Caltech
Student-Faculty Programs

Session F Abstracts

Controlling mist formation in droplet impact using megasupramolecules
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Controlling mist formation in liquid sprays is essential in many applications, including fuel safety. In the event of a crash, flammable hydrocarbons are sprayed outside the confines of the engine, generating an explosive air-fuel mixture. It has been previously demonstrated that adding dilute concentrations of ultralong polymers to fuel sprays decreases flammability by decreasing mist formation; however, the mechanisms by which these polymers decrease mist formation are not fully understood. To investigate these mechanisms, we study the effects of adding megasupramolecules to polyalphaolefin lubricant in the droplet impact flow configuration. Using high speed images of this impact, we quantify secondary droplet size distributions, droplet and bead fates, and local kinematics of pinchoff events. Secondary droplet sizes follow a gamma distribution up to 0.01 wt% megasupramolecules until transitioning to a bimodal distribution. This transition is due to the emergence of the beads-on-a-string morphology and subsides at higher concentrations due to longer filament lifetimes. Bead fates confirm this, showing that beads deposit on the solid substrate at higher megasupramolecule concentrations before they can pinch-off to form secondary droplets. All analyzed ligaments lie in the Rayleigh regime of the Ohnesorge diagram, allowing us to study their breakup behavior using simpler flow configurations, such as Rayleigh jets. This analysis confirms that megasupramolecules are effective in decreasing fine mist formation by increasing deposition of beads. Future studies should investigate how ultralong polymers change splashing behaviors, as droplet impact experiments show a transition from corona splash to levitating lamellar breakup and total deposition at higher concentrations.

Particle sedimentation in Newtonian and non-Newtonian fluids
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Mentors: Sujit Datta, Mohamed Abdelgawad, and Sujit Datta

Sedimentation is a fundamental process governing various industrial and natural phenomena. In Newtonian fluids, particle-particle interactions generate hydrodynamic fluctuations that produce velocity fluctuations and complicate sedimentation dynamics. Viscoelastic fluids, a type of non-Newtonian fluid, exhibit both viscous and elastic properties, and further complicate settling. Sedimentation in Newtonian and viscoelastic fluids is characterized using an experimental setup and flow analysis. Glass beads are suspended in each fluid, and videos of their settling are recorded and analyzed using particle image velocimetry. Velocity fluctuations, spatial autocorrelation functions, correlation lengths, fluctuation amplitudes, and cell dependence are calculated and plotted to characterize the settling. Preliminary results indicate that viscoelastic fluids produce shorter correlation lengths and smaller velocity fluctuations than Newtonian fluids across various volume fractions. Parallel fluctuations are larger than perpendicular fluctuations, while autocorrelation trends are similar between the two fluids. These results show differences in sedimentation dynamics between Newtonian and viscoelastic fluids and establish a foundation for continuing to investigate sedimentation in non-Newtonian fluids.

Gas compressibility in the compression-driven displacement of non-Newtonian fluids in a capillary tube
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When a low-viscosity gas displaces a more viscous liquid inside a narrow channel, the interface between them can become unstable and break into finger-like intrusions that reduce how efficiently the liquid is pushed out. Controlling this instability matters for processes ranging from oil recovery to industrial coating. Recent work has shown that the compressibility of the driving gas is a powerful and often overlooked way to stabilize the interface, since a compressible gas naturally softens the injection

and delays the onset of fingering. This project investigates how gas compressibility governs displacement in a capillary tube driven by a syringe pump, and extends the idea from simple liquids to non-Newtonian liquids, whose resistance to flow changes with how hard they are pushed. The displacing behavior is recorded through imaging and compared against theoretical predictions across a range of injection rates and reservoir sizes. By measuring how compressibility interacts with the unusual flow properties of complex liquids, the project aims to clarify the conditions under which such fluids can be displaced smoothly and stably.

Banding phenomena in rotating viscoelastic polymer solutions
Isaac L. Thompson
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Rotating horizontal cylinders are important to industrial processes including cement mixing, food processing, and pharmaceutical coating, and prior work on Newtonian fluids in this geometry has characterized how rotational drag, gravity, viscosity, centrifugal effects, surface tension, and inertial instabilities shape the resulting flow. Far less is known about how viscoelastic, non-Newtonian fluids, common in biological and industrial settings such as blood, toothpaste, and polymer solutions, behave under the same conditions. This project involved designing and building a custom rotating cylinder apparatus, featuring a sealed glass tube system with stable RPM control, and high-speed camera visualization, to directly compare Newtonian and viscoelastic fluid behavior. Using a 93% glycerol solution as a Newtonian baseline and a viscoelastic polymer solution as the non-Newtonian test case, we observe that the polymer solution develops axial bands that are absent in the Newtonian case, suggesting the bands originate from elastic rather than purely inertial or centrifugal effects. Kymograph analysis at 20, 100, and 200 RPM shows that band number and spacing depend on rotation rate, while multi-hour timelapses reveal that bands continue to coarse and merge over time. Preliminary trials with 100-micron glass beads suspended in the polymer solution show that banding persists in particle-laden systems as well. Future work will use a dimensionless parameter framework spanning cylinder geometry, fluid rheology, and particle properties to systematically map how tube dimensions, fluid type, and particle characteristics govern band formation.

