Engineering across Length Scales

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Abstract - **The Center for Advanced Engineering Fibers and Films (CAEFF) is a U. S. National Science Foundation Engineering Research Center. Parallel numerical simulation and experimental research thrusts involve faculty from over eight distinct academic disciplines. To support the research activities of students, a series of interdisciplinary courses, taught in many cases by multiple faculty from different disciplines, has been developed. Individually, these courses cover the spectrum of length scales from molecular modeling and polymer physics, through continuum modeling, and up to polymer processing. Taken as a series, they introduce students to the fundamentals necessary to solve complex research problems, and to the team-based approach required for challenges that emerge in a Center conducting research ranging from polymer synthesis to commercial-scale polymer processing. To enhance the integration of students from different academic backgrounds, e. g. numerical simulation and experimentation, these courses combine lectures, interdisciplinary team-based projects, and experiments. In this paper, we discuss the challenges and opportunities of teaching interdisciplinary courses, and comment on the integration of the concurrent research activities into the classroom experience. Finally, we address the responsibilities of a Research Center to expand its education offerings beyond the university campus to the broader industrial community that we serve.**

Index Terms – Continuum Modeling, Interdisciplinary, Length Scales, Molecular Modeling, Processing

INTRODUCTION

The Center for Advanced Engineering Fibers and Films (CAEFF) at Clemson University is one of approximately twenty Engineering Research Center funded by the U.S. National Science Foundation. Additional financial support comes from the State of South Carolina and from industrial partners with interests in polymeric materials. The vision of the CAEFF is to "be the international leader in the development of fibers, films, and related functional materials through integrated systems research and education programs that combine molecular understanding, process innovation, and multi-scale modeling to impact industry, academe, and society." To achieve this vision, parallel numerical simulation and experimental research thrusts involve faculty from over eight distinct academic disciplines and several universities, including core partners Massachusetts Institute of Technology and Clark Atlanta University. Coupled with the extensive research program is a broad-based education program that includes outreach to high-school students; undergraduate research opportunities; formal undergraduate and graduate level courses; and short courses for professionals in related industries. Here, we focus on the development and teaching of (primarily) graduate-level courses that prepare students to contribute to the research activities of the CAEFF. Of particular note in these courses is a focus on the multiple length scales that emerge, and an integration of students from a wide range of disciplines into each course.

Two of the core engineering disciplines, Chemical Engineering and Mechanical Engineering, typically incorporate research activities related to polymeric materials. In these fields, there is often a focus on either continuum-level or process-level length scales. In Polymer Science and Chemistry departments, research on polymers often focuses on new product (polymer) development, in which length scales characteristic of the molecular, or monomer, dimension are most important. Given the interdisciplinary research that an Engineering Research Center typically supports, it is imperative that there is an integration of research *across* length scales, and this concept motivates the development of a series of courses, that, taken together, provide students with the fundamental background to integrate concepts from a variety of disciplines into their research activities.

This teaching across length scales is being encouraged by several trends in current engineering research. First, computing power is increasing so that models can be developed with increasingly complex components. These complexities are frequently manifested by more details at smaller length scales. Second, high value added products are being designed in which the chemistry (and, increasingly, the biology), again at a molecular length scale, is being systematically manipulated. Third, empirical process and product development is being supplemented by computational fluid dynamics, for example, that builds upon continuum, rather than process, length scales. Taken as a whole, it is expected that teaching across length scales will become a more integral part of undergraduate, as well as graduate, engineering education, as is proposed by Armstrong [1] in work summarizing a series of workshops held by chemical engineering faculty and industrial representatives.

In this paper, we introduce and discuss a portfolio of interdisciplinary courses developed and taught within the Center for Advanced Engineering Fibers and Films. Taken individually, these courses offer the student the requisite background material to conduct research activities in a narrowly focused area. Taken as an integrated series of coursework, the classes provide students with an overview of the research activities within the CAEFF, and enable students to integrate their particular research interests and activities within the greater mission of the Research Center as a whole. Because of the *explicit* interdisciplinary nature of the courses, students from a variety of disciplines are encouraged to learn about different fields and build classroom (and ultimately, research-based) interactions with a wide range of collaborators. Furthermore, the series of courses enables a student to explicitly study, in a formal classroom environment, aspects of polymer science and engineering on length scales ranging from the Angstrom level found in chemical bonds through the meter scale encountered in industrial-scale polymer processing.

Our paper is organized in the following sections: (1) a discussion on the diversity of the backgrounds of student participants, motivating some of the course development and syllabi; (2) a description of the coursework through brief synopses as well as a discussion on the integration of the length scales relevant to the lectures, and, in some cases, the experiments; (3) a discussion, based upon characteristic length scales, on the integration of the coursework with research activities; (4) an introduction to the short courses for industry personnel, again with a focus on the length scales of interest; and (5) conclusions.

