Corrosion Inhibitor Modelling and Optimisation

Presented at the Institute of Corrosion

25th May 2021

Chetan Laddha

Juan Dominguez Olivo

Corrosion Inhibitor Technology Positioning

Status Quo

Current practices:
Inhibitor chemistry is a black-box provided by the chemical suppliers

Challenges:
- Gap in the ability to correlate inhibitor (CI) efficiency/performance with changing process conditions. Leads to conservative practices for corrosion inhibitor evaluation
- State-of-the art simulation and techniques cannot be applied to simulate CI performance
  - Unknown molecular structure of the inhibitor
  - Simulation assumes a “atomically flat” metal surface

Business impact:

Conservative dosage rates

High OPEX

Aspired Vision

- Mechanistic model for deriving the performance and efficiency of corrosion inhibitors
- Optimised inhibitor dosage rates
- Real-time correlation between dosage and operating envelope

➢ Inhibitor performance model based on electrochemical response from the presence of the inhibitor on the metal surface (doesn’t require information on inhibitor chemical composition)

Electrochemical model

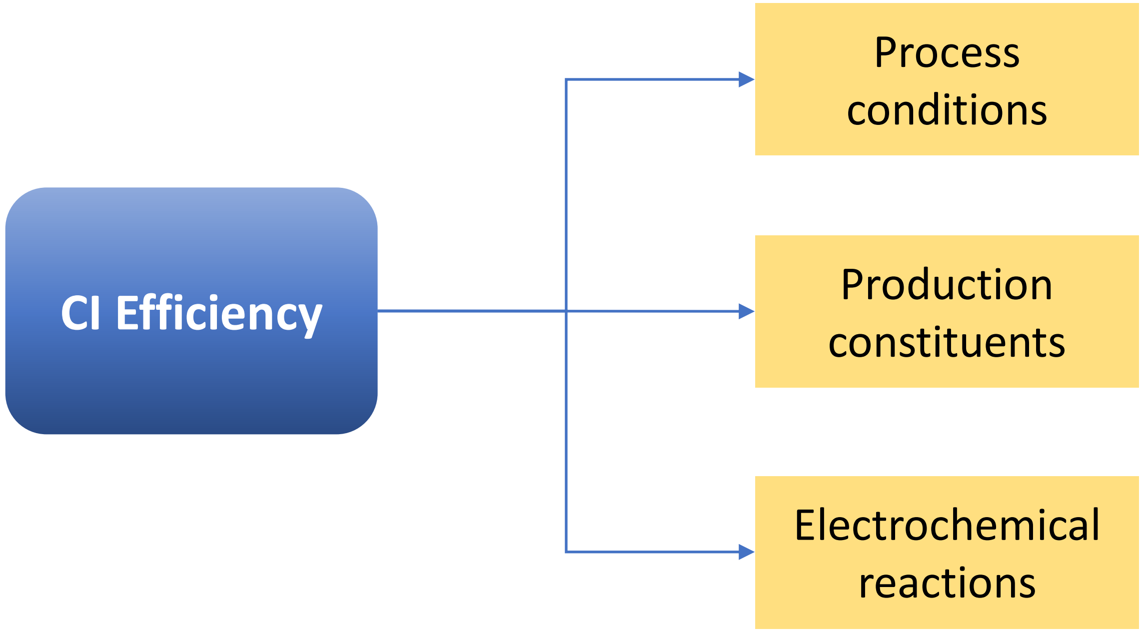
Inhibitor response testing

Mechanistic Inhibitor Model

Corrosion Inhibitor Technology Positioning

Widely acknowledged that the corrosion Inhibitor (CI) efficiency does vary with changing operating conditions.

However, there is a gap in the ability to accurately model or correlate the CI performance with changing parameters.



Note: Some general rules of thumb exist, such as the inverse correlation between corrosion rates and temperature, however the rest of the correlations are known to be highly **non-linear** and **fractal** in nature. These regimes drive the need for mechanistic modelling techniques.

Example of Corrosion Inhibition Assessment with the Current Inhibition Understanding: Effect of Velocity

Sinclair

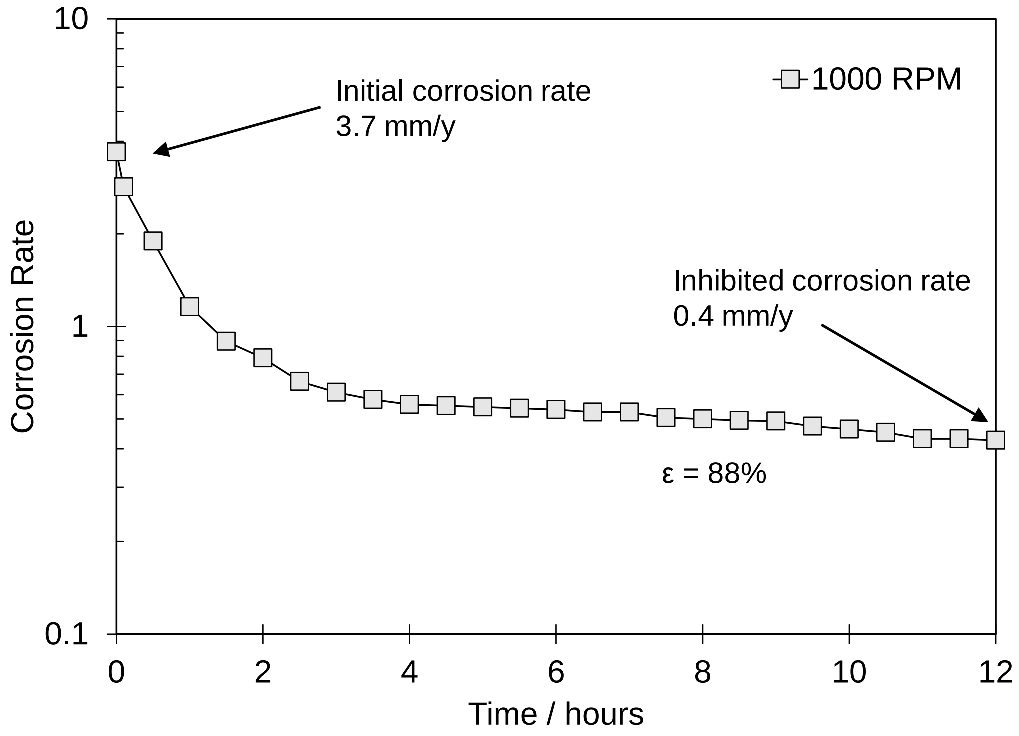
Effect of Rotational Speed (1/4)

