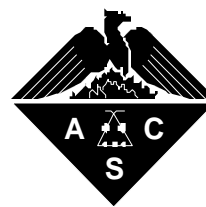


At the Interface of Science and Engineering



AMERICAN CHEMICAL SOCIETY

## SS&T NEWSLETTER

March 1, 2000

Becky Chamberlin, Editor

### **Gordon D. Jarvinen**

*Chair*

Nuclear Materials  
Technology Division  
Los Alamos National Laboratory  
505-665-0822  
gjarvinen@lanl.gov

### **James A. Ritter**

*Chair-Elect*

Dept. of Chemical Engineering  
University of South Carolina  
803-777-3590  
ritter@engr.sc.edu

### **Kent D. Abney**

*Vice Chair-Elect*

Chemical Science &  
Technology Division  
Los Alamos National Laboratory  
505-665-3894  
abney@lanl.gov

### **Gregg J. Lumetta**

*Treasurer*

Pacific Northwest  
National Laboratory  
509-376-6911  
gregg.lumetta@pnl.gov

### **Rebecca M. Chamberlin**

*Secretary*

Chemical Science &  
Technology Division  
Los Alamos National Laboratory  
505-667-1841  
rmchamberlin@lanl.gov

### **Kenneth L. Nash**

*Past Chair*

Chemistry Division  
Argonne National Laboratory  
630-252-3581  
nash@anlchm.chm.anl.gov

### Chair's Message

#### **SS&T in Y2K**

by Gordon Jarvinen

Now that the dire events that some predicted for Y2K have been safely avoided, I hope the year 2000 is proving to be a happy and prosperous one for you. Along with the onslaught of Y2K reporting, we have also seen a lot of looking back at the events of the 1900s and predictions and worrying about what we will face in the 2000s. The ACS is doing its share of prognosticating and certainly there is no lack of challenges ahead for humanity that will involve chemists in major ways to develop solutions. The "Millennium Special Report: Chemistry in the Service of Humanity," in C&E News Dec. 6 presented interesting overviews of some of these challenges and the exciting research and engineering that is addressing problems ranging from sustainable production of chemicals to the chemistry of the human brain. I thought many challenges for separation scientists were also apparent in these articles. Separation science and technology has important contributions to make from the scale of combinatorial chemistry methods using nanograms to petrochemical processing on the scale of billions of gallons.

Our program at the ACS Spring National Meeting in San Francisco certainly reflects the interdisciplinary nature and wide-ranging applications of separation science and technology. Symposia range from the fundamental, "Molecular-Level Characterization in

Separations" and "Equilibrium Modeling of Solution Speciation in Separations" to the practical, "Frank Derbyshire Memorial Symposium on Activated Carbon Separations" and "High-Level Waste Salt Alternative Separation Programs." A major programming theme of the San Francisco meeting is the "21<sup>st</sup> Century Celebration" and the symposium honoring the Separation Science and Technology Award winner, E. Philip Horwitz, fits right in, "Solvent Extraction and Ion Exchange in the 21<sup>st</sup> Century." Our Division program has additional symposia in this theme area, "Applied Chemistry for the 21<sup>st</sup> Century," "Catalysis for the Future," and "Emerging Technologies: Waste Management in the 21<sup>st</sup> Century." Come and join us at the Hilton for these and other interesting symposia!

Some developments within the I&EC Division will be of interest to our members as well. The former Materials Subdivision has been reorganized under the new chair Robert Haddon and is now the Advanced Materials and Nanotechnology Subdivision. This subdivision is planning a number of future symposia of potential interest to SS&T members including a symposium on "Functional Nanostructures" at the ACS meeting in August in Washington D.C. The Green Chemistry and Engineering Subdivision also has a number of symposia of interest including "Green Chemistry for the Reduction of Greenhouse Gases" at the San Francisco meeting and "Green

*Continued on page 2*

**Chair's Message**  
*Continued from page 1*

Chemistry: Applications in Academia and Industry" at the Washington D.C. meeting. The I&EC Division also is a cosponsor of the 4<sup>th</sup> Annual Green Chemistry and Engineering Conference to be held in Washington D.C., June 27-29. The I&EC Division continues to be active in the ongoing Vision 2020 process and a direct link to the Vision 2020 website can be found on the I&EC Division website. Several Vision 2020 workshops on separation technologies have been held and the summary reports from these workshops have been published or are in progress. These reports will be of considerable interest to the separations community.

