2006 Danckwerts Lecture

Modeling Polymeric Materials

During a one-on-one interview, Doros Theodorou, the Danckwerts Lecturer at AIChE's 2006 Annual Meeting, explained the more-complex aspects of the hierarchical computations for polymer characterization and the commercial relevance of his promising research. My PhD thesis aimed at predicting molecular packing and elastic constants of glassy polymers and could be described as one of the first successful applications of molecular modeling to polymers. Since then, the field of molecular modeling has exploded, with applications in all kinds of materials and properties, he said.

A professor of chemical engineering in the the Dept. of Materials Science and Engineering, National Technical Univ. of Athens, Greece, Theodorou recently co-edited a new book with fellow researcher Michael Kotelyanskii on simulation methods for polymers*. We simulate materials (mainly polymers and synthetic zeolites) on a computer using statistical mechanics and algorithms, based on the fundamental molecular sciences, in order to predict material properties from their chemical constitution. Knowledge of these properties is needed in the design of products with prescribed performance characteristics in end-use applications (*e.g.,* plastics with desired stiffness and strength as structural materials, better processability in the melt state, controlled permeability by atmospheric gases leading to prolonged shelf life of products packaged in them, adhesives that can bond different materials together, polymeric or inorganic membranes that can separate mixtures with high throughput and selectivity, etc.) and in the design of processes to make these products.

"It would be a great mistake to think of the content of chemical engineering science as permanently fixed. It is likely to alter greatly over the years, in response to the changing requirements of industry and to new scientific discoveries and ideas for their application."

P. V. DANCKWERTS, 1966

In general, predicting properties from chemical constitution is a formidable task. "Our computational approaches are often hierarchical, *i.e.,* operate at various levels of description, from the detailed atomistic to the macroscopic, utilizing systematic coarse-graining

Doros Theodorou, this year's Danckwerts Lecturer, grabs the attention of the audience with a discussion of his cutting-edge research — hierarchical computations for polymer characterization that can be used to efficiently predict the polymer's physical properties.

*Kotelyanskii, M. J., and D.N. Theodorou, Eds., "Simulation Methods for Polymers," Marcel Dekker, New York, 900 pp. (2004). ISBN 0824702476.

Visit http://comse.chemeng.ntua.gr for more information. This website contains a general introduction to his group's research projects.

(*e.g.,* from atoms to groups of atoms to entanglement networks to continuous media) to capture properties with currently available computational resources.

The input to molecular modeling calculations is the chemical constitution of a material, which consists of building blocks, such as molecules, atoms, ions, etc. These calculations predict how these building blocks arrange themselves in space, and what properties they give rise to. What molecular modeling can do is predict a wide variety of properties starting from the same fundamental input. It can also bring out the mechanisms, *i.e.,* why does a material exhibit the properties that it does?, and how are these properties expected to change if we change something in the constitution of the material.

Theodorou points out a particularly challenging task — computational prediction of physical properties for polymeric materials, because of the extremely broad spectra of length and time scales governing structure and molecular motion in these materials. For instance, a polymer has structure at the level of atoms and bonds (10^{-10} m), at the level of entire polymer chains (10^{-8} m), at the level of domains in a semicrystalline material or a phase-separated blend (10^{-6} m or higher). A piece of Teflon is white because it contains crystallites that can scatter light, *i.e.,* are of a length scale commensurate with the wavelength of light (10^{-7}–10^{-6} m).

At the atomic level we have bond vibrations with periods 10^{-14} s. Individual bonds in a polyethylene melt flip between trans and gauche states every 10^{-11} s or longer, depending on the temperature. As a result of these flips, chains can adopt a tremendously large number of conformations. Longer pieces of chains take longer to change their shapes. The time required for a chain to move by a length comparable to its size in a melt and thereby "forget" its previous shape is 10^{-3} to 1 s for usual molecular weights. On the other hand, a glassy polymer, such as polystyrene, polyethylene terephthalate (PET), or the polycarbonate in your CDs, undergoes very slow structural changes (physical ageing) with characteristic times of years (10^7 s). Between vibration of chemical bonds and physical ageing of a polymer glass, we have 21 orders of magnitude in time scale, which is quite impressive.

"This challenge can only be met through the development of hierarchical analysis and simulation strategies encompassing many interconnected levels, each level addressing phenomena from the detailed atomistic to the continuum microscopic over a specific window of time and length scales. Complementary technologies, such as group contribution methods for the estimation of properties, and high-throughput experimentation aimed at the massively parallel synthesis of materials of similar constitution and testing of their properties are valuable for validating modeling methods and also for realizing the design principles reached by the modeling.

