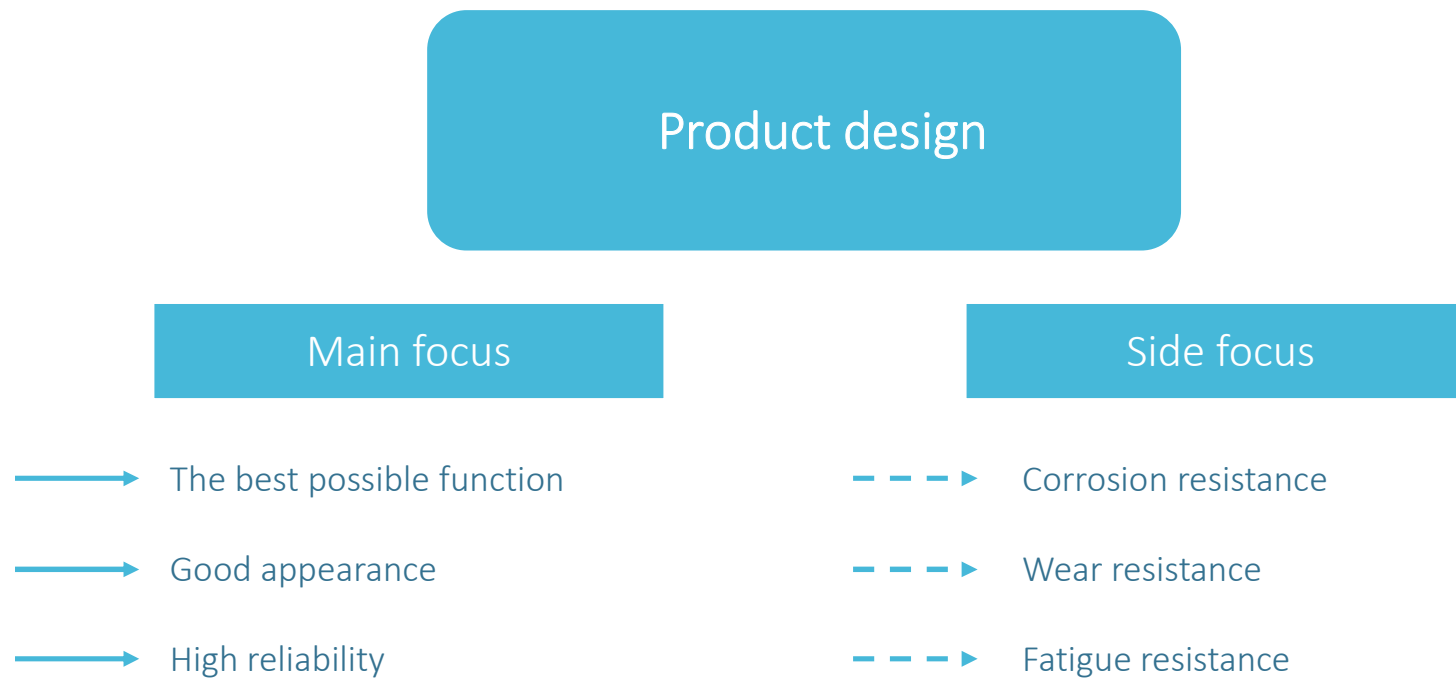


Initiating corrosion prevention during the design phase: utilizing Computer Aided Analysis to evaluate corrosion risks during material selection

Agnieszka Franczak, Florin Muntean, Romain Baudson, Bart Van den Bossche
Elsyca NV, Belgium

Automotive Corrosium Symposium
March 11-12/2024, Detroit, MI, USA

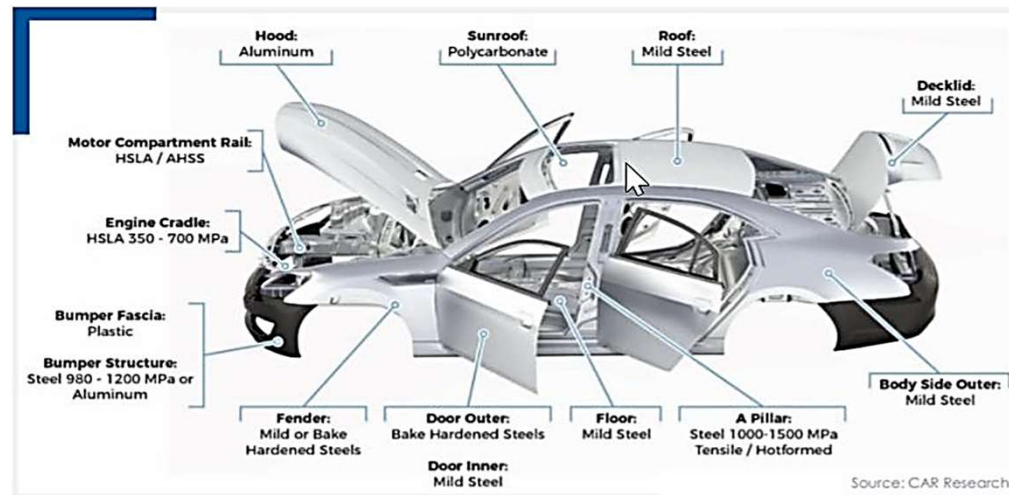
Achieve a long service life with the correct choice of material



Aggressive environment imposes very high demands on materials

Product challenges

New combinations of materials

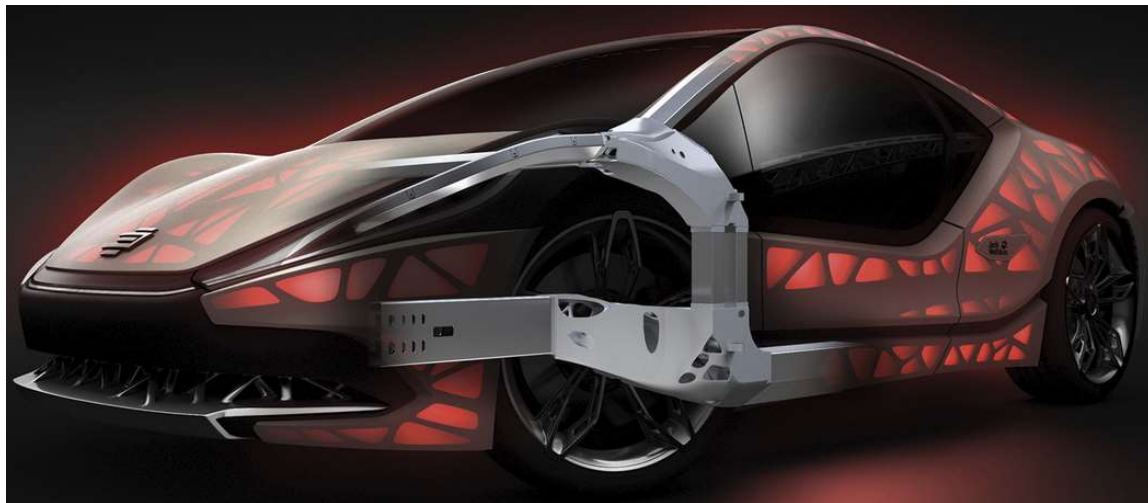


Example of a multi-material body-in-white, Alliance Project Horizon 2020.

Aggressive environment imposes very high demands on materials

Product challenges

New type of designs



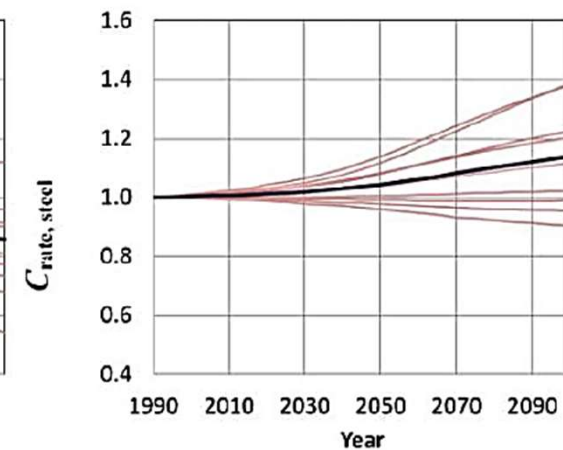
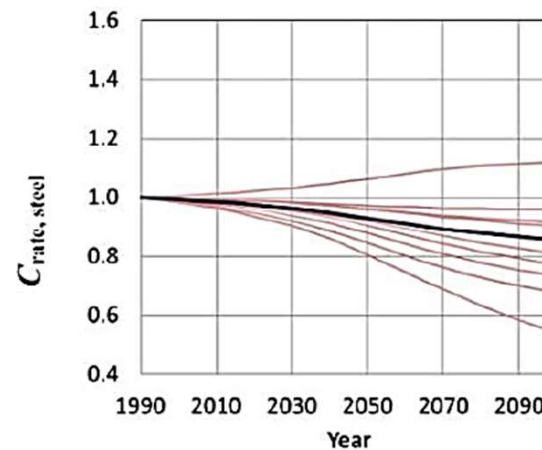
The EDAG Light Cocoon concept car showing the use of additively manufactured nodes combined with steel profiles in the NextGen spaceframe.