Overview of mechanistic model and kinetics

Hypothesis generation

Experimental evidence

pH4, 0.96 bar CO_2, 25˚C, RCE 300 rpm and 4500 rpm, 200 ppm CI Package K2

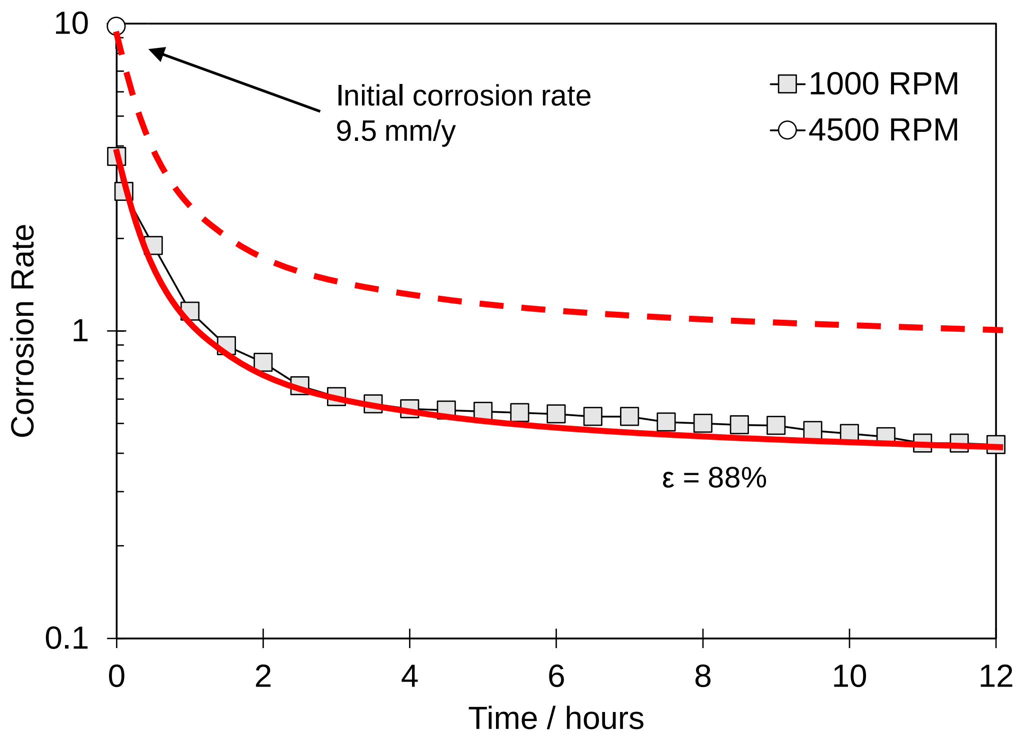


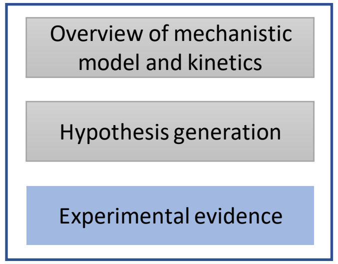
Common calculations in the assessment of CI

$$\varepsilon = \frac{CR_{uninhibited} - CR_{inhibited}}{CR_{uninhibited}}$$

Effect of Rotational Speed (2/4)

pH4, 0.96 bar CO_2, 25˚C, RCE 300 rpm and 4500 rpm, 200 ppm CI Package K2



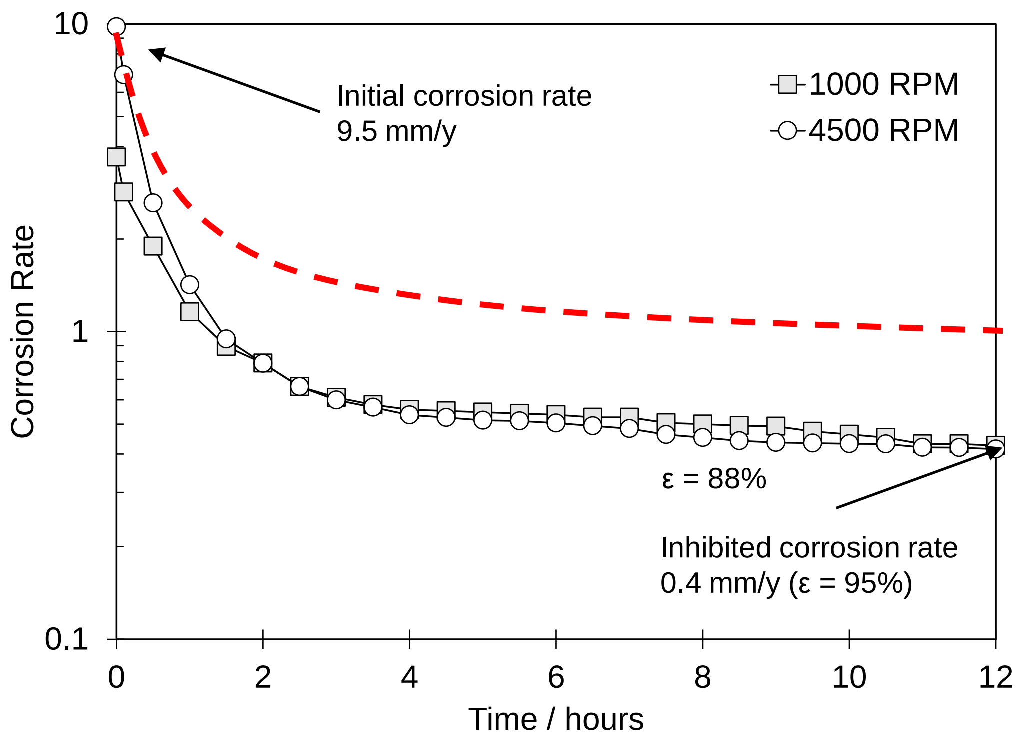


Common calculations in the assessment of CI

$$\varepsilon = \frac{CR_{uninhibited} - CR_{inhibited}}{CR_{uninhibited}}$$

Effect of Rotational Speed (3/4)

