Confidentiality Statement

Visible Light Activated Transparent Antimicrobial Coatings

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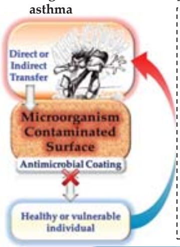
1. Antimicrobial Coating

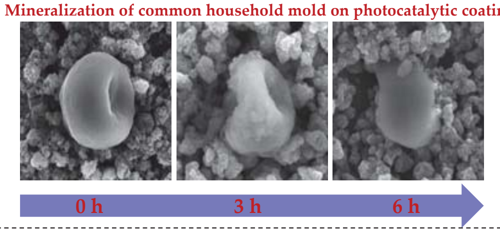
- 2 million infections
- 99,000 deaths

- 9 million U.S. children have been diagnosed with asthma



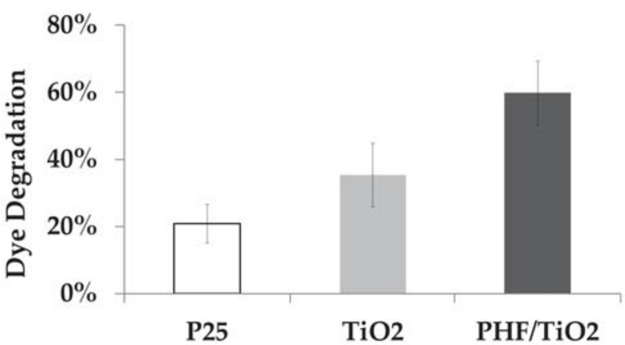
	Anti-adhesive coatings	Microbiocide releasing coatings	Polycationic coatings	Photocatalytic coatings
Commercial suppliers	Sharklet, Pilkington	AgION, SilvaGard	Microban	Italicement, Mitsubishi
Antimicrobial component	Does not kill microbes	Silver ions, Triclosan, etc.	Quaternary ammonium compounds	Light activated generation of free radicals
Mechanism of action	Prevents adhesion super-hydrophobic super-hydrophillic	Inorganic or organic molecules, ions or radicals kill microbes	Positively charged surface attracts & disrupts cell membrane	Free radicals degrade bacteria starting with cell membrane
Fate of inactivated microbes	Microbes are alive!!!	The dead microbe remains on the surface, thus continually masking the active area and reducing effective life		The microbes are mineralized. No loss of active area
Resistance development		Microbes develop resistance with time or repeated exposure		Microbes cannot develop resistance
Theoretical lifetime		The dead microbe stays on the surface reducing the lifetime		Everlasting
Spectrum of activity		Broad spectrum. Kills most of the bacteria, virus and some fungi		Kills all microbes
Toxins	Cannot destroy toxins			Toxins are also degraded
Major Limitation	Does not kill microbes	Does not kill all microbes		Thick, white coating required

Mineralization of common household mold on photocatalytic coating



4. Visible Light Active Photocatalyst

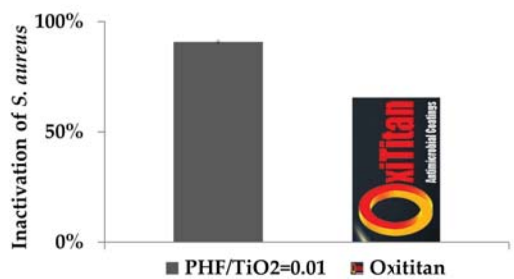
- Organic pollutant: Procion red MX-5B
- Fluorescent light: 2 W/m^2
- Exposure time: 6 hours



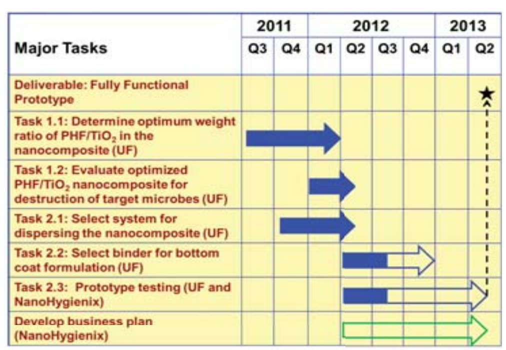
2. Product Criteria

- Transparent
- Visible light active
- Stable liquid formulation
- Compatible with commercial sprayers
- 90% of microbes (e.g., MRSA) inactivation in 12 hours (i.e., 2x faster than competition)

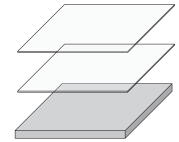
5. Inactivation of *Staphylococcus aureus* (surrogate for MRSA)



7. Timeline

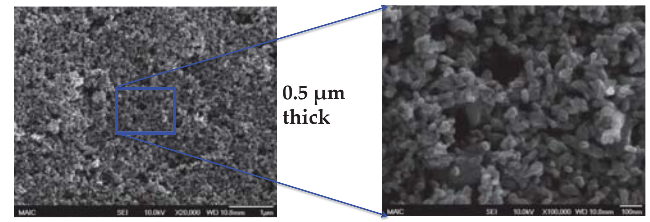


3. Transparent coating

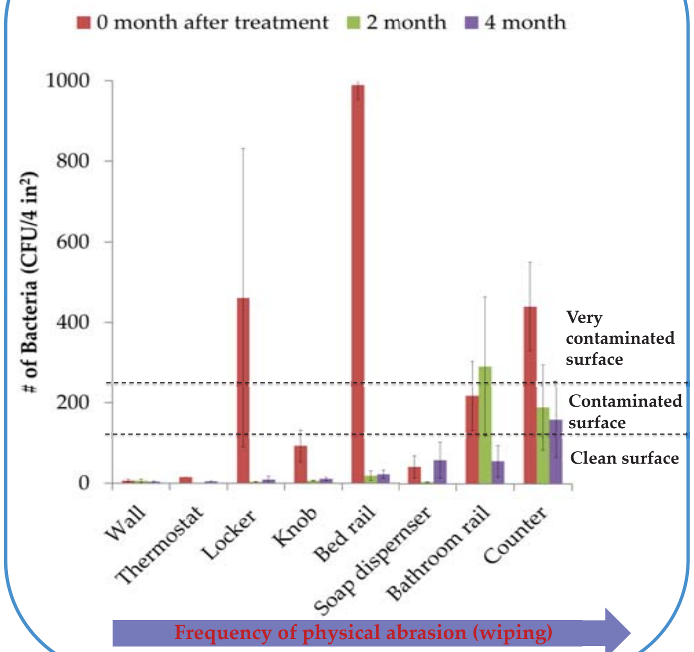


Active coating: PHF/anatase or anatase

Inert coating: rutile



6. Prototype testing



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Acknowledgements :

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Fall 2012 IAB Meeting – August 15-16, 2012

Particle Engineering Research Center

Fundamental Research Program: Foaming and Frothing Behavior of Green Surfactants and Fine Particulate Systems

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Angelina Georgieva, Parvesh Sharma and Brij Moudgil, University of Florida, Gainesville, FL 32611

Objective: Fundamental research will explore foaming/defoaming properties of green surfactants and fine particles. It will provide enhanced understanding of antagonistic and synergistic effects of hydrophobically modified fine particles and green surfactant formulations.

Market Motivation: Increased oil prices and environmental regulations signify the importance of developing renewable resources based foaming and defoaming modalities.

Broader Appeal: Foaming/defoaming formulations have important applications in mineral separations, detergency, boilers, paper, petroleum, paints, coating industry, biochemical separation, cosmetics, household industry and environmental remediation industries.

Industrial relevance: Global market for surfactants is forecast to reach $17.9 billion by 2015 with ever stricter environmental considerations.[1] There will be increased market demand 5.3% per year for environmentally friendly defoamers up to $2.77 billion total in 2015[2];

Advantages: Foaming is desirable criteria for:
- food industries: beer, ice cream and cappuccino beverage production
- Firefighting industries
- Household products (laundry detergents, dishwashing soaps).

Challenges: Foaming is detrimental for:
- Paper industries
- Petroleum industries
- Paint and coating industries
- Cement industry
- Waste treatment industries.

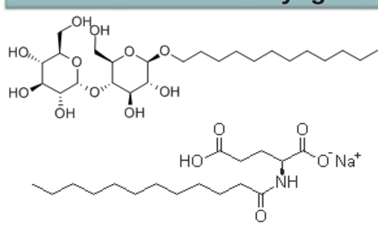
References: 1. Global Industry Analyst, Inc. : Surface Active Agents: A Global Strategic Business Report, 2010
2. BizAcumen, Inc.: Defoamers – World Market Review, 2010

Methodology Expertise:
- Production, characterization and surface modification of particles, frothing/defoaming (University of Florida);
- Colloids, foamability, froth stability, green surfactants, adsorptions and computational simulation (Columbia University)

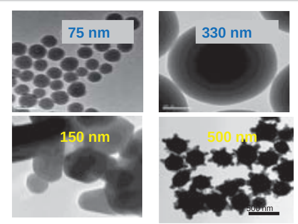
Methods: Colloidal dynamics acoustosizer for particles size; dynamic light scattering; zeta potential; macroscopic measurements of foam/froth stability; vibrational spectroscopy.

Systems:
- Sugar based and amino acid based green surfactants.
- Fine particulate systems of silica (SiO_2), kaolinite [$Al_2Si_2O_5(OH)_4$], calcite ($CaCO_3$), hydroxyapatites [$Ca_{10}(PO_4)_6(OH)_2$] and ferric(hydr)oxides [$Fe_{10}O_{14}(OH)_2$]

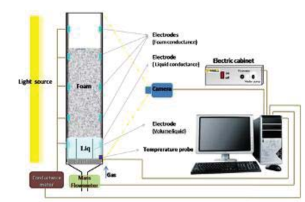
Green surfactants dodecyl maltoside & sodium dodecyl glutamate



Silica (top) & ferric hydroxide (bottom) nanoparticles



Foamscan for foaming property characterization



Timeline: June 2012 – July 2013	Q1	Q2	Q3	Q4
Columbia University	Physico-chemical characterization of green surfactants		Characterization of foamability of different surfactant mixtures	
University of Florida	Physico-chemical characterization of particles		Study of surfactant adsorption on the fine particles and evaluation of the effect on the foamability	

Acknowledgements: This material is based upon work supported by the National Science Foundation under Grant No. 1230637 & 1230680 and by the CPaSS industry members.

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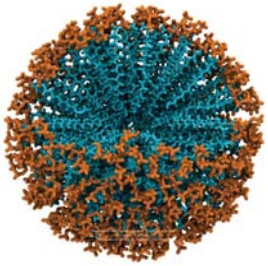
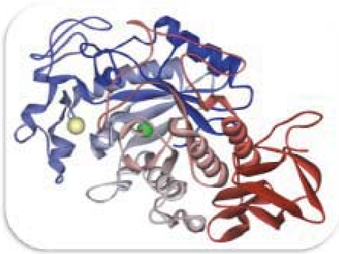
COLUMBIA UNIVERSITY IN THE CITY OF NEW YORK

Fall 2012 IAB Meeting – August 15-17, 2012

Protein / Colloid Interactions





Michael Chin
Columbia University

Center for Particulate & Surfactant Systems (CPaSS)
August 15-17, 2012

2) Impact – What can be gained?

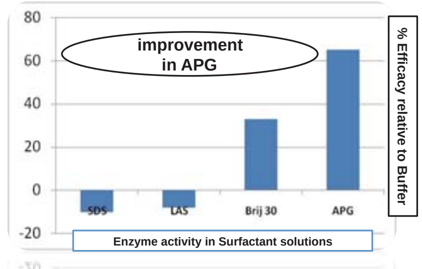
Improving cleaning properties of detergents featuring enzymes

Also: improving vaccine proteins in conjunction with $AlPO_4$ adjuvant particles

Objectives: Explore mechanism behind synergistic enzyme-detergent behavior

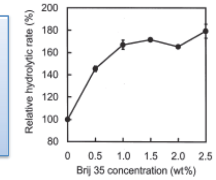
Challenges: Exploring changes in protein structures and function due to surfactant or colloid particles.