Source: <https://www.metal-am.com/articles/metal-3d-printing-in-the-automotive-industry/>

Aggressive environment imposes very high demands on materials

Product challenges

Environmental changes



Effects of climate change on corrosion rates for two cities: Melbourne (left) and Brisbane (right) (Nguyen et al., 2013).

Aggressive environment imposes very high demands on materials

Product challenges

Material costs

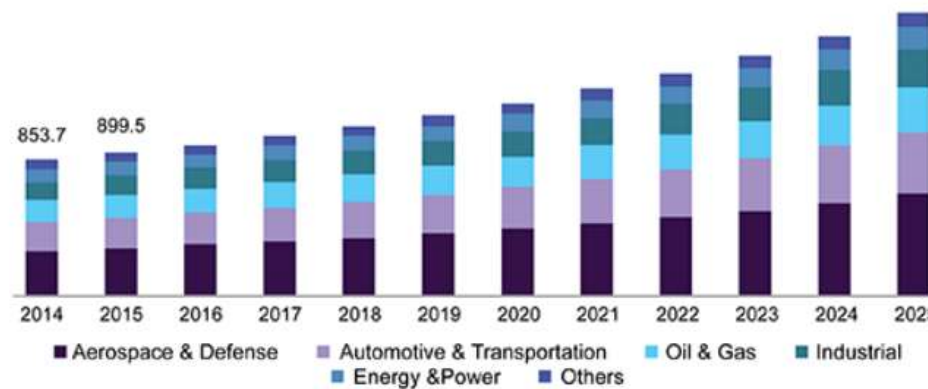
mitigated with:

Value engineering

Material substitution

Design optimization

U.S. corrosion resistant alloys market by end-use, 2014 - 2025 (USD Million)



Aggressive environment imposes very high demands on materials

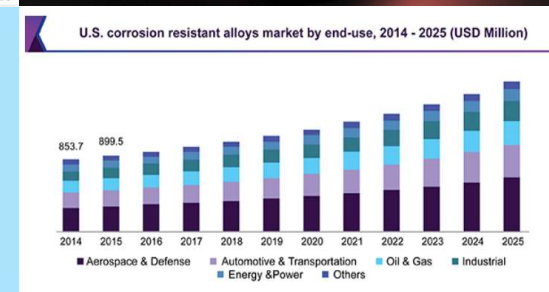
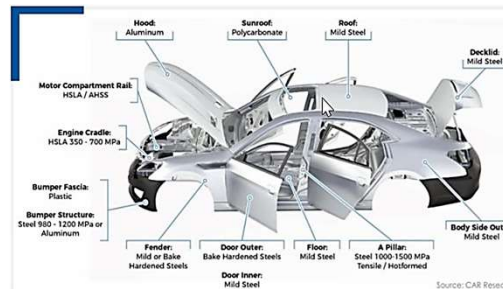
Product challenges

New types of designs

New combinations of materials

Environmental changes

Material costs



Digital transformation isn't important, it's imperative

Intelligent corrosion tool concept

REQUIREMENTS

1

A computational database architecture:

- storing and retrieving user-specified material properties and behavior,
- easy selection of material, corrosion mode, environment, and other user-definable contextual parameters.

2

With the ability to **gather key geometry** and materials information from a component drawing file, reading Standard Triangle Language (STL)-based drawings designed in commercial CAD software.

3

With the ability to **read multiple CAD drawings**, identifying materials and potential corrosion modes, automatically prepare model preprocessing files, and interface files.

4

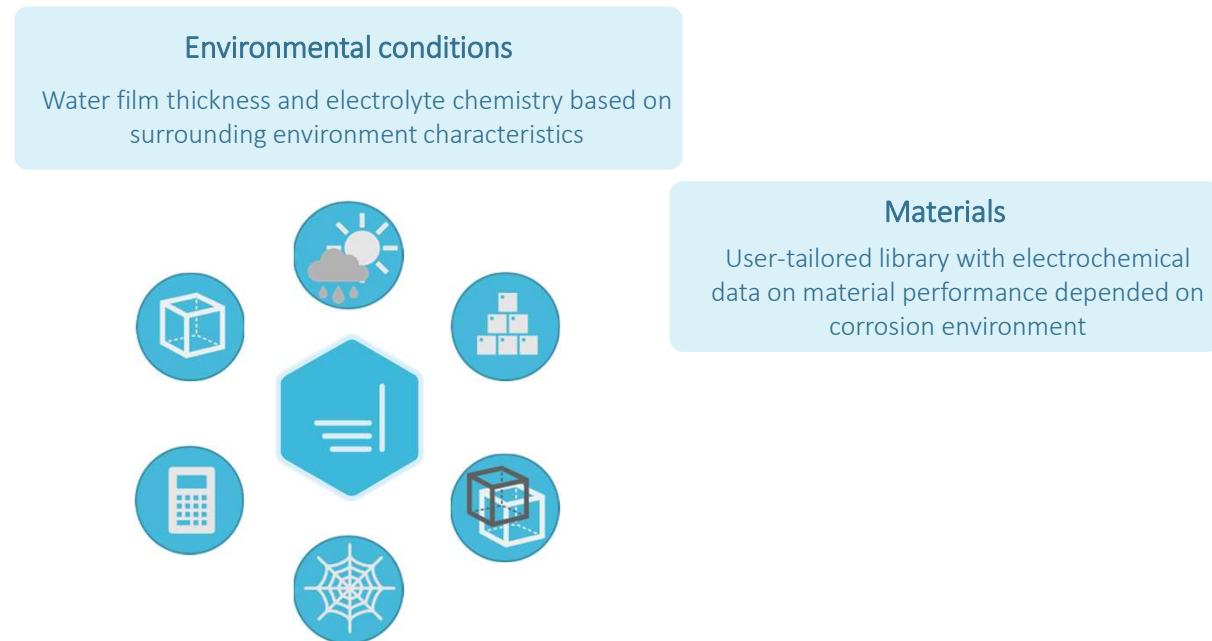
Incorporating logic to **evaluate drawings/designs** against the corrosion risks depended on environment and material properties.

Computer Aided Analysis:

a *dry* assistance in spotting corrosion risks when working on product design and material selection

Computer Aided Analysis approach

A *dry* concept of corrosion risk assessment

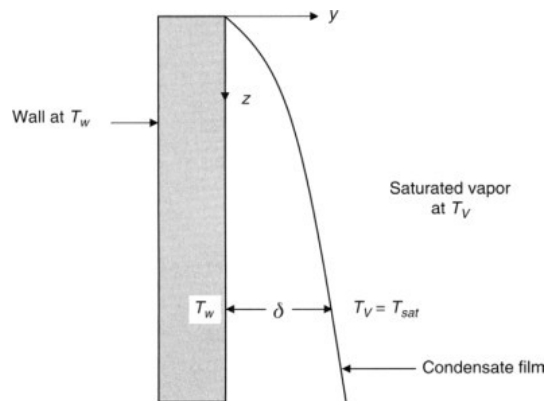


Computer Aided Analysis approach

Environmental conditions

Film thickness

Accelerated first guess of water film thickness based on environmental conditions and geometrical characteristics:



Nusselt equation

$$\delta = \left[\frac{4\mu_L k_L (T_V - T_w) z}{\rho_L (\rho_L - \rho_V) g \lambda} \right]^{1/4}$$

Chemistry

Electrical conductivity, oxygen diffusion coefficient and oxygen bulk concentration derived from environmental salinity concentration and temperature:

Conductivity

$$EC^{(0)} = \sum_i \Lambda_{m,i}^0 c_i = \left(\frac{F^2}{RT} \right) \sum_i D_i z_i^2 c_i \quad \text{Nernst-Einstein equation}$$

