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Awards Perry J. Yi-Hsien Cheng, Kansas State University, Probabilistic risk assessment of gold nanoparticles by integrating in vitro and in vivo toxicity with physiologically based pharmacokinetic modeling. Multistage modeling approaches for assessing cosmetic ingredients safety. Toxicology Physiologically based pharmacokinetic modeling of human exposure to perfluorooctanoic acid suggests historical non drinking-water exposures are important for predicting current serum concentrations. Toxicology and Applied Pharmacology , Combining transcriptomics and PBPK modeling indicates a primary role of hypoxia and altered circadian signaling in dichloromethane carcinogenicity in mouse lung and liver. Journal of Applied Toxicology 27 , The application of PBPK models in estimating human brain tissue manganese concentrations. Neurotoxicology 58 , Identifying populations sensitive to environmental chemicals by simulating toxicokinetic variability. Environment International , Quantitative bias analysis for epidemiological associations of perfluoroalkyl substance serum concentrations and early onset of menopause. Environment International 99 Predicting transport of 3,5,6-trichloropyridinol into saliva using a combination experimental and computational approach. Toxicological Sciences 2 , T Zurlinden and B Reisfeld. Eur J Drug Metab Pharmacokinet 42 , Award Title Perry J. This award is made possible by the Perry J. Research areas of interest include all aspects of biologically based modeling and simulation; they may include, but are not limited to: The competition is open to all current graduate and postdoctoral students whose abstract have been accepted by the SOT for presentation at the upcoming Annual Meeting. Applicants will be considered for all BMSS awards for which graduate students and postdoctoral fellows are eligible. The package should be submitted to Miyoung Yoon , as a single PDF file containing the following three items: A copy of the abstract. A page summary of the study with no more than 2 figures, discussing the rationale and scope of the study, significance of findings, and potential impact of the work on advancing toxicological science and biological modeling.

Chapter 2 : Research - Chemical and Biological Engineering

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The Bailey and Kipper groups lead efforts to experimentally synthesize new forms of polymers. Specifically, the Bailey Group uses small angle X-ray scattering SAXS to characterize new forms of hydrogel-based shape memory materials. For example, it is possible to X. Several examples of ongoing research are highlighted below: Multiplexed biomolecule and virus detection A local, evanescent, array-coupled LEAC sensor based on a compact, single-mode optical waveguide IOW is being developed by the Dandy, Lear, and Henry groups for multianalyte sensing of targets ranging from small biomolecules to virus particles. The LEAC sensor is a promising platform for point-of-care diagnostics. The sensor fabrication is compatible with trailing-edge complementary metal oxide semiconductor CMOS technology, which both lowers its cost and makes it possible to build a portable lab-on-a-chip system with silicon integrated circuits. As a label-free optical biosensor, it does not require reagents during operation. Furthermore, the LEAC approach is less sensitive to temperature or wavelength variations than resonance-based label-free optical biosensors, such as surface plasmon resonance biosensors or ring resonator biosensors. Molecular specificity is provided by probe molecules, e. Passive and active micromixing strategies It is recognized that mixing plays an important role in the growing use of microfluidic devices for lab-on-a-chip applications. For applications ranging from DNA separation and amplification to protein crystallization and kinetics studies, the performance of a lab-on-a-chip device is directly related to the rate at which two or more fluids can be mixed. Due to the small dimensions of microchannels as well as the limited range of obtainable linear flow rates, flow in microchannels is confined to the laminar regime and mixing is dominated by molecular diffusion. With the goal of further simplifying fabrication of a micromixer, we are developing a new method for achieving chaotic advection through application of a localized electric field perpendicular to the mean flow direction driven by a pressure gradient in a planar rectangular microchannel. The electric field, created by a potential drop across an integrated electrode gap, drives electro-osmotic flow EOF perpendicular to the main flow direction, thereby creating a secondary recirculation flow profile. Passive pumping Controlled pumping of fluids through microfluidic networks is a critical unit operation ubiquitous to lab-on-a-chip applications. Although there have been a number of studies involving the creation of passive flows within lab-on-a-chip devices, none have shown the ability to create temporally stable flows for periods longer than several minutes. We have developed passive pumping approach in which a large pressure differential arising from a small, curved meniscus situated along the bottom corners of an outlet reservoir serves to drive fluid through a microfluidic network. The system quickly reaches steady state and is able to provide precise volumetric flow rates for periods lasting many hours. Spatially resolved sampling The spatial and temporal distributions of diffusible molecules play an important role in a wide variety of biological and chemical processes. The formation and maintenance of these distributions is a complex function of the local fluid convection profiles, the diffusivities of the chemicals in question, and chemical reactions that take place. A microfluidic device capable of sampling multiple chemical messengers with a spatial resolution dictated by the extent and overall architecture of the tissue has been developed. Due to the precise fabrication methods of the underlying microfluidic architecture, the position of each sampling port can easily be modified to sample fluid from specific regions of interest within the sample reservoir. The device is readily fabricated using soft lithographic processes, where the degree of fluid sampling from each port is controlled via passive pumping techniques. The system is compatible with most transduction mechanisms that are easily incorporated into planar microfluidic systems, leading to a cost-effective solution for high-resolution, multi-analyte chemical analysis. Typically, bioparticle concentration and separation are accomplished through industrial or laboratory centrifugation, but when the particle size is very small and its density is comparable to the mixture medium, as with bacteria, virus and subcellular organelles, this approach can be problematic. A simple but robust platform able to provide

