

# AICHE-PITTSBURGH

## THE CATALYST

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## NOVEMBER 17 MEETING

### Designing amidine-based CO<sub>2</sub> sorbents - a computational and experimental study

John Kitchin

Department of Chemical Engineering

Carnegie Mellon

Atmospheric CO<sub>2</sub> concentrations are increasing by 1-2 ppmv/year due to CO<sub>2</sub> emissions from the combustion of fossil fuels for power generation and transportation. These emissions have been identified as a probable cause of climate change, and as a result we are now considering the capture and



sequestration of these emissions to minimize the effects of fossil energy utilization on the environment. Efficient methods for separating CO<sub>2</sub> from flue gas are needed to make the capture cost-effective and technologically viable. We are developing a sorbent-based approach to CO<sub>2</sub> capture in which molecular amines are supported on porous substrates. We have focused on a particular class of amines known as amidines and functional derivatives of amidines. We have used experimental methods to probe the role of moisture in the capture mechanism of CO<sub>2</sub>, the role of

the support in parasitic moisture sorption and the capture capacity of two amidines, DBU and DBN. A thermodynamic framework for evaluating the CO<sub>2</sub> capacity under different capture and regeneration conditions has been developed to show that each amidine is an optimal sorbent for different conditions. We have also used quantum mechanical calculations to explore the range of CO<sub>2</sub> capacities that might be possible from functionalized amidines. These functional groups modify the electronic and geometric environment around the CO<sub>2</sub> binding site through steric hindrance, hydrogen bonding and electron withdrawing/donating effects. We will discuss how these results are integrated in developing new CO<sub>2</sub> sorbents.

Continued on page 3

## UPCOMING EVENTS

October 23-24: Chemistry Week Celebration at the Carnegie Science Center (contact Julia at [Julia.A.Johnson@flexsys.com](mailto:Julia.A.Johnson@flexsys.com))

November 8-13: AIChE Annual Meeting, Nashville, TN

November 17: November program meeting, Waterfront Eat-n-Park (see this newsletter's notice)

January: Annual joint program with AMWA

January : Future City Competition, Carnegie Music Hall (AIChE awards "Most Creative Use of Recyclable Materials")

February: Job Searching for Chemical Professionals Workshop

February 16: Student Night

February 19-20: Engineers Week, Carnegie Science Center

### Please sign me up for the Pittsburgh Section of AIChE

Name \_\_\_\_\_

Company \_\_\_\_\_

Address \_\_\_\_\_

City \_\_\_\_\_ State \_\_\_\_\_ Zip \_\_\_\_\_

Business Phone \_\_\_\_\_

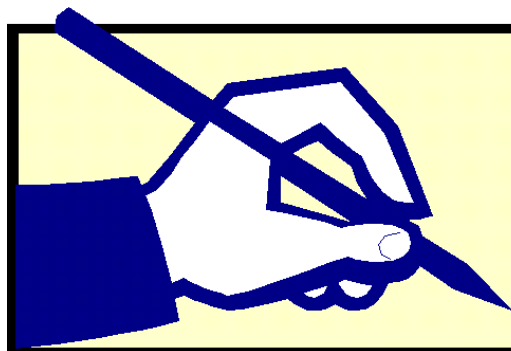
Residence Phone \_\_\_\_\_

Email \_\_\_\_\_

## BECOME A MEMBER OF AIChE-PITTSBURGH!

Local Section dues are \$20/year.

Contact Gary Hall: [gary.hall@sauereisen.com](mailto:gary.hall@sauereisen.com)



## LETTER FROM THE CHAIR

Dear Local Section Members,

I want to thank all those who have participated in our local section programs and volunteered in local technical activities. The individuals and companies whom we have asked, have accepted our invitation positively. We are grateful that they have contributed so much for membership and the local region.

You can look on the back of the newsletter and see our capable committee members, and notice some gaps in that list. In particular we need a Vice-Chair, Membership Chair, and Newsletter Editor. Please consider any of these positions, and let Chris Steffy know of your interest.

November 3 is Election Day. Its outcome impacts many chemical engineering-related issues such as biomedical, chemical processing, energy, and sustainability. However you choose to vote, it will be our duty to vote on November 3.