Diffusion

$$\log_{10} \left[\frac{D}{\text{cm}^2 \text{s}^{-1}} \right] = -4.410 + \frac{773.8}{T} - (506.4/T)^2 \quad \text{with } T \text{ in } [K]$$

Source: R.W. Serth, 11 - CONDENSERS, Editor(s): R.W. Serth, Process Heat Transfer, Academic Press, 2007, Pages 539-628,

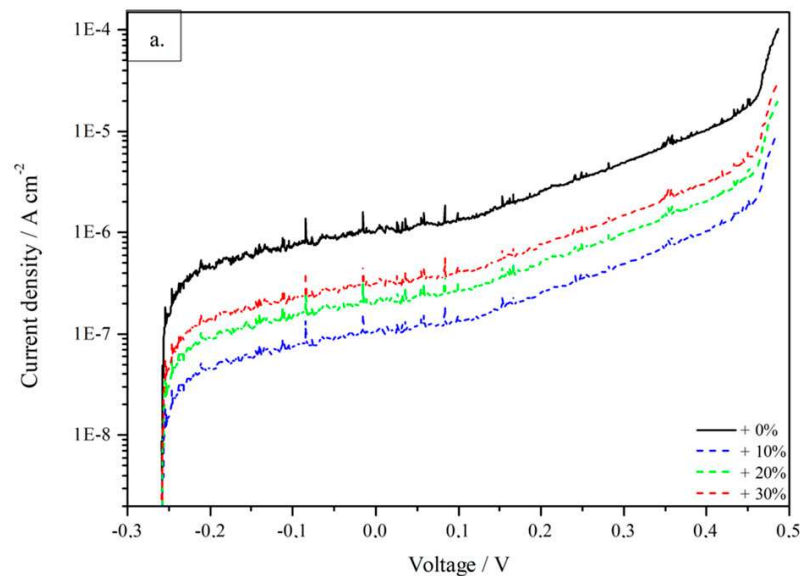
Han, P. and Bartels, D. M. (1996). Temperature dependence of oxygen diffusion in H₂O and D₂O. The Journal of Physical Chemistry, 100(13), 5597-5602.

Computer Aided Analysis approach

Materials – electrochemical data

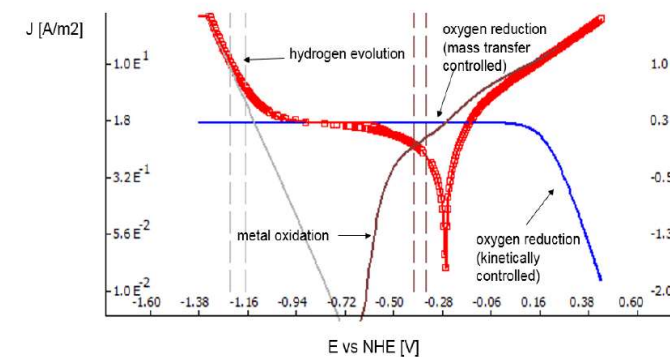
Galvanic corrosion

- Raw polarization data



Atmospheric corrosion

- Decomposed curves (metal oxidation, oxygen reduction and hydrogen evolution) are required



Reaction	Name	Stoichiometry	Modeling strategy
1	O ₂ reduction	$2 \text{H}_2\text{O} + \text{O}_2 + 4 \text{e}^- = 4 \text{OH}^-$	Spline or Butler-Volmer, mass transfer limited
2	H ₂ evolution	$\text{H}_2\text{O} + 2 \text{e}^- = \text{H}_2 + 2 \text{OH}^-$	Analytic Butler-Volmer
3	Metal oxidation	$\text{Me} + x \text{e}^- = \text{Me}^{x+}$	Spline

Computer Aided Analysis approach

Materials – electrochemical data

Atmospheric corrosion

- The Butler-Volmer expressions are mathematically expressed as:

Reaction	Name	Stoichiometry	
1	O ₂ reduction	$j_1 = k_{a1} \exp(\alpha_1 2F(V_1 - U - E_{o1})/RT) - k_{c1} [H^+] \exp(-\beta_1 2F(V_1 - U - E_{o1})/RT)$	Eq. 1
2	H ₂ evolution	$j_2 = k_{a2} \exp(\alpha_2 4F(V_1 - U - E_{o2})/RT) - k_{c2} [H^+] [O_2]_s \exp(-\beta_2 4F(V_1 - U - E_{o2})/RT)$	Eq. 2

- The theoretical limited current density can be calculated from:

$$j_{2\text{limRDE}} = -0.62 n F D^{2/3} \nu^{-1/6} \omega^{1/2} [O_2]_b \quad \text{Eq. 3}$$

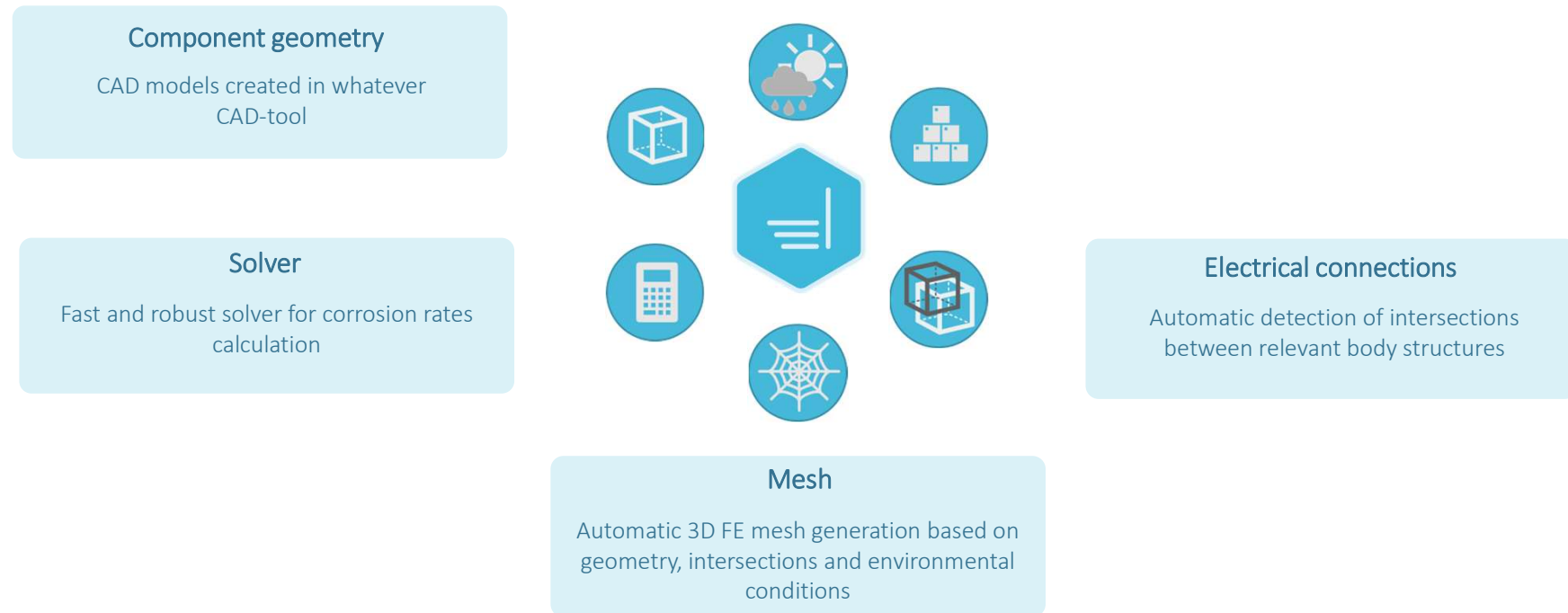
- The diffusion layer thickness can be introduced as:

$$j_2 = nFD \frac{[O_2]_s - [O_2]_b}{\delta} \quad \text{Eq. 4}$$

D	oxygen diffusion coefficient (m ² /s);
ω	rotation speed (rad/s);
ν	kinematic viscosity (m ² /s);
n	# of electrons exchanged in electrode reaction 2 (= 4);
F	Faraday's number (= 96500 C/mol);
$[O_2]_b$	oxygen bulk concentration (mol/m ³);
j	oxygen reduction mass transfer limited current density (A/m ²).

