Property Prediction Tools for Tailored Polymer Composite Structures

Merit Review: February 27, 2008

Academic Participants in the DOE Predictive Engineering Program:

Virginia Tech

University of Missouri

University of South Carolina

Northwestern University

University of Delaware

University of Massachusetts - Lowell

Simulation of Injection Molding of Polymers Reinforced with Short and Long Glass Fibers: *NSF DMI-052918*

Investigators: D. G. Baird and P. Wapperom, VA Tech

Improved the capability to predict fiber orientation as a function of injection molding conditions:

- Used an improved constitutive relation in which rheology and fiber orientation are coupled: included effect of fiber interaction, non-affine motion, and viscoelasticity.
- Constructed a rheometer for obtaining basic material parameters (e.g. Folgar-Tucker Constant)
- Developed a numerical simulation package incorporating the improved relation and including the advancing front.
- Confirmed prediction of orientation in a center-gate disk using confocal laser microscopy.

Present and continuing efforts:

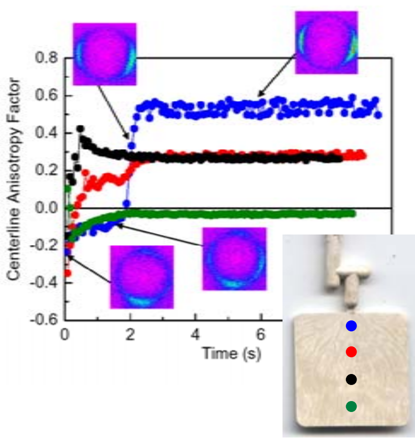
- Modify constitutive relation to include fiber flexibility-application to long fiber composites
- Predicting fiber orientation in gate region-3D simulation

Microstructural Modeling and Synchrotron Studies of Orientation Development in Injection Molding of Liquid Crystalline Polymers
(NSF DMI-0521823 & DMI-0521771)

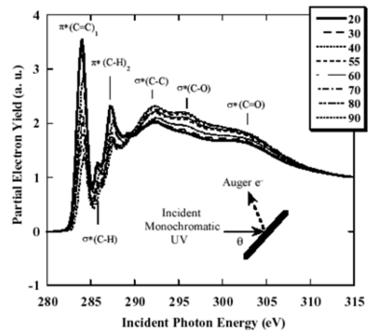
Wesley R. Burghardt
Northwestern University

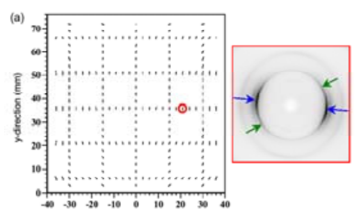
Robert A. Bubeck
Michigan Molecular Institute

1. Time-resolved, *in situ* x-ray scattering of molecular orientation *during* injection molding.

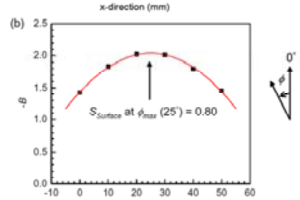


2. De-convolution of skin/core orientation distributions using surface-sensitive NEXAFS spectroscopy:



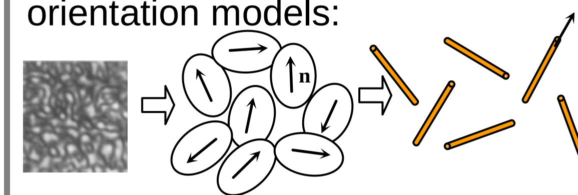


X-ray scattering (bulk)

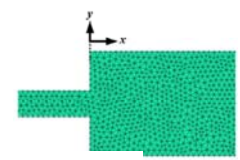


NEXAFS spectroscopy (surface)

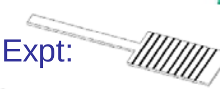
3. Process modeling of orientation in extrusion and molding, exploiting analogy between fiber & domain orientation models:

