Fundamental study of surfactant behavior at the metal/electrolyte interface for corrosion inhibition

Research Team: Akshay Rajopadhye (**arajopadhye@ufl.edu**), Melissa Andrews, Puneet Jawali, Yakov Rabinovich, **Brij Moudgil (PI, bmoudgil@perc.ufl.edu)**

Goal: To examine the fundamental surfactant structures at the metal/electrolyte interface leading to improved performance and cost effectiveness of surfactants and other additives used to inhibit corrosion in aggressive environments.

Previous findings:

- Role of Kelvin Probe Force Microscopy in studying the surfactant induced corrosion inhibitions
- Change in the surface potentials of metal samples due to corrosion

Current findings:

- Inferior mechanical properties of the individual component (BDMAC) as compared to model system (C12TAB).
- This is contrary to the current hypothesis & suggests the possibility of more than one mechanisms.

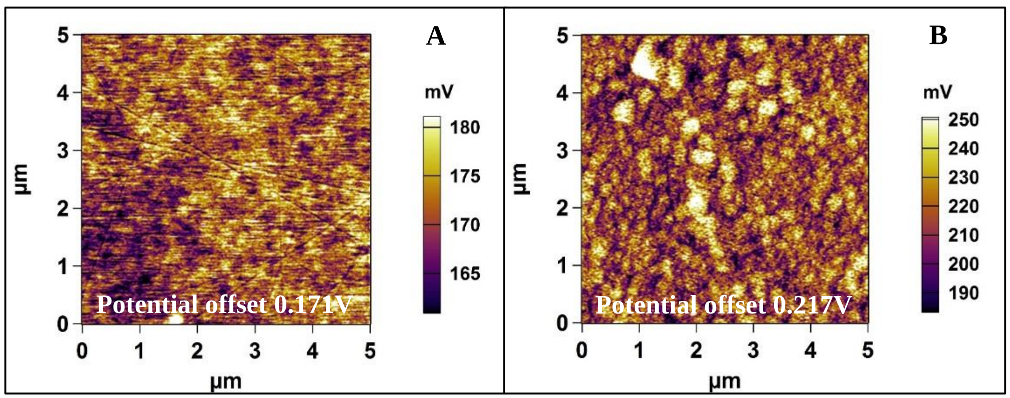


Figure: Surface potential images as obtained from Kelvin Probe Force Microscopy of: A. polished surface B. corroded surface

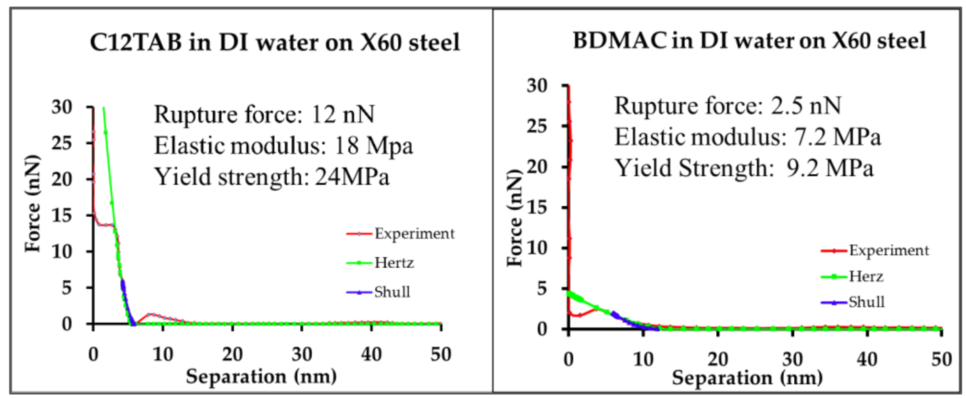


Figure: Mechanical properties of two surfactant-based inhibitor films as determined using AFM at concentrations well above their CMC

Future directions:

- Investigate imidazoline based inhibitor for it's mechanical properties at the steel-electrolyte interface
- Correlate the force measurements with the electrochemical properties

Principal IAB Sponsor(s): ExxonMobil, BP

UNIVERSITY of FLORIDA
The Foundation for The Gator Nation

COLUMBIA UNIVERSITY
IN THE CITY OF NEW YORK

EFFECT OF SURFACTANT STRUCTURE AND PROPRTIES ON ENZYME-SURFACTANT INTERACTIONS

Research Team: P. Somasundaran (ps24@columbia.edu), Derek Kim, Michael Chin

Goal: Investigate impact of surfactant structure and properties on enzyme functionality and dynamics to develop compatible enzyme-surfactant systems

Key Findings:

1. Enzyme activity enhanced by nonionic surfactants
2. Greatest increase at surfactant concentrations where loosely packed micelles are formed → Disorder in water structure → Greater enzyme flexibility → Higher activity
3. Activity decrease with addition of an anionic surfactant varied directly with its concentration

Future Directions:

1. Investigate enzyme activity change with proposed modifications to the surfactant system
2. Investigate differences in surfactant behavior, enzyme-surfactant binding, and colloidal interactions
3. Examine enzyme structural and dynamic changes with addition of surfactants