3) Observations



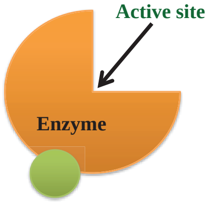
We observed protease enzyme in Brij-30 and APG digesting more substrate over a given period relative to the enzyme in just buffer

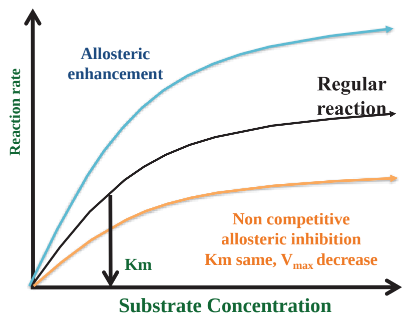
The same phenomena of non-ionic surfactants enhancing enzyme activity has also been noted in literature.
(Right) *Bacillus amyloliquefaciens* α-amylase (BAA) in the presence of Brij-35



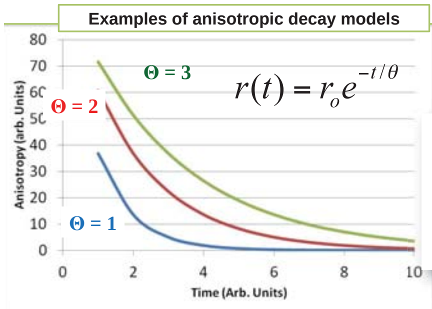
4) Hypothesis

Hypothesis:
Micelles interact with protein structure, influencing conformation in and possibly inducing greater active site flexibility through allosteric interactions, improving catalytic rate.



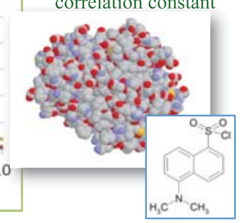


5) Method – Life Time Fluorescence Anisotropic Decay



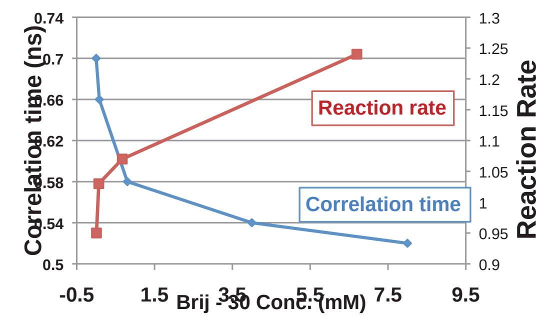
$$r(t) = r_o e^{-t/\theta}$$

r = anisotropy
t = time
θ = rotation correlation constant



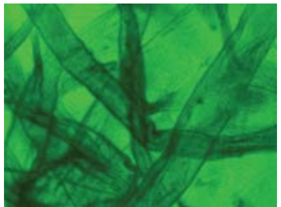
By attaching a fluorescent probe (dansyl) to the protein structure and exciting it with polarized light, we can observe the flexibility, or "wiggle room", of that particular part of the protein by measuring how quickly the probe reorients, resulting in diminishing anisotropy.

6) Linking Flexibility and Reaction Rates

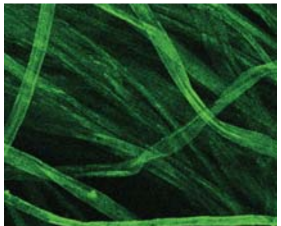


Using the decay correlation time as a measurement for the "stiffness" of the local protein structure, we can measure this structural property as a function of surfactant concentration. Here, a clear correlation between structure stiffness and maximum reaction rates can be seen

7) Imaging protein "stains" via fluorescence microscopy



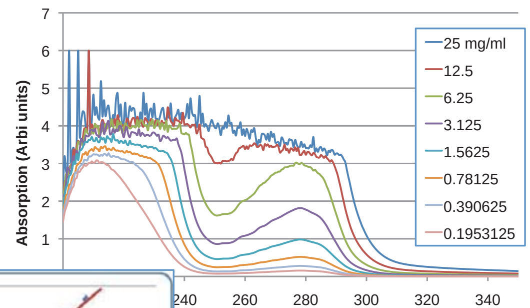
Fibers in FTC-Casein solution

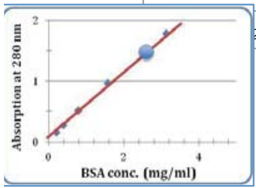


After drying

We are also utilizing fluorescence microscopy as a method of imaging fluorescently labeled proteins, to observe how they "soil" various fibers and how fiber size, shape, and surface properties may affect enzyme hydrolysis of these adsorbed proteins

8) Parallel project: Protein structure dynamics on $AlPO_4$





Above: Concentration standards of BSA measured by UV-Vis at 280nm. Linear intensity-concentration correlation fails past 5 mg/ml. **(left)** Measurement of supernatant BSA conc. after $AlPO_4$ particle separation (blue circle). Subtracting this value from known BSA concentration of original solution reveals approximately 48mg of BSA absorbed for every gram of AlPO4.

9) Summary and Future work

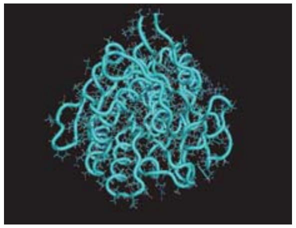
Findings up to date:

-Non-ionic surfactants can significantly increase catalytic rates
- This is seen at specific surfactant concentrations

- Surfactants can also affect binding efficiency
- Link found between enzyme flexibility and efficiency when in surfactant solutions
- Techniques and theory being extended to studying protein structure dynamics on ceramic particle surfaces

Future work:

-Molecular dynamic simulation to quantify degree of structure dynamics changes (right)
- NMR and 2D FTIR to measure water dynamics and the role they play in the interaction between colloid surface and protein.



DEM Study of Granular Shear Flows of Rod-like Particles

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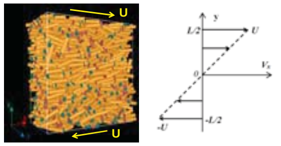
Introduction

- The flow of granular materials is widely found in pharmaceutical, mining and food industries, and a better understanding of granular flows can aid in the design and optimization of industrial processes.
- Although the particles in reality normally have non-spherical shapes, most of the early studies on granular flows were conducted using simple shapes for the particles such as spheres.
- The objective of this work is to explore the effect of particle shape on the flow behavior and the constitutive laws of granular shear flows of rod-like particles.

Methodology



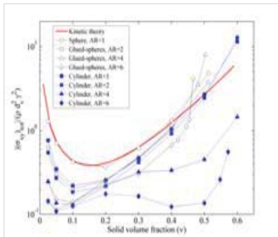
o Numerical model of granular shear flow of cylindrical particles. Periodic boundary conditions are applied in the x and z directions, and Lees-Edwards boundary condition is adopted in the y-direction.

- A soft-particle Discrete Element Method (DEM) is employed to model the simple shear flows of rod-like particles, in which the Hertz theory is used to describe the inter-particle contact forces.
- Damping is added to the contact forces to account for the energy dissipation in collisions. The coefficient of restitution is 0.95 due to the effect of damping.
- A number of particles with or without friction are randomly generated in a shear cell. The granular shear flow is initiated by applying a linear x-velocity (V_x) profile in the y-direction, and conducted in the absence of gravity and fluid media.
- Two types of rod-like particles are used:

(a) Glued-spheres particle (b) True cylindrical particle

Results and Discussion

➢ Stress tensors

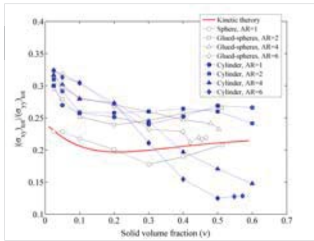


- The total stress tensors σ_{tot} can be expressed as a sum of kinetic and collisional components:

$$\sigma_{kin} = \rho\nu\langle CC\rangle$$

and

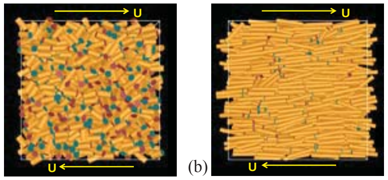
$$\sigma_{col} = \langle F_c l\rangle$$



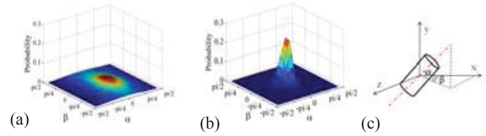
- At low solid volume fractions (ν<0.4), smaller stresses are obtained for the rod-like particles compared to the kinetic theory prediction for the spherical particle systems, due to the loss of translational energy to the rotational energy for the rod-like particles.
- At high solid volume fractions (ν>0.4), a sharp stress increase is observed for the glued-sphere particles, while low stresses are obtained for the elongated true cylindrical particles.

- The ratio of shear to normal stress is defined as the apparent friction coefficient of the bulk granular material.
- At low solid volume fractions, higher apparent friction coefficients are obtained for the rod-like particles compared to the spherical particles, due to the higher dissipation rate of translational energy.
- At high solid volume fractions, much lower apparent friction coefficients are obtained for the elongated true cylindrical particles.

➢ Particle orientational preference



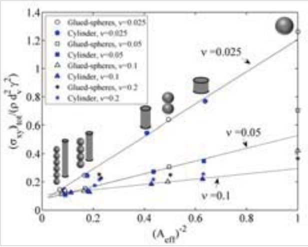
o Shear flows of true cylindrical particles with particle aspect ratios of (a) AR=2 and (b) AR=6. The solid volume fraction is 0.5.

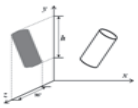


o Probability distributions of particle orientation as a function of α and β for true cylindrical particles with (a) AR=2 and (b) AR=6 , in which angles α and β are illustrated in (c).

- Particles with large aspect ratios show an orientational preference with the major/long axes aligned horizontally in the flow direction.
- This particle alignment becomes more significant as particle aspect ratio increases and/or solid volume fraction increases.
- The interference of particles and the bulk flow stream is minimized by this particle alignment. Therefore, smaller stresses and smaller apparent friction coefficients are obtained for the true cylindrical particles with large aspect ratios at high solid volume fractions.

➢ Stresses in dilute flows





o Effective projected area:

$$S_{eff} = \langle h\rangle \cdot \langle w\rangle$$

o Normalized projected area:

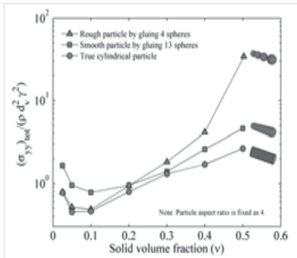
$$A_{eff} = \frac{S_{eff}}{d_v^2}$$

- For the dilute granular flows:

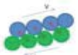
$$\text{Stresses} \propto (\text{Fluctuating velocity})^2 \propto \left(\frac{1}{\text{Collision frequency}}\right)^2 \propto \left(\frac{1}{\text{Projected area}}\right)^2$$

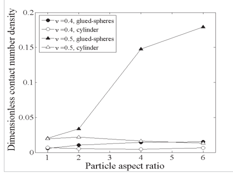
- Linear relationship between the stresses and $(A_{eff})^{-2}$ is obtained for the dilute flows of the rod-like particles with various particle aspect ratios.
- Thus, the projected area may be used to account for the effect of particle shape on the granular flows.

