The Graduate Association of Chemical Engineers held its sixth annual graduate symposium on March 9, 2005, to highlight the research activities of chemical engineering graduate students. The symposium consisted of a collection of individual student talks of approximately twenty minutes each, as well as a luncheon. Cash prizes were awarded to the winning presenters in each section as judged by faculty members.

Congratulations to Marissa Fallon, Marco Verwijs, O. Berk Usta, and Ashish Gupta for winning their respective sections. Each winner received $60.

Many thanks to Dr. Robert Dean of the Department of Civil and Coastal Engineering for his keynote presentation on tsunamis and Florida's beach systems.

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**Multi-Scale Modeling of Biomembrane Deformations**

Speaker: Eric May

Eric May and Atul Narang
Department of Chemical Engineering, University of Florida

The goal of this research is to determine what role, if any, changes in chemical composition inside of biomembranes play in deforming the shape of cells. Certain types of Eukaryotic cells respond to chemical stimuli in the environment by moving toward the source of the chemo-attractant. During this process, known as chemotaxis, it has been observed that certain chemicals, especially the class of molecules known as phosphoinositides localize at the leading edge of these crawling cells. In this work, using a course grain molecular model, molecular dynamics simulations of lipid bilayer structures were conducted. From these simulations the bending modulus can be determined by analyzing the thermal fluctuations the bilayer. We have studied what effect adding phosphoinositides into a dipalmitoyl phosphatidyl choline (DPPC) bilayer has on the bending modulus. The bending modulus determined from these simulations can then be fed into a continuum scale model for predicting the shape of cells based upon the minimization of bending energy for a given ratio of the surface area to volume of the cell.

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**Winner of Session 1**

Drug Detoxification by Liposomes
Nanoparticles can potentially separate hydrophobic compounds from aqueous solutions by either adsorption on the surface or absorption into the particle. Such separations can be important in a variety of applications, such as removal of toxic substances from the blood stream. We study the separation of amitriptyline, which is a common cause of overdose-related fatalities in the United States, from aqueous solutions by dimyristoyl phosphatidylcholine (DMPC) liposomes. The amount of drug that is taken up by the liposomes is determined through use of a UV spectrophotometer. The effect of pH and liposome concentration on the drug uptake by liposomes at the solubility limit of the drug is determined. The results of the study are used to determine the area per molecule of the adsorbed drug on the liposomes. The results show that at the solubility limit, DMPC liposomes sequester approximately 70 – 100% of the drug present in the solution. We conclude that the amount of drug uptake is independent of pH, which is consistent with the fact that DMPC liposomes have no net charge. The area of a drug molecule on the liposome’s surface is calculated to be about 25 Å²/molecule, which suggests that the drug may be adsorbing to the surface of the liposomes in a bilayer configuration.

The role of phospholipid signaling in neuronal polarity generation

Speaker: Ved P. Sharma

Ved P. Sharma and Atul Narang
Department of Chemical Engineering, University of Florida

Within 1-2 days of their birth, new-born neurons undergo neuritogenesis, i.e., they become polarized into distinct axons and dendrites. There is a growing interest in understanding the signaling mechanisms involved in neuritogenesis, mainly because the major events in neural aging and many neurodegenerative diseases, like Alzheimer's disease starts with progressive loss of neuronal polarity. Although little is known about these mechanisms, our analysis of the experimental literature suggests that they are strikingly similar to the phospholipid signaling mechanism used by motile cells for sensing chemotactic gradients. We will present initial experimental data which shows that the key elements of the signaling pathways in neuritogenesis are similar to those in chemotactic gradient sensing. Signaling mechanisms in chemotactic gradient sensing have been intensively studied for several years and are relatively well understood. Equipped with this knowledge, our group has developed a quantitative model that successfully explains the polarization of motile cells by integrating the reaction mechanisms of the signaling pathway with the equally important, but less studied, transport mechanisms such as intracellular diffusion. To the extent that the signaling mechanisms are similar, this study would yield similar quantitative insights into the molecular mechanism of neuritogenesis.