Industrial Relevance: Home and Personal Care, Cosmetics, Foods, Pharmaceuticals, Renewable Energy

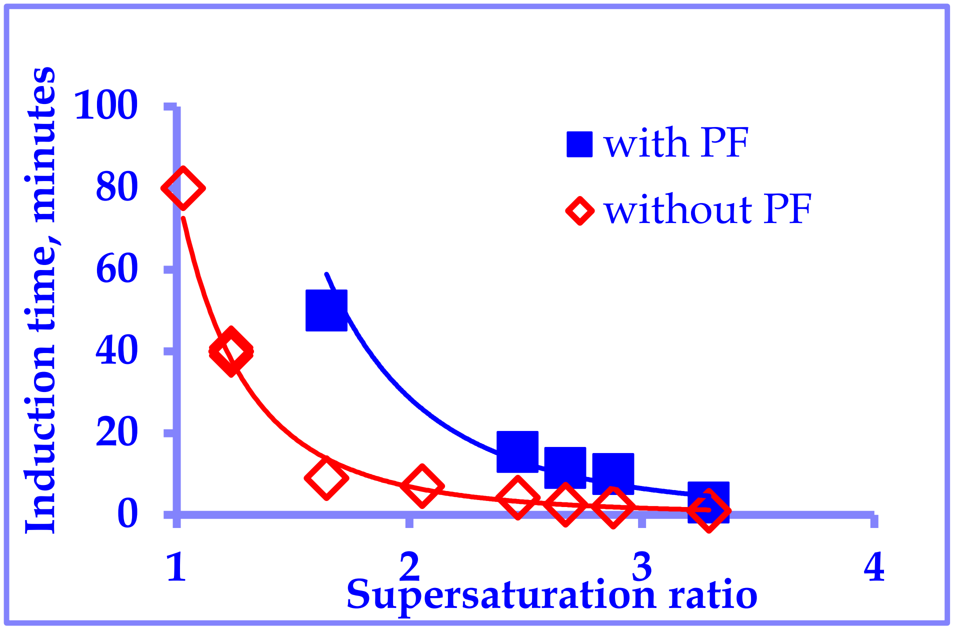
Inhibition of Scale Formation by PHOSFLOW® reagents developed by Cytec-Solvay Group: Fundamentals and Applications

Research Team: Brij Moudgil (bmoudgil@perc.ufl.edu, 352-846-1194), Juan Tanquero, Elsayed Abdelaal, Hassan El-Shall, Mohamed Helmy, John Carr

Goal: Understand the mechanisms that govern the effect of the PHOSFLOW® reagent on inhibition of scale formation in phosphoric acid production.

Previous Findings: None

Current Findings:



- **PHOSFLOW® increases induction times at all tested supersaturations.**
  - Calculations indicate limited surface interactions between PHOSFLOW® and crystallites
- **Precipitates formed in lab match the composition of those collected in industry**
  - Verified using XRD
- **Preliminary tests show that PHOSFLOW®**:
  - Reduces crystal size
  - Narrows crystal size distribution

Future Directions:

- Complete quantifying inhibition effects of PHOSFLOW®
  - Crystal size distribution measurements
- Begin investigation of PHOSFLOW® mediated scale inhibition mechanism
  - Supersaturations tests, SEM, XRD, and AFM

Principal IAB Sponsor(s): Cytec-Solvay Group

UF UNIVERSITY of FLORIDA The Foundation for The Gator Nation

PaSS

COLUMBIA UNIVERSITY IN THE CITY OF NEW YORK

Investigating bacterial removal from biological surfaces

Research Team: Brij Moudgil (bmoudgil@perc.ufl.edu, 352-846-1197), Vignesh Nandakumar, Andrea Pulgar, Huang Chenan, Robert Rautenkranz, Oreana Ramirez, Wu Guohui, Prem Chandar and K. Ananth

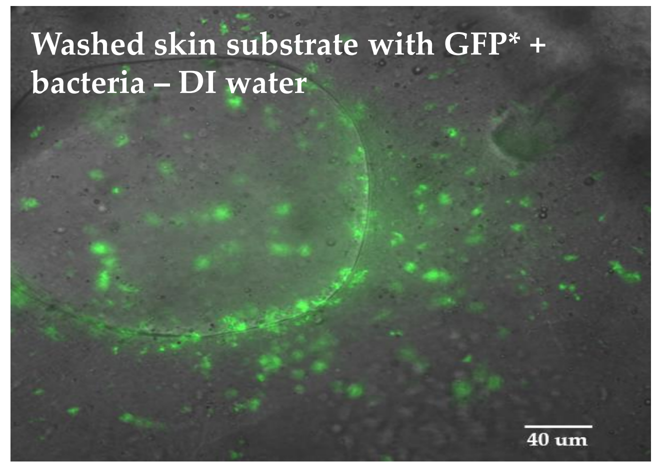
Goal: Project intends to enhance the disinfection potential of commercial hand wash agents through enhanced removal of microbes.