Theodorou is working with software developers for materials design that have already incorporated his methods into their commercial products. Examples are Accelrys, Inc. (San Diego, CA, and Cambridge, U.K.), and the recently founded company Scienomics SARL in France. We work closely with industrial researchers in order to develop methods and software appropriate for solving their materials design needs. For example, we have worked with BP in Naperville, IL, on permeability-related problems, with DSM Research BV in the Netherlands on adhesion and interface-related problems, and with Mitsui Chemicals in Japan on polymer equilibration methods. Although we are not a company, we welcome collaborations with industry — industrial problems are a great source of inspiration for us. Our primary need is for able and motivated young scientists and engineers (working as PhD students and post-docs) willing to embark on the development of these methods and their implementation on specific industrial problems. "This is far from routine work; it needs inspiration and dedication. I find it fascinating to enlist one's basic scientific knowledge and mathematical skills in order to understand and predict why materials behave the way they do, he concludes. CEP

8th Annual Chem-E-Car Competition

Racing to the Finish Line

The pressure was on, as students participating in the 8th Annual Chem-E-Car Competition — a highlight of the AIChE National Student Conference (Nov. 11–13, 2006; San Francisco, CA) — raced against the clock to optimize their cars after learning that this year's load was 10 mL of water and the target distance was 75 ft. For those unfamiliar with the event, students are given only one hour to tweak their shoe-box-sized cars, which are powered by a chemical or biological reaction. The competition consists of two runs, of which the best run is used to determine the winner of the competition. All award winners are listed in the box below.

After the first round, the Univ. of Dayton was in the lead, coming in just 22 in. shy of the 75-ft target distance. Right behind was the Univ. of Puerto Rico, registering a first run of 70 ft and 11 in., while Ohio State Univ. came in at 70 ft and 3 in. But, since it's the best run, and not the best average run that wins the competition, the title of top performer was still up for grabs.

In the end, the Univ. of Puerto Rico edged out the Univ. of Dayton by coming a mere 12 in. away from the specified distance. Meanwhile, the Univ. of Maine at Orono, which was in 12th place after the first run, came in third place with an impressive second run of 72 ft and 9 in.

This year's top three finishers used fuel cells to drive their cars. The Univ. of Puerto Rico's car, dubbed CoKi, used a proton-exchange-membrane (PEM) fuel cell that converted hydrogen and oxygen into water to provide a DC voltage to power a 0.5–3.0-V motor. The hydrogen fuel was supplied by an electrolyzer, which separated deionized water into gaseous oxygen and hydrogen that were stored in two cylinders mounted onto the chassis of the car. To ensure the containment of the gases in these cylinders during fueling, quick-release check valves were placed on the cylinders' inlets.

While hydrogen fuel cells have been the popular source for powering these miniature cars for the past several competitions, the Society of Biological Engineers (SBE) challenged students to think outside of the box and develop a car using a biological reaction. Winning the SBE-sponsored award for Best Use of a Biological Reaction to Power a Car was the Univ. of Minnesota. The car, named Gopher 2.1, used a propulsion system based on the enzymatic breakdown of hydrogen peroxide.

The University of Puerto Rico wins the 8th Annual Chem-E-Car Competition with its hydrogen fuel-cell powered car, CoKi.

Also new this year was a strong emphasis on safety. Recently, the AIChE Board required that a student leader and chapter advisor from each team receive AIChE-sponsored safety training before participating in regional or national AIChE Car Competitions. In total, 84 schools sent representatives to the Nov. 11, Car Competition Safety Workshop, conducted by the Safety and Chemical Engineering Education (SAChE) Committee.

SAChE also sponsored an award for Inherent Safety in Design. Winning this award was Michigan Technological Univ.'s car, Winter Wind, which used a hydrogen peroxide and catalase reaction in a pressure vessel to drive a pneumatic motor. According to the team, "the pressure vessel was rated beyond what we planned on doing with it and includes all of the necessary safety precautions and hardware."

The next round of competitions will be held in connection with the Spring 2007 regional student conferences, to be held at eight or nine schools beginning in March. Local section leaders may wish to contact regional conference host schools to offer their assistance as competition judges, corporate sponsors, speakers, etc.

FINAL RESULTS

Top 3 Performers
1. University of Puerto Rico
2. University of Dayton
3. University of Maine

Most Creative Drive System
University of Minnesota

Most Consistent Performance
University of Puerto Rico

Spirit of the Competition
University of Puerto Rico

Honorable Mention:
North Carolina State University

Top 3 Posters
1. University of Minnesota
2. University of Akron
3. University of Puerto Rico

Inherent Safety in Design
Michigan Technological University

Best Use of a Biological Reaction to Power a Car
University of Minnesota

Golden Tire Award
Oklahoma State University

Career Advice and Engineering Resources: Keys to the New Student Website

Compared to a decade ago, today's chemical engineering students are a lot more knowledgeable when it comes to surfing the Web. Plus, prices of laptops have dropped tremendously, so it's not an unusual sight to see a classroom of students with laptops in front of them, rather than a notebook and pen.

Keeping up with the times, AIChE has revamped its student website to give it a more attractive look and feel that should be appeal to today's generation of web-savvy students. But improved appearances are only just a part of the change — the new student website also comes with a lot more features that students can use to help them with their studies or even to potentially advance their budding careers.