STUDENT BACKGROUNDS

In this paper, we focus on graduate-level coursework offered through the interdisciplinary CAEFF. Students come from a wide range of academic disciplines (see Table I), and as such bring a wide range of skill sets to the CAEFF courses. These differences are both a challenge and an opportunity. For example, we find that some (incoming Mathematical Sciences) students do not know what a polymer is, and must be introduced to this concept and some typical visual representations before they can understand the mathematical framework, succeed in a class, or conduct an associated research project. Therefore, in each class some early lectures and assignments are dedicated to providing a basic introduction to the topic prior to commencing with the graduate-level coursework. While this may be review for some students, it ensures that for the majority of the course lectures, every student has the appropriate fundamental background necessary.

TABLE I
DISCIPLINES REPRESENTED IN CAEFF

Institution	Discipline
Clemson	Chemical and Biomolecular Engineering
	Materials Science
	Mechanical Engineering
	Chemistry
	Mathematical Sciences
	Physics
	Computer Science
	Bioengineering
	Electrical and Computer Engineering
MIT	Chemical Engineering
Lehigh	Chemical Engineering
Clark Atlanta	Chemistry
McGill	Chemical Engineering
Illinois	Mechanical Engineering

The positive aspect of these various student backgrounds is that students can work together and teach one another outside of the lecture by building upon the skills that each student brings to the class. For example, a Chemistry student may bring a detailed knowledge of polymer structure and behavior (at the monomer length scale) to a group of Engineering students who more commonly approach problems from the continuum length scale. This exchange of ideas enhances the learning for all students, and introduces the broad spectrum of ideas and approaches that so often leads to important scientific advances.

COURSES OFFERED

In this section, we introduce each of the courses offered through the Center for Advanced Engineering Fibers and Films. Table II provides course titles, the institution at which each course is offered, and the primary length scale associated with the material covered in the course. As the lead institution in the CAEFF, most of the courses are offered at the Clemson campus. To encourage students to enroll in a broad range of classes, most CAEFF courses are cross-listed in several of the disciplines represented within the Research Center.

TABLE II
COURSES OFFERED THROUGH CAEFF

Location	Title	Length Scale
Clemson	Molecular Modeling of Polymers	Molecular
Clemson	Diffusion through Polymers	Molecular
Clemson	Polymer Physics	Molecular
MIT	Molecular Modeling	Molecular
Clemson	Fiber and Film Systems: Modeling and Simulation	Continuum
Clemson	Rheology	Continuum
Lehigh	Rheology	Continuum
Clemson	Introduction to Fiber and Film Systems	Processing
Clemson	Techniques for Characterizing Fiber and Films	Multiple
Lehigh	Polymer Science and Engineering	Multiple

Because of the broad range of academic departments involved in the CAEFF at Clemson, most of the course offerings include students from several of the academic disciplines represented in Table I. In most classes, students are encouraged to work with each other on homework problems. Team-based projects are assigned over the semester. Again, these teams are interdisciplinary to encourage the sharing of ideas and to foster later research collaborations between both research groups and academic disciplines. An example of how this works may be found in the modeling courses. The chemists understand how polymer architecture affects thermal behavior; the engineers understand the effect of processing variables, and the mathematicians have the computational background necessary for solving systems of equations numerically.

As discussed above, length scales investigated within the research framework of CAEFF range from those associated with polymer processing (meters) to the bond length between atoms in a polymer backbone (Angstroms). Figure 1 demonstrates how the research activities span these scales, and how the coursework is organized to then provide both compartmentalized and broad-based content. As a consequence, students may cover the spectrum of length scales in their classes or devote their studies to a particular area.

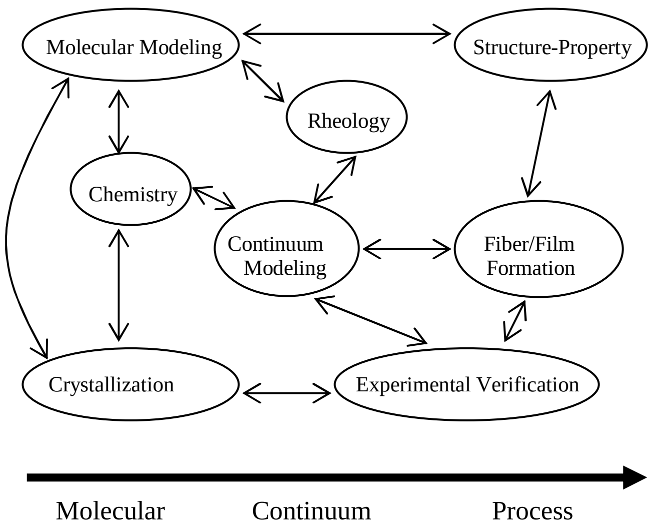

FIGURE 1
THE IMPACT OF LENGTH SCALES ON CAEFF RESEARCH AND COURSE DEVELOPMENT.