significant improvements over current concentration techniques is needed. The use of microfluidics has streamlined many traditional laboratory techniques, due to the advantages of ease to operation, low-cost, and miniaturized size. In the specific application to bioparticle concentration and separation, inertial focusing is a very promising approach that relies solely on channel geometry and intrinsic hydrodynamic forces exerted on particles in a dilute suspension as they are transported in laminar flow with a non-uniform velocity profile. We are investigating the use of this inertial microfluidics technique to separate micron and sub-micron bioparticles based on their size, and to incorporate the approach with digital microfluidics and cytometry. Professor Charles Henry At present, three distinct project areas exist within the Henry group. Paper-based microfluidic analytical devices are employed to understand occupational and environmental exposure to pollutants in atmospheric aerosols such as particulate matter and heavy metals. This involves the coupling of microfluidic devices with electrochemistry, colorimetry or electrophoresis, for the low cost and sensitive analysis of relevant biological targets. These are employed for a range targets and systems from environmental monitoring to global health. Professor Matt Kipper The Kipper research lab develops new functional biomaterials by advancing technology along several research themes that are inspired by biological materials. More specifically, the Kipper research lab develops techniques for exploiting inherent compatibility and functionality amongst biocompatible materials, functional biomaterials, and biologically derived materials, by designing new biomaterials from biologically-derived materials. A class of biologically derived polymers called polysaccharides, pose unique challenges and offer tremendous opportunity for development of function into biomaterials. They are challenging, because a lack in sequencing and synthesis technology has hindered the progress in this area. However, this offers an opportunity. By introducing polysaccharides into biomaterials we can simultaneously introduce many functions into a biomaterial, including cell adhesion ligands, guidance of cell migration, stabilization and delivery of biochemical signals, anti-microbial activity, and moieties that spatially organize other biomolecules. Another research theme explored in the Kipper research lab are techniques for engineering assemblies of biomolecules across length scales. A distinguishing feature of biology is that function is intimately dependent upon structure. Particularly, at the molecular, nanoscopic, and microscopic length scales, specific functions are organized inside organelles in cells, at interfaces and membranes, and in the pericellular and extracellular spaces. This organization and compartmentalization of function gives rise to emergent biological properties. We develop new processing methods for organizing biological macromolecule, like polysaccharides, into new nanomaterials with prescribed two-dimensional, and three-dimensional organization. This enables us to derive structure-property-function relationships that can be used to develop design principles for biologically inspired materials. The third research theme explored by the Kipper research lab is tissue engineering, orthopedics, and cardiovascular materials. These themes converge when we develop new materials for biomedical applications. Currently we are developing materials that stabilize and deliver otherwise very unstable biochemical signals cytokines , materials that guide adult stem cell differentiation, and materials that have multiple specialized functions for orthopedics and cardiovascular applications. We are also contributing to the development of new materials for biosensors, for stem cell cultivation and expansion, and materials with advanced optical and photonic properties. Professor Brian Munsky Dr. Previously, such noise was considered a nuisance that compromised cellular responses, complicated modeling, and made predictive understanding all but impossible. However, different cellular mechanisms affect these cellular fluctuations in different ways, and it is now clear that these fluctuations contain valuable information about underlying cellular mechanisms. The Munsky Group focuses on utilizing this information to gain predictive understanding of new biological phenomena. Along these lines, we have studied natural and synthetic transcriptional regulation pathways in bacteria, yeast and mammalian cells. Notably, the Munsky Group is heavily involved in q-bio, or Quantitative biology, an emerging interdisciplinary field that encompasses many different approaches to modeling, understanding, predicting, and manipulating biological processes. Professor Christie Peebles The Peebles Group works in the areas of metabolic engineering, secondary metabolism, regulatory networks, and systems biology in plants,