pH4, 0.96 bar CO_2, 25˚C, RCE 300 rpm and 4500 rpm, 200 ppm CI Package K2



Overview of mechanistic model and kinetics

Hypothesis generation

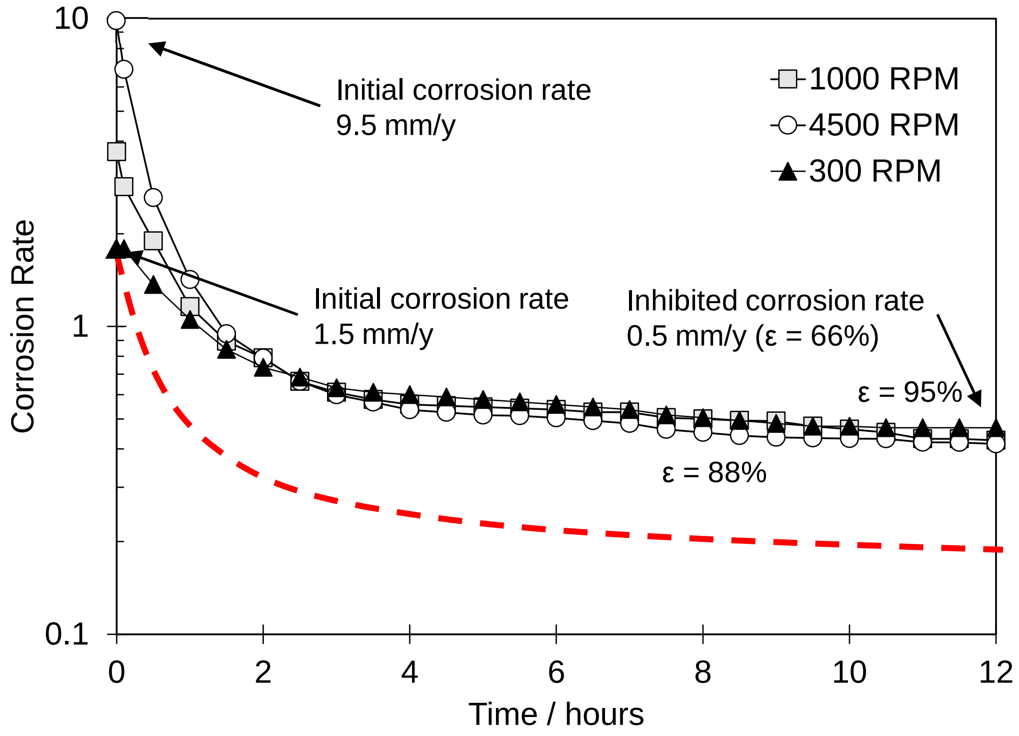
Experimental evidence

Common calculations in the assessment of CI

$$\varepsilon = \frac{CR_{uninhibited} - CR_{inhibited}}{CR_{uninhibited}}$$

Effect of Rotational Speed (4/4)

pH4, 0.96 bar CO_2, 25˚C, RCE 300 rpm and 4500 rpm, 200 ppm CI Package K2



Overview of mechanistic model and kinetics

Hypothesis generation

Experimental evidence

Common calculations in the assessment of CI

$$\varepsilon = \frac{CR_{uninhibited} - CR_{inhibited}}{CR_{uninhibited}}$$

Speed	Efficiency / %
4500 RPM (5 m/s)	95
1000 RPM (1 m/s)	88
300 RPM (0.4 m/s)	66

Rotational Speed – Key Observations

Key Observations:

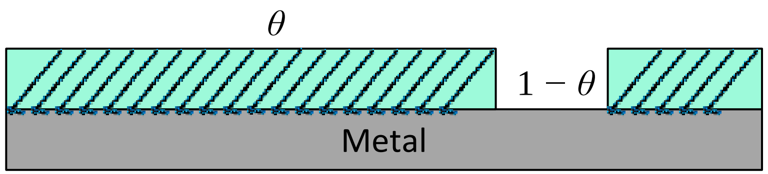
- The efficiency seems to change depending on the effect of velocity / rotational speed.
- Kapusta, B. Pots, and Connell[1] proposed more than 2 decades ago that a corrosion inhibitor would be evaluated by their final corrosion rates rather than efficiency coefficient.
- The empirical observation from Kapusta arises a question: why does a corrosion inhibitor have such a behavior? This behavior will be the same if we change pH rather than velocity? What about temperature?
- Fortunately, there is a better way to evaluate the performance of a corrosion inhibitor and answer those questions: evaluate the corrosion mechanisms affected by the inhibitor[2].

[1] Kapusta, S. D., Pots, B. F., & Connell, R. A. (1999, January). Corrosion management of wet gas pipelines. In *CORROSION 99*. NACE International.
[2] **Dominguez Olivo, J.M.**, Young, D., Brown, B., & **Nesic, S**. (2020, August). An Improved Methodology to Assess the Performance of Organic Corrosion Inhibitors. In *CORROSION 2020*. NACE International.

Example of Corrosion Inhibition Assessment with an Improved Methodology: Effect of Velocity and Concentration

Inhibitor Model Based on the Concept of Blockage

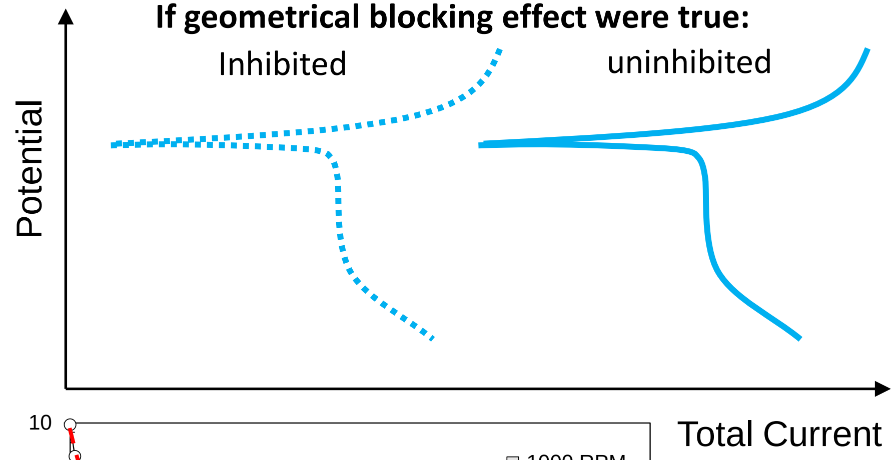
Underlying Assumption: Diminution of Active Surface Area

