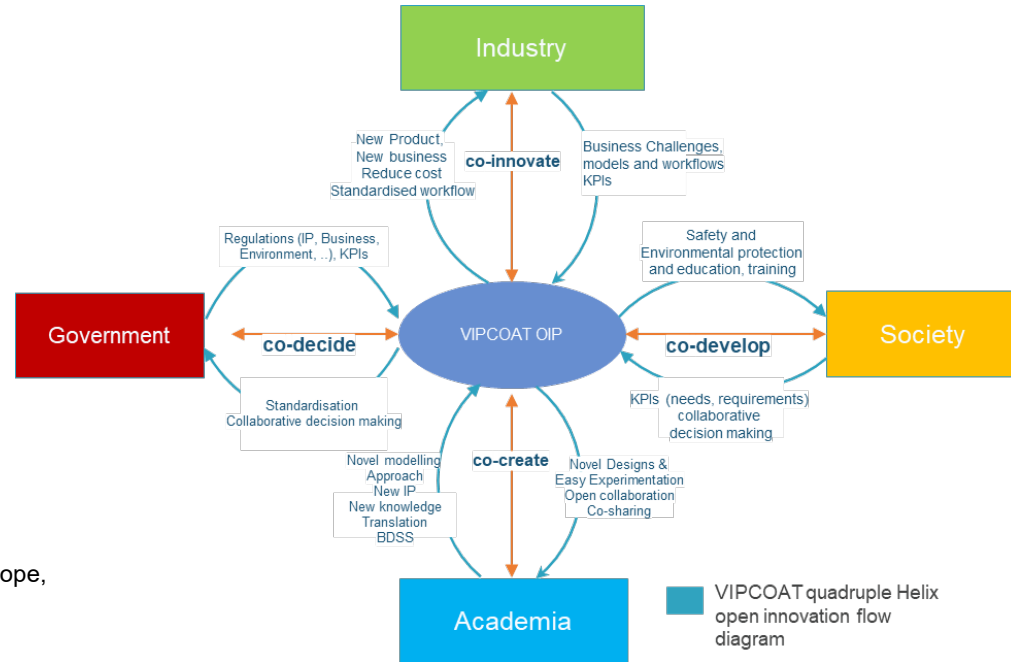
P. Klein, H.A. Preisig, M.T.Horsh, N.Konchakova, Ontology and semantic net based technology applied to smart corrosion protection modelling & simulation, Semantic Web, *submitted*, 2022

OPEN INNOVATION PROCESS

Interaction protocol through VIPCOAT OIP



- Build and maintain a **community of co-innovators**.
- **Exchange information** → ontology defines the language / standard and the software interfaces.



N.Konchakova , P. Klein, et al. Position Paper: Open Innovation in Horizon Europe,
<https://zenodo.org/record/5848552#.YftcKt8o9hE>

CONCLUSION

- Ontology development: use case
- Domain specific ontology for active protective coating where applicable derived from EMMO
- Workflows for models and data connections
- Model topology / ProMo use
- Open Innovation Framework





FOR PEOPLE AND THEIR
FUTURE ENVIRONMENT



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Thank you.



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