A Mathematical Model for Ophthalmic Drug Delivery by Contact Lenses
Approximately 90% of all ophthalmic drug formulations are now applied as eye-drops. While eye-drops are convenient and well accepted by patients, about 95% of the drug contained in the drops is lost due to absorption through the conjunctiva or through the tear drainage. Ophthalmic drug delivery via contact lenses is more effective because it increases the residence time of the drug in the eye. An increase in residence time will lead to a larger fractional intake of drug by the cornea. In this talk we model the drug release from the contact lens into the thin tear fluid of the eye sandwiched between the cornea and the contact lens (i.e., the Post Lens Tear Film or POLTF), and the mass transfer of the drug in the tear film. The motion of the contact lens, which is driven by the eyelid motion during a blink, enhances the mass transfer in the POLTF. We use regular perturbation methods to obtain the Taylor Dispersion coefficient for mass transfer in the POLTF. The diffusion of drug in the gel is assumed to obey Fick’s law and the diffusion in the gel and the mass transfer in the POLTF are combined to yield an integral-differential equation that is solved numerically by finite difference. Results show that the dispersion coefficient of the drug in the post lens tear film is unaffected by the release of the drug from the gel. Furthermore, simulation results show that drug delivery from a contact lens is more efficient than drug delivery by drops. However soaked contact lenses can only deliver drugs for a few hours and thus cannot be used for extended ophthalmic drug delivery.

The Role of Nucleotides in Bacterial Growth

When a chemostat is perturbed from its steady state, it displays complex dynamics. For instance, if the identity of the growth-limiting substrate is switched abruptly, the substrate concentration and cell density undergo a pronounced excursion from the steady state that can last several days. These dynamics occur because certain physiological variables respond slowly. In the literature, several physiological variables have been postulated as potential sources of the slow response. We have been addressing this problem by systematically exploring the role of these variables. In previous work, we studied the role of transport enzymes, and we showed that transients starting from low transport enzyme levels could be quantitatively captured by a model taking due account of transport enzyme synthesis. In recent work, we studied the role of ribosomes or RNA which catalyzes the synthesis of biomass. This study was motivated by same kind of lag in growth rate observed in dilution rate shift up experiment and continuous to batch shifts experiments, where dilution rate used in the experiments, the transport enzyme was not the limiting growth factor. We showed that observed transients could be captured by a model by taking due account of ribosome synthesis. In this work, we have tried to answer the question that how the cell decides on the metabolic regulation of the substrate uptake, whether the substrate should go to growth, respiration, excretion during the growth phase or the cell should cease the growth during the starvation. We have used the nucleotide tri-phosphate (NTP) or adenine nucleotide tri-phosphate (ATP) as physiological controlling parameter
and extended our model. Simulations of the model show good agreement with both the steady states and the transients observed in experiments. Specifically, the model predictions are in good agreement with the steady state and transient profiles of the cell density, substrate concentration, RNA, proteins, transport enzymes, and ATP.

First Principle Calculation Study for the Decomposition of N-imido Tungsten Nitride Precursors

Speaker: YongSun Won

YongSun Wong and Timothy J. Anderson
Department of Chemical Engineering, University of Florida

Successful MOCVD growth of tungsten nitride (WNx) thin films has been reported using three similar kinds of single-source precursors – phenylimido complex Cl4(CH3CN)W(NPh) (1), isopropylimido complex Cl4(CH3CN)W(NiPr) (2), allylimido complex Cl4(CH3CN)W(NC3H5) (3). In order to theoretically validate the design strategy of these precursors – determine the impact of imido ligand on properties of the deposited film – and elucidate gas phase homogeneous decompositions of precursor molecules in the earlier stage of growth, computational chemistry based on density functional theory (DFT) was employed in the calculation of bond energy and thermodynamic properties, transition state identification, etc. Calculated Gibbs free energy vs. temperature plotting verified that the acetonitrile trans ligand (CH3CN) cleavage, believed as the first step of entire reaction process, for all of three complexes readily happened in the low temperature range of 400 ~ 500 K. Then, chlorine cleavages through homogeneous s-bond metathesis with hydrogen were suggested as the next step with the search of relevant transition complexes. Qualitative natural bonding orbital (NBO) analysis and quantitative bond energy calculation were used to support that 1 has the strongest N-imido bond and slightly weaker W-N bond, corresponding to the lowest nitrogen content in the deposited film over the entire growth temperature range. Moreover, it was also shown that 2 has relatively stronger N-imido bond than 1, matching with the results of positive ion electron-impact (EI) and negative ion electron-capture chemical ionization (NCI) processes and corresponding to the positive offset of nitrogen content in the film from 3 to 2 above the crystallization temperature range (> 500°C).