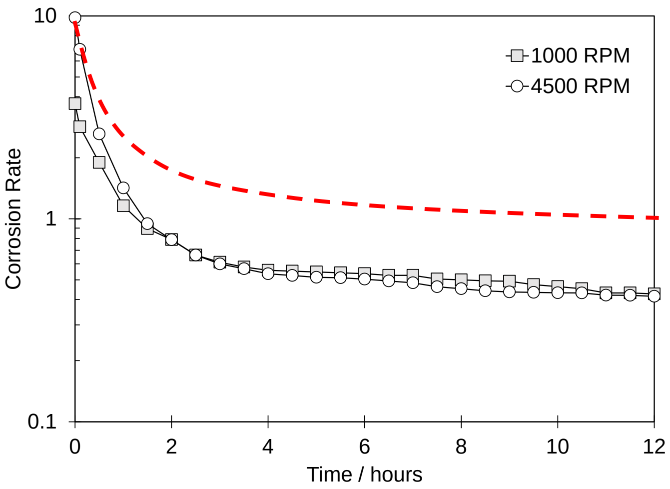


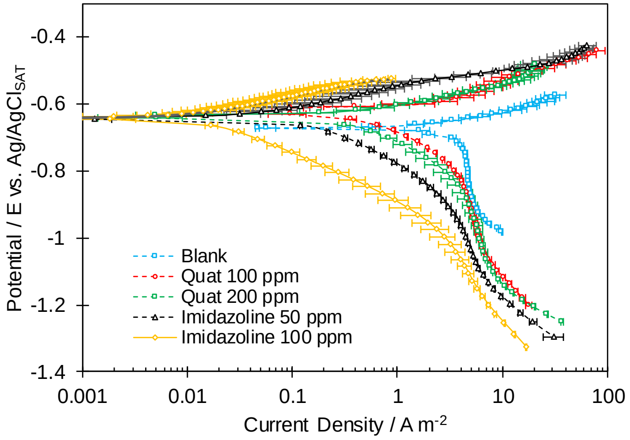
$$CR_{inhibited} = (1-\theta)CR_{uninhibited}$$

$$\theta = \varepsilon = \frac{CR_{uninhibited} - CR_{inhibited}}{CR_{uninhibited}}$$

Charge transfer and limiting currents are diminished in a blocked/ partially blocked electrode[1,2]



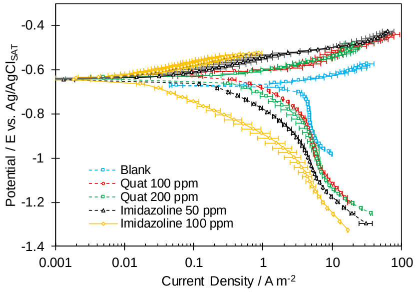


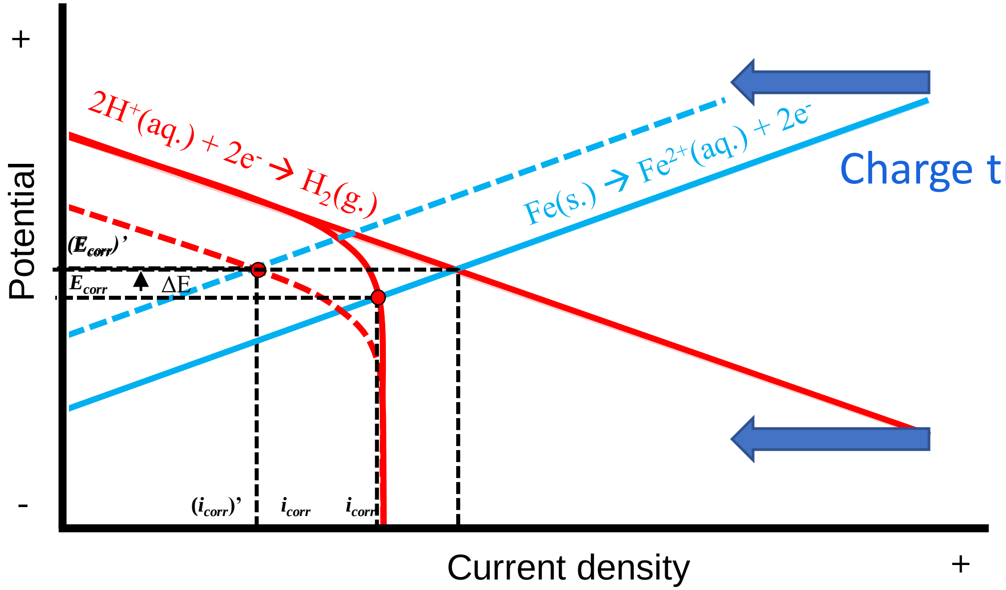


1. Amatore, C., Savéant, J. M. & Tessier, D. Charge Transfer at Patially Blocked Surfaces. A Model for the Case of Microscopic Active and Inactive Sites. *J. Electroanal. Chem.* **147,** 39–51 (1983).
2. Reller, H., Kirowa-Eisner, E. & Gileadi, E. Ensembles of microelectrodes. *J. Electroanal. Chem.* **138,** 65–77 (1982).