bacteria and yeast for the production of bio-based chemicals and fuels. More specifically these areas can be divided into 2 main applications: One area focuses on the metabolic engineering of cyanobacteria for fuels and chemical while the second area focuses on plant metabolic engineering to produce pharmaceuticals. Today, that work, funded in part by seed money from the Colorado Center for Biorefining and Biofuels, involves manipulating the genetic structure of a microorganism called cyanobacteria, which is believed to have been a building block to the development of life on Earth two to three billion years ago. Using newly developed metabolic engineering tools and methods for controlling gene expression, Peebles and her research team at CSU are exploring whether some genetically engineered form of a microorganism such as cyanobacteria can someday emerge as a building block for biomass-derived fuels and chemicals. Cyanobacteria are believed to be the first organisms capable of oxygenic photosynthesis. According to Peebles, while still largely unexplored as a production source for commercial biofuels and biochemicals, they possess several qualities that make them especially promising in those pathways. Peebles and her CSU team are also investigating two pathways involving cyanobacteria, one designed to yield free fatty acids for producing biodiesel and chemicals mainly for human health applications , and the other designed to yield terpenoids, also to produce biofuels and chemicals that may prove valuable in the human health arena, such as in the development of drugs for treating cancer Cyano-bacteria can double their biomass in four to eight hours, as compared to several days for popular biomass feedstocks such as corn, notes Peebles. Professor Ashok Prasad The Prasad Group works on several projects at the interface of the physical sciences and engineering with biology, using mathematical and computational methods as well as experiments. Research areas of interest to the group include cellular biomechanics and the determination of cell shape, the theoretical properties of signaling and gene transcription networks, synthetic biology, especially in plants, identification of network aberrations in cancer using machine learning, and genome scale metabolic modeling. The group has developed methods for quantitative image analysis to distinguish between some types of cancer cells, and is currently working to extend these methods more generally. Prasad is interested in developing techniques for measuring the physical parameters of the cellular cytoskeleton using microrheology, and relating them to cellular phenotype, motility and cytoskeletal properties. In synthetic biology the group works on developing synthetic circuits in plants, in collaboration with plant synthetic biologists at CSU. In cancer network analysis, Dr. Prasad collaborates with researchers in the College of Veterinary Sciences to help uncover the signatures of drug sensitivity of cancers. The group also works on understanding p53 dynamics and mitochondrial dynamics in cancer cells. In metabolic modeling, Dr. The research group also collaborates closely with many experimental groups across campus. Professor Kenneth Reardon Professor Brad Reisfeld The Reisfeld Group investigates the disposition of foreign chemicals environmental toxicants and drugs in humans and their effects on human health. In other words, models are developed to better understand and predict how drug molecules are distributed throughout bodies, as well as how they affect the organs and tissues, as well as how the body processes the small molecules. Additional efforts are made to study the role of the immune system in responding to foreign molecules xenobiotics. Ultimately, such models can guide targeted experiments to analyze and predict how human beings will react to and process xenobiotics. At the most detailed molecular level this includes modeling specific cytochrome P isozyme reaction rates and ligand binding. The Snow Laboratory is engaged in Biological Engineering. The focus in these cases is engineering at the level of biological macromolecules and assemblies thereof rather than engineering at the cellular level. One strength of the department is the ability to engineer functional nanostructures by taking advantage of biomolecular engineering approaches. Specifically, the Snow Lab engineers proteins that serve as building blocks within larger assemblies, respectively protein crystals and viral phage capsids. Both groups use protein engineering and chemical biology methods to optimize the resulting protein assemblies. The Snow Lab is engineering porous protein crystals as scaffolds in which the position of guest macromolecules can be programmed. Applications include advanced catalytic materials by loading enzymes and enzyme mixtures , advanced biodegradable biosensors by conditionally confining fluorescent proteins , oxygen carrying materials by loading hemoglobin , deep tissue in vivo

