



# Rocky Mountain AICHE News

May 2003

Volume 12 Number 8

## May Section Meeting: Computational Chemistry In The Development Of Separation Processes

Although the computational chemistry has its roots at least as far back as the 1960's, it wasn't until the late 1970's that it began to be commercialized significantly. Since that time, its application to chemistry and engineering research and development has grown tremendously. In combination with experimental work, computational chemistry can be used to minimize the costs of developing new separation processes. As one example, the selection of solvents for extraction processes took three months using computational chemistry to supplement the experimental effort versus one year using more traditional techniques.

Our talk this month will be given by local AIChE section member Dr. Mark Plummer. Dr. Plummer will discuss four of the major chemical mechanisms that control separation processes: structure minimization in the removal of sulfur compounds from gasoline, size exclusion in the separation of xylene and naphthol isomers, and polarity/charge transfer mechanisms in the de-adsorption of hydrocarbons off catalysts. In all cases, computational chemistry was used to reduce the development time and costs of these processes.

Since retiring from Marathon Oil in January 2001 after nearly 40 years of service at the Petroleum Technology Development Center in Littleton, Dr. Plummer has worked as an independent consultant through his company, MPr&d, LLC. A 1997 National Medal of Technology nominee, Dr. Plummer holds thirty U.S. patents.

## May Section Meeting

**Speaker:** Dr. Mark Plummer  
MPr&d, LLC

**Topic:** Computational Chemistry In the  
Development Of Separation  
Processes

**Date:** Tuesday, May 20

**Time:** 6:00 Doors open  
6:30 Dinner Served  
7:00 Presentation begins

**Location:** Renaissance North Room  
Mary Reed Building on the DU  
University Park (main) campus  
2199 S. University Blvd.  
303-871-2000

**Cost:** \$15 (half price for students and unemployed)

Please RSVP by **Friday, May 16th**. Indicate your name, phone number, and number of attendees by e-mailing Kevin Milliman at [kevin.milliman@earthtech.com](mailto:kevin.milliman@earthtech.com). Alternatively, you may leave a voice mail for Kevin at 303-804-2374.

*Get Involved in Your  
AIChE Rocky Mountain Section*

Yes, it's that time of year again. As we start to wrap up the 2002-2003 academic calendar year, it is time to elect officers for the 2003-2004 year.

**We are in particular need of a volunteer for the Program Chair position for 2003-2004.** The Program chair is a vital position because the Program Chair, with some assistance from the other officers, arranges the monthly Section meetings from September through May. The Program Chair gets, free of charge, one year of exhilarating activity, opportunities to meet new people, and the attainment of personal gratification and growth that cannot be attained in any other way (and, by the way, your back pain will go away and your lawn will stay green without water!!). In all seriousness, the Program Chair position is a good opportunity to meet new people and to help keep the Rocky Mountain Section active and interesting. After one year, the Program Chair (also known as the Vice-Chair) typically moves on to the Chair position for the following year.

If you are interested in the Program Chair position for next year, please call Kevin Milliman (303-804-2374) or James Meyer (720-201-0148) for more information.

*If you are interested in any other of the officer positions for next year, or want to try your hand at the newsletter editor position next year, also please contact James Meyer for more info.*

**Awards Presented at the 2003 Colorado  
Science and Engineering Fair**

By Natalie Van Tyne, P.E.

The AIChE Rocky Mountain Section sponsored two special awards for outstanding projects in areas related to chemical engineering at the 2003 Colorado Science and Engineering Fair, held on April 10-12, 2003 at the Colorado State University campus in Fort Collins. A first place award for \$100 was given to Jessica Gaver, Deer Trail CO, for her project in Environmental Sciences, Senior Division, entitled, "Designing and Testing Solids to Remove Arsenic". She conducted an extensive study on the effect of pH on the removal of arsenic from soil, involving the design of experiments to characterize the differences in both pH and valence levels (+3 vs. +5) for arsenic compounds found in soil contaminated with mine tailings. The second place award was given to John Heermann, Haxtun, CO, for "Oil Pollution Solution II", in which he built a device for removing contained oil spills from water surfaces, combining a knowledge of surface effects with solutions to both mechanical and materials handling problems. John's project was also entered in the Environmental Sciences category, Junior Division. Both John's and Jessica's projects were continuations of past projects, with expansion into areas previously uninvestigated, and each clearly built on past experience and insight to produce new studies with outstanding depth of understanding and attention to detail. The Section congratulates them on their achievement, with encouragement to pursue careers in chemical engineering.