I. Introduction to Fiber and Film Systems

This course is designed to provide students with an introduction to polymeric fibers and films. An interdisciplinary, systems approach is used to explain how the processing variables in the system affect the structure and properties of the resulting fiber and films. The specific learning objectives are to provide students with an introduction to the following aspects of fiber and film manufacturing: polymers; extrusion; fiber spinning, film extrusion; and structure-property relationships. As such, the process length scale dominates the course context, although continuum quantities are discussed in terms of fiber/film properties. Incorporated into this introductory course are visits to industrial facilities.

II. Molecular Modeling

This course is devoted to providing students with a solid foundation in classical simulation techniques, and then applying these techniques to engineering applications. Topics covered include: statistical mechanics; intra- and inter-molecular potentials; molecular dynamics, Monte Carlo methods; atomistic simulation techniques; and applications to gas transport and x-ray diffraction. Obviously, the dominant length scale is molecular, and there is a connection made with numerical simulations and experimental measurements such as degree of crystallinity. The Engineering Research Center contributes software developed "in-house" for both lecture examples and team-based student projects.

III. Diffusion through Polymers

The primary goal of this course is to teach students the fundamentals that govern the mass transfer of small and large molecules in polymeric materials such as films. The class starts with Fickian diffusion, and moves on to more complex models for polymeric systems including semi-crystalline materials and polymer-polymer systems. The theoretical, molecular level framework is integrated with continuum approaches. Predictions are discussed in terms of direct experimental data.

IV. Polymer Physics

The focus of this course is to introduce students to classical and contemporary approaches to polymer physics, with a focus on the structure and properties of polymer solutions. The course starts with the structure and dynamics of isolated polymer chains, and progresses to dilute, semi-dilute and entangled systems as well as bulk behavior. In this progression, the material begins with the dynamics of single chains, and over the semester additional interactions, both polymer-polymer and polymer-solvent, are considered. Concepts required include statistical mechanics through the continuum approximation. Theoretical derivations are used to interpret experimental structural measurements including light and neutron scattering.

V. Fiber and Film Systems: Modeling and Simulation

This course introduces students to a broad range of continuum level modeling, and is co-taught by Mathematical Sciences and Chemical Engineering faculty. Introductory lectures are devoted to aspects of polymer physics, fluid mechanics, and computational methods. Then, a wide range of constitutive equations is introduced, beginning with simple empirical models and progressing to detailed models based upon various concepts of polymer deformation and interactions. Through this model development, students must come to grasp polymer dynamics on a local, molecular scale in order to predict quantities at the continuum level. Several team-based projects are interspersed through the semester. Teams typically include both mathematicians with strength in computational methods and engineers with greater knowledge of fluid mechanics and polymers. Ultimately, students use the CAEFF software developed "in house" to predict process level fiber or film systems using detailed continuum level constitutive equations based upon a molecular understanding of polymer physics.

VI. Rheology

The field of rheology is concerned with describing the flow and deformation of matter on a continuum length scale. In this course, students are introduced to standard rheological flow geometries and measurement techniques in a lecture format. They learn the fundamental rheological properties such as shear and extensional viscosity, storage and loss moduli, and characteristic relaxation times. Knowledge of rheological properties serves two distinct purposes. First, rheological results give insight into the performance of a particular polymer in a typical processing geometry. Hence, rheology serves as a bridge between the continuum and process length scales. Second, rheological measurements describe fundamental material properties of polymeric materials. Thus, these measurements are direct inputs into the continuum level modeling undertaken by the CAEFF, and link numerical studies with "real" materials. In addition, detailed molecular modeling is able to predict properties such as the shear viscosity, and therefore rheology provides the connection between the length scales of single monomers and continuum parameters. A team-based, month-long experimental project in which students fully characterize a representative polymer is a highlight of the course. By measuring flow properties and determining model parameters from the experimental results, students must make the connection between the simulation and experimental realms.

VII. Techniques for Characterizing Fiber and Films

This course introduces students to measurement techniques for fiber and film structure and properties. Parameters of interest include: mechanical/tensile properties; DSC, TGA and DMA; birefringence, spectroscopy and microscopy; and process parameters such as velocity, diameter and temperature as a function of position within the fiber or film. Clearly, this material covers the entire range of length scales ranging from atomic structure to process conditions. As in the rheology course, there are complementary foci in terms of both the theoretical underpinnings of different techniques and the hands-on experience of laboratory exercise. In addition to the instruction on experimental techniques, students learn (1) how to connect experimental measurements to molecular structure; and (2) how experimental validation at the process level is used to evaluate predictions in the continuum-level modeling.