Kinetics of Inhibited Corrosion (Unchanged Limiting Current)

Model Equations for Inhibited Kinetics[1]





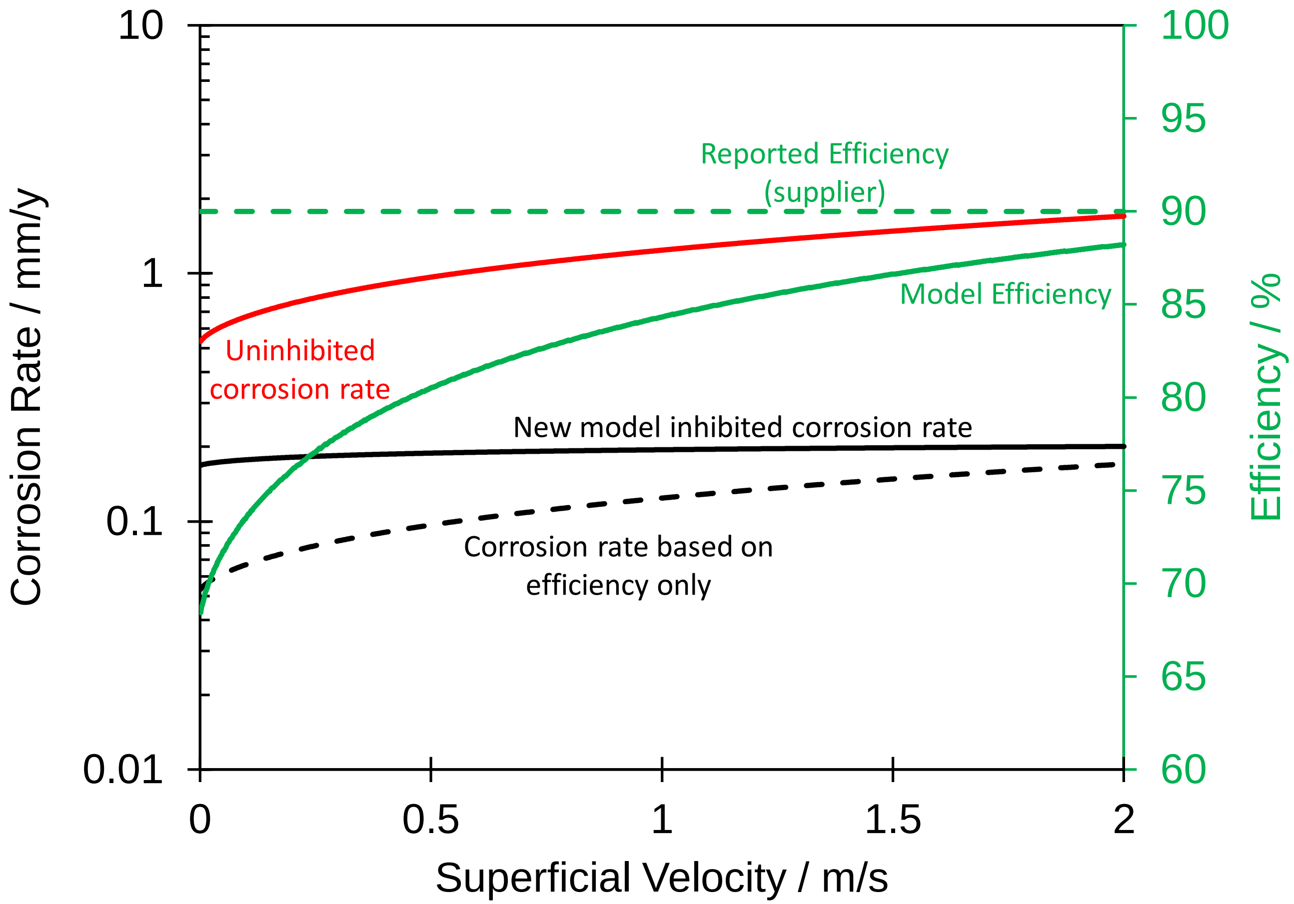
Charge transfer equally affected

[1]**Dominguez Olivo, J.M.**, Brown, B., Young, D., & **Nesic, S**. (2019, May). Electrochemical Model of CO_2 Corrosion in the Presence of Quaternary Ammonium Corrosion Inhibitor Model Compounds. In *CORROSION 2019*. NACE International.