➢ Effect of surface roughness



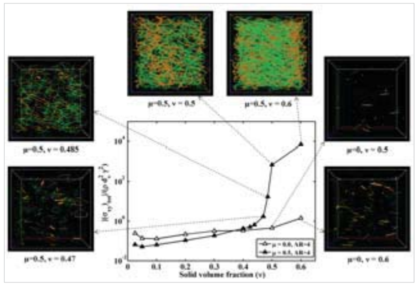
o Strong interaction between two rough glued-spheres particles:





- A smoothed glued-spheres particle is generated by using more constituent spheres which could have overlaps with their neighbors.
- Strong interaction can occur between two rough glued-spheres particles when they pass each other. Thus, high contact number densities are obtained for the glued-spheres particles with rough surfaces, in particular at a high solid volume fraction.
- As a result, at high solid volume fractions the stresses increase as the surfaces of particles become rougher.

➢ Effect of particle friction coefficient



o A comparison of stress curves with and without inter-particle friction.

o The snapshots show the corresponding plots of force chains, which are obtained by using straight lines to connect the centers of mass of each pair of particles in contact.

- At low solid volume fractions, smaller stresses are obtained for the frictional particles (μ=0.5) due to the loss of kinetic energy during the process of sliding friction.
- At high solid volume fractions, a sharp increase in stress is observed for the particles with friction (μ=0.5). As the sharp increase occurs, a continuous structure of force chains is formed throughout the whole shear domain.
- For the flows of frictionless particles, the inter-particle collisions occur much less intensely and only a few force chain lines are observed even at high solid volume fractions.

Conclusions

- The particle shape (in terms of particle aspect ratio and surface geometry) has a significant impact on the constitutive relations of stress tensors and the flow behavior.
- The DEM method is an effective tool to explore the constitutive laws of granular flows with non-spherical particles, which can then be applied to the continuum modeling of some industrial powder-handling processes (e.g. fluidized particle bed, blast furnace etc.).

Acknowledgement

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PREDICTING GAS-SOLID BUBBLING BED FLOWS USING CONTINUUM MODELING

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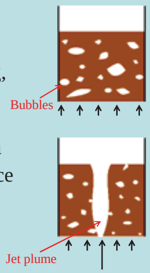
Bubbling Bed Flows

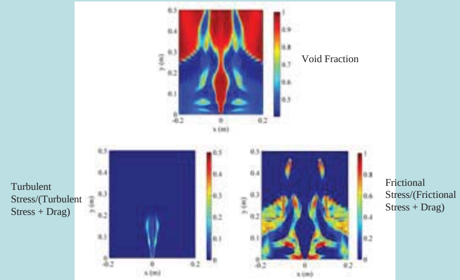
- Uniformly Fluidized Bed
  - To mix gas and solids
  - Employed in industries for drying, granulation, coating, heating and cooling
- Fluidized Bed with Jet Injection
  - To introduce reactants and enhance mixing
  - Employed frequently in coal and biomass gasification



Continuum Modeling

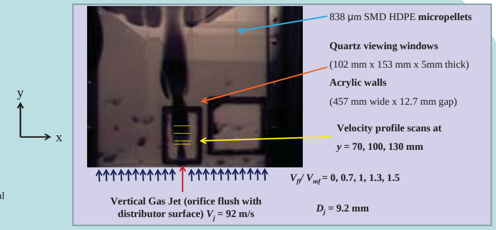
- Particles assumed to form a continuous fluid-like phase
- Volume averaged continuity and momentum equations for gas and solid phases
- Successfully applied– pneumatic conveying, fluidized beds, cyclones, hoppers
- Currently no general set of closure models which will work for all types of flows
- Thorough understanding of closure description necessary to ensure reliability and improvement

High Speed Jet Injected into a Fluidized Bed



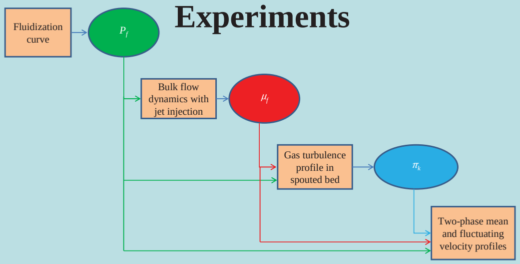
Turbulence is significant in the dilute jet plume region
Friction is significant in the dense bubbling regions

Experimental Data



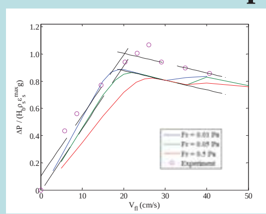
1. Pressure drop fluidization curve without jet
2. Videos revealing bulk flow pattern with jet
3. Detailed mean and fluctuating velocity measurements within dilute jet plume region using Laser Doppler Velocimetry

Determining Closures based on Increasing Complexity of Experiments



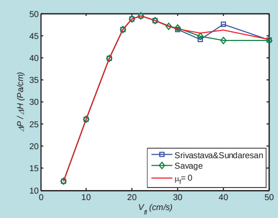
MFIX

Determining Empirical Constant in Frictional Pressure Expression



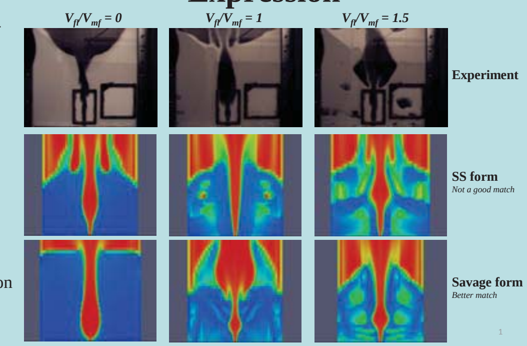
- Increasing ***Fr*** decreases the slope of the packed bed pressure drop accompanied by an increase in the minimum fluidization velocity prediction
- ***Fr*** = 0.05 Pa predicts closest agreement with experiment

Determining Empirical Constant in Frictional Pressure Expression

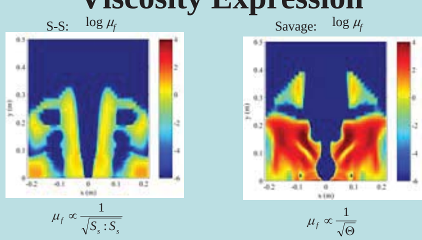


- Verifying the independence of frictional viscosity expression

Determining Frictional Viscosity Expression



Determining Frictional Viscosity Expression



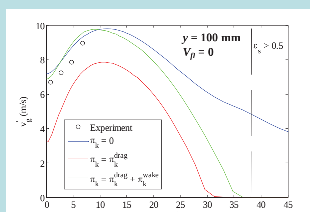
$\mu_f \propto \frac{1}{\sqrt{S_s : S_s}}$ $\mu_f \propto \frac{1}{\sqrt{\Theta}}$

In dense regions subjected to high shear, the viscosity is under-predicted

Viscosity is better predicted by this relationship

- Because of better emulsion behavior captured by Savage frictional viscosity model, it is chosen in the continuum model

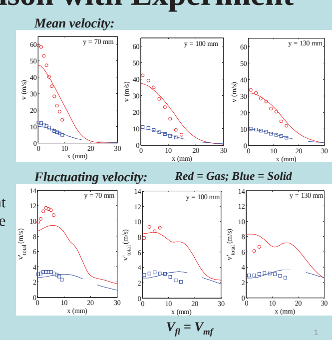
Determining Gas Turbulence Modulation



- Effect of instantaneous particle drag on turbulence able to avoid unrealistically high fluctuations in dense regions
- Including effect of wakes predicts the magnitude of gas fluctuations better

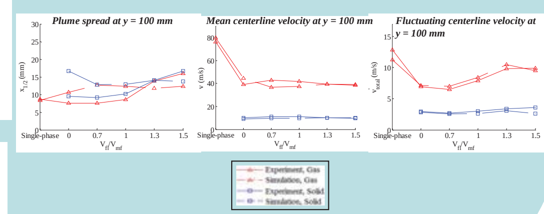
Comparison with Experiment

- Velocity fluctuations due to bubbling emulsion action added to intrinsic turbulence
- Match between simulation and experiment generally good
- Deviation at low height attributed to round pipe in experiment which has been neglected in simulation



$V_{fl} = V_{mf}$

Comparison with Experiment



- Simulation able to capture mean and fluctuating velocity along the centerline reasonably well
- Only a fair match with regard to plume spread
- Mismatch in plume spread at $V_{fl} = 0$ attributed to static effects causing an inward sloping top surface in experiment

Acknowledgement: This material is based upon work supported by the US Department of Energy-National Energy Technology Laboratory

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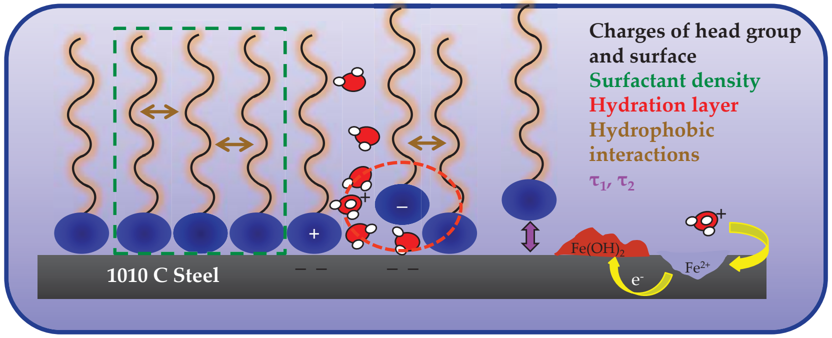
Investigative Tools for Studying Surfactant–Surface Interactions in Corrosion

Eric Bidinger, Neha Saxena, Megan Hahn, Zhao Han, Michael Powers, Yakov Rabinovich, Vijay Krishna, Kevin Powers & Brij M. Moudgil
Particle Engineering Research Center, University of Florida; Gainesville, FL 32611

Motivation

- The total annual estimated direct cost of corrosion in the U.S. is **$276 BILLION**
- **3.1% OF NATION'S GDP** is spent on corrosion management

"Corrosion Costs and Preventive Strategies in the United States," Report FHWARD-01-156



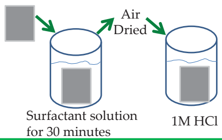
Objective

Examine structure and dynamics of inhibitors at the solid/liquid interface

Dissolution Method

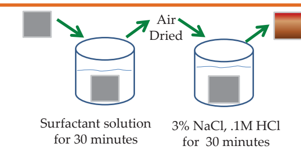
For glass in 1M NaOH
$2NaOH + SiO_2 \rightarrow Na_2SiO_{3(aq)} + H_2O$

For Steel coupons in 1M HCl
$Fe + 2\,HCl \rightarrow FeCl_2 + H_2$

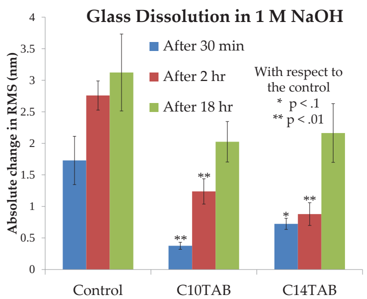


Corrosion Method

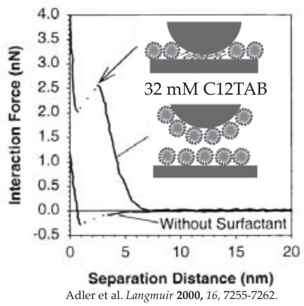
$Fe(OH)_2 \rightleftharpoons FeO + H_2O$
$Fe(OH)_3 \rightleftharpoons FeO(OH) + H_2O$
$2FeO(OH) \rightleftharpoons Fe_2O_3 + H_2O$



Atomic Force Microscopy

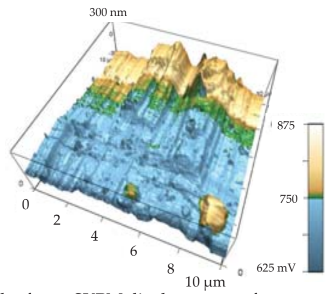


- C10TAB inhibits dissolution slightly better than C14TAB



Adler et al. *Langmuir* **2000**, *16*, 7255-7262.