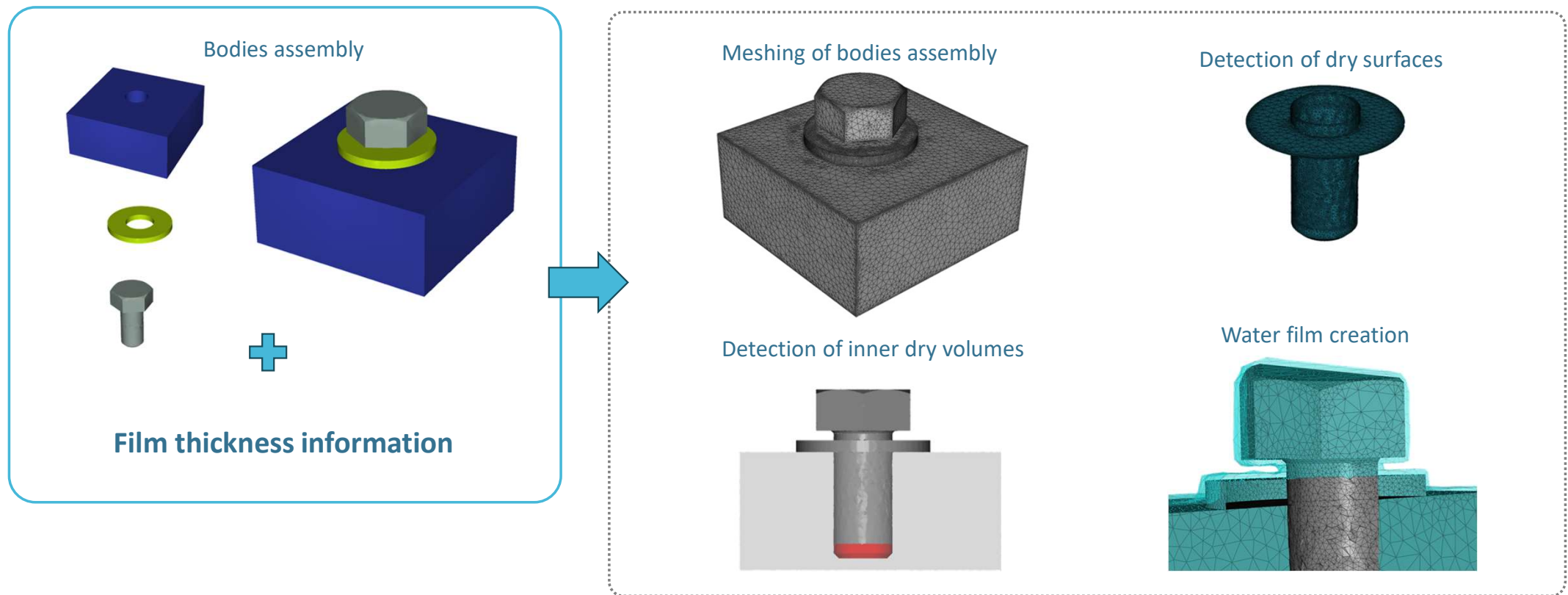
Computer Aided Analysis approach

A *dry* concept of corrosion risk assessment



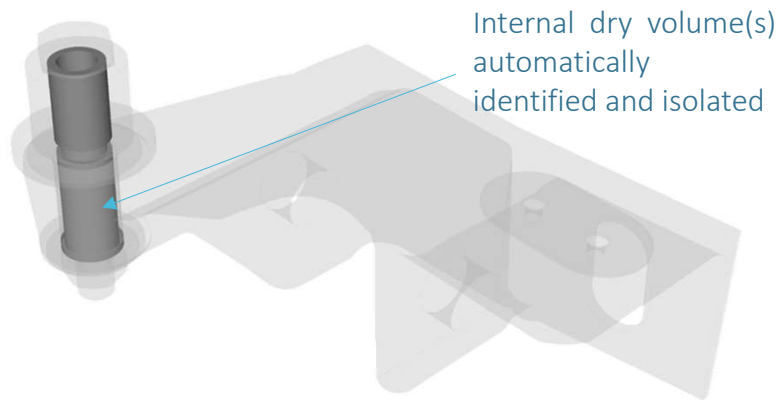
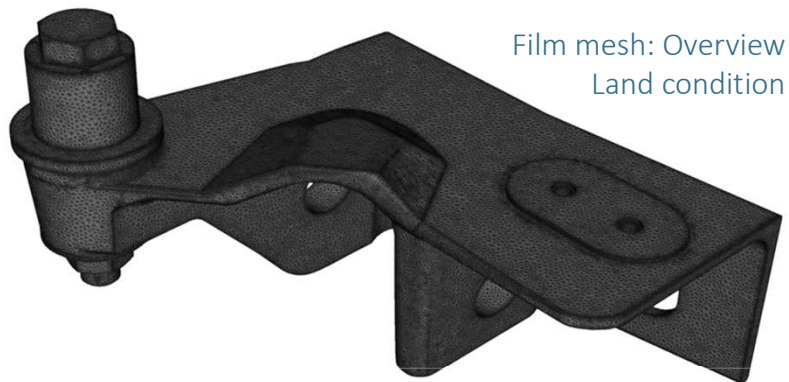
Computer Aided Analysis approach

Automatic pre-processing



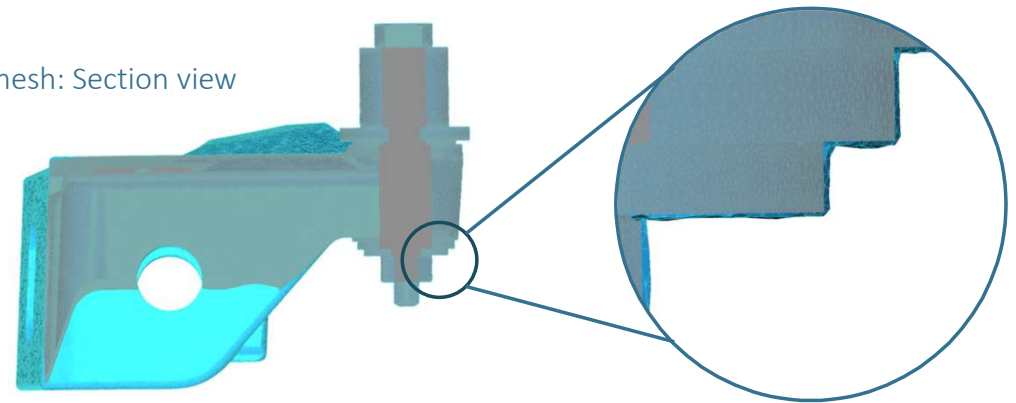
Computer Aided Analysis approach

Meshing step



Conditions	Land	Coastal	User Defined	User Defined with Sea water
Film thickness [mm]	0.147	0.161	0.182	0.182
FE Mesh: # Nodes	343 838	341454	335 779	335 779
FE Mesh: # Elements	996 575	985 640	961 653	961 653
Meshing Time [min]*	12	11	11	-
RAM Consumption [GB]*	1.57	1.56	1.57	-

