From Nano- to Macro: Modeling and Simulation of Industrial Processes and Products with Inclusions

David A. Jack, PhD
Visiting Assistant Professor
Department of Industrial and Manufacturing Engineering
Florida State University

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This research seeks new analysis and design procedures to effectively, and efficiently, represent the relationship between process and product for composites with a wide variety of engineering inclusions spanning a broad size spectrum, from nano- to macro-, where the coupling between inclusion orientation and melt flow are tantamount to the effective final product representation.

Composites have enjoyed widespread industrial use, and with recent advances in the fabrication of materials with nano-scale inclusions, it is becoming increasingly important for the design engineer to have accurate and effective tools to aid them in the creation of advanced multifunctional products. The demand for accurate process and product prediction methods has significantly increased with the demand for high performance materials, and as computational capabilities exponentially increase, it seems reasonable that this need may be within computational feasibility. Unfortunately, the models developed over two decades ago for predicting inclusion orientation have been known to drastically over predict the alignment rate and were formulated for rigid inclusions with low aspect ratios. It is even more surprising that existing theories remain employed, even though they are known to have limitations both in their material representation and in fiber orientation kinematics. These limit the design engineer to, at best, a qualitative insight to the final product capabilities, and thus the engineer will remain unable to fully understand the relationship between process and product.

This presentation will begin with a classical study into the equations of motion for fiber inclusions within a melt flow and introduce the work developed from presenter's currently funded research which seeks to formulate relevant constitutive equations of motion for rigid inclusions. The classical closure dilemma is introduced, and results from several of the presenter's published closures are discussed. Recent work in the area of spherical harmonic expansions seeks to alleviate, entirely, the closure issue, which plagues many classes of engineering problems, and preliminary results will be presented. The work transitions to the prediction of structural properties and presents a statistical study relating inclusion orientation to the material stiffness tensor. During the seminar, analytic expressions that relate the orientation distribution function to the expectation and the variance of the stiffness tensor will be discussed.

The talk concludes with recent work in the area of conductivity predictions for neat CNT networks (buckypapers) based on the presenter's work with the AFRL. Previous methods yielded results several orders of magnitude from the observed results and were unable to accurately capture experimental trends with varying volume fraction, length and diameter distributions, or CNT alignment state. The presented model is the first physics-based modeling technique to address the relationship between macroscale (bulk) planar electrical conductivity and stochastically dependant, orientationally biased, freestanding neat single walled nanotube (SWNT) networks (buckypapers). Results from the nanostructure variations correspond with results previously available in the literature, both theoretical and experimental observations. The power emission study results suggest failure of these conductive networks will be initiated at a current loading density less than $1/50^{th}$ and $1/100^{th}$, respectively, than would be expected from a classical perspective for a metallic network and for a metallic/semi-conductive network.