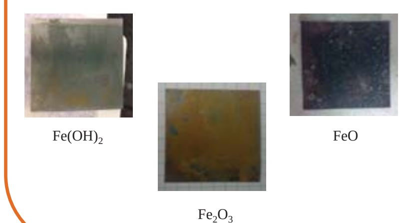
- Force curves demonstrate strength of micelle layer, with forces increasing with chain length of surfactant

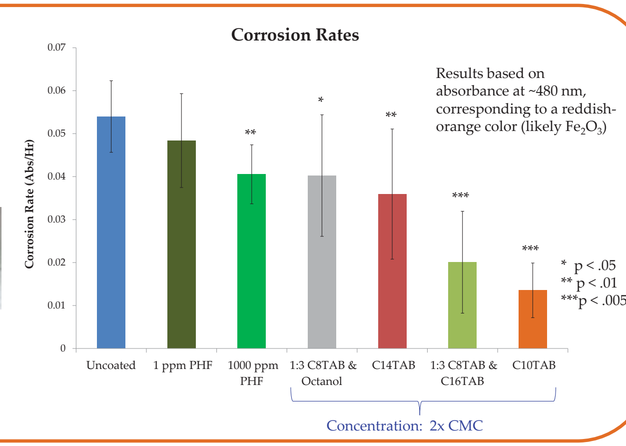


- SKPM displays areas of corroded (blue) and pristine (yellow) metal surface

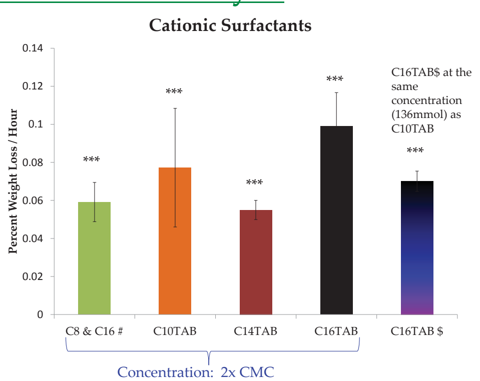
Reflectance

- Can identify different corrosion products (ex. hydroxides, oxides, pyrites)
- All groups show corrosion inhibition, except for 1 ppm PHF

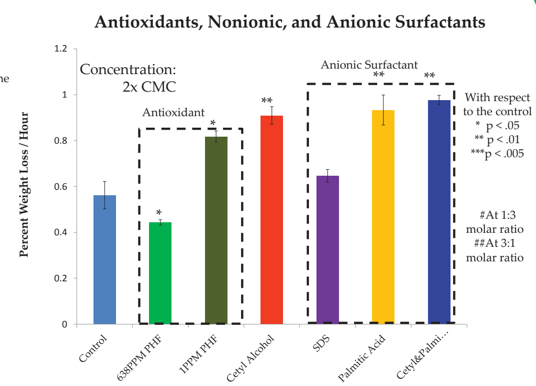




Gravimetric Analysis



- Dissolution inhibition is dependent on surfactant concentration
- C8TAB and C16TAB inhibits more than C16TAB alone



- Anionic surfactants promote dissolution because they chelate Fe^{2+}

Summary

- AFM can be used to determine surfactant structures and local electronic structure
- Reflectance can be used to determine corrosion species
- Gravimetric is the most sensitive technique to determine corrosion/dissolution rate
- Cationic surfactants inhibit dissolution better than anionic and nonionic surfactants

Future Work

- Determine the influence of surfactant packing density on corrosion pathways leading to hydroxides, oxides, pyrites and carbonates
- Investigate the effect of temperature and flow velocity on surfactant adsorption and corrosion inhibition
- Determine the effect of particles in suspension (e.g., sand, clay or rust) on surfactant mechanism of corrosion inhibition

Acknowledgements: M. Q. Landenberger Foundation; Particle Engineering Research Center, Major Analytical Instrumentation Center, Water Reclamation & Reuse Laboratory

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Deposition of Benefit Agents on Skin from Emulsion Cleansers upon Dilution

Jose Martinez Santiago, P. Somasundaran

Earth and Environmental Engineering Department, Columbia University, New York, 10027

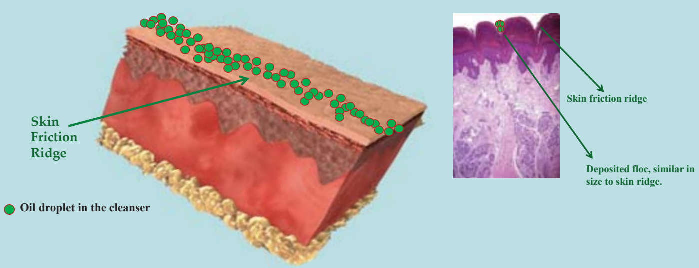
Objective: To optimize deposition of beneficial agents (oil) on skin from rinse-off emulsion cleansers

Challenges: Polymer induced flocculation upon dilution is a complex process due to numerous factors, including dilution factor, interaction between polymer and surfactant, pH, and the interaction of other ingredients in the cleanser.

Industrial Relevance: Obtaining a fundamental understanding of flocculation in emulsion cleansers upon dilution will lead to streamline-driven processes for defining the right composition of industrial formulations containing polymers, surfactants, and oils, and will help optimize deposition of beneficial agents in skin.

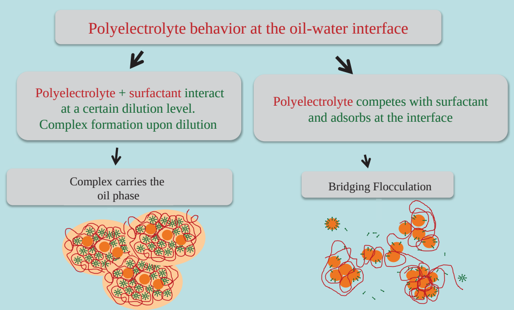
Broad Appeal: Fundamental models and theories developed will be helpful to product developers and formulators in industries where flocculation is a key process; such as personal care household, pharmaceuticals, mining technologies, etc.

Deposition of benefit agents on skin from emulsion cleansers



- Upon dilution (cleanser rinsing stage), flocs are formed due to polymer present in the system.
- If flocs are similar in size to friction ridges of skin, deposition is favorable

Why flocculation upon dilution? Possible mechanisms for polymer induced flocculation

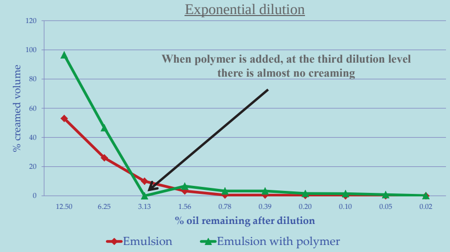


Experimental
Studying Polymer behavior at O/W interface

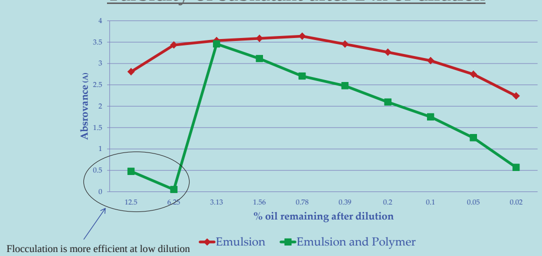
System: Stock emulsion formulated with:
Polyelectrolyte: Guar grafted with hydroxypropyl trimethyl ammonium chloride (Jaguar polymer)
Surfactant: Sodium lauryl ether sulfate (SLES) and Glyceryl Distearate
Oil phase: Petrolatum (mixture of hydrocarbons)

Experimental creamed volumes after 24h of dilution

Exponential dilution



Turbidity of subnatant after 24h of dilution

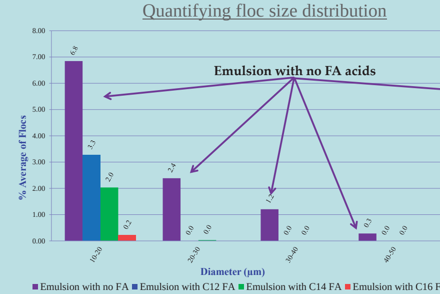


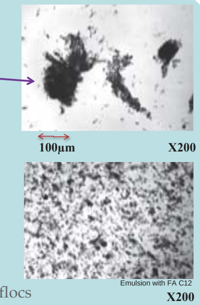
Flocculation is more efficient at low dilution
At third dilution (3.13 % w/w oil) flocculation efficiency decreases significantly.

- **When no polymer is present, creaming decreases following dilution scheme**
- **When Polymer is present, polymer and surfactant may interact (opposite charge) and inhibit flocculation**

Effect of fatty acids on flocculation

Quantifying floc size distribution





- Upon dilution, emulsion with no FA developed bigger flocs
- The longer the FA chain length, the smaller the flocs formed

Suggestions for modeling flocculation of diluted emulsions under shear flow

from von Smoluchowskii equation for aggregation

Loss or disappearance of particles or aggregates | Growth of aggregates

$$\frac{\partial n(v,t)}{\partial t} = -\int_0^{\infty} \alpha(v,u)\,\beta(v,u)\,n(v,t)n(u,t)du + \frac{1}{2} - \int_0^{v} \alpha(v-u,u)\beta(v-u,u)n(v-u,t)n(u,t)du$$

Collision frequency:
1. Brownian motion
2. Applied Shear
3. Differential creaming

Collision efficiency:
1. Van der Waals at.
2. Electrostatic rep.
3. Hydration rep.
4. Bridging at.
5.Hydrophobic at.
6.Steric (adsorbed polymers)
7.Depletion (non ads. polymers or micelles)

New! Forces due to P-S interaction

$$-S(v)n(v,t) + \int_v^{\infty} S(u)\gamma(v,u)n(u,t)du$$

Loss of aggregates due to fragmentation | Generation of aggregates due breakage of larger ones

n Number of particles or aggregates
v Particle volume
u Aggregate volume
t Flocculation time
α Hydrophobic attraction
β Collision Frequency factor
S Fragmentation rate constant
γ Breakage distribution function

Conclusions

- **Studying polymer and surfactant interactions at the o/w interface is very important to understand flocculation in emulsions that undergo dilution**
- **As seen in the bulk, polymer and surfactant interact at certain dilution level perturbing the flocculation process.**
- **Polymer and surfactant forces should be added to population balance eq. for flocculation**

Acknowledgement: This material is based upon work supported by the National Science Foundation under Grant No. 0749481 and by the CPaSS industry members.

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Dilute Suspension Flow Studies Using LDV

Sarah Elizabeth Mena and Jennifer Sinclair Curtis

Department of Chemical Engineering, University of Florida; Gainesville, FL 32611

Objectives: To acquire novel nonintrusive experimental data for slurry flow over a range of operating conditions and system parameters.
To develop Novel CFD models for slurry flow and to incorporate these models into CFD software.

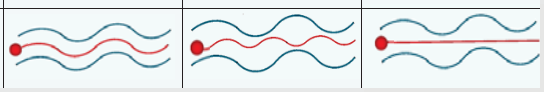
Two-phase flows are prevalent across a diverse range of industrial and geophysical processes including fluidized bed reactors, pneumatic and hydraulic conveyors, and sedimentation units.

The presence of a second phase has an effect on the momentum, heat and mass transport properties of the flow. Knowledge of the behavior of two-phase flows is required for the development of accurate transport models that will help reduce problems with settled/stationary particles, improve the design of new slurry lines, and help determine optimum operating conditions in existing lines.