imaging by loading infrared fluorescent proteins , high surface area conductive materials via in crystallo synthesis of conductive polymers , anchored DNA nanotechnology via installation of guest oligonucleotides , and new approaches to crystallographic structure determination by loading guest molecules of unknown structure. Modeling is a strong branch of the department; multiple research groups specialize in diverse mathematical or computational modeling strategies. The Snow Lab develops software to model and design proteins www. These simulations range from atomic detail molecular dynamics simulations including explicit water molecules to coarse grained simulations simulating the assembly of multiple nucleic acid strands. One of the key applications for these molecular simulations is to validate designed proteins prior to experimental testing. To simulate events that occur on longer time scales or length scales Snow group researchers use implicit solvent, Brownian dynamics, and Markov State models. To accelerate the expensive computations, the Snow group uses graphics cards GPUs. Another specialty is using continuum electrostatics calculations Poisson Boltzmann to understand subtle energetic effects involving screening of charge-charge interactions. The Snow Lab also has a long standing interest in explicitly modeling cytochrome P structure and reaction specificity. Example applications for the methods described above are to assess the risk associated with exposure to environmental pollutants, or to optimize drug regimens. The Snow Lab also engineers polymers. First, the expressed polypeptides proteins that are the building blocks for their [Bionanotechnology] efforts are themselves polymers. More important, however, are the efforts in both groups to synthesize highly controlled polymers by covalently linking together proteins as templated by non-covalent assembly. The Snow Lab is also interesting in modeling transport in the particular context of understanding and controlling the diffusion of guest molecules within porous crystals.

Chapter 3 : Modeling the Kinetics of Biological Activity in Fermentation by saeid kalantari on Prezi

The approach employs kinetics of the drug-receptor interaction based on mass action law, whereby biological response is considered as proportional to the receptor modification, and the time.

Chapter 4 : First-order and pseudo-first-order elimination kinetics.

Kinetic parameters (constants that are associated with the kinetic rate expressions for the system) Stoichiometric parameters (define the stoichiometric relationships in the reactions or biological activity).

Chapter 5 : The role of the gut microbiota in the toxicity of foodborne chemicals - WUR

[Kinetics of the biological activity of xenobiotics]. [Article in Slovak] BalÃ¡z S, Rosenberg M, SturdÃ-k E, AugustÃ-n J. PMID: [PubMed - indexed for MEDLINE].

Chapter 6 : [Kinetics of the biological activity of xenobiotics].

Modelling the Kinetics of Biological Activity in Fermentation Systems. Modelling the Kinetics of Biological Activity in Fermentation Systems, in Practical.

Chapter 7 : Society of Toxicology

The second part gives the mathematical description of a simple monophasic pseudo-first-order two-compartment model, which allows a quantitative kinetic analysis in the case of both initial compound and metabolite elimination.