VIII. Polymer Science and Engineering

This course is designed to introduce to students the three core areas of polymer science and engineering: polymerization kinetics; polymer physics and characterization; and polymer processing. These topics necessarily cover the multiple length scales discussed in this work. By starting with kinetics and synthesis, students learn how the polymer is constructed from the basic monomer components. Polymer physics and characterization is then introduced based upon an understanding of polymer structure and conformation. Later lectures focus on processing polymeric materials and structure-property relationships, and require an understanding of the continuum-level parameters that emerge from polymer physics. As with many CAEFF courses, the processing component focuses on systems and examples drawn from the fiber and film industries.

INTEGRATION WITH RESEARCH ACTIVITIES

The CAEFF is organized around two research thrusts. Thrust 1 is devoted to the numerical simulation of polymer dynamics and fiber and film processes. A continuum-level simulation package, FiSim, is in continuous development and is designed to model the fiber and film processes from the extruder to the final material properties. Thrust 2 is devoted to experimental verification and process/product development. These two broad research activities are highly intertwined, most obviously through the experimental verification (at the molecular (x-ray), continuum (rheology), and process (velocity) length scales) of the FiSim numerical simulations in model geometries with well-characterized materials.

This integration between modeling and experimental techniques is also explicit within the course offerings as well. At Clemson, the core, introductory class for the CAEFF is "Introduction to Fiber and Film Systems." This course gives participants an overview of polymer processing, with a focus on fiber and films. It is ideal for students with diverse backgrounds to be introduced to the terminology encountered throughout CAEFF research activities. The "Fiber and Film Systems: Modeling and Simulation" course explicitly introduces students involved in both numerical and experimental work to the FiSim software, as well as a broad array of constitutive models based upon characteristic length scales. The Rheology courses teach students how to experimentally obtain continuum-level parameters for the modeling of polymer processing. Finally, the courses that focus on the molecular length scales provide students with knowledge of the underlying physics of polymer dynamics that are manifested in continuum- and process-scale behavior.

SHORT COURSES

Short courses offer a direct method of knowledge transfer between the Research Center environment and the industrial community. The CAEFF has developed short courses that are available both as stand-alone offerings and as add-ons to conferences. These courses integrate the experimental and numerical research conducted within the CAEFF, and offer participants the opportunity to examine industrial processes from a fundamental, rather than empirical, basis.

As with the traditional coursework, attention is paid to the full spectrum of length scales, although there is a definite focus on the process level. Table III shows a typical outline of a one-day short course.

TABLE III
FIBER SPINNING SHORT COURSE OUTLINE

Topic
Overview of melt spinning
Process stages
Process variables
Structure-property relationships
Experimental characterization and verification
Rheology
On-line measurement
Post-mortem
Mathematical modeling of melt spinning
One-dimensional model with flow-enhanced crystallization
Parameter fitting
Two-dimensional modeling
Hands-on case study simulations
FiSim software
Using the polymer database

Presentations start with a process-scale introduction to the geometry of interest. A more limited-scope component focuses on the molecular and process reasons for structure-property relationships. The experimental characterization lectures include both process scale measurements as well as (continuum) parameter measurement using rheological techniques. The subsequent modeling lectures build upon molecular-level information (such as crystallization phenomena) to introduce the continuum-level modeling contained within the FiSim software package. A significant portion of the short course is devoted to active, hands-on learning by the attendees with the software package. In this activity, participants can directly probe the impact of a wide range of variables such as crystallization rate (molecular length scale), viscosity (continuum length scale), and draw ratio (process length scale) on fiber or film formation. Ultimately, our goal is to provide short course participants with the fundamentals at the molecular and continuum level necessary to make informed decisions on process design on an industrial scale.

CONCLUSIONS

Engineering polymer processes is no longer confined to process-specified length scales and empirical product design. Rather, an integrated approach building upon numerical simulation and experimental validation offers the opportunity for lower-cost, more reliable development. To achieve this goal, it is necessary for the engineer to understand physical behavior on length scales ranging from the molecular level through industrial processes. A broad-based series of courses has been presented to prepare students for careers in polymer fiber and film processing. By demonstrating how the information obtained at one length scale is relevant to model or process development at other scales, these courses prepare a new generation of engineer for work at the frontiers of science. The interdisciplinary nature of the Research Center, in which students from a range of science and engineering disciplines interact and collaborate in classes, further integrates the different length scales into research activities.

ACKNOWLEDGMENT

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REFERENCES

[1] Armstrong, R.C., "A Vision of the Curriculum of the Future", *Chemical Engineering Education,* 40, No 2., 2006, 104-109.