Particle Flow Classification

A method to quantify the response of particles to fluid fluctuations is the Stokes number, defined as:

$$St = \frac{particle\ response\ time}{fluid\ response\ time} = \frac{U_f \cdot \rho_s \cdot d^2}{18 \cdot \mu \cdot D}$$

Stokes Number	1-10	10-40	>40
Regime	Viscosity dominated	Intermediate	Collision dominated
Behavior			

There is a lack of experimental data for the viscous-dominated (Stokes ~1) and transitional regimes (Stokes ~5-30).

Experimental Facility

A unique pilot flow facility was constructed and is fully functional for the investigation of turbulent two-phase flows. The equipment, depicted in Figure 1, can accommodate a wide range of flow rates, particle sizes and concentrations.

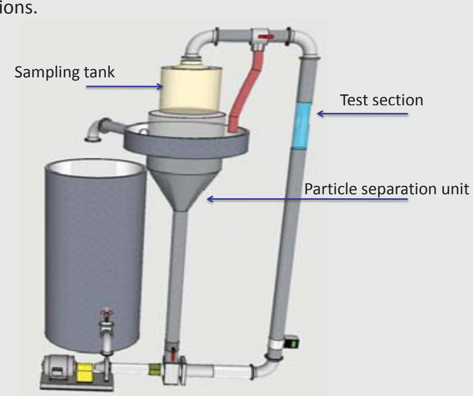


Figure 1 Diagram of the pilot scale slurry facility

Experimental Technique: Laser Doppler Velocimetry

Flow data will be acquire using non-intrusive laser Doppler velocimetry (LDV). The principle of operation is depicted in Figure 2. LDV is a high resolution laser based technique that can be used to obtain instantaneous and averaged velocity measurements. LDV is one of the most popular methods for the measurement of local velocity.

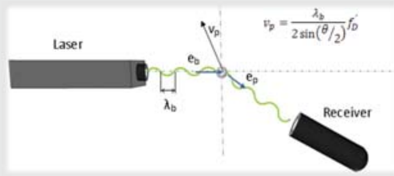


Figure 2 Principle of Operation LDV/PDPA

Phase Doppler Particle Analyzer (PDPA) is used to measure the size of the particles in the flow and provides a discrimination technique between the solid and liquid phases

Experimental Particles: Dense Slurries

One of the limitations of LDV is its inability to measure concentrated solutions of solids in liquids.

This can be overcome through closely matching the refractive index of the solid to the liquid phase. An extensive literature review was conducted to select possible candidates for IR matched systems with Sodium iodine (NaI) solutions with borosilicate glass or silica gel particles being two of the most promising.

Preliminary testing showed that NaI solutions with borosilicate beads can be used to study slurries with volume fraction between 9.9%-12.8%.

Figure 3.1 Silica gel beads and NaI solution

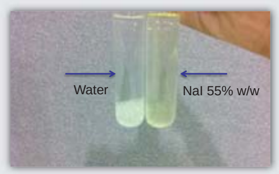


Figure 3.2 Borosilicate beads and NaI solution

Experimental Particles: Non-spherical

Few applications in industry deal with homogeneous distributions of spherical particles. That is why non-spherical particles, such as sand or crushed glass, will be tested in an effort to establish the effect that shape has on the flow.

The first set of experiments for non-spherical particles were conducted using crushed glass with a size distribution of 0.4-0.8 mm. The Stokes number was around 3 with a Reynolds number of approximately 200,000.

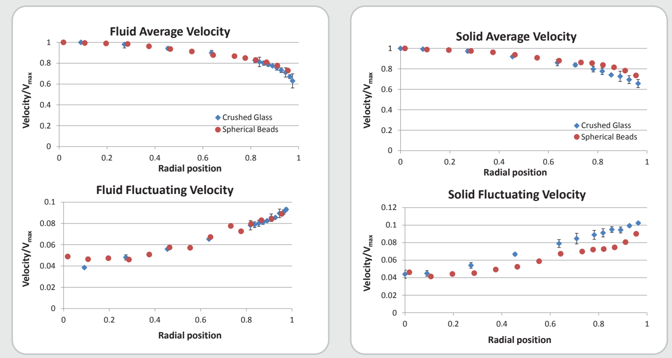


Figure 4. Results for crushed glass experiments compared to results from spherical beads. Error bars shown are calculated over three runs for the crushed glass.

Even at this low Stokes number there is an appreciable difference between spherical and non-spherical particles that confirms the importance of the study of shape effects in the slurries.

Future Work

For the non-spherical particles, the next step is to increase the Stokes number and observe the effects of particle shape in the intermediate Stokes regime. Also, we will be exploring the effect of particle size distribution (i.e. by considering bimodal mixes of smaller and larger particles).
For the concentrated slurries we will be conducting tests in the pilot scale loop using the NaI-borosilicate system

Acknowledgement: This material is based upon work supported by the National Science Foundation under Grant No. 0749481 and by the CPaSS industry members.

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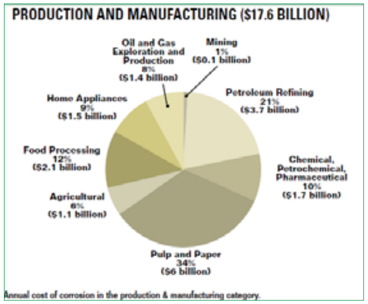
Corrosion Reversal via TiO_2 Photocatalysis

Michael Powers, Zhao Han, Neha Saxena, Eric Bidinger, Megan Hahn, Kevin Powers, Vijay Krishna and Brij Moudgil
Particle Engineering Research Center, University of Florida; Gainesville, FL 32611

Industrial Significance of Corrosion

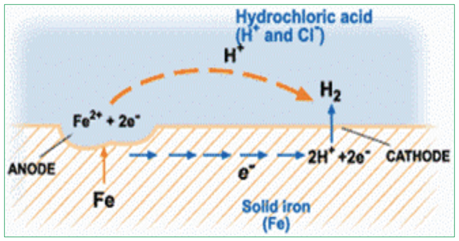


3.1% of nation's GDP is spent on corrosion management.

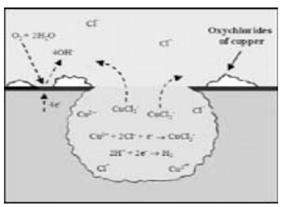
The total annual estimated direct cost of corrosion in the U.S. is $276 billion.

"Corrosion Costs and Preventive Strategies in the United States," Report FHWARD-01-156

Corrosion Mechanism

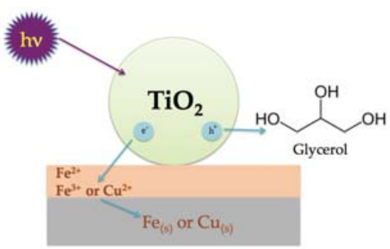


- Lattice matching between CuO and Cu, and FeO and Fe allows for corrosion reversal in copper alloys and steel, respectively.



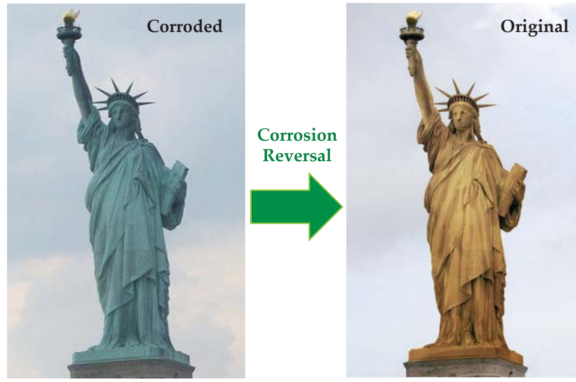
Photocatalysis for Corrosion Reversal

- Photons excite electrons from the valence to conduction band.
- The holes are taken by glycerol molecules.
- The electrons reduce the oxidized metal.



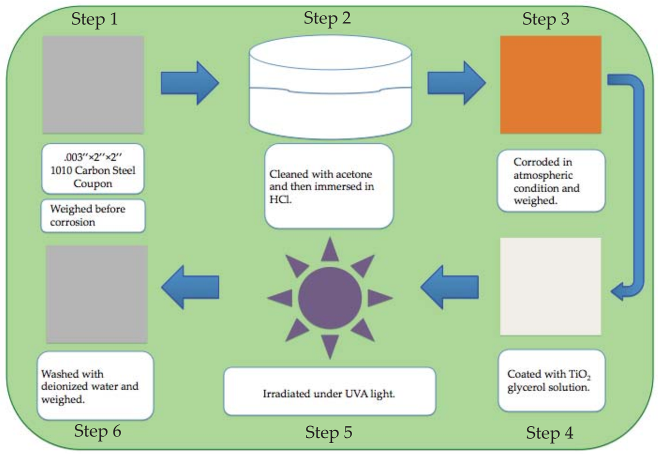
Objective

To investigate the reduction of metal oxides via TiO_2 photocatalysis



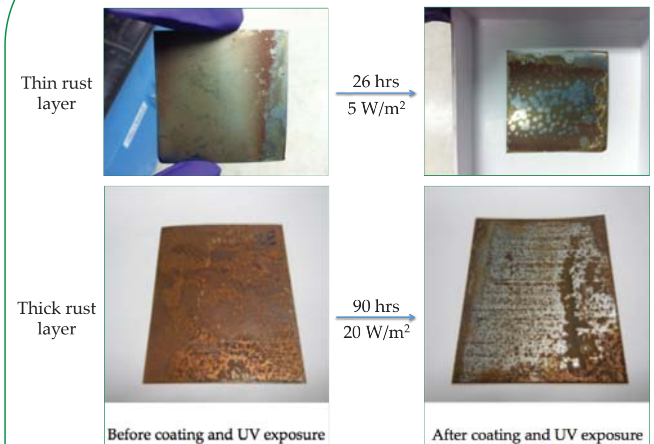
"The Statue of Liberty Before It Was Green" Posted by Benjamin Starr
http://www.visualnews.com/2011/09/02/the-statue-of-liberty-before-it-was-green/

Materials and Methods

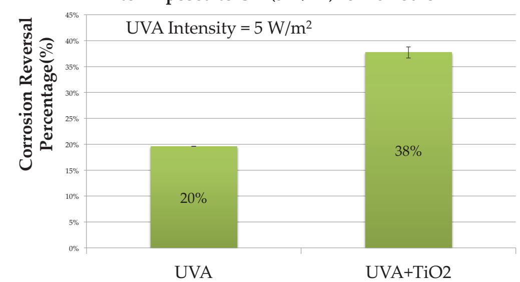


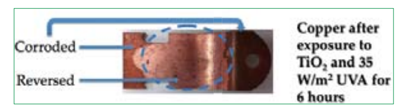
Acknowledgement: This material is based upon work supported by the National Science Foundation under Grant No. 0749481 and by the CPaSS industry members.

Results



Corrosion Reversal in 1010 Carbon Steel After Exposed to UV (5W/m²) for 26 hours





Copper after exposure to TiO_2 and 35 W/m^2 UVA for 6 hours

Future Work

- Demonstrate photocatalytic corrosion reversal in steel and copper alloys in outdoor environment
- Determine the maximum thickness of oxidized metal that can be reduced with photocatalysis without loss of material
- Investigate the effect of lattice parameters of oxidized and pristine metal for corrosion reversal
- Develop transparent and visible light active photocatalytic coatings for corrosion reversal

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Particle Process Analytical Technology (PPAT) - Summary

J. Zhou, P. Sharma, S. Svoronos, A. K. Saha, M. Hahn, G. Scheiffele, and K. Powers

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INTRODUCTION

Process analytical technology (PAT) has been defined by the FDA as a mechanism to design, analyze, and control pharmaceutical manufacturing processes through the measurement of Critical Process Parameters (CPP) which affect Critical Quality Attributes (CQA). PAT allows manufacturers to produce products with consistent quality and also helps to reduce waste & overall costs. The application of PAT in particle science is still an unexplored area. By using PAT, both quality and control over particle synthesis systems can be improved.