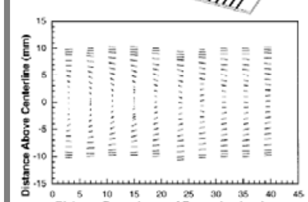


$$\frac{D}{Dt}\langle \mathbf{nn}\rangle = \boldsymbol{\omega}^T\cdot\langle \mathbf{nn}\rangle + \langle \mathbf{nn}\rangle\cdot\boldsymbol{\omega}$$
$$+\lambda(\mathbf{D}\cdot\langle \mathbf{nn}\rangle + \langle \mathbf{nn}\rangle\cdot\mathbf{D} - 2\langle \mathbf{nnnn}\rangle : \mathbf{D})$$
$$+\,\textit{Interaction term}$$

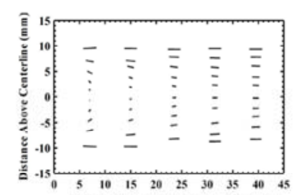


Expt:





Calc:



Award DMI-0522221

"A Hierarchical, Structure-Oriented and Stochastic Approach to Model Liquid Molding Processes"

T.D. Papathanasiou (PI), Chemical Engineering, U. South Carolina (papathan@engr.sc.edu)

RESEARCH OBJECTIVE

Develop models for the hydraulic permeability (K) of fibrous media, taking explicit account of the underlying microstructure and its variability.

APPROACH

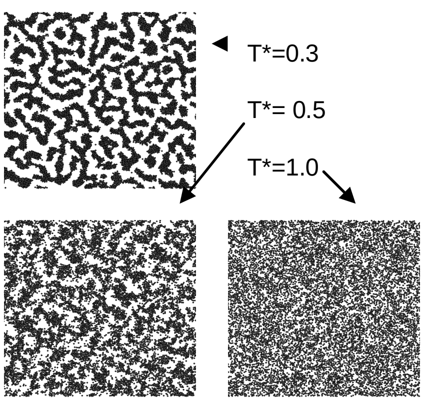
Our approach is computational. A large number of simulations have been carried out, using a parallel implementation of the Boundary Element Method, in microstructures consisting of ~10^3 fiber cross-sections placed within a containing unit-cell by a Monte Carlo procedure. This allows a direct and unambiguous correlation between (K) and the microstructure of the fiber arrays.

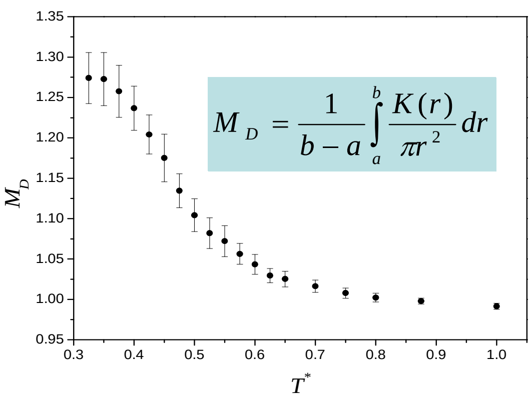
BROADER IMPACT

Quantitative structure-permeability correlations for fibrous media will allow for optimal design of fabrics used in liquid-molded composite materials. This will advance the technology of high-performance composites.

MICROSTRUCTURE GENERATION & CHARACTERIZATION

We use a NVT-Monte-Carlo process to create microstructures showing various degrees of clustering. The process temperature (T*) correlates to a structural metric (M_D) derived from Ripley's K-function K(r)





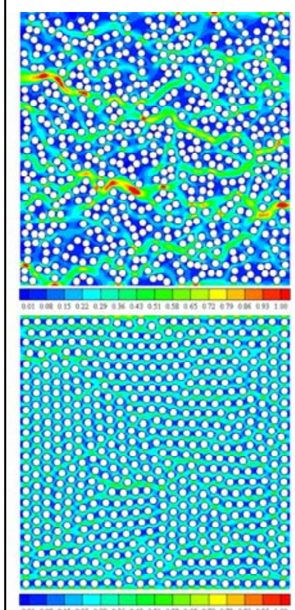
KEY RESULT

We find that the permeability (K) of random fiber arrays correlates to the underlying microstructure, namely the mean nearest inter-fiber distance ($\langle\delta_1\rangle$) according to:

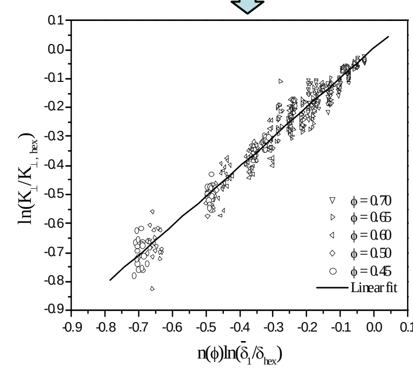
$$\frac{K}{K_{hex}} = \left(\frac{\langle\delta_1\rangle}{\delta_{hex}}\right)^{n(\phi)}$$

where K_{hex} and δ_{hex} are functions of porosity only

Flow speed contours across two arrays of 576 fibers, having 70% porosity. The two arrays differ only in the extent of local aggregation, reflected in the value of ($\langle\delta_1\rangle$); their permeabilities are different.



Results of several hundred simulations scaled as above. (K) decreases as the extent of local aggregation ($\delta_1 < \delta_{hex}$) increases



Center for Composite Materials

Department of Mechanical Engineering

Modeling Compression Resin Transfer Molding (CRTM)

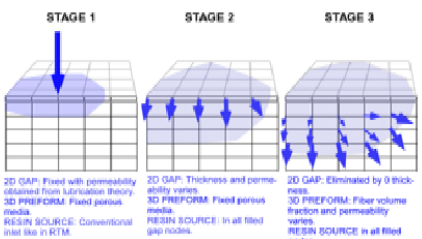
by Suresh Advani and Pavel Simacek

Process and Constitutive Models

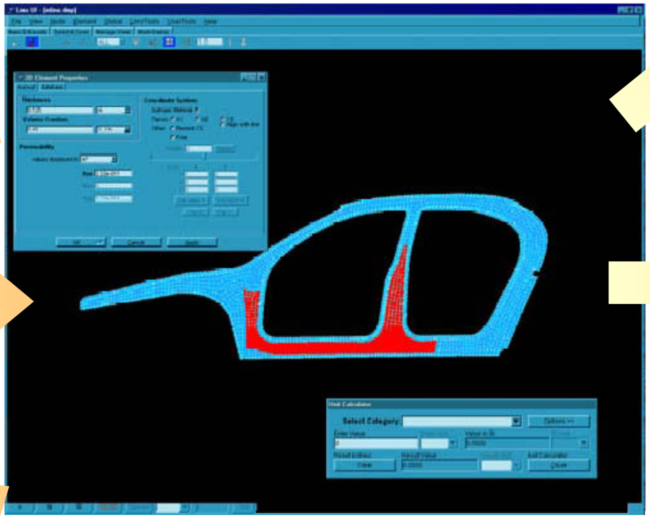
$$\phi_F \cdot \frac{\partial s_F}{\partial t} + \frac{\partial \phi_F}{\partial t} \cdot s_F + \phi_M \cdot \frac{\partial s_M}{\partial t} + \frac{\partial \phi_M}{\partial t} \cdot s_M = \nabla \cdot \frac{\mathbf{K}}{\eta} \cdot \nabla p$$

$$\dot{s} = C \left(\frac{(p+p_c)}{s_f} - \frac{p_0}{s_f \cdot (1-s_f)} \right)$$

Numerical Methods

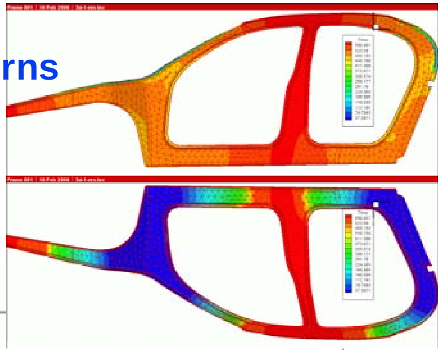


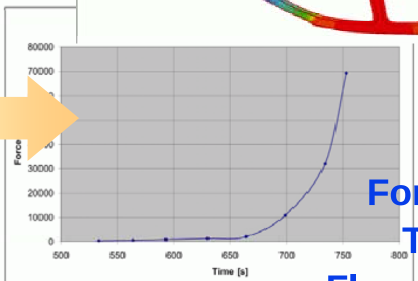
Numerical Modeling & Computer Implementation