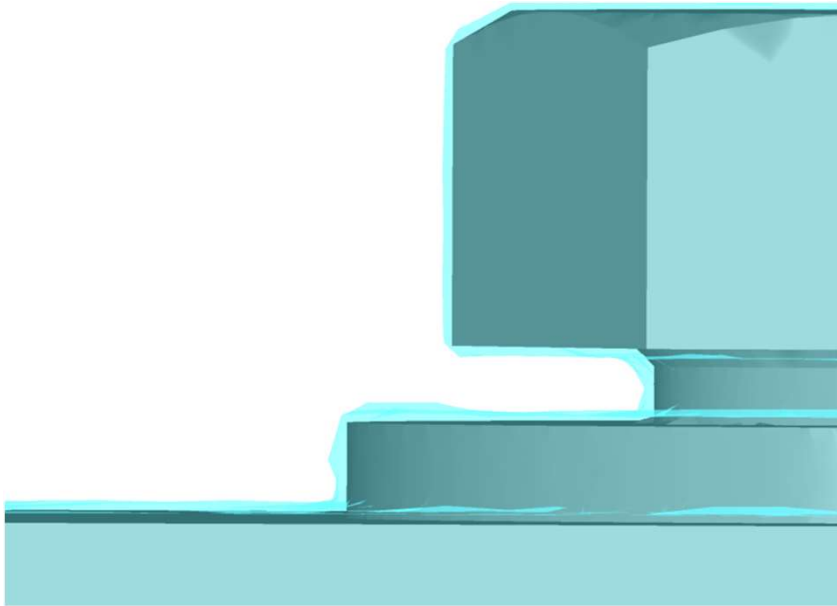
Film mesh: Section view



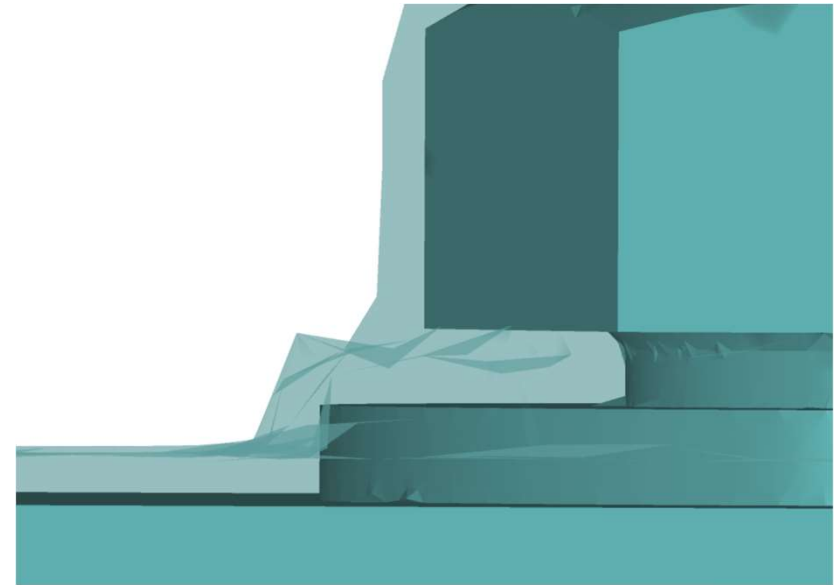
*Machine characteristics: **Processor:** 11th Gen Intel(R) Core(TM) i7-11850H @ 2.50GHz | **Installed RAM:** 16.0 GB (15.7 GB usable)

Computer Aided Analysis approach

Water film definition



Water film thickness 0.1 mm



Water film thickness 0.5 mm

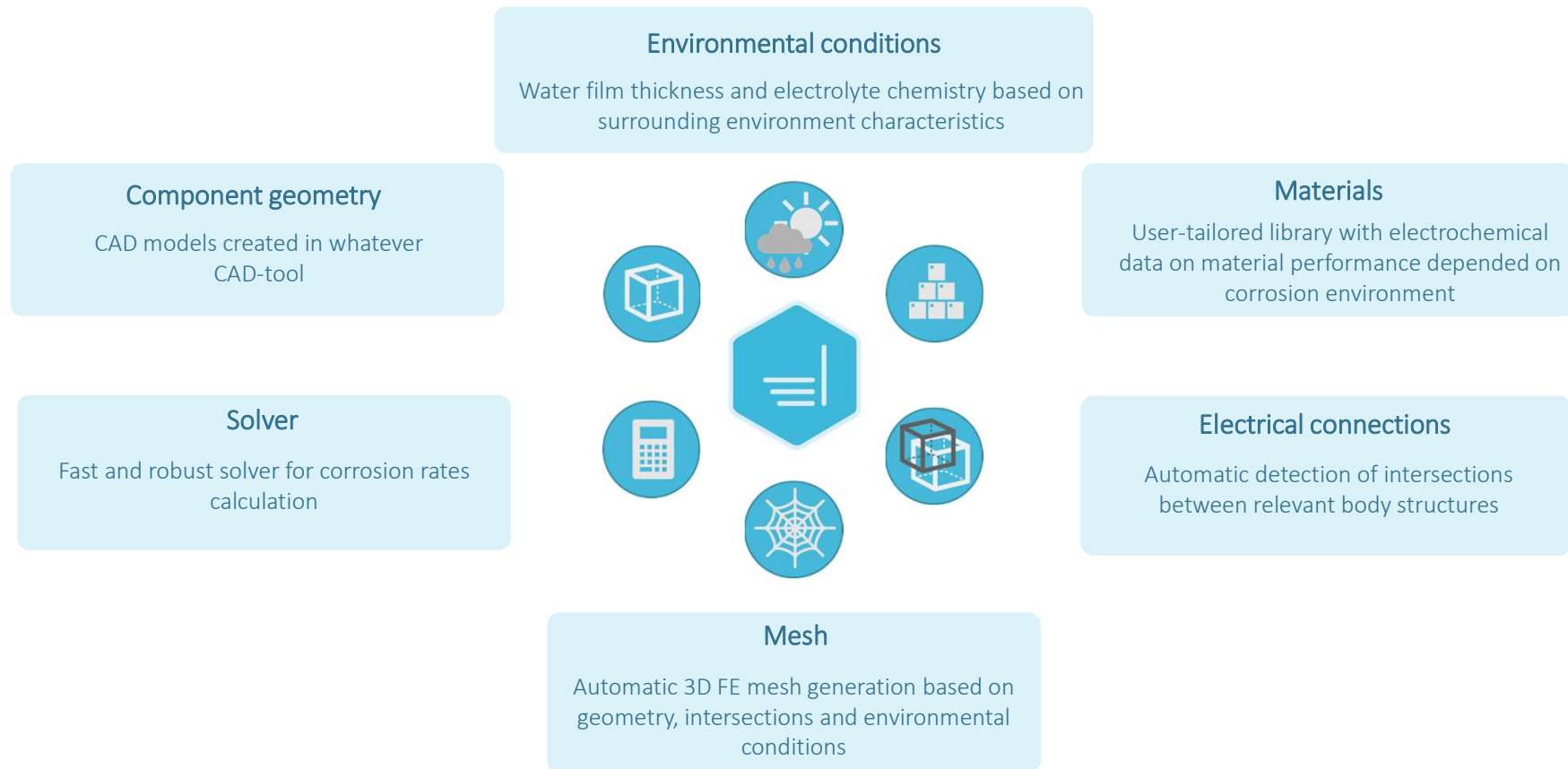
Computer Aided Analysis approach

Parameter definition

The screenshot displays the 'Elsyca CorrosionManager' software interface. On the left is a 'Project Dashboard' sidebar with a search bar and a list of icons for 'Import Geometry', 'Select Material', 'Environmental Conditions' (highlighted with a blue circle and a red arrow), 'Define Connections', 'Mesh', 'Solve', and 'Result'. The main workspace is divided into three panels: 'Environmental Conditions', 'Component Characteristics', and 'Electrolyte Film Characteristics'. The 'Environmental Conditions' panel contains four icons (factory, palm tree, wave, and person) with the wave icon selected. Below these are sliders for 'Air temperature [°C]' (set to 10), 'Atmospheric pressure [Pa]' (set to 101325), 'Salinity [g/l]' (set to 30.00), and 'Relative humidity [%]' (set to 100). The 'Component Characteristics' panel has sliders for 'Air/Component temperature difference [°C]' (Minimum: -20, Maximum: 20), 'Characteristic length [m]' (set to 1.000), and 'Characteristic angle [°]' (set to 45). The 'Electrolyte Film Characteristics' panel lists parameters: 'Water film thickness [mm]' (0.170), 'Electrical conductivity [S/m]' (1.622), 'O2 diffusion coefficient [m²/s]' (1.331e-9), 'O2 bulk concentration [mol/m³]' (0.2927), and 'Wetted time fraction [%]' (50). At the bottom are '< Back' and 'Next >' buttons.

Computer Aided Analysis approach

A *dry* concept of corrosion risk assessment



Computer Aided Analysis approach

A dry concept of corrosion risk assessment

✓ A computational database architecture.

