Distinction in the Major (DITM) Projects 2007

1. Effect of charged nanoparticles on protein separations in gel electrophoresis (Dr. Stretz)
2. Fate of drug delivery nanoparticles from hospital effluent in surface water (Dr. Stretz)
3. Supercritical CO2 deposition of ceramic nanoparticles on surfaces in ordered arrays (Dr. Stretz)
4. X-ray and neutron diffraction methods for measuring strain in cement-based materials (Dr. Biernacki)
5. Micro-scale separation of nano-particles (Dr. Biernacki)
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17. Puddle formation flows in low Reynolds number viscous flows (Dr. Arce)
18. Modeling cell mobility through a porous network (Dr. Carpen)
19. Mixing drop instability (Dr. Arce and Dr. Carpen)
20. *Other projects may be possible, discuss with individual professors*

SEE BELOW FOR FURTHER DETAILS

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Dr. H. Stretz:

1. **"Effect of charged nanoparticles on protein separations in gel electrophoresis"**- Gel electrophoresis is used both on the analytical scale and bulk scale to separate protein mixtures such as would be found in drug preparations. The transport of proteins is being modelled by our group using principles of electokinetic flow. Experimentally we are attempting to insert charged nanoparticles along the route of the protein to cause a charged field to exist orthogonal to the external field, and potentially aide distinguishing similar proteins. Additionally if these particles are ~50 nm apart, you can get into issues of larger proteins with a larger radius of gyration having to stretch to get through the nanochannel, and there will be a force associated with that stretching that causes larger molecules to resist movement, providing another basis for separation.

2. **"Fate of drug delivery nanoparticles from hospital effluent in surface water"** - The fate of certain organic nanoparticles/colloidal drugs in surface water is being experimentally probed. We wish to know what happens to colloidal drug particles in the water column as a function of : ionic strength, pH, humic acid interactions, temperature, UV light. If the colloidal particles continue to exist as colloids, their environmental fate could be to absorb certain contaminants in the ecosystem, accumulate and transport such to drinking water treatment facilities.

3. **"Supercritical CO2 depostion of ceramic nanoparticles on surfaces in ordered arrays"** - Ordered arrays of gold and silver nanoparticles have been achieved on surfaces common to the electronics industry, eg: silicon wafers. We wish to understand the deposition of charged ceramic nanoparticles which might be nonspherical, hoping that we can get deposition on one surface because of surface energy matching but simultaneous patterning/failure to deposit because of a mismatch in surface energy. If this can be achieved, we will be able to order nanoparticles eventually around macroscopic carbon fibers, protecting them from erosion in much the same way marbles in a bed of sand are more stable than marbles on a smooth table.

Dr. J. J. Biernacki

1. **X-ray and neutron diffraction methods for measuring strain in cement-based materials** – X-ray and neutron diffraction can be used to measure the distance between atoms in crystalline materials. These atomic distances are altered when loads (stresses) are applied to a material. Unique facilities at Oakridge National Laboratory (ORNL) and Brookhaven National Laboratory (BNL) will be used to make measurements on cement, mortar and concrete samples.

2. **Micro-scale separation of nano-particles** – Nano-particles can be separated by size and electric charge using electrophoresis. Tiny micro-fluidic devices will be tested and their performance compared to computational model predictions. Both models and experimental methods will be explored.

3. **Kinetics of blast furnace slag hydration** – The use of waste and byproduct materials as partial cement replacement in concrete has been practiced for decades. Uncertainty in the behavior of such blended-cement materials, however, is an obstacle to more widespread use. Electron microscopy and direct image analysis has become a viable alternative too more traditional calorimetric or gravimetric methods for conducting chemical kinetic analysis.

Dr. D. P. Visco

1. **Molecular Design using the Signature Molecular Descriptor** – The Signature molecular descriptor, in conjunction with the I-QSAR technique, is a powerful tool to use in the design of molecules in a variety of industries. We have already used this in several problems including development of non-ozone-depleting blowing agents and in drug design. Since the technique is not limited to a specific class of compounds, virtually any problem can be explored. For this project, you can help decide which problem you would like to solve. Where applicable, experimentation with the Biology and Chemistry Departments will be utilized to verify the results of the work. Multiple students can work on this project since each individual problem brings with it unique challenges to overcome.

2. **Evaluation of Transferability of Parameters in Molecular-Based Equations of State** --Molecular-based equations of state allow the user to add in terms into the model depending on the type of interactions expected in the system Unfortunately, it is a common occurrence that a non-polar compound and a polar compound (say pentane and pentanol) which are modeled the same, except an extra term on the pentanol to account for the polarity, can have widely different parameters that are supposed to describe just the non-polar part on each molecule. This is a problematic situation since it limits the transferability of those parameters to other types of systems. This study will look at the effect of this phenomenon on mixture predictions and evaluate a new technique to arrive at an optimal parameter set.