OBJECTIVE

To develop procedures, methods and integrated systems for measuring selected particle morphologies (size, shape and state of dispersion) and then to implement PAT into product quality control procedures, leading to better precision and lower cost.

ACCOMPLISHMENTS

Stober silica:

✓ Demonstrated precision and reproducibility when changing size parameters as well as the ability to make more precisely controlled particle size distributions.

System improvement:

✓ Achieved on-online control

✓ Integrated pressure &temperature control, Integrated in-line size measurement by dynamic light scattering (DLS), laser diffraction (LD) and spectrofluorometer

Gold particles:

✓ Tested synthesis of gold colloids

Quantum dots:

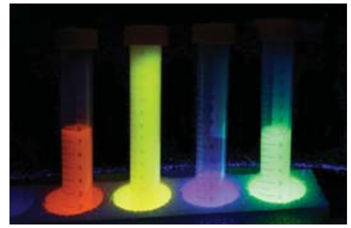
✓Implemented first flow CdTe hydrothermal synthesis, scale-up and coating.

✓Achieved precision control over QD emission and CDS coatings

Dye doped stober silica

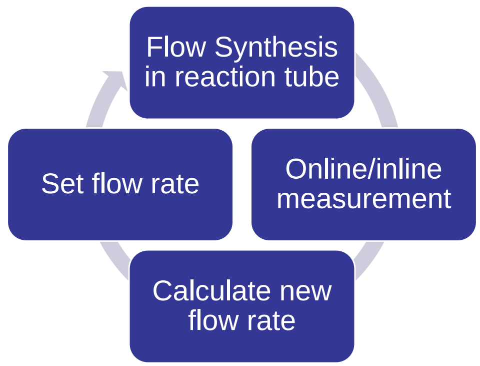
Mix dye molecules with TEOS precursor

- Chemical bonding
  - FITC (Green)
  - MCA(Blue)
- Physical adsorption
  - Rubpy (Red)
  - R6G (Yellow)



112nm 171nm 370nm 338nm
(Mean volume size)

Process Control Flow Chart



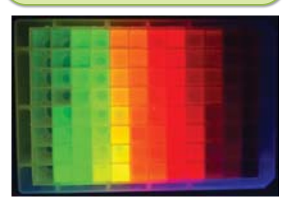
CdTe quantum dots

Hydrothermal method

Advantages
- Water dispersibility
- High quantum yield
- Good photostability
- Low cost of precursor

Characteristics
- Emission range: 500nm – 800nm
- Quantum yield: 40%-60%

Controllable parameters
•Temperature (up to 190°C)
•Reactant concentrations
•**Residence time (3sec to 1min)**

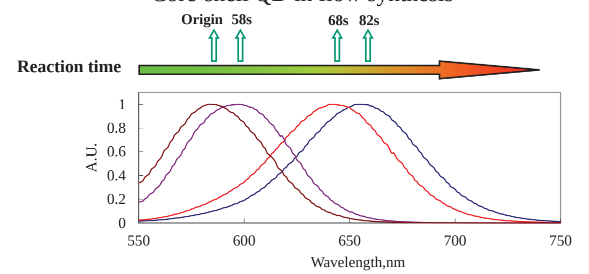


96 samples w/ 2nm interval

CdTe/CdS core/shell quantum dots

Continuous emission wavelength change with increasing CdS shell thickness controlled by flow reaction time

Core-shell QD in flow synthesis



Other potential control parameters: Temperature, pH, Na_2SO_3 concentration

SUMMARY

- Flow manufacturing system shows great promise for precision synthesis of a variety of high-value added particulates and nano systems.
- Convenient tool for expanding the understanding of current synthesis system.
- Significant interest-good potential for many other hydrothermal syntheses.
- Augments CPaSS's particle engineering programs

FUTURE WORK

- Explore different QD chemistries and other promising hydrothermal reactions
- Scale up to produce more than 10-20 g/day

ACKNOWLEDGEMENTS

- Particle Engineering Research Center (PERC)
- Center for Particulate and Surfactant Systems

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IAB-I/UCRC – August 15, 2012

Investigation of surfactant-stratum corneum interactions: Drying Stress and Raman studies

Parag Purohit[1], Annamaria Vilinska[1] and P. Somasundaran[1]

Department of Earth and Environmental Engineering, Columbia University, NY 10027

Objectives: To study effects of common surfactants on stratum corneum biomechanical properties and determine the role of SC lipids on stress relaxation behavior of stratum corneum

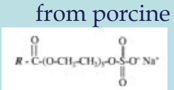
Challenges: Develop methods to measure mildness of next generation cleanser systems

Industrial Relevance: Knowledge generated from SC-surfactant interactions will help design milder surfactant systems in personal care industry

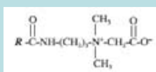
Broad Appeal: Understanding of SC barrier function is vital to Pharmaceutical/ drug delivery applications and the knowledge of thin film behavior has importance in paints/ coatings industry

Materials/Methods

- Stratum corneum separated from porcine skin



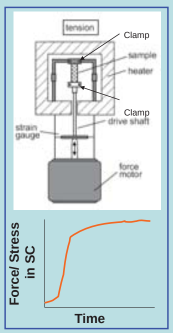
Sodium Lauryl Ether sulfate, SLES



Betaine, LAPB

Dynamic Mechanical analyzer

- The specimen as a thin film is loaded between the clamps and kept under initial load (enough to straighten but not allowing significant stress)
- The change in force is measured as a function of drying time
- Stress-time plots are recorded for period of 4-6 hours

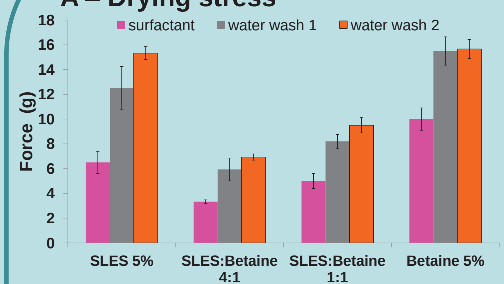


Raman spectroscopy

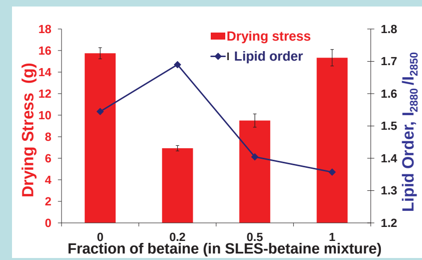
- Effect of surfactant binding to Stratum corneum: Protein and lipid structure
- Lipid-order by I_{2880}/I_{2850} ratio : Monitor lipid structural changes
- Lipid/Protein ratio (by I_{2880}/I_{2933}): Monitor lipid extraction potential

Important results

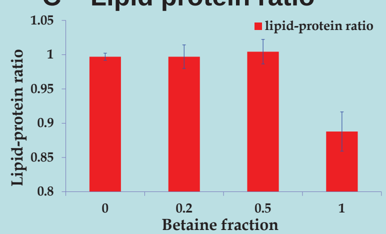
A – Drying stress



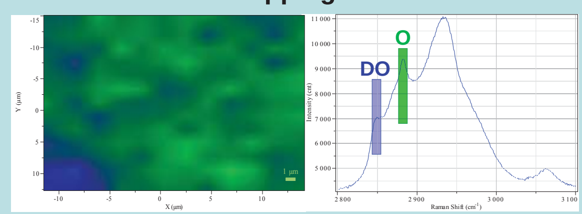
B – Lipid order by Raman



C – Lipid protein ratio



D – Raman mapping



A. Mixed surfactant treatment generates lower drying stress in SC
B. Optimum performance (lower drying stress + better lipid rigidity) is observed at 1:4 Betaine : SLES → Minimum damage to SC lipids
C. Betaine extracts SC lipids as seen from lower lipid/protein ratio
D. Raman mapping : A technique to understand effect of surfactants on localized skin regions, e.g. to map extent of lipid disorder (DO) upon treatment

Summary

Drying stress and lipid mobility studies measure the damage potential of surfactant treatment on SC. The future work will focus upon developing and testing next generation surfactant systems

Acknowledgement: This material is based upon work supported by NSF under Grant No. 0749481 and by Unilever Research (a CPaSS industry member).

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Fall 2012 IAB Meeting – August 15-16, 2012

ATR-FTIR Spectroscopy to Evaluate Skin Mildness of Consumer Care Products

Manoj Varshney, Parvesh Sharma and Brij M Moudgil

Particle Engineering Research Center, University of Florida; Gainesville, FL 32611

Industrial Relevance: US occupies one third of the global surfactant market. With rising affluence and disposable income in China and India, two of the largest populated countries, the global demand of surfactant in consumer market is estimated to be $ 17 billion in 2012. Sustainability is a desired goal in this industry and many major surfactants players are trying to add more "green-ness" into their products such as bio-propylene glycol and bio-based ethylene oxide surfactants. Such green surfactants independently may be safe to the skin, but it is not necessary that after adding other inactive and active ingredients , the formulation remain mild to the skin. It is essential that there should not be any adverse synergy among formulation excipients, which reduce the skin barrier property and deliverer the unwanted chemicals to the circulatory system . ATR-FTIR is a sensitive technique to access the following:

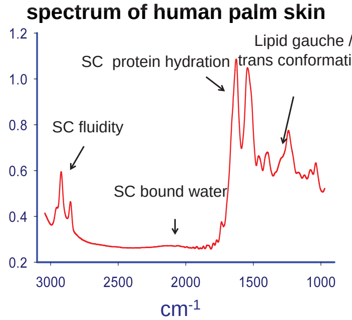
- **Skin Mildness (by measuring dryness of stratum corneum (SC)**
- **Skin Permeability (by monitoring SC lipid fluidity and protein interactions)**

It is strongly recommended to validate the IR results with skin cells viability MTT assay for the skin irritancy and corrosiveness effects.

FT-IR Skin Mildness Markers

- ✓ Detection of lipid conformational changes (by monitoring the alteration in methylene bands intensities and vibration frequencies)
- ✓ Protein Hydration Study (by monitoring amide bands and bound water vibrational frequencies)
- ✓ Formulation effect on SC permeability (measuring skin flux and permeability)

ATR-FTIR Spectroscopy of Stratum Corneum (an illustrative example)

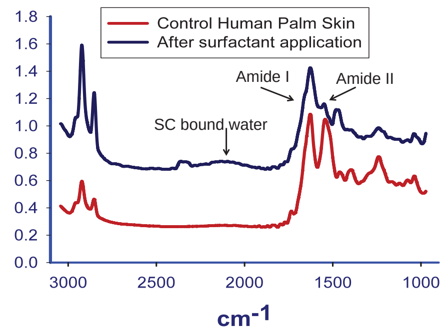


Spectrum important points that are related with SC barrier efficacy :

1. Change in methylene band intensities, provides lipid alkyl chain lateral order packing
2. Shift in vibration frequencies of methylene provides gauche/trans ratio
3. Change in Amide I and Amide II bands and bound water band gives SC hydration / dehydration

Preliminary Results

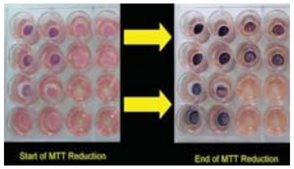
Effect of CTAB of on SC



1. No shift in lipid bands at 2920cm-1 and 2850 cm^{-1} – good for skin mildness
2. However, a small intensity ratio from 1.17 (control) to 1.26 (CTAB treated) shows that CTAB induced a slight alteration in lateral packing
3. CTAB enhances 2100 cm-1 band peak area , means protein hydration.
4. The trans fraction is quantified using the trans and gauche absorbance at 1340 cm−1 and 1370 cm−1, respectively.