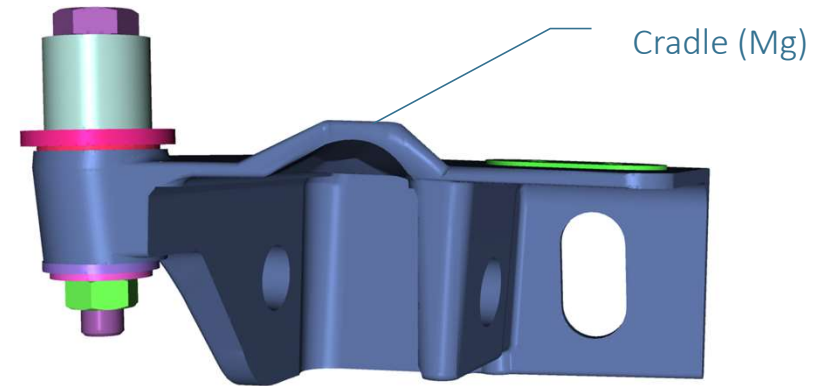
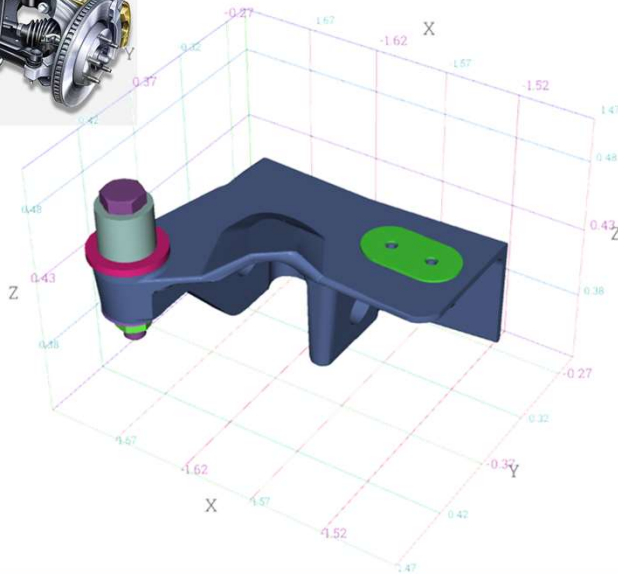
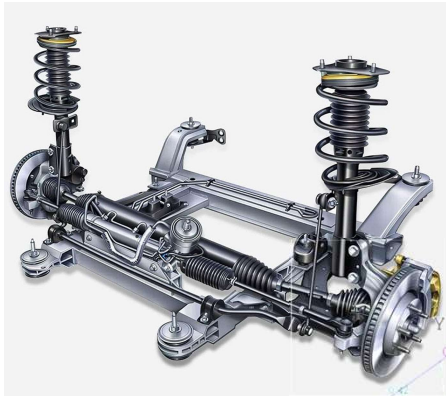
✓ Ability to gather key geometry from STLs.

✓ Ability to read multiple CAD drawings, identifying materials, corrosion modes, automatic pre-processing.

✓ Logical evaluation of drawings/designs against the corrosion risks.

Computer Aided Analysis approach

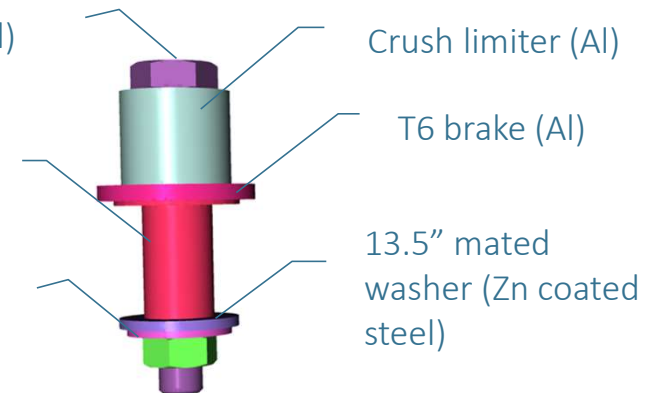
Logical evaluation of the corrosion risks



Bolt
(Zn coated steel)

Sleeve (Al)

washer (Zn
coated steel)



Crush limiter (Al)

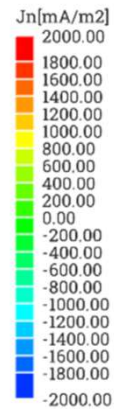
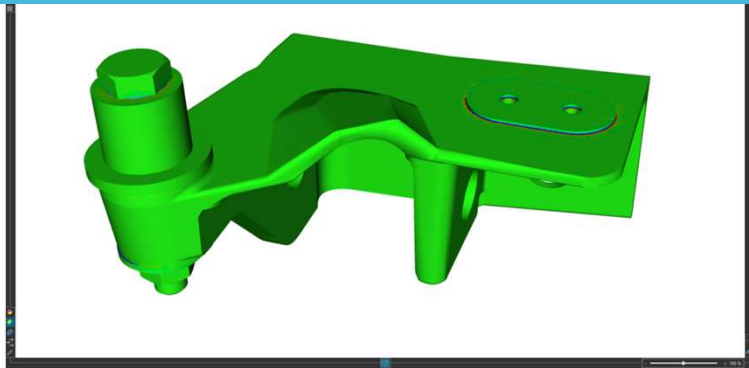
T6 brake (Al)

13.5" mated
washer (Zn coated
steel)