Capabilities of the Model

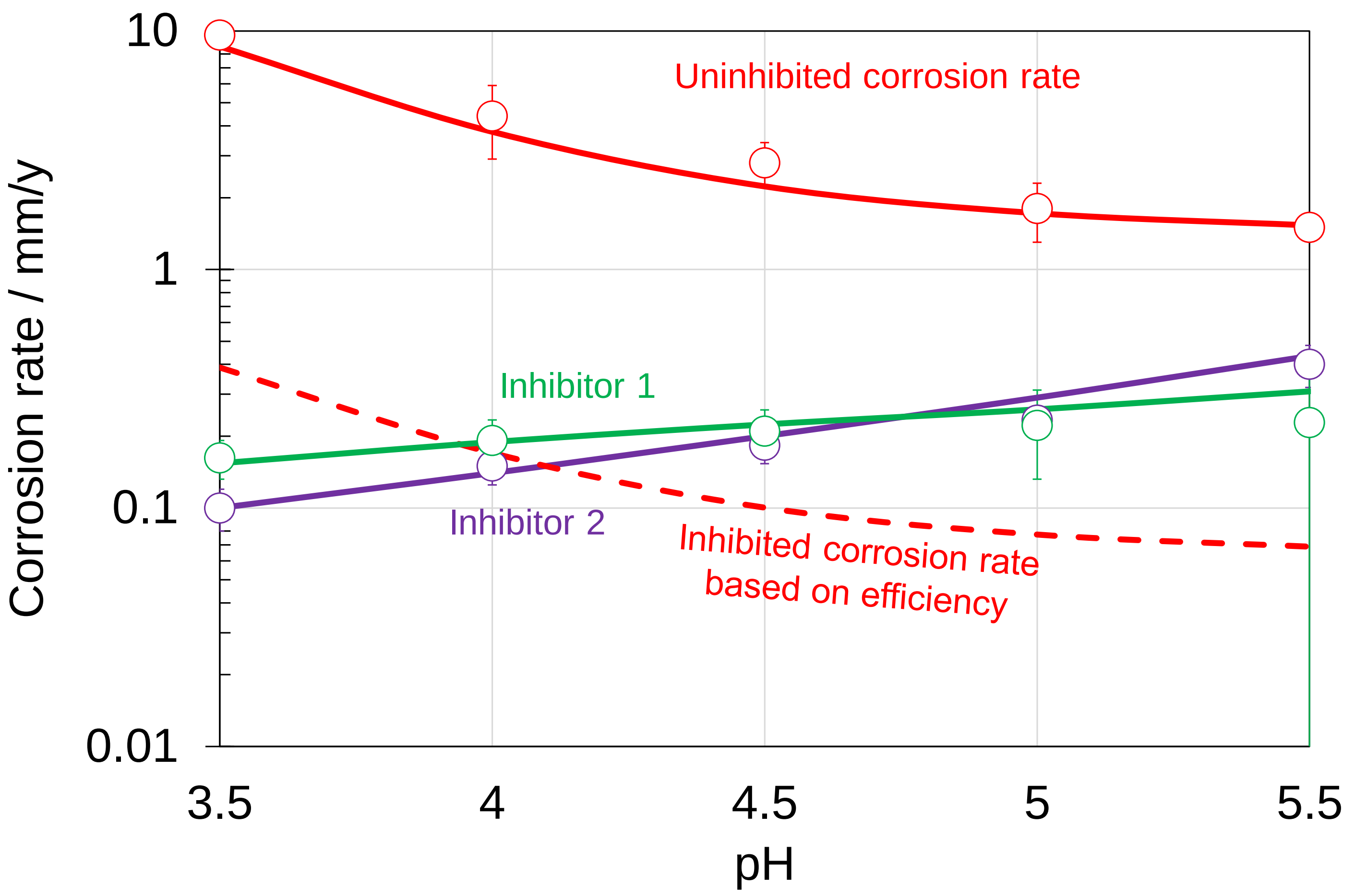
Modelling Effect of Rotational Speed

Corrosion Inhibitor Operating Window Extrapolation: Changing Flow



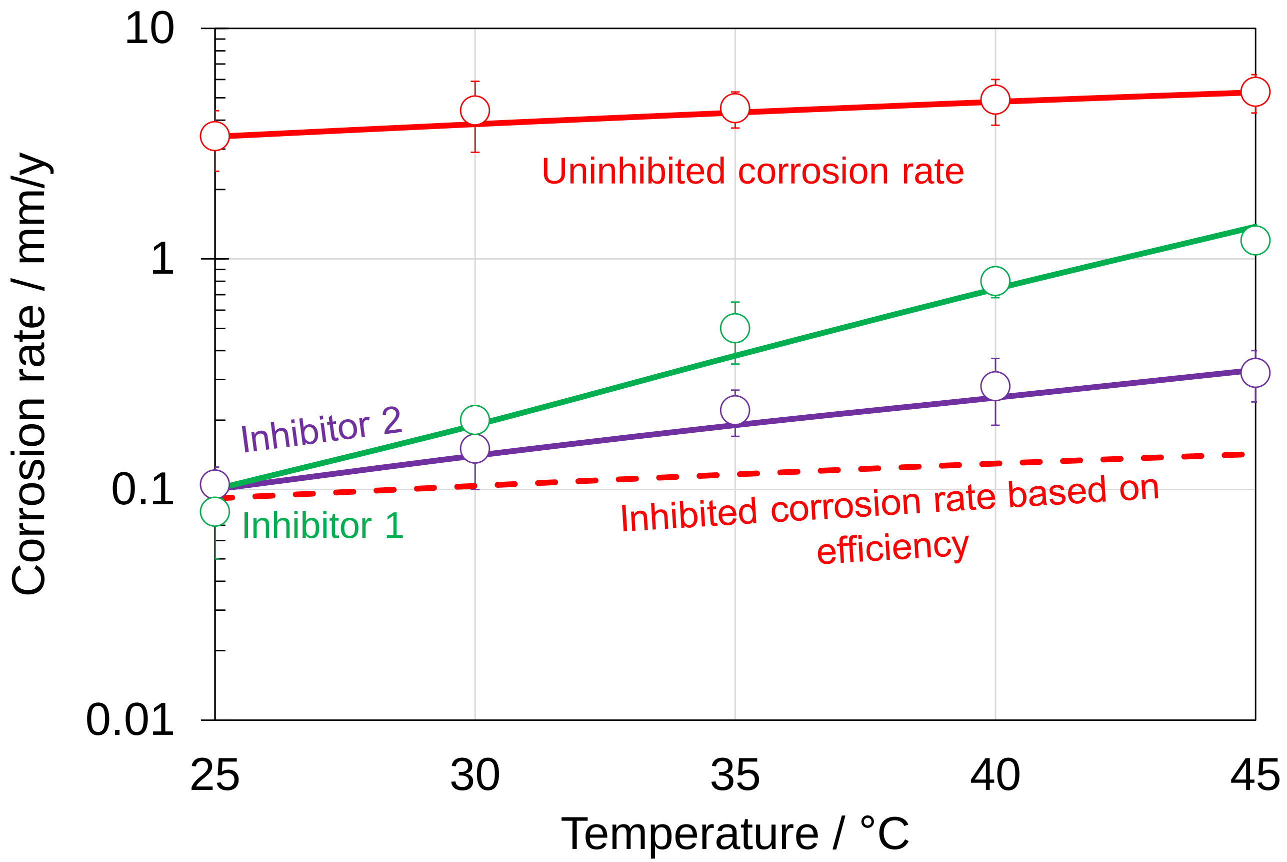
Modelling Effect of pH