Current Findings:

- Removal of microbes from skin - lot of room for improvement
- Fluorescence spectroscopy - technique to differentiate between bacterial removal and kill
- Bacterial interactions with skin substrate result in reduced wash off from skin substrates

Future Directions:

- Establish confirmatory techniques like qPCR to differentiate between kill and wash off.
- Examine remnant bacteria on artificial skin substrate for kill using fluorescence microscopy.
- Investigate why removal of bacterial from skin substrate is independent of starter inoculum.



Skin substrate after wash off using water and soap show high numbers of remnant bacteria

Principal IAB Sponsor(s): Unilever

UF UNIVERSITY of FLORIDA
The Foundation for The Gator Nation

Pass

COLUMBIA UNIVERSITY
IN THE CITY OF NEW YORK

GREENER SURFACE ACTIVE AGENTS
Structure/Property/Performance Relationships

Research Team: Jun Wu and Prof. Somasundaran

GOAL

Comparison between greener *vs* conventional surfactants for structure/property/performance relationships of greener surfactants

Previous Findings

Viscosity Difference of greener surfactants with structure variations
Micellar evolution: spherical to worm-like micelle by ultracentrifugation
Worm-like micelle networks lead to viscoelascity properties
Synergism between greener surfactants enhances foamability and stability
New effective packing parameter formula with interaction information
Developed decontamination foam to fight Ebola virus
Spectroscopic methods to study packing of surfactants at interface to identify the driving force of the synergism

Current Findings

Understanding the effects of solvent polarity on size and shape of micelles

Future Directions

Elucidate mechanism how the polarity or interactions of medium affect micellization

Principal IAB Sponsor(s): Personal Care Companies

Interactions of surfactants and mineral oils with stratum corneum

Research Team: P. Somasundaran (ps24@columbia.edu, 212-854-2925), Parag Purohit, X. Lei

Goal: To study the damage processes in SC by common surfactant and solvent systems and devise strategies for mitigation

Current Findings:

- Water content effects studied using spectroscopic methods
- Water retention correlated to generation of drying stress in SC
- Effect of emollient oils on SC studied by ESR spectroscopy method
- Effect of pH and contact time evaluated on the SC properties
- Surfactant penetration in SC studied using depth profiling
- Residual surfactant studies using deuterated systems
- Effect of additives on skin proteins using ESR

Future Directions:

- Effect of polar/ non-polar oils on surfactant retention in SC
- ESR investigation of SC- surfactant interactions
- Modelling surfactant-SC interactions

Principal IAB Sponsor: Unilever

Engineering Kaolin Properties for Different Applications with a New Focus on Enhancing their Behavior in Ceramic Processing

Research Team: Brij M. Moudgil (bmoudgil@perc.ufl.edu, 352-846-1194), Shuaishuai Yuan, Hassan El-Shall

Goal: Investigate the kaolin properties that have a direct and indirect impact on the ceramic behavior. Understanding the correlation between particle characteristics and processing performance will lead to guidelines to achieve most effective processing condition.

Previous Findings: (New focus)

Current Findings: (New focus)

Future Directions:

Task 1. Characterization Study involving:

Particle size and size distribution will be determined using light scattering technique as well as Scanning Electron Microscope (SEM), b) Mineralogical and chemical analysis, c) Image analysis for shape and shape distribution analysis, d) Surface charge characteristics (zeta potential measurements)

Task 2. Identification of rheological behavior of high solid content kaolin slurries such as:

Relative viscosity, b) Thixotropic behavior, c) Effect of various dispersants , d) Determination of Critical Moisture Content (CMC), e) Plasticity, f) Modulus of Rupture (MOR), and g) Resistance to Cracking

Task 3. Data Analysis:

Correlation of particulate systems' characteristics with the rheological behavior of their high solid content slurries will be performed to clarify the desired characteristics for cost effective ceramic processing.

Principal IAB Sponsor(s): Sumicol

Dispersions of high solid content slurries

Research Team: Jason E. Butler (jbutler@che.ufl.edu, 352-392-2591), Hassan El-Shall, and Brij Moudgil

Goal: Advance the ability to accurately and rapidly predict the dynamics of concentrated slurries.

Previous Findings: We have identified the need for a more clear description of the origin of irreversibilities and relevant mechanisms that control dynamics and rheology:

1) Simulations have indicated that contact interactions play a role, despite previously assumptions.
2) Measurements of rheology and structure indicate the existence of short-ranged interactions that are non-hydrodynamic.
3) Initial attempts at validation indicate that using simplified simulations can give accurate predictions of slurry dynamics.

Current Findings: Contact interactions do occur, despite the classical assumption that lubrication singularities prevent solid-solid contacts. This has important implications for modeling slurry dynamics, particularly for non-colloidal particles suspended in viscous fluids.

Future Directions:

1) Extending the model and concepts to assess whether the model can predict dynamics in non-uniform shearing flows.
2) Measurements have been performed for tube flows and will be compared to simulation outputs.
3) Rheological characterizations and dynamics studies are being performed on more general slurries to test the model (rods, instead of spheres, for example).
4) A macroscopic set of equations , that can be used for a wide range of slurries on non-colloidal particles, will be developed based upon the detailed experimental and modeling outcomes.