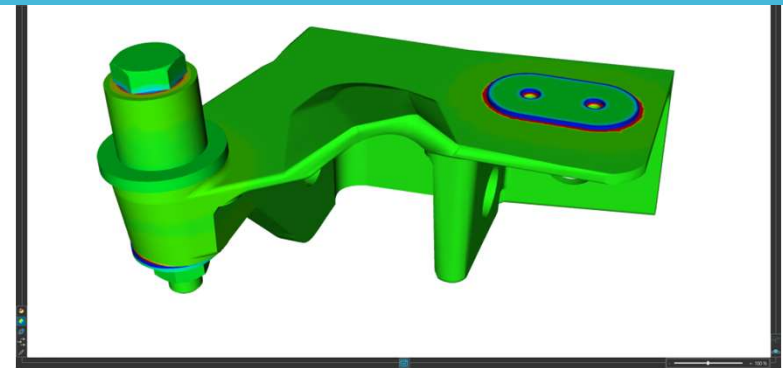
Computer Aided Analysis approach

Logical evaluation of the corrosion risks

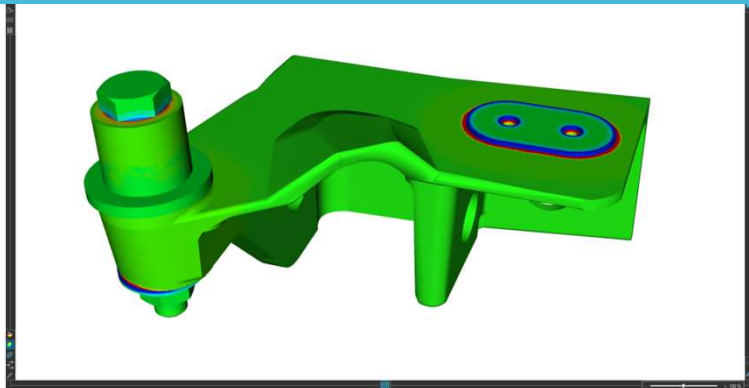
Land



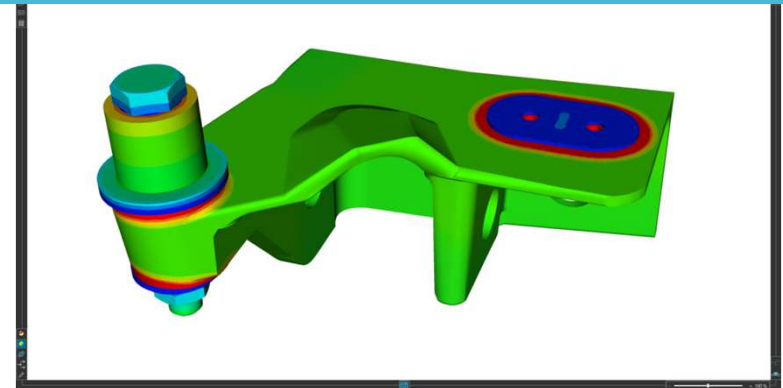
User Defined



Coastal



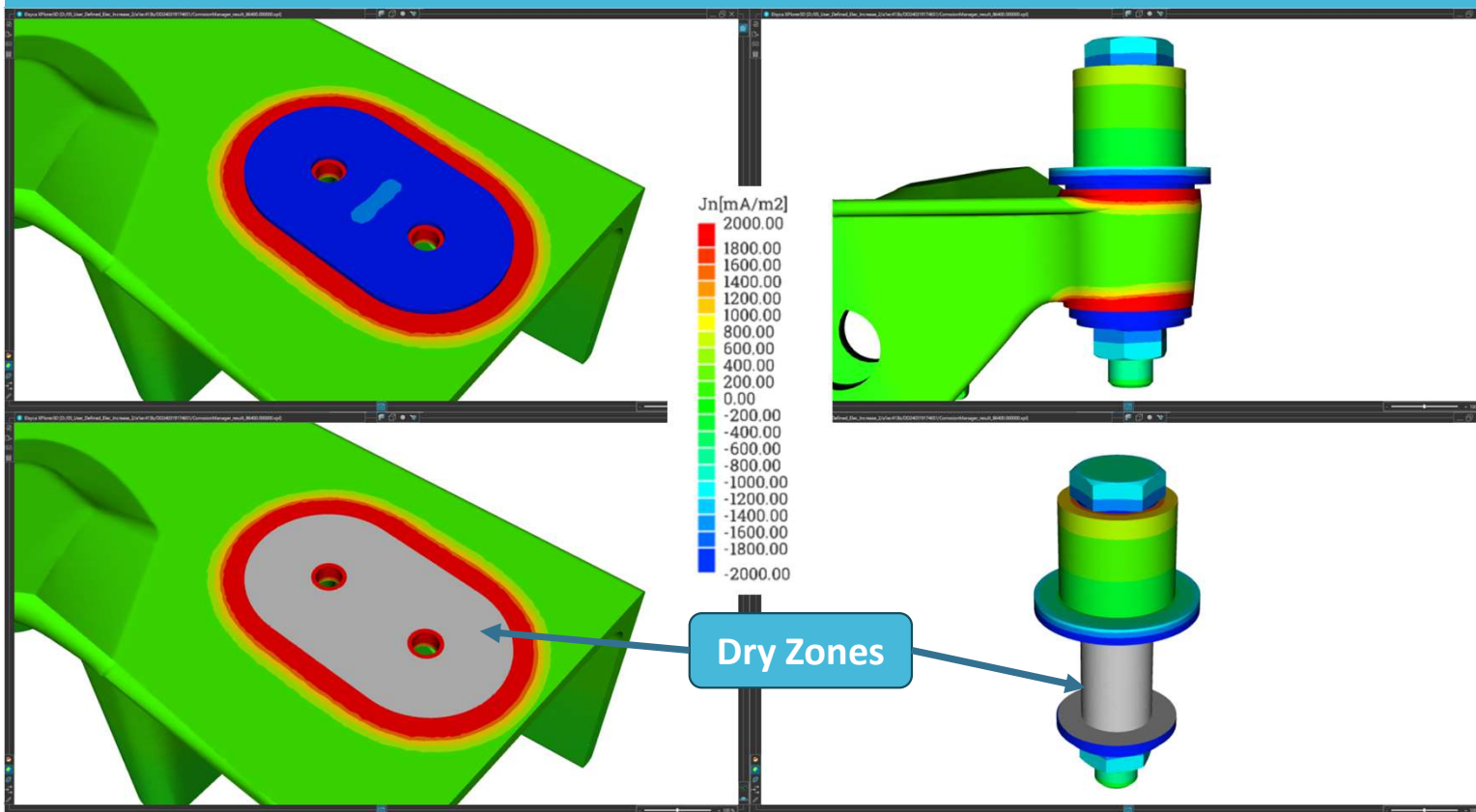
User Defined with sea water



Computer Aided Analysis approach

Logical evaluation of the corrosion risks

User Defined with Sea Water



Film thickness [mm]

0.182

Film Electrical Conductivity [S/m]

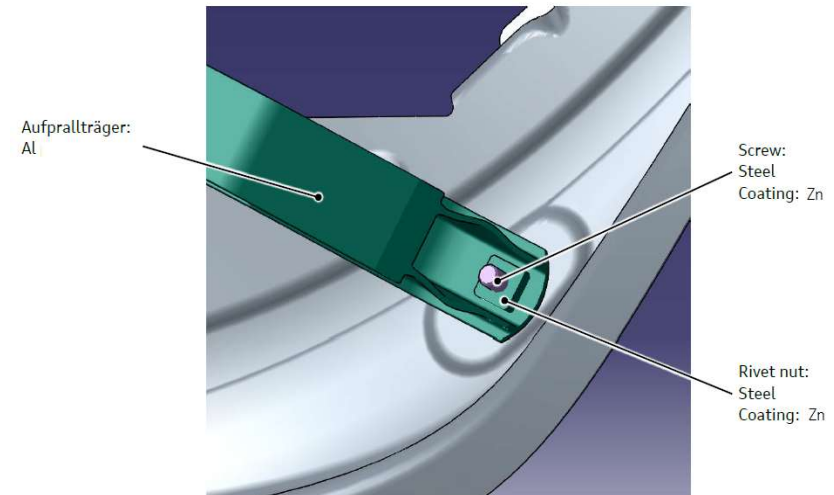
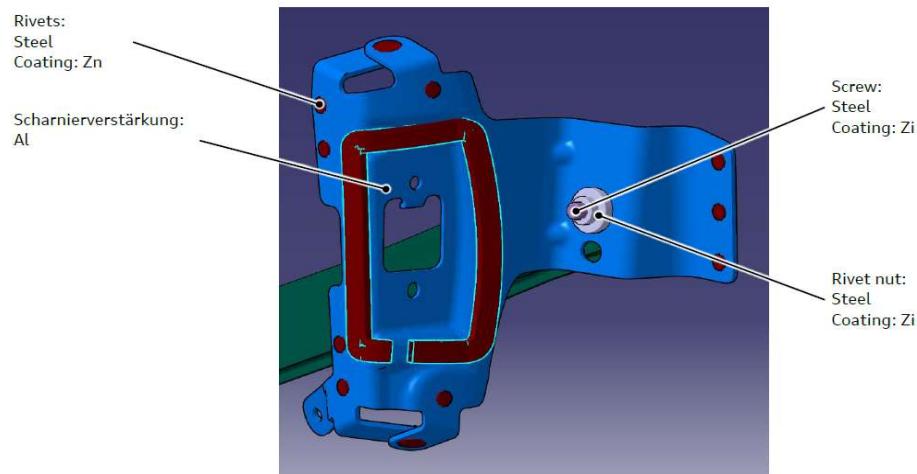
5

Computer Aided Analysis:

Audi A6 example

Computer Aided Analysis approach

Multi-material body – Audi A6 door structure

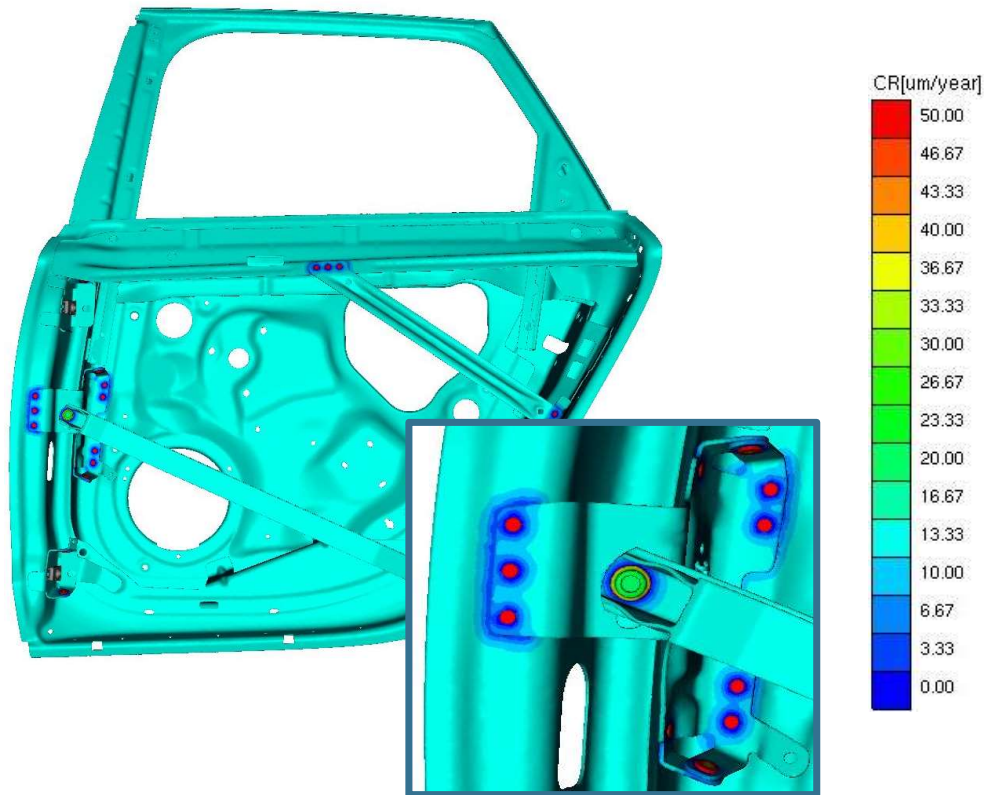


Simulation parameters:

- materials involved: Al, hot-dip galvanized steel, Zn coating (d = 100 mm)
- industrial environment – electrolyte conductivity 0.1 S/m, thin film thickness 80 nm
- average temperature – 25°C
- average humidity – moderate

Computer Aided Analysis approach

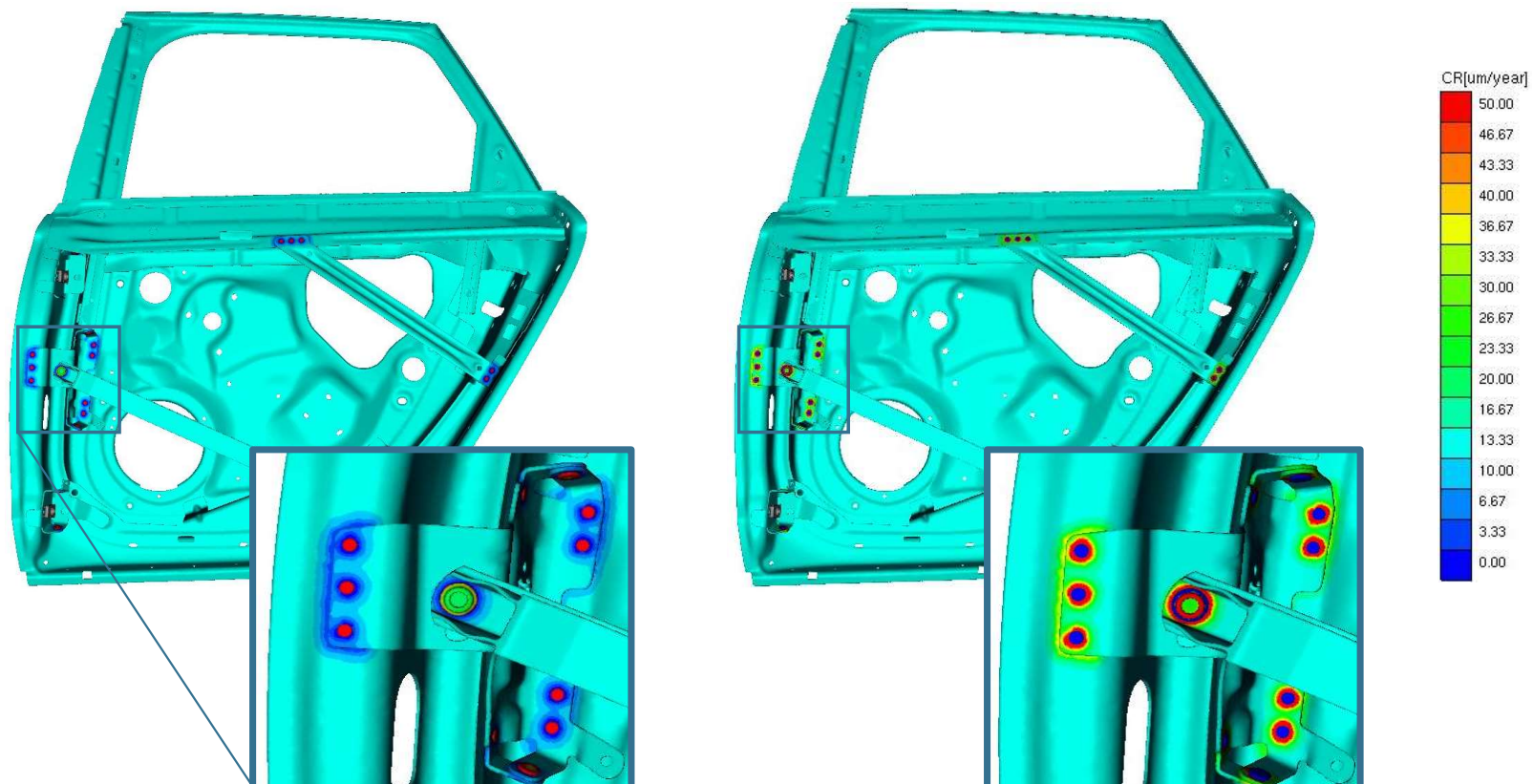
Multi-material body – Audi A6 door structure



- Hot-dip galvanizing protects Steel cathodically: Zn is anodic to the Steel base metal and is placed in the circuit to corrode in place of the base metal.
- Zn will initially sacrifice itself until a protective layer of rust will develop on Steel.
- Under atmospheric conditions of moderate humidity, contact between a galvanized surface and Al is unlikely to cause substantial incremental corrosion .

Computer Aided Analysis approach

Multi-material body – Audi A6 door structure

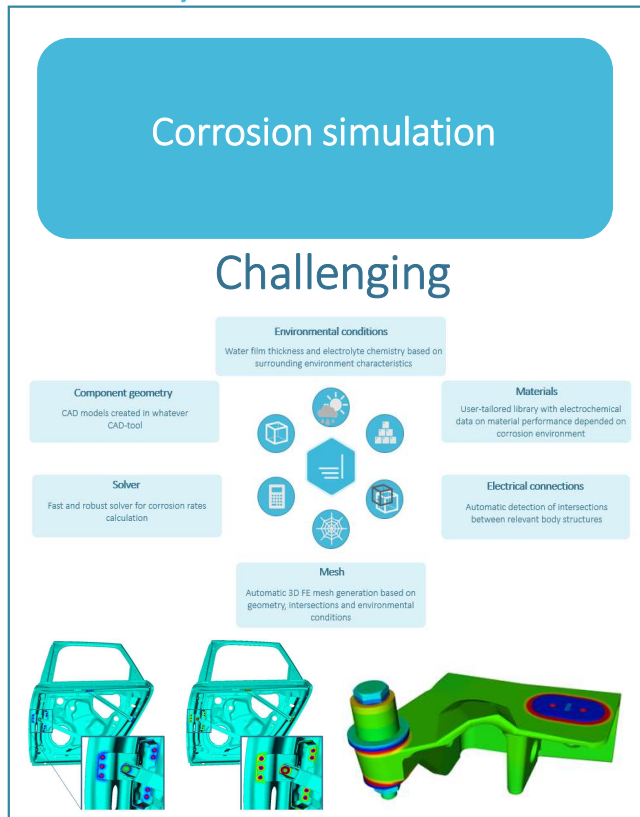


Atmospheric corrosion simulation – 30 days

Atmospheric corrosion simulation – 365 days

Computer Aided Analysis in corrosion risk assessment at a design stage

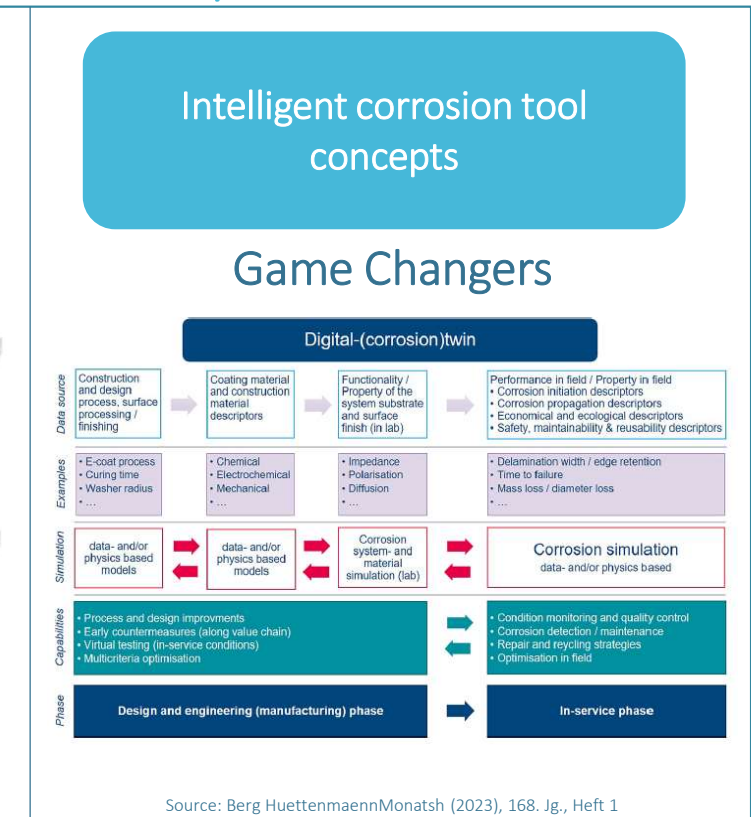
Takeaway n°1



Takeaway n°2



Takeaway n°3



Thank you!



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The electrochemical reference | in software & engineering.

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