Skin Epiderm Test

Validate the IR findings by gold standard Skin Cells MTT assay



From: http://www.iivs.org/

The test product is considered to be irritating to the skin if the tissue viability (purple color 570 nm) after exposure & incubation is equal (≤) to 50% of control .

Skin Epiderm is a gold standard test for skin irritancy but it is quite cumbersome and need about four days to complete the assay.

Summary: Increased lipid fluidity and protein hydration indicate that CTAB perturbs the SC and increase skin permeability. ATR-FTIR technique provides a quick method for screening mildness of surfactant and related consumer products.

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Particulate Systems for Controlled Release of Insect Repellent to Mitigate Citrus Greening

Aarthi Narayanan, Parvesh Sharma, Manoj Varshney, Hassan El-Shall, and Brij Moudgil
University of Florida, Gainesville, FL

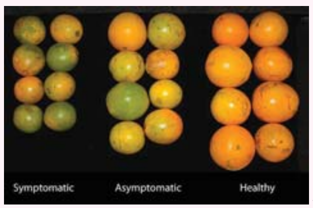
Overall Objective

Develop engineered particulate systems for crop protection

Develop particle platforms (silica, clay, polymer, emulsions) for controlled release of protecting agent (pesticide, herbicide) or delivery of micronutrients, employing GRAS materials.

Background

- Citrus greening –threatens $ 9 B Industry in Florida
- Bacteria (*Candidatus Liberibacter asiaticus*) transmitted by an insect Asian citrus psyllid (*D. Citri*).



Slisz et al J Proteomics 2012

- Leads to deformed and bitter citrus fruits
- No Cure known

Current mitigation strategies

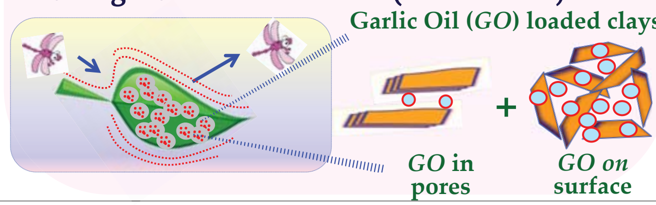
1. Quarantine infected trees
2. Insecticidal formulations
3. Natural enemies
4. Particle Film Technology

Challenges:
- Complete coating required;
- Lack of rain-fastness

Apple leaves coated (Particle film technology)

CPaSS Strategy - Novelty

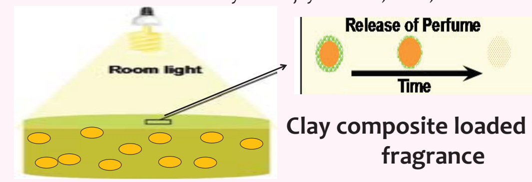
- Presence of insect repellents in the clay coatings would prevent infestation even with partial coating
- Addition of appropriate adjuvants enables the coatings to withstand rainfall (rain-fastness)



Broader implications of the approach

- Consumer products, Paints and coatings etc.
  1. Visible light activated fragrance release from clay composites

Cartoon courtesy : Dr. Vijay Krishna , PERC, UF

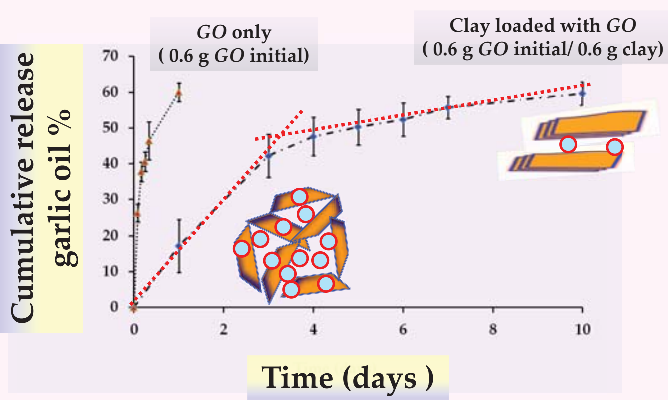


Clay composite loaded with fragrance

  2. Odor control - incorporate functional nano particles (e.g. copper speckles) in clay
  3. Indoor pollution control - incorporate catalysts (e.g. Manganese oxide) in clay composites to remove volatile organic compounds
- Oil, Wastewater treatment, mining industries (Sorption of oil, organic contaminants, toxins)

Preliminary results

(a) Extended release of garlic oil from the clay



- Estimated garlic oil release time ≈ 3 weeks
- Extended release of insect repellent from pores and surface

(b) Rain-fastness of the clay coatings

(a) Immediately after spraying

(b) regular water sprays and rainfall conditions (Average precipitation June = 16 cm)

- Coatings sustain regular water sprays and rainfall conditions
- New leaves emerged from the plant after a week and the plant continues to grow

Summary

- Demonstrated encapsulation and extended release properties
- Demonstrated rainfastness of extended release coatings

Future work

- Determine effect of hydrophobic clay coatings on plant growth, phytotoxicity
- Encapsulate /release of insecticide (e.g. Imidacloprid in poly caprolactone)
- Test formulation at lab scale/ greenhouse
- Field-tests

Acknowledgments

This material is based upon work supported by the National Science Foundation under Grant No. 0749481, CPaSS Industry members, Mr. Travis Murphy and Mr. Ben DeVries (Citrus Growers)

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The Development of the Greenness Index

Yang Shen[1], Chi Lo[1], D. R. Nagaraj[2], Raymond Farinato[2], P. Somasundaran[1]

[1]Earth and Environmental Engineering, Columbia University, New York, NY 10027; [2]Cytec Industries, Stamford, CT 06904

Greenness needs to be defined and evaluated before implementing holistic Green or Greener processing practices.
However,
- *No widely accepted definition*
- *Each industry has its own unique attributes, and thus a specific definition*
- *Each industry is composed of various components, and they should all be evaluated systematically*

The goal here is to develop a **Greenness Index** tool in which
- *Reagent is the starting point for the definition and evaluation*
- *Other factors, such as water, energy, cost, could be evaluated as affiliated to reagent*

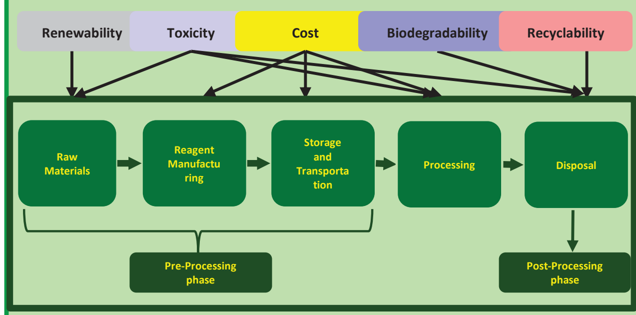
The **Greenness Index** will be capable of being:
- *Used to define and evaluate Greenness*
- *Applied to a specific industry by incorporating industry-specific characteristics*

Intellectual Motivation: *a first tool to define and evaluate the Greenness comprehensively using multi-disciplines*

Industrial Relevance: *the Greenness Index will avail companies evaluate their processing practice and make improvements to achieve sustainability goal cost-efficiently*

Broad Appeal: *the Greenness Index will be applicable to various industries by incorporating industry-specific principles*

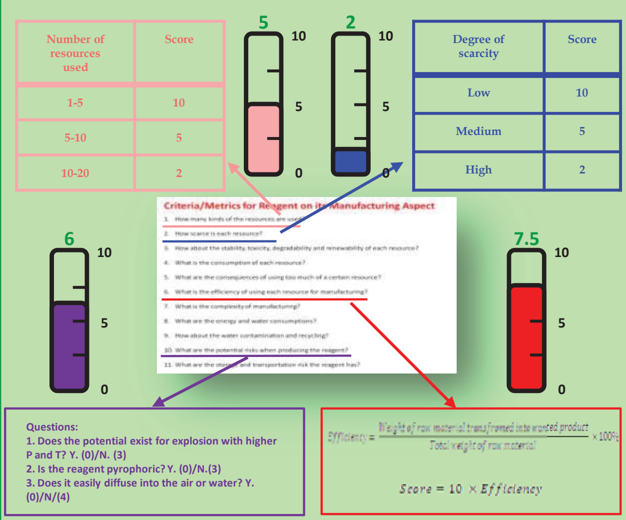
How to do a simplified LCA for the reagent



How to assign a score for the criterion/metric

Number of resources used	Score
1-5	10
5-10	5
10-20	2

Degree of scarcity	Score
Low	10
Medium	5
High	2



Questions:
1. Does the potential exist for explosion with higher P and T? Y. (0)/N. (3)
2. Is the reagent pyrophoric? Y. (0)/N.(3)
3. Does it easily diffuse into the air or water? Y. (0)/N/(4)

$$Efficiency = \frac{Weight\ of\ raw\ material\ transfromed\ into\ wanted\ product}{Total\ weight\ of\ raw\ material} \times 100\%$$

$$Score = 10 \times Efficiency$$

Overall Roadmap/Methodology (5"A"s)

1. Attain a comprehensive list of criteria/metrics which are able to evaluate and the Greenness of the reagent
- ❖ *By conducting a full or simplified LCA (Life Cycle Analysis) for the reagent*

2. Assemble the permissible limit for each criterion/metric
- ❖ *From EPA, OSHA, ACC, Clean Water Act…*

3. Acquire the information on the behavior of the reagent corresponding to each criterion/metric
- ❖ *From extant database and database*
- ❖ *From experimental tests*

4. Assign a score for each criterion/metric
(by comparing the permissible limit and the behavior of the reagent)
- ❖ *By using the standard algorithms*

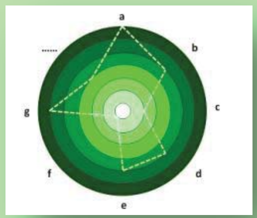
5. Achieve the overall Greenness Index of the reagent by multiplying weighting factors to the scores
- ❖ *Different weighting factors can result in different GI for the same reagent*

How to present the Greenness Index

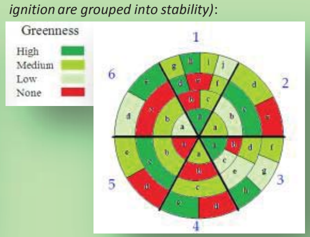
(1) A value:

Greenness Index = 82.00/100.00

(2) Spider Diagram
(each metric can be seen):

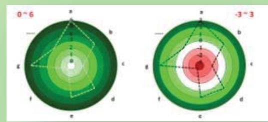


(3) Detailed Diagram
(each metric is grouped, such as explosion and ignition are grouped into stability):



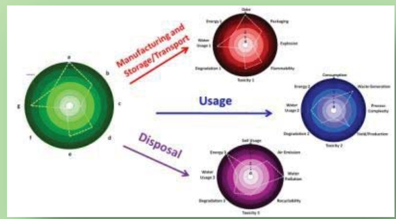
Challenges and Modifications

1. The scoring scale for each criterion/metric



(1) *Should negative values be assigned?*
(2) *What value should be given when there is no information for that criterion/metric?*

2. The dividing of the spider diagram into three layers



(1) *It is more legible from each layer divided according to life cycles*
(2) *It is easier to apply complicated algorithms on each layer*
(3) *It is possible to make comparisons w/not necessarily the overall Greenness Index but w/ the layer(s) flexibly*

3. Appearance of the same criterion/metric on three layers

(1) *Emphasizing the criteria/metrics that are highly concerned throughout the entire life cycle*
(2) *Enabling the analysis/calculation with different algorithms in different phases*
(3) *Realizing the comparison of various reagents in different phases with one criterion/metric*

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The Role of Greener Surfactants in the Mixed Surfactants/Polymer System

Yang Shen and P. Somasundaran

Earth and Environmental Engineering, Columbia University; New York, 10027

Challenges

1. With an increasing pressure put on the industrial manufacturers, there is an evitable need to incorporate Greener Alternative in their formulations without sacrificing performances or increasing cost.
2. Greener Alternatives are made from the environmentally benign sources (e.g., plants and bacteria) and most of their properties are unknown since they are distinct from those made from petroleum based sources that have been widely studied.
3. Robust models for describing and predicting the behaviors of the surfactants/polymer system are still in demand, especially when the Greener Surfactants involved

Goals:

1.Understand how the Greener Surfactants contribute to the interactions between the mixed surfactants and polymer
2.Model these interactions
3.Develop the structure-property-performance relationships
4.Reduce dosages (*of surfactants or polymer*) without compromising the performance (e.g., *high viscosity*)

Characterization of the Interactions and Complexes Formed

- **Interaction Process**: Turbidity, Polarity, Surface Tension, Zeta Potential
- **Properties of Complexes**: Size and Shape, Structure, Bonding Type

Intellectual Motivation:

A model will be developed for the list of Greener Surfactants based on the structure -property –performance relationships.