Numerical Predictions

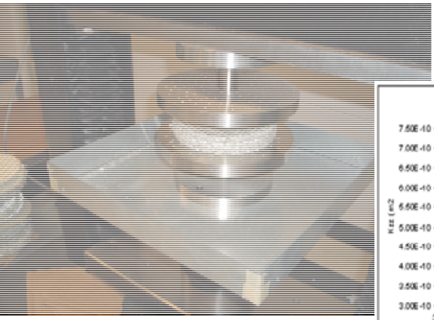
Flow Patterns

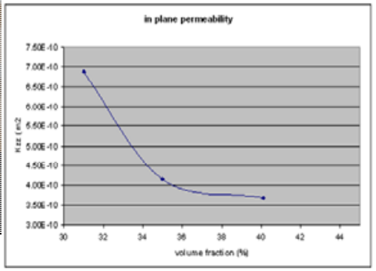




Forces, Time, Flowrates

Material Characterization





Experimental Verification

Achievement

Model to predict flow patterns and forces of P4 fabrics in CRTM

Incorporating Higher Order Tensors in the Computation of Polymer Composite Mechanical Properties (NSF Grant: DMI-0522694)

Douglas E. Smith
University of Missouri

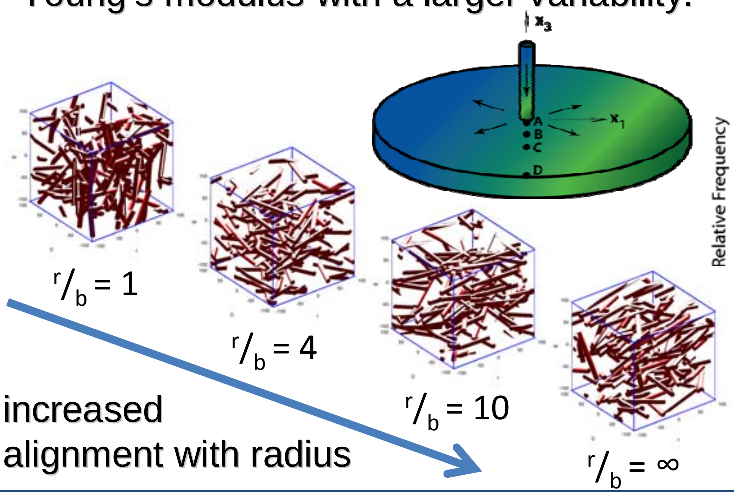
Research Objective

Develop a predictive capability that incorporates higher-order orientation tensors to evaluate elastic mechanical properties of short- and long-fiber reinforced polymer composites.

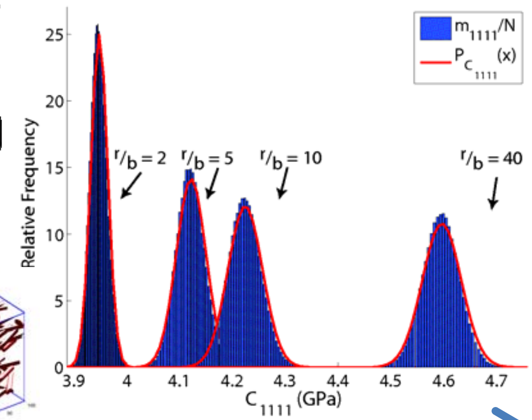
Milestones

- Mean and variance of elasticity matrix computed from 4^{th} through 8^{th} order orientation tensors and orientation distribution functions for short fiber composites.
- Analytical expressions for mean and variance verified with Monte Carlo simulation.
- Three-dimensional voxel-based finite element method developed for computing elastic properties for short (completed) and long (in progress) fiber polymer composites.

Center-gated disk short-fiber orientation simulations show that fibers tend to align in the radial direction with increased radius, resulting in a higher Young's modulus with a larger variability.



