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Multi-Scale Composites; Manufacturing; Structure/Property Correlations

Prof. Papathanasiou received his PhD (Chemical Engineering) from McGill University (1991), his Diploma (Chem. Eng.) from NTUA in 1985 and his MSc in Chemical Engineering from the University of Calgary (1987). He is currently Professor and Deputy Head of Department at Uth, Mechanical Engineering. Prior postings include Assoc. Professor of Chemical Engineering at the University of South Carolina, USA (1997-2008), Unilever Lecturer, Chemical Engineering, Imperial College, UK (1992-1997), Director's Post-Doctoral Fellow, Los Alamos National Laboratory, USA (1991-1992) and Research Scientist at ALCAN Intl. R&D Center in Kingston, Canada.

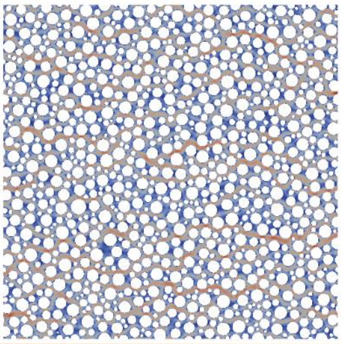

Figure 1: Velocity field for transverse flow across a model biomaterial, representing collagen taken from healthy connective tissue, exhibiting a bimodal fiber size distribution [1].

RESEARCH INTERESTS & ACTIVITIES

I am interested in the investigation of processing-structure-property relationships in composite materials, as a prerequisite to optimal manufacturing and product design. Processes of interest involve flow into complex cavities or channels (injection molding, calendering), flow through fibrous media of complex internal structure (liquid molding, pultrusion),transport through fibrous biomaterials such as connective tissue or collagen, or transport in filled systems, including platelet nano-composites. Key to our approach is the use of computation to investigate the influence of microstructure on the details of the flow fields (processing-microstructure correlations) as well as on the details of concentration, thermal or stress fields (microstructure-property correlations). In addition we are interested in developing and testing realistic CAD models for composites manufacturing processes, with recent emphasis in die- and pin-assisted pultrusion. My work has been funded by the EU as well as by the US-NSF, US-DOD, US-ONR and US-DOE. Specific projects:

1 *Micro-Scale Flows in Fibrous Media and Fibrous Biomaterials [1-7]:* We are interested in the computational investigation of flow patterns (e.g Figure (1)) in fibrous media of complex internal structure, encountered in diverse applicatios, such as in transport through connective tissue or in liquid molding of high performance composites, and the determination of how such patterns are affected by the microstructural details of these media. Both Stokes' and finite Reynolds-number flows are considered, for generalized Newtonian as well as for micropolar fluids [1]. An immediate objective is the development of quantitative models for the effective permeability (K) of fibrous media as function of microstructural parameters. This involves differentiating between various hard-core arrays (usually lumped together under the heading "random") as well as identifying the point in microstructure evolution at which a fibrous medium's resistance to flow is significantly affected by clustering. A large part of this effort involves proposing and testing microstructural metrics that correlate with the observed trends in (K). Achievements include the development of predictive models which relate measures of microstructural randomness to the deviation of (K) from that of regular arrays.

2 *Flow through Dual-Scale Porous Media [8-9]*: Such media are ubiquitous in the area of composites fabrication, where different types of reinforcement in different stages of orientation and aggregation are combined to produce preform architectures with optimal processability and products with optimal on-site performance. Besides elucidating micro-scale flow patterns, we are interested in developing and testing models for their effective permeability. Example flows in such dual-porosity media are shown in Figure (2).

3 *Transport across filled systems [10-15]:* We are using high performance computing (based on the BEM and the FVM) to investigate the manner in which the efficacy of filled systems is affected by their internal structure. Systems of interest include flake-filled membranes and particulate/fiber composites in which the dispersed phase shows various degrees of aggregation. An example of transport across a particulate containing 10,000 individual particles, the aggregation state of which is determined by the parameters of the NVT-MC algorithm used in its generation, is shown in Figure (3.a). Concentration contours for diffusion across a material filled with 50000 randomly placed and randomly oriented impermeable flakes at very high concentration ($\alpha\varphi$=10) are shown in Figure (3.b) and a 3D geometry containing 2000 flakes in (3.c). These illustrate the coupling between local inhomogeneity and macroscopic homogeneity and are the key in understanding the manner in which microstructure alters the effective properties of the composite.