Winner of Session 2

Stick-Slip in Powder Flow, A Quest for Coherence Length

Speaker: Marco Verwijs

Marco J. Verwijs¹, Kerry Johanson², Spyros Svoronos¹
Department of Chemical Engineering¹ and PERC², University of Florida

Stick-slip is a step-wise or pulsating flow of granular material. In industries this phenomenon can cause problems in processes as bin discharge and dye filling for tabletting. Bins can honk or quake up to failure due to stick-slip. If stick-slip occurs during dye filling, there will be a large deviation in the tablet mass or concentration. The mechanism that causes stick-slip is not known. A mechanism is
proposed where a stick-slip event is a collapse of the powder structure. Therefore, the particle surface roughness and inter-particle forces seem to be of eminent importance. In this research the deformation of Corn Starch and Polystyrene powder are measured in a Schulze Shear Cell and a uniaxial tester and the stick-slip during the processes recorded. The experiments show a clear increase in magnitude and length scale of the stick-slip events with increasing stress. The length scale at a low normal stress is about one particle diameter, and this increases to several diameters at higher loads. This seems to be an indicator for the structure change in the powder. At low stresses individual particles cause stick-slip, while at higher stresses particle clusters deform. This might be an indicator of the (change in) coherence length of the powder. The project will be continued using the Atomic Force Microscope to measure inter-particle forces. Using Discrete Element Modeling a connection will be made between the microscopic particle properties and the macroscopic stick-slip event.

In-situ Investigation on Reaction Pathway and Kinetics for a-CuInSe2 Formation from the Various Precursors

Speaker: Woo Kyoung Kim

Woo Kyoung Kim and Timothy J. Anderson
Department of Chemical Engineering, University of Florida

Chalcopyrite a-CuInSe2 (CIS) and its alloys with Ga or S is one of the most promising absorber materials for high efficiency thin film solar cells. While there have been several studies on the mechanism for synthesizing CuInSe2 absorber films, the detailed reaction pathways are not fully understood, partly due to the complex phase evolution and defect chemistry present in the material system. A systematic study of the growth mechanisms for various precursor structures in the CuInSe2 (CIS) system should assist the selection and development of a cost-effective and high performance CIS growth process. The reaction pathway and kinetics of a-CuInSe2 formation from the bilayer precursor films (e.g., glass/InSe/CuSe and glass/In2Se3/CuSe) and from the selenization of metallic precursor (glass/Mo/Cu-In) were investigated using time-resolved, in-situ high-temperature X-ray diffraction. Precursor films were deposited on thin glass (or Mo-coated glass) substrates (Corning #7059) in a migration enhanced molecular beam epitaxial (MEE) deposition system. These films were then temperature ramp annealed while monitoring the phase evolution. For the observation of selenization process, selenium powder was placed in the XRD sample holder chamber. During the selenization of Cu-In/Mo, the generation of CuSe followed by transformation of CuSe to CuSe2 at higher temperature was observed. The formation of CuInSe2 was observed to be initiated at a temperature between 250 and 300oC. The kinetic parameters were estimated using the Avrami and parabolic diffusion controlled reaction models.

InGaAs Metal-Semiconductor-Metal Optoelectronic Mixers for Eye-Safe LADAR Applications

Speaker: Soohwan Jang

Soohwan Jang¹, Timothy J. Anderson¹, P. Shen², N. W. Emanetoglu², S.J. Pearton³, and Fan Ren¹
An InGaAs metal-semiconductor-metal (MSM) based frequency-modulated continuous wave (FM/cw) laser detection and ranging (LADAR) system was demonstrated. For battlefield applications, an eye-safe LADAR is required, and 1.55 μm wavelength is preferred. Typical Schottky barrier heights on InGaAs are quite low (~0.1-0.2 eV), leading to high dark current of the MSM devices and, hence, to low signal-to-noise ratio. To reduce the dark current, the Schottky barrier height must be enhanced. Higher energy bandgap, lattice-matched InAlAs Schottky enhancement layers (SEL's) grown on top of the InGaAs layer were employed to improve the barrier height. Photodetectors using Schottky enhancement layers were shown to yield low dark current, high responsivity, and high bandwidth. To improve the performance of MSM photodetectors or OE Mixers, the signal-to-noise ratio was maximized by minimizing dark current and by minimizing the parasitic capacitance of the MSM device. Dark current and parasitic capacitance were further minimized by using “smart designs” for the MSM device by decreasing finger width, by removing the semiconductor layer underneath the final metal, or by using low-k material beneath the final metal. A self-mixing, Metal-Semiconductor-Metal Photo Detector (MAM-PD) has been designed and fabricated to extend the LADAR operating wavelength to 1.55 μm to enhance the detection signal response.