Industrial Relevance:

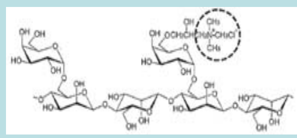
The model developed will serve to provide the scientific bases for selecting the Greener Surfactants for industrial formulations.

Broad Appeal:

Interactions of surfactants/polymers in the presence of Greener Surfactants have the capabilities of applying in various fields, e.g., personal care, detergency, oil recovery, mineral processing and so on.

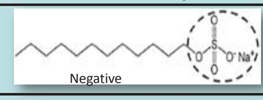
Main Materials

Jaguar C17



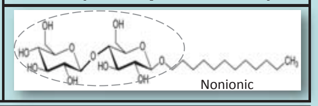
Positive, long hydrophobic chain

SDS (sodium dodecyl sulfate)



Negative

DM (dodecyl maltoside)



Nonionic

Systems of different surfactants ratios with 0.1%wt Jaguar

SDS:DM	1:0	0.1mM DM	3:1	1:1	1:3	0:1

Current Progress

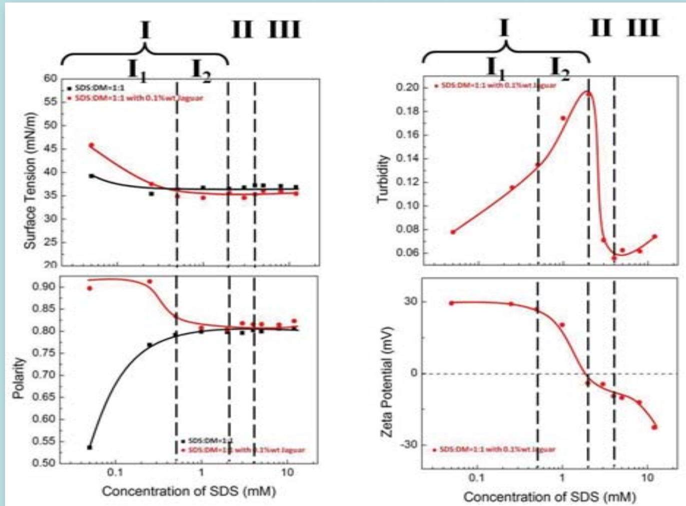
Observations:

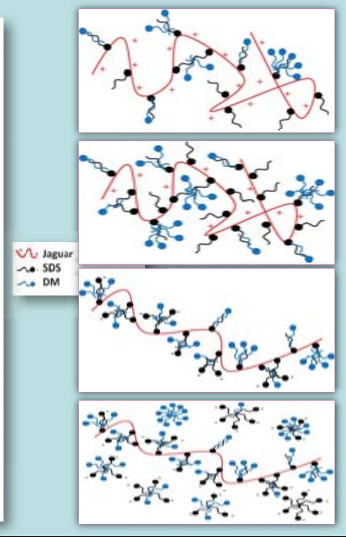
1. ST and Polarity both reached constancy at low concentrations of surfactants.
2. The constant value for ST was close in presence or absence of Jaguar; and so was Polarity.
3. Turbidity increased, decreased and then increased again.
4. Maximum turbidity appeared around the IEP of the system.

Results and Discussions:

1. The surface components on the surface in the presence or absence of Jaguar might be the same (i.e., SDS, DM and SDS/DM hemimicelles).
2. The properties of the complexes formed during the Interaction process are significantly affected by DM (compared to the case of Jaguar/SDS which is not shown here, the presence of DM with the ratio SDS:DM=1:1 results in changes in Turbidity only, not in Polarity).
3. The properties of the complexes formed in this system are crucial to understand the effect of DM.

Qualitative Model Development for the Interaction Process of the System: SDS:DM=1:1 with 0.1%wt Jaguar





I_1: ST ↓, Polarity ↓, Turbidity ↑, ZP (+) ↓

- SDS/DM:
  - Start to form micelles
  - Adsorbs on Jaguar together with mixed micelles
- Jaguar:
  - highly coiled
  - might be further compacted by interacting with surfactants/their micelles

I_2: ST →, Polarity →, Turbidity ↑, ZP (+) ↓

- SDS/DM:
  - form micelles
  - Adsorbs on Jaguar mainly in the form of mixed micelles
- Jaguar:
  - highly coiled
  - might be further compacted by interacting with surfactants micelles

II: ST →, Polarity →, Turbidity ↓, ZP (-)↓

- SDS/DM:
  - form micelles
  - Adsorbs on Jaguar in the form of mixed micelles
- Jaguar:
  - stretches

III: ST →, Polarity →, Turbidity ↑, ZP (-) ↓

- SDS/DM:
  - mainly form micelles and stay in the solution
- Jaguar:
  - might be got a little compacted in the presence of mixed surfactant micelles

Near-Future Plans

For SDS:DM=1:3 and 0:1 with 0.1% wt Jaguar:
- To study the interaction process
  - *To see how it changes with varying SDS/DM ratios*

For SDS:DM=1:1 with 0.1% wt Jaguar:
- To study the size and shape of the various complexes
  - *To further characterize the interactions between Jaguar/SDS/DM*

Long-Term Plans

To study the Jaguar/SDS/DM system in terms of the size, shape and structure of complexes as well as the bonding type:
- To find out the effect of DM
- To model the Jaguar/SDS/DM interactions
- To explore the possibility of replacing SDS

To examine other Greener Surfactants

Steric stabilization of particulate systems in high ionic strength environments

Annamaria Vilinska
PI: P. Somasundaran
Columbia University, New York

Center for Particulate & Surfactant Systems (CPaSS)
Fall 2012 IAB Meeting
Columbia University, New York, NY
August 15-16, 2012

Introduction

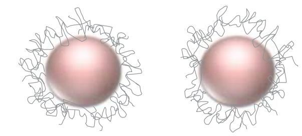
Stabilization colloidal dispersions

Electrostatic stabilization	Polymeric stabilization	
Coulombic repulsion Long range, but sensitive to pH and ionic strength	**Steric stabilization** - macromolecules attached on the particle	**Depletion stabilization** - macromolecules are free in solution

In case of several industries higher electrolyte concentrations are involved (paper and pulp, ceramics, pharmaceutics, mineral processing) and Polymeric stabilization is necessary.

Steric stabilization

- Useful where the Coulombic interactions are insufficient to ensure stability
- Effect depends on the type of polymer, molecular weight, composition, mixture of polymer with surfactant, and sequence
- The amount required for stabilization in extremely high ionic strength is significantly higher

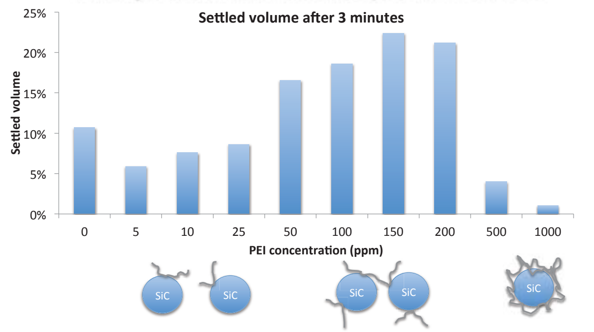


Materials and Methods

- SiC suspended in concentrated $NiSO_4.6H_2O$ solutions were studied
- 2 types of SiC particles - 1 µm and 45-55 nm
- Polyethyleneimine (PEI) was used as a dispersant
- PEI: branched, two molecular weights – 1 300 and 60 000 MW
- Solid concentration kept at 2%w and at pH 3.5
- The stability is reported as a percentage of settled volume after some time – 3 or 120 minutes

Results

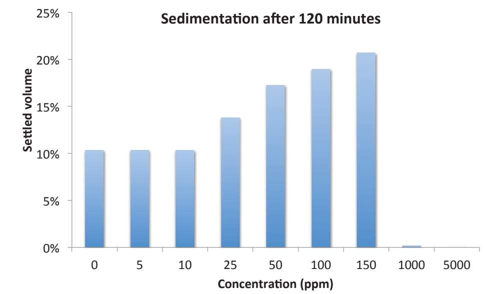
Coarse particles: Silicon Carbide, 1 µm, 60 000 MW PEI



60 000 PEI is a slight dispersant around (5-25 ppm), flocculant around (50-150 ppm) and good dispersant at 1000 ppm

Results

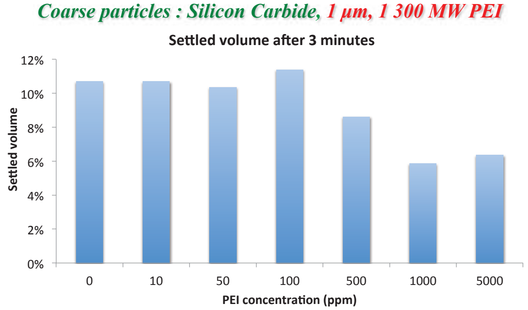
Fine particles: Silicon Carbide, 45-55 nm, 60 000 MW PEI



Low polymer concentrations (25-150 ppm) reduces stability, 1000 and 5000 pm stabilize the system

Results

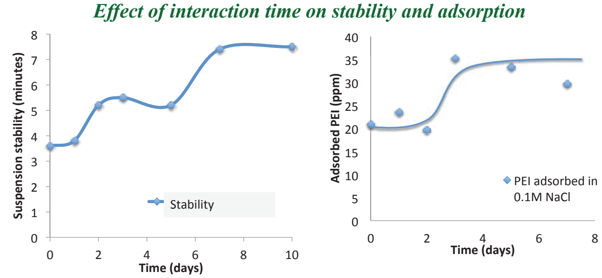
Coarse particles : Silicon Carbide, 1 µm, 1 300 MW PEI



The effective concentration of 1 300 MW PEI is over 500 ppm

Results

Effect of interaction time on stability and adsorption



Adsorbed amount and suspension stability increased after 2 days
Stability is a function of PEI adsorbed on the surface of SiC

Summary

- **60 000 PEI slight dispersant around (5-25 ppm), flocculant around (50-150) and good dispersant at 1000 ppm for both particle sizes**
- **1 300 PEI has weaker dispersive properties**
- **Dispersion stability maintained after filtration and redispersion**
- **Dispersion stability increases after prolonged conditioning time**

Future plans

- **Polymer pretreatment – sequence changes**
- **Other polymers, mixtures of polymers and surfactant**
- **Polymer characterization – size, aggregation**

Acknowledgment

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Disclaimer