We need your ideas and enthusiasm for future programming and other Subdivision activities. The Program Committee and the Executive Committee meet on Sunday, March 26, in the Hilton Hotel, Union Square 8, from 5:30-6:30pm and 6:30-8:30pm, respectively. Drop by

if you can or send ideas and suggestions to members of these committees.

**"Thank You" from the New SS&T Officers**

The new group of officers wish to express their gratitude to last year's team for all their efforts and their continuing participation in many cases. Ken Nash becomes Past Chair, but continues his excellent work on behalf of the Division in many ways, including serving on an ad hoc budget committee for the Division. We want to thank Doug Way again for his leadership as he leaves the Past Chair post. Andy Bond has done a great job as Secretary. We want to recognize Dave Rockstraw's efforts both as Membership Committee Chair and for developing the Subdivision's website. We thank these individuals and the Committee members listed below for their work on behalf of the Subdivision, and look forward to their continuing help and guidance in the future.

**Thanks to the 1999 SS&T Officers and Committee Members!**

**Officers:**

Kenneth Nash, *Chair*  
J. Douglas Way, *Past Chair*  
Gordon Jarvinen, *Chair-Elect*  
James Ritter, *Vice-Chair-Elect*  
Gregg Lumetta, *Treasurer*  
Andrew Bond, *Secretary*  
David Rockstraw, *Membership Chair*  
Spiro Alexandratos, *AICHE Liaison*

**Executive Committee  
Members-at-Large**

Bruce Moyer  
John Scamehorn  
Paul Smith  
Kent Abney  
Dick Bartsch  
Steve Cramer  
Dale Ensor  
Ralph Gatrone  
Robin Rogers  
Wally Schulz

**Programming Committee**

Gordon Jarvinen, *Chair*  
Kent Abney  
Spiro Alexandratos  
Dick Bartsch  
Andy Bond  
Steve Cramer  
Mark Dietz  
Dale Ensor

Gregg Lumetta  
Bruce Moyer  
Ken Nash  
Robin Rogers  
Jim Ritter  
Dave Rockstraw  
John Scamehorn  
Doug Way

**2000 SS&T Officers and Committee Members**

*Contact information for SS&T officers appears on the front page. We invite you to contact us with your ideas and concerns.*

**Officers:**

Gordon Jarvinen, *Chair*  
Kenneth Nash, *Past Chair*  
James Ritter, *Chair-Elect*  
Kent Abney, *Vice-Chair-Elect*  
Gregg Lumetta, *Treasurer*  
Rebecca Chamberlin, *Secretary*  
David Rockstraw, *Membership Chair*  
Spiro Alexandratos, *AICHE Liaison*

**Executive Committee  
Members-at-Large**

Bruce Moyer  
John Scamehorn  
Paul Smith  
Kent Abney  
Dick Bartsch  
Steve Cramer  
Dale Ensor  
Ralph Gatrone  
Robin Rogers  
Wally Schulz  
Andy Bond  
Doug Way

**Programming Committee**

Jim Ritter, *Chair*  
Kent Abney  
Spiro Alexandratos  
Dick Bartsch  
Andy Bond  
Becky Chamberlin  
Steve Cramer  
Mark Dietz  
Dale Ensor

Amudhu Gopalan  
Gordon Jarvinen  
Gregg Lumetta  
Bruce Moyer  
Ken Nash  
Dave Rockstraw  
Robin Rogers  
John Scamehorn  
Doug Way

**Electronic Distribution of Newsletter Available**

Past SS&T Subdivision Newsletters are archived on the Web at <http://membership.acs.org/s/sst/default.htm>. If you would prefer to receive this newsletter by email (pdf format), please send your email address to the secretary, Becky Chamberlin at [rmchamberlin@lanl.gov](mailto:rmchamberlin@lanl.gov).