4 Realictic Modeling of Polymer/Composites Manufacturing Operations [15-19]: We are interested in developing and using realistic CAD models for polymer manufacturing processes (Figure (4)), especially processes which make use of flow and geometry to achieve the infiltration of a resin into a fibrous/porous scaffold. Our objective is to combine large numbers of CAD results in order to propose and test explicit process models relating material and process parameters to fabrication outcomes – in the case of pin-assisted pultrusion, such a model for the extent of resin infiltration was recently proposed in [16]. In addition, we are interested in coupling fluid mechanics and material deformability (flow/structure interactions) in pultrusion and liquid molding.

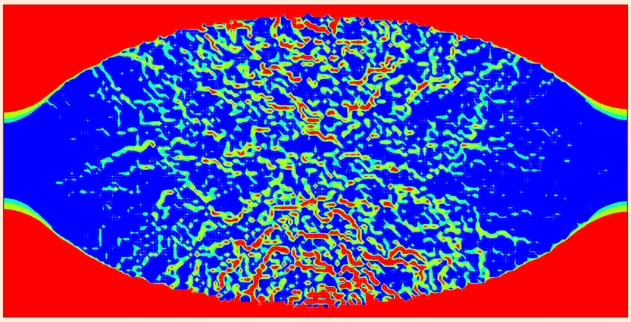

Figure 2: Distribution of interstitial fluid speed in a dual porosity material, consisting of a square array of fiber bundles, each containing 11000 individual filaments. Colors indicate dimensionless fluid speed levels (red for u>0.0.1, blue for u<0.025 and green for intermediate values).

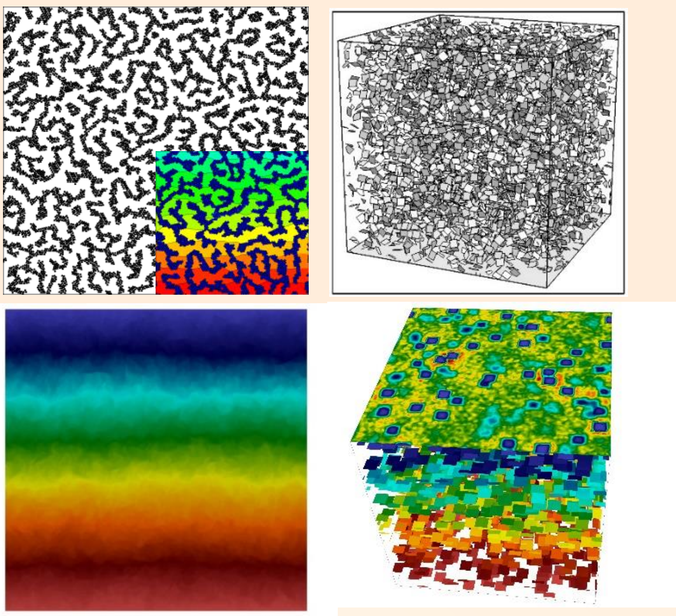

Figure 3: Distribution of concentration in random filled systems. Top Left, (3a) is a co-continuous particulate composite. Bottom left (3b) is 2D system containing 50,000 randomly placed and oriented flakes. Bottom Right, is a layered 3D flake composite. Top Right, 3D geometry containing 4000 randomly placed and oriented flakes (3.c)

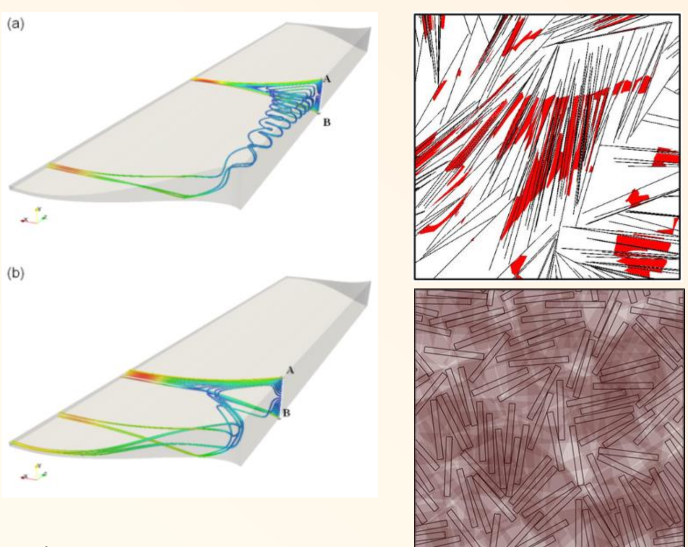

Figure 4:
(Left) Predicted non-intuitive fluid trajectories (3D Calendering of a polymeric melt) showing that the sides of the calendered sheet originate in the interior of the fed material [17].
(Right) Sample synthetic dense nematic structures (top) and space polarization (bottom) during the coverage of a surface with rod-like particles of high aspect ratio [9].