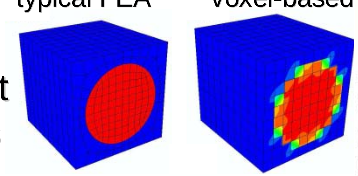
increased alignment with radius

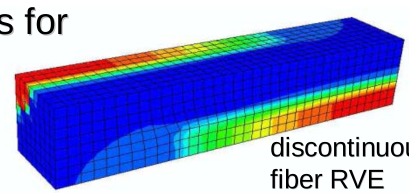


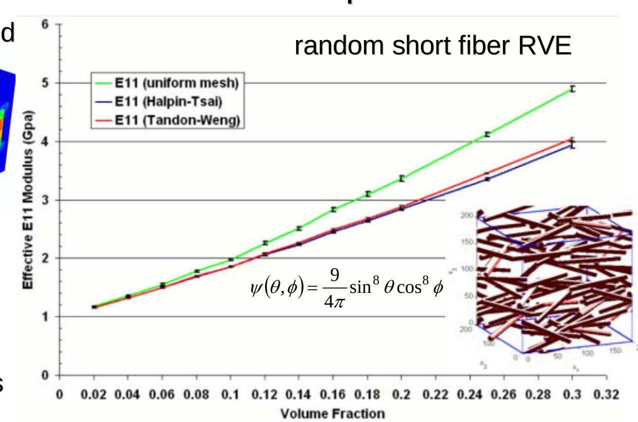
increased mean & variance

Fiber interaction within the composite structure is more accurately modeled with voxel-based finite element modeling approach, yielding higher than expected modulus values for short fiber composites.

representative volume element (RVE) captures desired mechanics for periodic structures







$$\psi(\theta,\phi)=\frac{9}{4\pi}\sin^8\theta\cos^8\phi$$

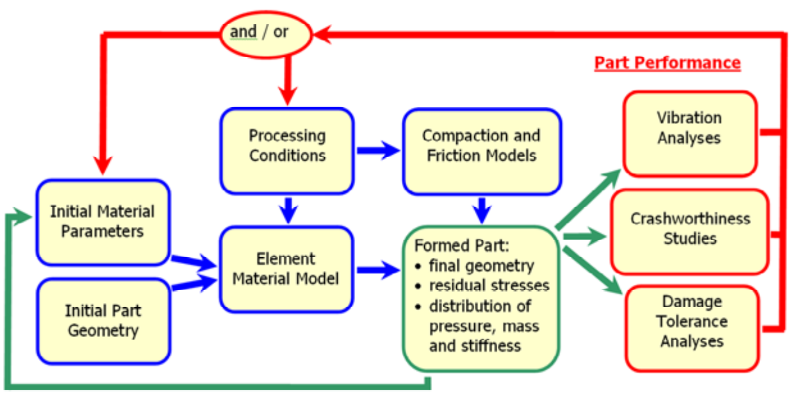
DES FEB08

Linking Process-Induced Properties to Thermoplastic-Matrix Woven-Fabric Composite Performance

NSF Grant # DMI-0522923 – NSF Program Name: MPM
Principal Investigators: James A. Sherwood, Julie Chen, Larissa Gorbatikh
UML Students: Corey Morris, Konstantine Fetfatsidis, Lisa Gamache, James Kremer
Advanced Composite Material and Textiles Research Laboratory
Department of Mechanical Engineering, University of Massachusetts Lowell

Goal of Research is to develop a widely-accepted integrated design tool:

- That will be used by the automotive industry and
- That will link the process-induced properties to product performance
  - o By capturing all of the critical material-processing mechanisms that occur during the thermostamping process for this class of commingled polypropylene-fiberglass woven-fabric composites,
  - o By predicting the magnitudes of the material properties and the distribution of these properties in a formed part of complex geometry, e.g. a floor pan or bumper of a car, as a result of the manufacturing process,
  - o By giving insight as to the potential damage tolerance of the formed part, and
  - o By allowing the output of this design tool to be seamlessly used for subsequent finite element analysis of the part for in-service load conditions—either as a single component or integration into a vehicle system.



Flowchart for the integrated design tool