**Breathers and ballistic energy transfer in a nonlinear lattice system**

Speaker: Valere Chen

Valere Chen and Dmitry Kopelevich
Department of Chemical Engineering, University of Florida

Heat transfer in nano-scale materials is the critical issue in the performance and stability of nanoelectronic devices and, hence, understanding the heat transfer mechanism on this scale plays an important role, as nano-materials are currently being integrated with various semiconductor devices. Fourier’s Law, commonly used to calculate heat transfer, is found to be invalid in nano-size materials and devices, which is explained by the fact that the ballistic transport of heat carriers is more dominant than their diffusive transport on this small scale. The goal of this work is to investigate the ballistic energy transfer in quasi-one dimensional nano-materials, such as carbon nanotube (CNT). To this end, we will investigate nonlinear lattice vibration modes and their contribution to the heat transport. In order to develop a method for acquiring nonlinear solutions for CNTs, we first study the Fermi-Pasta-Ulam (FPU) lattice system. For this nonlinear system, we obtain intrinsic localized time-periodic modes known as breathers. The steady state solutions are obtained from the nonlinear equations of motion by using the perturbation theory, Newton’s method, and the Poincare map. The stability of a steady-state solution is examined by the Floquet analysis. The analysis of the stationary structures is complemented by molecular dynamics (MD) simulations of heat relaxation. We show that (1) the structures of breathers observed in the MD simulations are consistent with the solution from Newton’s method, (2) the lifetime of breathers is very long, and (3) the energy is localized in these breathers after the lower-frequency phonons fade away and, therefore, are expected to significantly contribute to the thermal properties of the system.
Nano-Bio Particulate Systems: Stability Analysis of Propofol Microemulsions

Speaker: Dushyant Shekhawat
Dushyant Shekhawat and Dinesh Shah
Department of Chemical Engineering, University of Florida

Propofol (2,6-diisopropylphenol) is an intravenous general anesthetic, having several favorable anesthetic characteristics, including antiemetic effect and rapid emergence from unconsciousness without drowsiness. Current formulations of propofol contain it in macroemulsion form, which has various side effects. In this study we have formulated various oil in water microemulsion consisting propofol (oil), biodegradable non-ionic pluronic polymers, and ionic fatty acid salts. Various properties of these microemulsions, like particle size, stability on dilution, and pH etc. were measured as a function of time, which shows that these systems are stable. Anesthetic studies of these stable microemulsion systems were done using randomized crossover design in rats, which indicate that these microemulsions are as good as current system in term of various anesthetic properties.

Winner of Session 3

Lattice-Boltzmann Simulations of Single Polymer Chains in Periodic and Confined Geometries

Speaker: O. Berk Usta
O. Berk Usta, Tony Ladd, and Jason Butler
Department of Chemical Engineering, University of Florida

We have developed an efficient and accurate algorithm to simulate long single polymer chains in solution. The method combines the fluctuating lattice-Boltzmann solution [1,2] for the fluid phase with a micromechanical model of the polymers consisting of point particles with hard-sphere excluded volume which are connected by FENE spring potentials. A simple friction term [3] couples the point particles to the lattice-Boltzmann method which solves the Navier-Stokes equations with thermal fluctuations. The method accounts for inter-particle hydrodynamic interactions, hydrodynamic interactions with the walls, and the correlations of Brownian motion between the polymer beads. Geometries ranging from simple periodic boundaries to more complicated channel and contraction flows are possible. The implementation of boundaries for confined geometries is easily achieved through simple bounce back rules at boundary nodes for the fluid and hard sphere exclusion for the solid phase. In this work we present results for equilibrium and dynamic properties of a single polymer chain ranging from 16 up to 1024 beads.