Selected Publications (underlined for corresponding author)

1 E.G. Karvelas, A. Tsiantis and T.D. Papathanasiou, "Effect of Micropolar Fluid Properties on the Hydraulic Permeability of Fibrous Biomaterials", Computer Methods and Programs in Biomedicine,185, 2020,1050135.

2 C. Erisken, A. Tsiantis, T.D. Papathanasiou, E.G. Karvelas, "Collagen Fibril Diameter Distribution Affects Permeability of Ligament Tissue: A Comparison Between Healthy and Injured Tissues", *Computer Methods and Programs in Biomedicine,* 196, 2020, 105554

3 X. Chen and T.D. Papathanasiou, "The transverse permeability of disordered fiber arrays: A statistical correlation in terms of the mean interfiber spacing", Transport in Porous Media, **71**(2), 233-251, 2007

4 X. Chen and T.D. Papathanasiou, "Micro-Scale Modelling of Axial Flow through Unidirectional Disordered Fiber Arrays", Composites Science and Technology, **67**, 1286-1293, 2007

5 X. Chen and T.D. Papathanasiou, "On the variability of the Kozeny constant for saturated flow across unidirectional, disordered, fiber arrays", Composites Part A: Manufacturing and Applied Science, **37**(6), 836-846, 2006

6 T.D. Papathanasiou, B. Markicevic and E. Dendy, "A computational evaluation of the Ergun and Forchheimer equations for fibrous media", Physics of Fluids, **13**(10), 2795-2804, 2001

7 B.Bijeljic, M.D.Mantle, A.J.Sederman, L.F.Gladden and T.D.Papathanasiou , "Slow flow across macroscopically semi-circular fibre lattices and a free flow region of variable width - visualisation by magnetic resonance imaging", Chemical Engineering Science, Vol.59(10) pp. 2089-2103, 2004

8 A. Tsiantis and T.D. Papathanasiou, "A general scaling for the barrier factor of composites containing layered flakes of square, circular and hexagonal shape", *International Journal of Heat and Mass Transfer*,2020

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12 A. Tsiantis and T.D. Papathanasiou, "An Evaluation of Models and Computational Approaches for the Barrier Properties of Coatings Containing Flakes of High Aspect Ratio", Journal of Coatings Technology and Research, 16 (2), 521-530, 2019

13 T.D. Papathanasiou and A. Tsiantis, "Orientational Randomness and its Influence on the Barrier Properties of Flake-Filled Composite Films", Journal of Plastic Film and Sheeting,33(4), 438-456, 2017

14 M.S. Ingber and T.D. Papathanasiou, "A Parallel-Supercomputing Investigation of the Stiffness of Aligned, Short-Fiber-Reinforced Composites using the Boundary Element Method", International Journal for Numerical Methods in Engineering, **30**, 3477-3491, 1997

15 Dobri, A. , Y. Wang and T.D. Papathanasiou, "Transient heat transfer in fibrous composites: A semi-analytical model and its numerical validation", *Numerical Heat Transfer: Part A*, 77(9), 840-852, 2020

16 N. Polychronopoulos and T.D. Papathanasiou, "Pin-Assisted Resin Infiltration of Porous Substrates", Composites Part A – Applied Science and Manufacturing, **71**, 126-135, 2015

17 N. Polychronopoulos, I. Sarris and T.D. Papathanasiou, "3D Features in the Calendering of Thermoplastics: A Computational Investigation", Polymer Engineering & Science, **54**,1712-1722, 2014

18 N. Polychronopoulos and T.D. Papathanasiou, "A Novel Model for Resin Infiltration in pin-assisted Pultrusion", Polymer Composites, 38(12), 2653-2662, 2017

19 N. Polychronopoulos and T.D. Papathanasiou, "Fluid Penetration in a Deformable Permeable Web moving past a Stationary Rigid Cylinder", Transport in Porous Media, **116**:393-411, 2017

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