# SS&T Programming for the San Francisco ACS Meeting

March 26-30, 2000

All Industrial and Engineering Chemistry sessions will be held in the Hilton Hotel.

<b>Symposia Overview</b>	<b>Sun</b>	<b>Mon</b>	<b>Tues</b>	<b>Wed</b>	<b>Thur</b>
Applications of Molecular Mechanics to Metal Complexes	D	D			
General Posters	E				
Activated Carbon Separations		D			
Molecular-Level Characterization in Separations		D	D		
ACS Award In Separations Science and Technology			D	D	
Equilibrium Modeling of Solution Speciation in Separations				DE	D
High-Level Waste Salt Alternative Separation Programs					A

A = Morning; D = Morning and Afternoon; E = Evening

## **Separation Science & Technology Award Honoring E. Philip Horwitz: Solvent Extraction and Ion Exchange in the 21<sup>st</sup> Century**

*Sponsored by IBC Advanced Technologies, Inc. and Millipore Corp.*

Phil Horwitz (Eichrom Industries, Inc., Darien, IL) will present his award address, "Forty Years of Radiochemical Separations" Tuesday morning at 8:45 in the Hilton Continental 2 Room. In addition, invited presentations featuring recent advances and future challenges in solvent extraction and ion exchange will be given by many of Phil's friends and colleagues.

## **Applications of Molecular Mechanics to Metal Complexes**

*Organized by: Benjamin P. Hay (Pacific Northwest National Laboratory) and Mark Zimmer (Connecticut College)*

This symposium focuses on how molecular mechanics calculations are being used to address issues in coordination chemistry. The emphasis is on model application rather than model development. With access to efficient desktop computers and the development of new software products, this has been a rapidly expanding field. As a result, contributed papers cover a wide range of topics including structure prediction, conformational analysis, metal ion recognition and ligand design, kinetics and mechanism of catalysts, and bioinorganic chemistry.

## **Frank Derbyshire Memorial Symposium on Activated Carbon Separations**

*Organized by: David A. Rockstraw (New Mexico State University), Marit Jagtoyen (Center for Applied Energy Research, University of Kentucky) and Christopher A. Toles (U. S. Department of Agriculture)*

Sessions on activated carbon separations will include discussions of the use of novel feedstock materials, unique manufacture techniques, the physical properties of the resulting materials, and the separation isotherms of activated carbons generated by these techniques. The session is a memorial in honor of Frank Derbyshire, a co-organizer of the symposium who passed away in August 1999.

## **Molecular Level Characterization in Separations**

*Organized by: Rebecca Chamberlin (Los Alamos National Laboratory) and Rich Barrans (PG Research Foundation, Darien, IL)*

This symposium will focus on the use of molecular-level characterization methods to understand the structural and thermodynamic factors governing chemical separations. Topics include spectroscopy, crystallography, surface characterization, theoretical modeling, chemical kinetics, and related studies of aqueous and non-aqueous systems.

## **Equilibrium Modeling of Solution Speciation in Separations**

*Organized by: Bruce A. Moyer (Oak Ridge National Laboratory) and Mamoun Muhammed (Royal Institute of Technology, Stockholm)*

This symposium will examine the state-of-the-art in modeling of speciation and equilibria in solutions with special emphasis on separations. It will focus primarily on the recent developments of methodologies for the determination and deduction of speciation in solutions; including aqueous and non-aqueous solutions. The symposium will provide a chance for the solution chemistry community to review the available computer codes developed for the calculation of solution equilibria. Overviews of some of these programs will be highlighted and discussed. The application of speciation and equilibrium data over a wide range of temperature and composition will be addressed. Some of the most known equilibrium calculation algorithms and databases and its use for separation processes will be presented. Hands-on software demonstrations will be given.

## **High Level Waste Salt Alternative Separation Programs**

*Organized by: Mark J. Barnes, Westinghouse Savannah River Company*

Papers will be presented relating to the three Salt Alternative Programs (i.e., Small Tank Tetraphenylborate, Crystalline Silicotitanate, and Grout) being investigated for the separation of cesium, strontium, and the actinides from high level waste at the Department of Energy's Savannah River Site.