pH 3.5 to 5.5, 0.96 bar CO_2, 30°C, RCE 1000 rpm

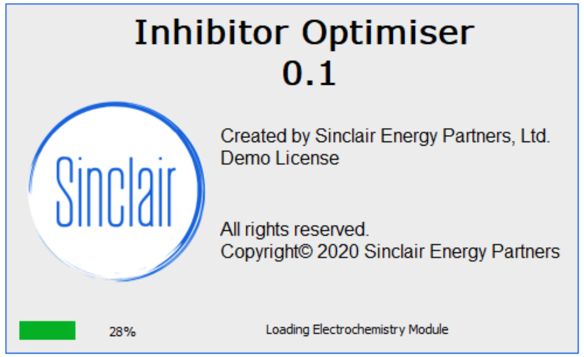


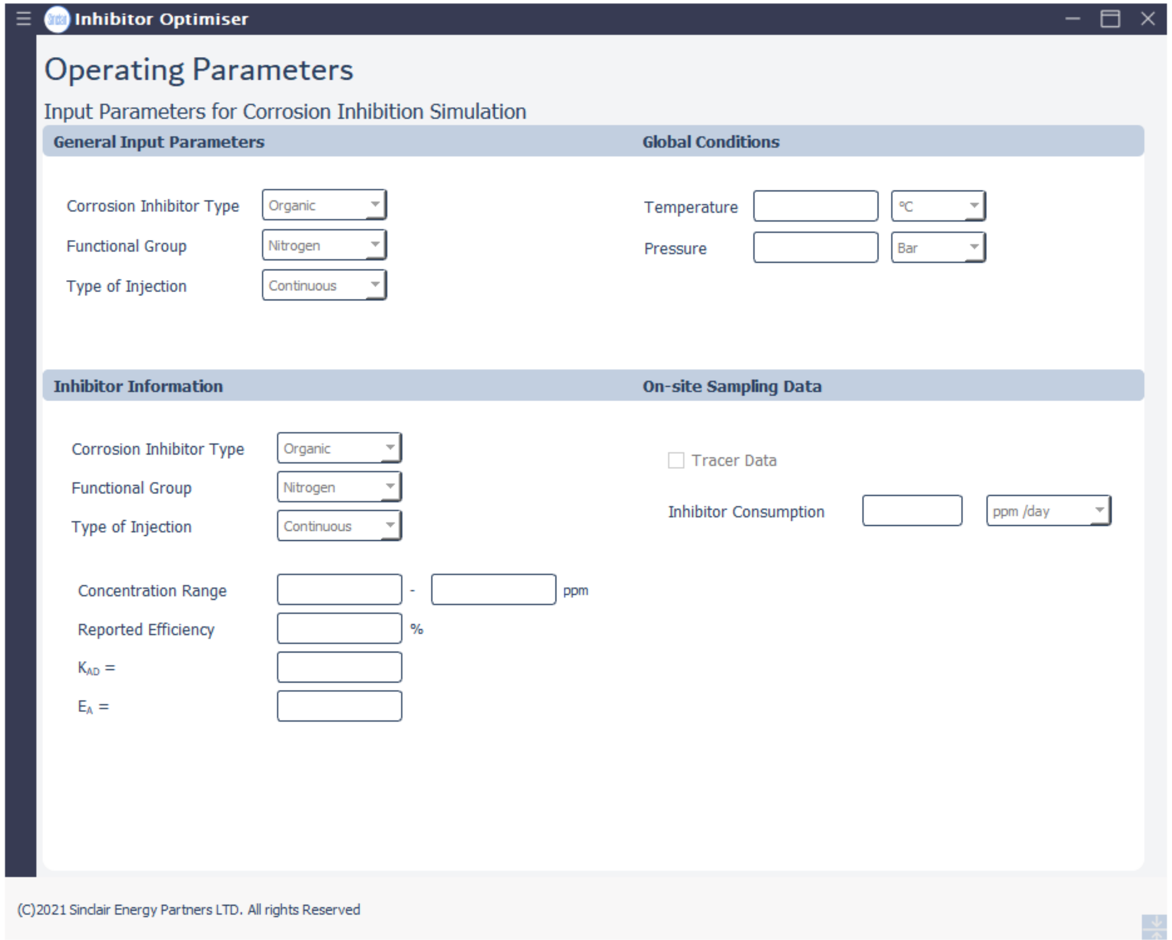
Capabilities of the Model

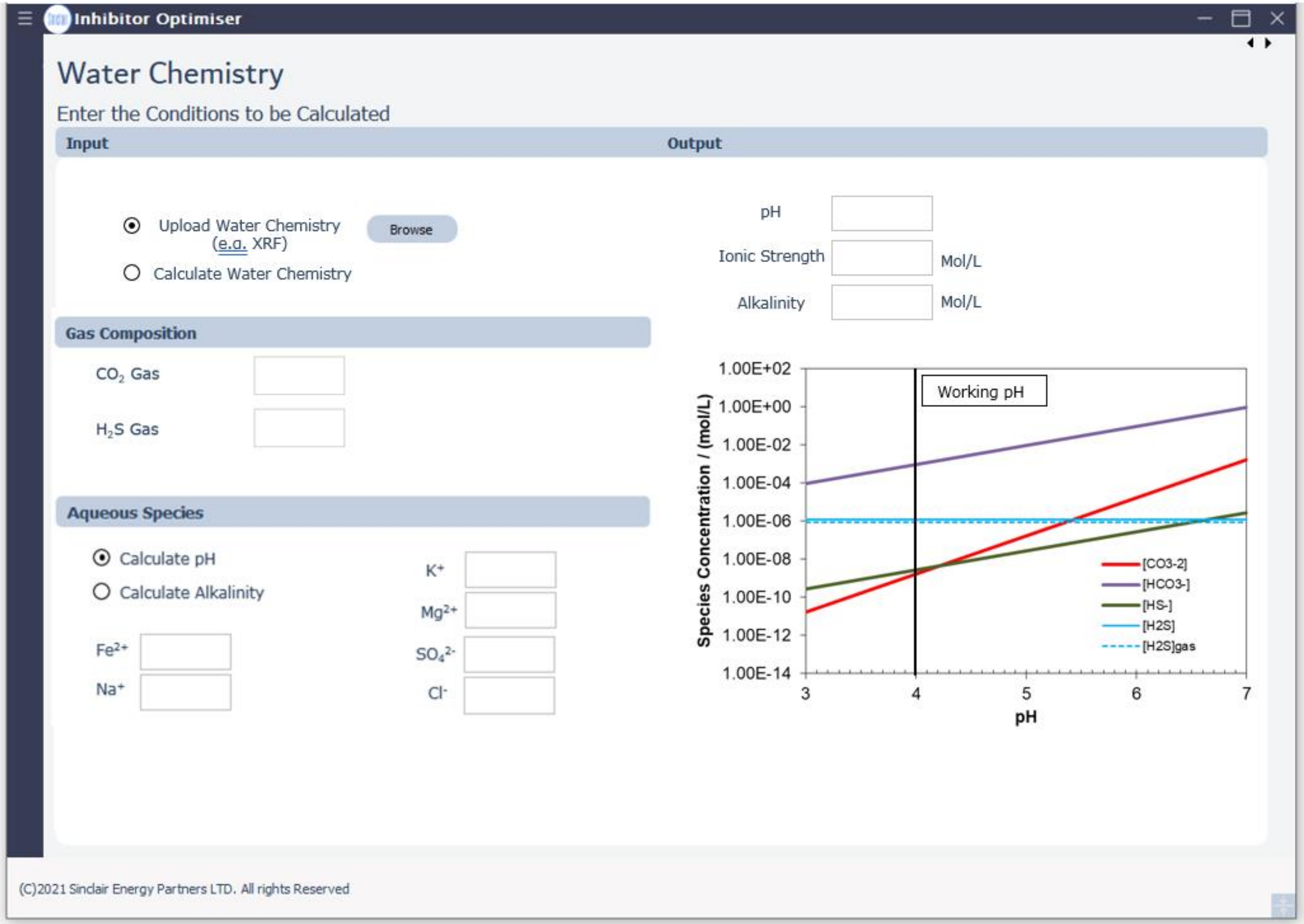
pH4, 0.96 bar CO_2, 25 - 45°C, RCE 1000 rpm