Computational Study of Micellar Systems

Speaker: Gunjan Mohan
Gunjan Mohan and Dmitry Kopelevich
Department of Chemical Engineering, University of Florida
Ordered molecular structures arising from self-assembly of amphiphilic molecules, such as nano-scale clusters of molecules, spherical micelles, worm-like micelle, bilayers, vesicles and complex hexagonal packed structures play an important role in biological and industrial processes. The main goal of this study is to investigate the dynamics of structural transitions in the self-assembled systems. Here we investigate the mechanism of micelle fusion. The process of fusion of micelle is modeled as rare events. The underlying assumption is that there is a time-scale separation between few slow and many fast degrees of freedom. Coarse-grained molecular dynamics and kinetic approach method are the main building blocks of our simulation methodology. The dynamics of interaction of micelles is decomposed into fast (noise) and slow (reaction coordinates) parts. The dynamics of the process is described by the Fokker-Planck equation. The kinetic approach method is used to obtain the drift and diffusion coefficient required to construct the Fokker-Planck equation from a series of bursts of short-time simulations. The free energy of interaction between two micelles is reconstructed from the effective Fokker-Planck equation.

Importance of Dynamic Surface Tension on the Residual Moisture of Textiles

Speaker: Daniel Carter

Daniel Carter and Dinesh Shah
Department of Chemical Engineering, University of Florida

The Laplace equation for capillary rise predicts that the capillary rise is proportional to the surface tension of the air-liquid interface. The use of a tailored rinse additive has the potential to significantly alter the surface tension of solutions thus leading to a decrease in the capillary rise which can then be related to the residual moisture content (RMC) of fabrics. It would be expected that as surfactant concentration is increased and surface tension decreases, then the RMC of fabrics would also decrease. However, a peak is observed in the RMC of fabrics before the critical micelle concentration (CMC) occurs. Prior to the CMC, it is thought that rapid adsorption of surfactant is occurring on the fabric surface leading to a decrease in bulk monomer concentration. The decrease in free monomer concentration due to adsorption should result in an increase in the equilibrium surface tension of the residual solution. Since the equilibrium surface tension measurement provides adequate time for all available monomers to diffuse to the air-liquid interface, the measurement of dynamic surface tension would be another way to amplify the reduction of free monomer in the residual solution due to low residence time of bubbles created during the measurement process. During the laundry process, detergents are used during the wash cycle and residual detergent will carry over into the rinse cycle. It is important that the concentration of the residual detergent does not fall into the range of concentrations where there is an increase in RMC to avoid an increase in drying time and energy costs.

Interfacial Instabilities During the Solidification of a Pure Material from Its Melt

Speaker: Saurabh Agarwal

Saurabh Agarwal, L.E. Johns, and R. Narayanan
Department of Chemical Engineering, University of Florida
Moving fronts occur in a number of technological applications such as secondary oil recovery, chemical vapor deposition, electrodeposition, crystal growth of compound semiconductors, and in solidification. In this presentation, the physics of solidification of a pure material is considered. Solidification of a pure substance is a typical ‘moving front’ phenomenon where the speed and direction of the front determine its stability, and hence, the state at which an erstwhile planar front will become non-planar in morphology. It is found that a pure material, when subject to phase change, may give rise to a non-planar interface. The conditions depend upon the manner in which the latent heat is removed, geometry and the thermo-physical properties as well as the imposed temperature differences. If the front turns out to be unstable we seek to understand the physics leading to this instability as well as the physics after the instability sets in as a control variable (degree of undercooling) is manipulated. In particular we are interested in studying the effect of interfacial tension, diffusion, fluid flow and geometry on the instability arising in a moving solidification front. We propose a simple model for pure solidification which is solved to get what is called the base solution. The base solution is then perturbed to investigate the fate of small perturbations given to a moving front. We first predict the critical value of the control variable that leads to the instability. A weak nonlinear method (using dominant balancing) is then invoked to describe the dynamics of a pure solidification system in the vicinity of such a phase change instability.

