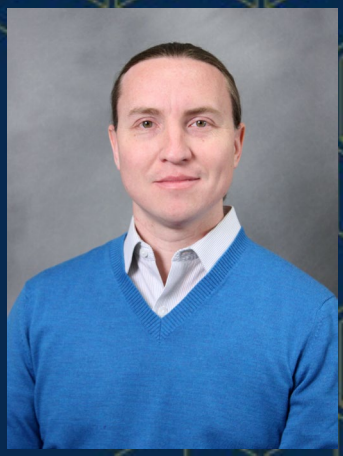
Materials Science and Engineering Department

Spring Seminar Series

Multi-scale Modeling, Simulation and Characterization of Particulate Products Processing and Performance: Driving Innovation of Pharmaceutical Products Through Mechanistic Understanding



Prof. Marcial Gonzalez
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April 10, 2024
11AM-12PM | Hill Seminar Room (LeBow 240)

Powder compaction plays a relevant role in many pharmaceutical, food, ceramic and metallurgical manufacturing processes, so much so that microstructure evolution during consolidation has direct impact on the end-product properties and performance. This process involves a variety of coupled physical mechanisms at the particle-scale (e.g., elasto-plastic deformations, formation of solid bridge, friction, and fracture) that govern the properties and performance of the final product (i.e., tablet hardness, swelling, disintegration and dissolution for pharmaceutical powders pressed into solid tablets for oral administration). Therefore, it is of paramount importance to fundamentally understand these coupled mechanisms in order to optimize manufacturing processes and to improve product design. Predictive multi-scale modeling and simulation of microstructure formation and evolution during compaction of granular solids, and the performance of the compacted heterogeneous solid, requires research efforts in three main fronts. First, the development of predictive constitutive models of inter-particle and particle-pore interactions that account for high levels of confinement and a variety of physical mechanisms. Second, the development of concurrent multi-scale strategies that combine a detailed description of the granular scale with the computational efficiency typical of continuum-level models. Third, the experimental characterization of particle's mechano-chemical properties required in the model. In this Seminar, I will present progress in these three fronts, including: (i) nonlocal contact formulations that overcome the typical, but unrealistic, assumption that contacts are independent regardless the confinement of the granular system, (ii) a quasi-static particle mechanics approach which concurrently solves for contact forces at the granular scale, for nonlocal deformations at the mesoscale, and for equilibrium at the macroscale, (iii) a pore-scale model that enables the investigation of swelling, disintegration and dissolution from simulated tablet microstructures, and (iv) characterization techniques that utilize modeling and experimental methodologies in lockstep coordination with each other at the particle scale.

Marcial Gonzalez is an Associate Professor of Mechanical Engineering at Purdue University since 2014. He has worked with undergraduate students in mentoring, advising, and counseling activities across campus, and in courses and independent research studies. Gonzalez is the winner of the Robert W. Fox Outstanding Instructor Award that is presented annually to a junior faculty member in the School of Mechanical Engineering who has demonstrated excellence in the classroom. He has also received six Seeds of Success. He works to empower underrepresented minority community college students who demonstrate the desire and ability to pursue graduate studies in STEM fields. He obtained his BS in Mechanical Engineering at University of Buenos Aires, MS and PhD in Aeronautics at Caltech.

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