As we work to recover from the recession, keep in mind the opportunity to employ co-op students from Carnegie Mellon, University of Pittsburgh, West Virginia University and Youngstown State University. I continue to be impressed with their capability and resolve to work through difficult problems. One who went through such a program had become my boss's boss, and so you should expect that our regional chemical engineering students, co-ops in particular, can contribute substantially in ways to find and serve your clients and improve your company

Paul Brezovec

## NOVEMBER 17 MEETING (FROM PAGE 1)



John Kitchin completed his PhD in Chemical Engineering at the University of Delaware in 2004 under the advisement of Dr. Jingguang Chen and Dr. Mark Barteau. He received an Alexander von Humboldt postdoctoral fellowship and lived in Berlin, Germany for 1 ½ years studying alloy segregation with Karsten Reuter and Matthias Schefler in the Theory Department at the Fritz Haber Institut. John began a tenure-track faculty position in the Chemical Engineering Department at Carnegie Mellon University in 2006. At CMU, Professor Kitchin's research focuses on CO<sub>2</sub> capture, adsorption behavior, and electrochemical energy conversions, and. He is coordinating a major research effort within the National Energy Technology Laboratory Institute for Advance Energy Solutions (NETL-IAES) in CO<sub>2</sub> capture, sequestration and risk management that includes 12 faculty members and 18 graduate students. Professor Kitchin also uses computational methods to study adsorbate-adsorbate interactions on transition metal surfaces, which is funded by DOE-BES. Finally, his research group is developing electrochemical energy conversion technologies including fuel cells, electrochemical gas separations and hybrid hydrogen generation/CO<sub>2</sub> sorbent regeneration systems.

Where: Eat 'n Park Restaurant 245 E. Waterfront Drive, Homestead - (412) 464-7275

When: November 17, 2009

0600: Registration

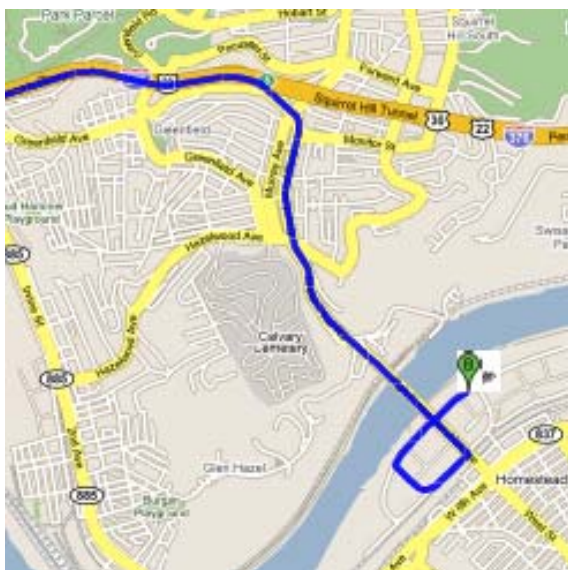
0615: Order your dinner from Eat 'n Park menu

0715: Presentation

Register: Limit is 30 attendees

\$15/student, \$20/member, payable at door

Reserve your spot by sending your contact information to Gary Hall at [gary.hall@saureisen.com](mailto:gary.hall@saureisen.com)

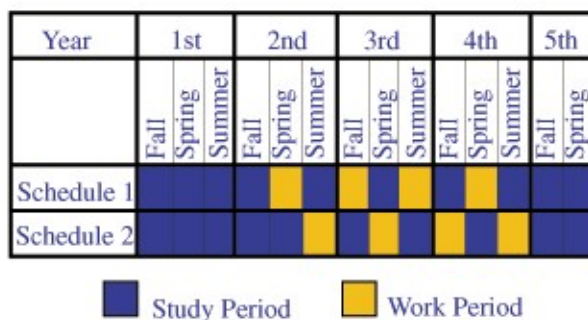


1. Head southwest on Grant St toward Oliver Ave
2. Turn right toward Grant St
3. Turn left at Grant St
4. Turn right to merge onto I-376 E toward Monroeville
5. Take exit 5 toward Squirrel Hill/Homestead
6. Merge onto Beechwood Blvd
7. Continue on Browns Hill Rd
8. Continue on Pgh Homestead Bridge
9. Turn right at E Main St
10. Slight right at Waterfront Dr E
11. Turn right to stay on Waterfront Dr E

## THE CO-OP EXPERIENCE AT WEST VIRGINIA UNIVERSITY – IS IT FOR YOUR COMPANY?

The Cooperative Education ("Co-op") Program in the West Virginia University (WVU) College of Engineering and Mineral Resources (CEMR) involves students alternating classroom study and work in a professional atmosphere during their college experience. These students are generally above-average in dedication and performance, as they have volunteered and been selected for this program. The Co-op program benefits participating companies as it allows them an extended period of time to evaluate these superior students while they are in an actual professional atmosphere. The students benefit because they obtain professional employment experience -- and earn a good paycheck -- while they are earning their degree. While a wide range of companies nationwide offer Co-ops to our students, we are interested in expanding the number of local companies participating in this exciting program.