A Mathematical Model for Tear Balance

Speaker: Heng Zhu

Heng Zhu and Anuj Chauhan
Department of Chemical Engineering, University of Florida

In this study we develop a mathematical model that can predict the steady state tear film thickness and the dynamic tear film thickness and the solute concentrations after instillation of a solute-laden fluid in the eye. The mathematical model developed in this study is a tear mass balance. It incorporates a tear drainage model and a model that relates the tear film thickness to the meniscus radius of curvature. To predict the solute concentrations, the tear mass balance is coupled with the solute mass balance. The differential equations for the unsteady balances are solved numerically. The model predicts that the tear film thickness depends on a number of physiological factors such as rates of tear production and evaporation, geometry and modulus of the canaliculi, and surface tension and viscosity of tears, and varies from about 3 to 15 μm. The model also predicts that the drainage time for an instilled volume of 15 μL is 1283 seconds. Additionally, the time required for the tracer concentration to decay to 1% of the value immediately after instillation of drug-laden 40 μL drop is 2480 seconds. Similarly, the time for intensity decay for a radioactive tracer after 25 μL instillation is 1566 seconds. Also, the model predicts that the fraction of the instilled drug that reaches the cornea is about 1.3% for topically application of timolol. The predicted results agree reasonably with the reported experimental results, at least qualitatively. The model developed here can serve as a useful tool to evaluate the effect of various parameters on the tear volume and thus can be used in the development of dry eye treatments.

Stability of Elliptical Liquid Bridges: An Experiment
Aliquid bridge is a region of liquid suspended between two solids. These bridges occur within natural and technological contexts. For long enough cylinders in zero gravity, the bridge collapses at what is known as the Plateau limit, i.e. the bridge becomes unstable when its length exceeds its circumference. This limit is reached when there is a balance between the stabilization effect of longitudinal curvature and the destabilization effect caused by transverse curvature. In this presentation, the effect of distortion of the circular end plates to the nearby elliptical ones is studied.

The circular disks can be distorted to an ellipse by many ways: usually by either keeping the area of the circle constant, or by keeping the perimeter constant, which determines the shape of the elliptical liquid bridge. Our aim is to find out the critical length of a static elliptical liquid bridge where the bridge collapses and compare it with the critical length of a cylindrical bridge by requiring that the volume of the elliptical bridge suspended between the plates 'L' apart be equal to the volume of the nearby right circular. We conclude that elliptical liquid bridge is more stable than a circular liquid bridge. Several cases are studied and comparisons are made.

Winner of Session 4

Molecular Modeling of Transport across a Surfactant-Covered Oil-Water Interface in Microemulsions

Speaker: Ashish Gupta

Ashish Gupta and Dmitry Kopelevich
Department of Chemical Engineering, University of Florida

Microemulsions are the most promising of colloidal systems for drug delivery and drug detoxification. Both these processes involve transport across a microemulsion interface. In spite of the importance of transport across a surfactant-covered oil-water interface in microemulsions, the detailed mechanism of this process is not clearly understood. The goal of the proposed work is to use molecular dynamics (MD) simulations to obtain a detailed understanding of transport across a microemulsion interface. For this purpose, we first prepare model microemulsion systems. We observe that the spontaneous self-assembly of surfactants-oil-water systems, starting from a random mixture of same, is a good way to reproduce the phase behavior of microemulsion systems. Depending on the initial concentration of surfactant, oil and water, we observe the formation of oil-in-water (O/W) and water-in-oil (W/O) spherical and cylindrical microemulsion droplets and surfactant monolayer. The time scale of formation of these structures is of the order of 60 ns and hence is readily accessible by direct MD simulations. The surface tension and surface coverage of surfactant monolayers and spherical microemulsion droplets is close to experimentally measured values. We also observe that the surface tension decreases with increase in surfactant length and surface coverage. Since it is anticipated that the structure and dynamics of the microemulsion interface play an important role in solute transport, we investigate the microemulsion interface structure. We obtain the pore size distribution in a surfactant monolayer and spherical O/W microemulsion interface and the pore size evolution with time. We observe large volume pores in the
system and random fluctuations in the pore sizes. We shall use this data to systematically characterize the microemulsion interface structure which will help us predict the transport rate of solute across microemulsion interface. In order to estimate kinetics of solute movement, we run simulations with the hydrophobic solute initially placed near an oil-water interface with and without surfactants. We observe that the hydrophobic solute moves from water phase to oil phase in approx. 1 ns when no surfactants are present. The timescale of solute movement with the surfactant monolayer present appears to be out of reach of direct MD simulations. Hence we use an alternative method of constraining the hydrophobic solute at different depths of the microemulsion interface and integrate the average force on solute to obtain the free energy of the hydrophobic solute as function of depth across the microemulsion interface.