The main highlights of the relaunched website include:

• "Ask the experts" advice — Need a little help with an engineering problem or maybe seeking some guidance on potential career choices? The new website now connects students with an industry professional or professor who can offer his/her insights.

• Internships-only area — Many students who want an edge over their colleagues try to get some work experience prior to graduating. Scouring the Web for internships may be one way to do this, but it can be quite time consuming to visit all of the various sites. The AIChE student website now has a newly designated area that is just for internship postings.

• Career tools for life — Using ExecuPlanet's CareerToolsPLUS, get strategic guidance and access to the top job sites, employer and HR posts, and also get advice and support to build a solid resume, and more.

• Wealth of engineering data — Powered by Knovel, the e-library offers 24/7 access to numerous interactive scientific references, handbooks, standards, databases, charts, and graphs.

Other new features include: discussion board; online calendar; RSS feed; instant messaging; student blogs; podcasts; and much more. Check it out for yourself at www.aiche.org/students.

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OBITUARIES

Robert J. Booker, 74, Pasco, WA

Richard J. Cordovano, 64, Sun City West, AZ

Benjamin L. Harris*, 89, Glen Arm, MD

Mehmet Uz, 53, Easton, PA

* AIChE Fellow

2007 AIChE Conference Calendar

For information and registration details, visit www.aiche.org/conferences or call Customer Service at 1-800-242-4363 or 1-212-591-8100 (outside the U.S.)

SBE's First International Conference on Biomolecular Engineering (ICBE)
January 14–18 • Coronado Island Marriott Resort • Coronado Island, CA

SBE's Conference on Accelerating Biopharmaceutical Development*
March 12–19 • Loews Coronado Bay Resort • Coronado Island, CA

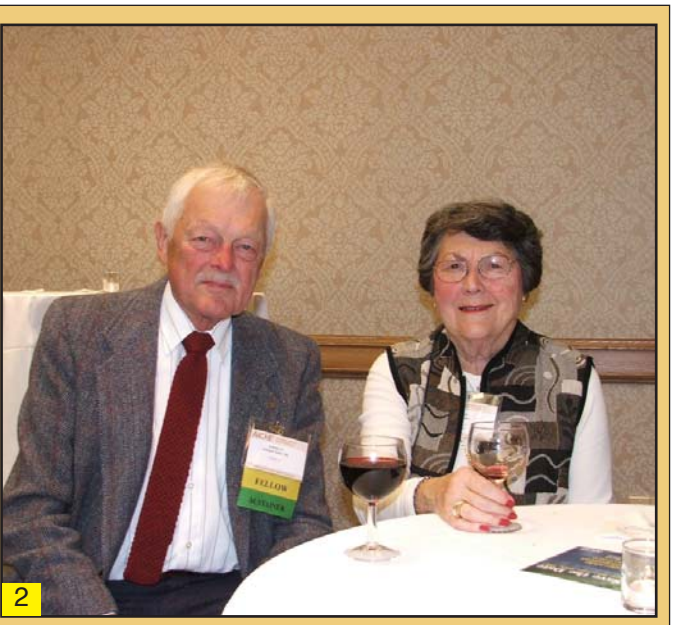
2007 AIChE Spring National Meeting*
April 22–26 • Houston Hilton & George R. Brown Convention Center • Houston, TX

2007 AIChE-ACS Management Conference
April 25–27 • Houston Hilton • Houston, TX

SBE's 3rd International Conference on Bioengineering and Nanotechnology (ICBN)
August 12–15 • Biopolis, Singapore

2007 Ammonia Conference
September 16–20 • Hyatt Regency, Las Vegas • Henderson, NV

*Call for papers is now open. Visit www.aiche.org/conferences for more information.



1. Fellow New Yorkers *Joe Porcelli* (left) and *Neil Yeoman* (right) catch up at the meeting.

2. *Mr. and Mrs. Emmett Miller* share a toast.

3. Former AIChE Treasurer *Dave Rosenthal* (center) meets with past presidents *Bill Byers* (left) and *Jeff Siirola* (right).

4. President-Elect *Dale Keairns*, Society for Biological Engineering Executive Director *June Wispelwey*, and *Ray Cocco* socialize at the welcome reception.

5. *Joyce* and *Phil Winkler* (left) (center) chat with *Terry Langevin* (right) at the Board of Directors Reception.

6 and 7. At the Student Conference Bash, the students who got lucky at craps, blackjack and other casino games took home iTunes as prizes.

8. Chemical engineering students cheered from the sidelines at the annual AIChE Chem-E-Car Competition (see story on p. 14).

9. Newly elected treasurer *Scott Love* takes a moment to pose for a photo with his wife.

10. An enthusiastic *Angelo Perna* (second from right), a ChE professor at New Jersey Institute of Technology, inspires future chemical engineers.