User Interface Overview







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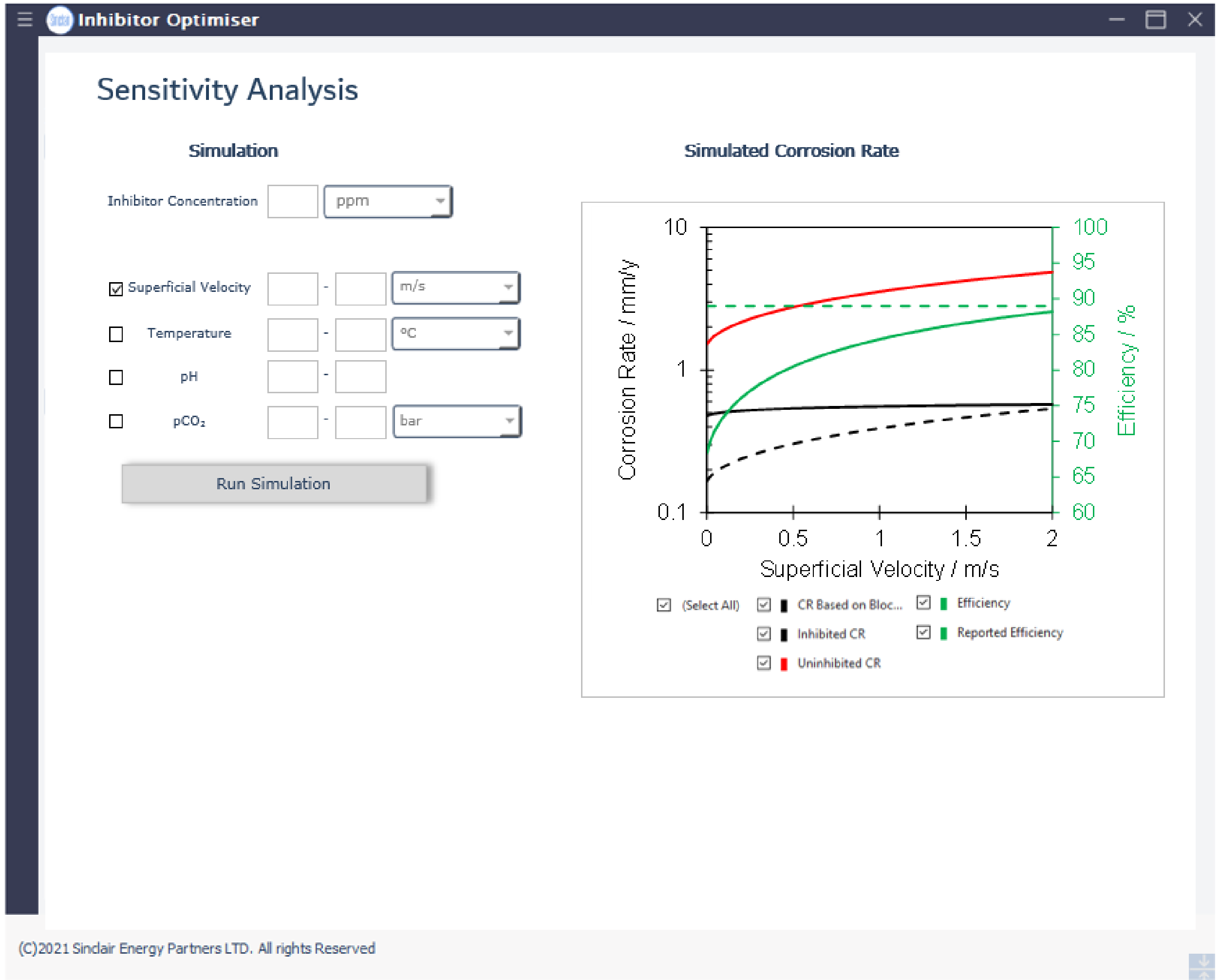

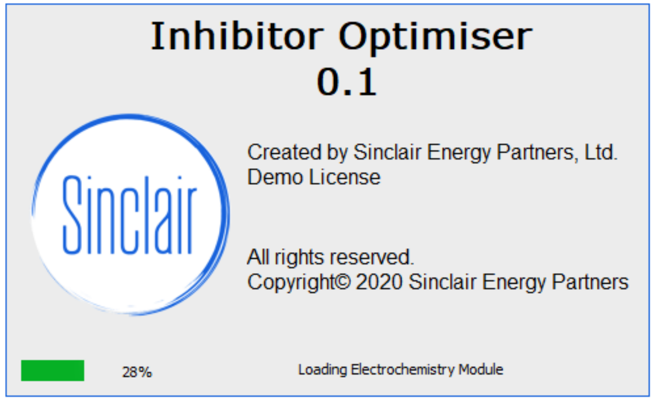

Current Deployment and Future Work

Inhibitor Optimizer

Current Capabilities

- Model the inhibited corrosion rates under different operating conditions
- Model IOW for inhibition performance
- Aid the selection of corrosion inhibitor(s)
- Integrated sensing and modeling capability

Future Developments

Short Term

- Effect of H_2S and corrosion inhibitors enhancers (e.g. thiols)
- Effect of organic acids
- Machine learning implementation

Long Term

- Impact of using hydrates inhibitor in combination with corrosion inhibitors
- Effect of scales and corrosion product layers
- Scale inhibitor modelling

Assumptions / Limitations

- This model predicts the best possible outcome of a corrosion inhibitor (maximum efficiency)
- The model assumes constant bulk concentration of the corrosion inhibitor.
- Batch treatment is not included

Thank you

Sinclair Energy Partners Ltd.
9 Queen Elizabeth Way,
Woking, GU22 9AG
United Kingdom
+44 749 076 4492

www.sinclairenergy.co.uk

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