**UPCOMING MEETINGS**

*May is the last AIChE meeting for the 2002-2003 program year. There will be no meetings through the summer. Next meeting is scheduled for Tuesday, September 16th. Have a great summer!*

## *AIChE Meetings*

**2003**

June 22-25	Process Develop. Symposium Poconos, PA
Sept 4-5	Engr. & Construc. Contracting Scottsdale, AZ
Sept 15-18	Safety in Ammonia Plants Orlando, FL
Sept 23-25	CCPS Int'l Scottsdale, AZ
Nov 16-21	2003 Annual Mtng San Francisco, CA

**2004**

Apr 25-Apr 29	2004 Spring Nat'l New Orleans, LA
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For further information, contact  
National AIChE.

### National AIChE Contact Info

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## *Rocky Mountain AIChE Officers*

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Kevin Milliman	Vice-Chair / Program	303/804-2374
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Craig Wildemuth	Treasurer	303/791-6307
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The objectives of AIChE are to advance chemical engineering in theory and practice, to maintain a high professional standard among its members, and to serve society, particularly where chemical, engineering can contribute to the public interest.

## **Articles for Upcoming Newsletters**

Please submit articles for future newsletters to the editor at [mmoes@ekiconsult.com](mailto:mmoes@ekiconsult.com). Let us know of interesting technical items you're working on or are familiar with, what is happening in the Chemical Engineering programs or AICHE Student Chapters at the universities in the Section, unique and useful web sites, or any other information your fellow Section members may find of interest.

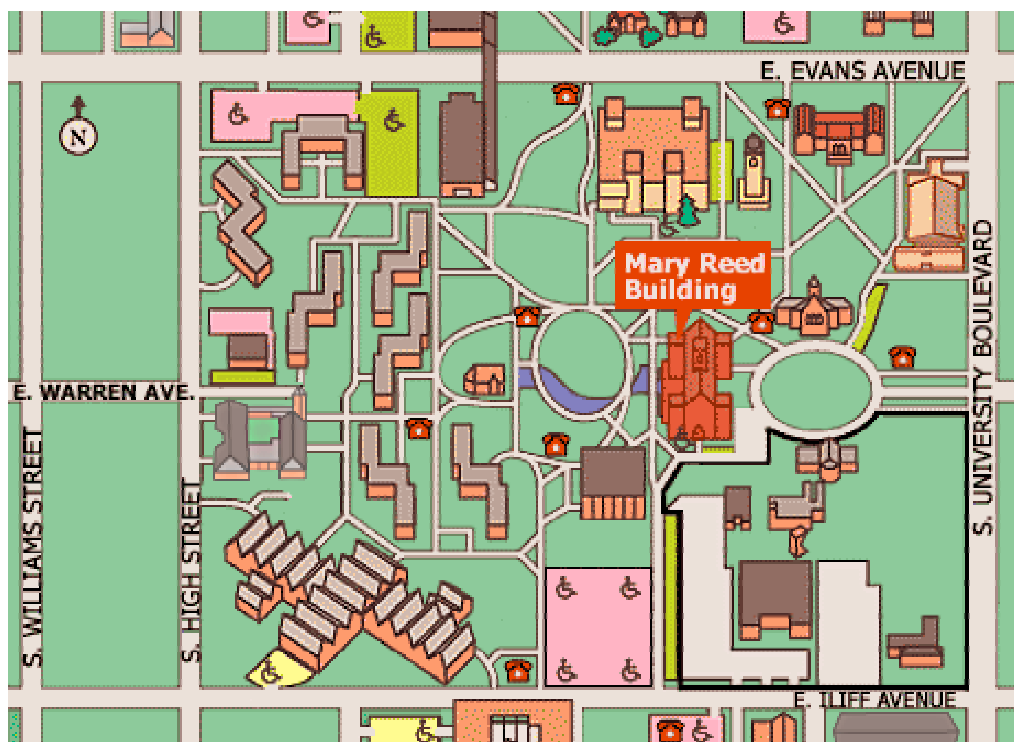
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**DIRECTIONS:**

From downtown, take I-25 south to University Blvd. Drive south on University Blvd about 2 ½ blocks. Turn right into the campus, then the first right onto the circle drive. Travel 2/3 around the circle, then take the right turn onto a road which parallels the south side of the building. There will be 3 hour metered parking on this road so **BRING COINS!**