3. **Evaluation of a Method to Calculate Phase Equilibrium by Solving the Differential Form of the Equilibrium Constraints** – Phase equilibrium modeling problems are normally solved either by equating fugacities or minimizing the Gibbs free energy. In this work we propose a new way to solve the phase equilibrium problem by treating the equilibrium constraints in differential form. Recent work in our group has shown that this new technique might have advantages over the traditional technique in certain types of problems. This study will look to explore that issue in more detail.

4. **Effect of Mixture Property Predictions on the Pure Component Parameterization Process** -- Equations of state are ubiquitous in the chemical process industry and are mostly used during process analysis. The prediction of mixture properties from equations of state are dependent on how the pure component parameters were found. In this work, we explore the sensitivity of the mixture predictions done in this manner using complex, state-of-the-art, approaches.

Dr. V. Subramanian

1. **Modeling capacity fade and lifetime of Lithium-ion Batteries for Satellite Applications** - The lithium-ion battery is an ideal candidate for satellite applications because of its high energy/power density and operating voltage. Thermal runaway, leakage of current, side reactions, capacity fade, etc., may cause lithium-ion batteries to fail. Some of these events might happen because of unplanned or man-made events (e.g., overcharge, uncontrolled discharge/charge of lithium-ion batteries). To evaluate this time dependent and unexpected behavior of lithium-ion batteries in satellites, we need exact models along with capable solvers that can predict discharge curves, state of charge, state of health and capacity fade accurately and efficiently. We attempt to do this by combining various mathematical and experimental techniques. Together all these tasks aim to predict the future behavior of lithium-ion batteries efficiently and accurately. The successful development and implementation of an efficient model and computational schemes will help cement the way for using Lithium-ion batteries in satellites efficiently, effectively and safely.

2. **Exploratory Research - A Novel AC Impedance Model for Understanding Transport and Kinetics Limitations of Electrochemical Devices** - To improve the electrochemical devices towards meeting the energy needs of the future; there is a need to fundamentally understand the behavior of electrochemical systems. Physics based AC impedance modeling is a powerful technique to extract useful information from Li-ion batteries and other electrochemical devices. A typical AC impedance model involves multiple partial differential equations in multiple domains. To overcome the numerical and computational difficulty associated with these models, this project aims to develop the next generation of high-efficient novel closed-form solutions for the AC impedance models of electrochemical devices. The novel numeric symbolic solution (NSS) is numerical in the spatial coordinate and closed-form in all the system parameters. This exploratory research demonstrates the development and importance of the technique using a simplified Li-ion battery model and its AC impedance response. The advantage of NSS is that it will give more insight into the behavior of the system when compared to a pure numerical solution and is computationally more efficient compared to both numerical and analytical solutions for parameter estimation from experimental curves.

Dr. C. S. Wang

1. **Metal-air batteries using concrete as an electrolyte** (with Dr. Biernacki) - Zn-air and Al-air batteries normally use an alkaline solution as an electrolyte. Concrete is a

solid alkaline material. It can conduct OH- and can be used as a solid electrolyte for the metal-air batteries. Concrete Zn-Air battery will be served as both structural and functional materials.

Dr. P. Arce

1. **The effect of charged nanoparticle channels on the analysis of proteins by gel electrophoresis** (with Dr. Stretz): The work will involve experimental work and some theoretical-computational effort.

2. **Pulsed corona discharge reactors in either gas or liquid phase decontamination of organic contaminants** - The work is mostly experimental on the liquid phase but most modeling on the gas phase.

3. **Biological microflows in the human body** - Mostly modeling.

4. **Puddle formation flows in low Reynolds number viscous flows** - Mostly experimental/some theoretical efforts.

Dr. I. C. Carpen

1. **Modeling cell mobility through a porous network** - The complexity of biological behavior is ultimately driven by fundamental physics. This project is a theoretical/computational effort to examine cell behavior by looking at cell motion through a porous media (i.e. a tissue or fibrous network) from the point of view of a particle that interacts with its surroundings through a set of simple attachment/detachment rules, and whose basic motion is thermally driven (Brownian). The work will involve simulations.

2. **Mixing drop instability** (with Dr. Arce) – When a drop of fluid is introduced into another fluid with different properties, various interesting phenomena can be observed. This is a primarily experimental project wherein a system of slightly miscible fluids will be studied.