Improving stability of peptide displaying Tobacco Mosaic Virus-Like Particles
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Mentors: Gözde S. Demirer and Andres Heredia

Tobacco Mosaic Virus Virus-Like Particles (TMV VLPs) are a promising evolutionarily adapted, yet non-infectious plant delivery system due to their unique physiochemical characteristics. TMV VLPs consist of a single coat protein (CP) that assembles into nanorod particles, which can be modified by fusing peptide cargo to different regions of the CP. However, this challenges the proper assembly of TMV VLP and can potentially cause their aggregation. This work aims to engineer the VLP scaffolds that best tolerate the peptide addition to their surface, by investigating: (1) how CP net charge and (2) stoichiometry of fusion CP within a VLP affects assembly and aggregation. The latter is explored using the Foot-and-Mouth Disease 2A skip-sequence, whereby both wild-type-like and fusion coat proteins can be co-expressed to assemble together into chimeric TMV VLPs. Our VLP characterization data supported previous findings that altering pI will disrupt TMV nanorod assembly, as our more basic CP fusions exhibited a hypothesized truncation event of their SpyTag cargo. By integrating these two approaches to reduce cargo occupancy and improve steric considerations, while also making CP charge closer to wild-type, this work demonstrates a promising strategy to re-design the scaffold of a natural plant pathogen for plant benefit.

Molecular dynamics simulations for nanoconfined ion transport
Carl J. Crum
Mentors: Kara D. Fong and Edward Chen

Upscaling global lithium harvesting for clean energy demands advanced separation technologies like nanofiltration, which rely on selective ion transport through nanometer-wide channel pores. Inside nanoscale confinement, intense ion-ion interactions and anisotropic dielectric screening invalidate classical dilute-solution models, compelling the use of an Onsager transport framework to account for correlated ion motion. In this project, we performed molecular dynamics simulations in LAMMPS to

compare unconfined bulk liquids against nanoconfined electrolytes across single-salt and mixed-salt solutions containing monovalent and multivalent cations. By calculating Onsager transport coefficients from particle displacements obtained through our MD simulations, we evaluated fundamental transport metrics, such as ionic conductivity, transference numbers, self-diffusion coefficients, and solution ionicity, while benchmarking bulk simulation densities against experimental literature. These results establish a control dataset and refine non-equilibrium transport theories, providing essential physical insights to optimize membrane selectivity for sustainable lithium extraction.

Breaking down the concentration-dependent dielectric response of lithium battery electrolytes using atomistic simulations
Chung Wang Lam
Mentors: Kara D. Fong and Nidhish Lella

Lithium-ion batteries find themselves in various areas of application, from small personal electronic gadgets to mass energy storage solutions and aerospace engineering. The dielectric constant, derived from the general dielectric response of the medium, is a crucial thermodynamic parameter of battery electrolytes, as it controls the strength of all electrostatic interactions. In turn, it affects the effectiveness of ionic conduction in the electrolyte. In accurately predicting properties of battery electrolytes, the dependence of dielectric constant on the battery salt concentration needs to be understood. So far, experimental measurements through dielectric spectroscopy have confirmed a non-monotonic dependence, but its physical origin is still unclear. Here, we utilise molecular dynamics simulations to study such a phenomenon in the cases of $LiAsF_6$ in DMC and $LiPF_6$ in 3:7 (by weight) EC:EMC. By studying the separate contributions to the dielectric response by solvent-solvent, ion-solvent, and ion-ion interactions, we provide an atomistic understanding of the physical mechanisms underlying the concentration-dependent dielectric response in terms of the competition between two effects: the formation of ion pairs and the destruction of solvent dipole correlations by free ions. The result provides insight into the design and engineering of similar lithium-based electrolytes.

Fixing nitrogen, faster: A reproducible, high-throughput approach to lithium-mediated ammonia synthesis
Ali Raza Sial
Mentors: Karthish Manthiram and Gangsan Lee

Ammonia synthesis via the Haber-Bosch process consumes about 1–2% of global energy and contributes ~1% of global CO_2 emissions, motivating ambient, electricity-driven alternatives. Lithium-mediated nitrogen reduction (Li-NRR) offers such a route, coupling nitrogen reduction to renewable electricity in a gas diffusion electrode (GDE) system. This project advanced two interdependent objectives: independently reproducing the Lab's Li-NRR results to validate the platform ahead of journal submission, and engineering a high-throughput reaction system to make Bayesian optimization of the reaction's multidimensional parameter space tractable. GDE cells were run under potentiostatic control, with ammonia quantified by ion chromatography and independently cross-validated by UV-Vis spectroscopy. Reproduced Faradaic efficiencies and ammonia production rates matched the original dataset in both magnitude and trend across varying pressure conditions, and agreed between both quantification methods, establishing a trusted experimental baseline and clearing the path to publication. In parallel, we designed and validated a leak-tight, quick-connect cell that maintains stable pressure under prolonged operation, laying the groundwork to scale throughput from 1-2 toward a target of 8 experiments/day. Together, this validated baseline and throughput infrastructure position the project to begin experiments that will feed a Bayesian optimization model, with the goal of identifying optimal operating conditions for ambient Li-NRR.

Constructing a SNIPR-based genetic circuit for non-invasive acoustic imaging of glioblastoma-specific antigens
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Mentors: Mikhail G. Shapiro and Ann Liu

Abstract withheld from publication at mentor's request.