The program is available to all undergraduate majors in the college: Aerospace Engineering, Biometric Systems, Chemical Engineering, Civil Engineering, Computer Engineering, Computer Science, Electrical Engineering, Industrial Engineering, Mechanical Engineering, Mining Engineering, and Petroleum and Natural Gas Engineering. Co-op students work three or four work periods throughout the five-year combined program, most often with the same employer (if both parties agree). Typically, Co-op students begin working either in the middle of their sophomore year or immediately following it, as shown in Figure 1. Juniors can also begin a Co-op following their fall semester; however, starting any later than that would require a special arrangement between the employer, the student, and the Co-op Office. Companies wishing to participate in an atypical co-op rotation are welcome to contact the Co-op Office. Examples of atypical rotations would be a Spring-Summer or a Summer-Fall work period. Availability of these rotations will depend on the engineering discipline, the company and the individual student.



**Figure 1: Typical Co-op Schedules**

Overall, industrial participants are better prepared to evaluate potential employees and have first crack at the more-marketable graduates. Participating students and employers almost unanimously agree that the Co-op experience is worthwhile, and they are the program's best ambassadors. If you are interested in participating in the WVU CEMR Cooperative Education Program, we would love to talk to you. Please contact the Co-op Coordinator, Lloyd Ford, via email at [Lloyd.Ford@mail.wvu.edu](mailto:Lloyd.Ford@mail.wvu.edu) or by phone at 304-293-4370.

*Editor's note: this is the first of a continuing series of articles about the Cooperative-Education programs at schools located in our local section area; others will follow.*

## OCTOBER 23-24: CHEMISTRY WEEK CELEBRATION

We are looking for volunteers for the AIChE booth at the National Chemistry Week celebration at Carnegie Science Center. The event will be held on Saturday, October 24 from 10am to 5pm. Volunteers are needed for the following shifts: 9:30-1:30, 1:00-5:00, or 9:30-5:00. Volunteers will receive free lunch and parking. To volunteer or for more information, please contact Julia Johnson at 724-258-2776 or [Julia.A.Johnson@flexsys.com](mailto:Julia.A.Johnson@flexsys.com)



## WESTERN PENNSYLVANIA'S ENERGY HERITAGE AND FUTURE SYMPOSIUM

AICHE-Pittsburgh co-sponsored, with the ACS (American Chemical Society) Energy Technology Group, a symposium titled "Western Pennsylvania's Energy Heritage and Future" to celebrate the pioneering work in our area that led to the development of the worldwide petroleum industry. The symposium, which was held at the Heinz History center on August 26, featured presentations on the history of the petroleum industry in Western Pennsylvania and prospects for its future. The highlight of the event was presentation of an ACS Historic Chemical Landmarks Plaque commemorating the development of the first one-barrel distillation unit for refining crude oil by Samuel Kier in downtown Pittsburgh in the 1850s. The plaque will be mounted permanently on the terrazzo wall at the USX Tower, at Seventh Avenue and Grant Street, near the location of the Kier still.

The next day, in Titusville, PA, a companion event was held to commemorate Edwin Drake's achievement in drilling the world's first oil well on August 27, 1859. Past AIChE president and local section member Dale Kearns spoke in Titusville and a second ACS Historic Landmark Plaque was presented.

Among the organizers were local section members Paul Brezovec, Gary Hall, Dale Kearns, and Jim Miller



ACS plaque commemorating Samuel Kier presented to Al Mann by ACS President Tom Lane



(L to R): Paul Brezovec, Gary Hall, Mordecai Treblow, Tom Lane, Tom Ruppel, Al Mann and Jim Miller at the Heinz History Center

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## 2009 AICHE PITTSBURGH SECTION SCHOLARSHIP

Congratulations to Mathew Payne, a WVU student, recipient of the 2009 AICHE Pittsburgh Section Scholarship of \$1,500. Keep posted for the request for applications in 2010.

## **AIChE-Pittsburgh Executive Committee 2009-2010**

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Open

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