**2000 International Chemical Congress of  
Pacific Basin Societies  
(PacifiChem 2000)**

December 14-19, 2000 in Honolulu, HI

***Separations Science: Trends for the New  
Century***

Separations are ubiquitous in chemistry research and in industry. Modern separation science often has to take into consideration the environmental impact of the separations process as well as the efficacy of the separation itself. The proposed symposium will bring together researchers from several Pacific rim countries with research thrusts in new separation technologies and the fundamental basis for those technologies.

The symposium will stimulate interest and discussion into how new technologies and new environmental regulations will affect separation science in the academic laboratory and in modern industry. The symposium is tentatively divided into five specific areas of interest:

- Green Separation Science and Technology
- Crystal Engineering of Porous Solids
- Ion Selective Polymers
- Industrial Separations
- Analytical Separations

*Organizers:*

Prof. Spiro D. Alexandratos, Department of Chemistry, University of Tennessee at Knoxville, Knoxville, TN 37996-1600 USA; Ph. 423-974-3399; Fax 423-974-3454; email alexsd@utk.edu

Prof. Akinori Jyo, Department of Applied Chem. & Biochem., Faculty of Engineering, Kumamoto University Kumamoto 860, JAPAN; Ph. +81-96-342-3053; Fax +81-96-342-2052; email jyo@gpo.kumamoto-u.ac.jp

Prof. Robin D. Rogers, Department of Chemistry, The University of Alabama, Tuscaloosa, AL 35487 USA; Ph. 205-348-4323; Fax 205-348-9104; email RDRogers@Bama.UA.edu

Prof. Mike Zaworotko, Faculty of Arts and Science, University of Winnipeg, 515 Portage Avenue, Winnipeg, Manitoba, CANADA; Ph. 204-786-9764; Fax 204-783-7981; email Mike.Zaworotko@uwinnipeg.ca

***Fall 2000 ACS Meeting***

Washington, DC  
August 20-24, 2000

No SS&T programming is scheduled for the Fall meeting. However, SS&T members may be interested in the call for papers from the NUCL Division, on page 6.

***Spring 2001 ACS Meeting***

San Diego, CA  
April 1-5, 2001

**SS&T Award Symposium Sponsored by IBC  
Advanced Technologies, Inc. and Millipore Corp.**  
Organizers to be determined.

**Fundamentals and Applications of Anion  
Separations** Bruce Moyer, Oak Ridge National Laboratory, P. O. Box 2008, Oak Ridge, TN 37831; Ph. 423-574-6718; Fax 423-574-4939; email moyerba@ornl.gov. See call for papers on page 5 of this newsletter.

**Separations in Environmental Analysis.** Organized by Dale D. Ensor, Department of Chemistry, Box 5055, Tennessee Technological University, Cookeville, TN 38505; email densor@tntech.edu and Martha Wells, Tennessee Technological University Water Resource Center, Box 5033, Cookeville, TN 38505; email mjmwells@tntech.edu.

*Great Symposium Ideas in Search of an Organizer!*

Contact Jim Ritter (ritter@sc.edu, phone 803-777-3590) if you are interesting in organizing any of the following symposia or suggesting potential organizers.

- **Applications of Dendrimers to Separations**
- **Nonbiological Combinatorial Separations**
- **Ultrafiltration**

***Planned Topics for 2001-2002***

**Polymer Supported Reagents: Fundamental  
Studies in Separation Science and Organic  
Synthesis.** Spiro Alexandratos, Department of Chemistry, University of Tennessee, Knoxville, TN 37996; Ph. 423-974-3399; Fax 423-974-3454; email alexsd@utk.edu.

**Field-Enhanced Separations.** James Ritter, Department of Chemical Engineering, University of South Carolina, Columbia, SC 29208; Ph. 803-777-3590; email ritter@engr.sc.edu.

*More Great Symposium Ideas in Search of an Organizer!*

- **Closed Loop Applications for Industrial Wastewater.** Organizer TBD.
- **Separations in Support of Carbon Management.** Organizer TBD.
- **Isotope Separations.** Organizer TBD.

## Fundamentals and Applications of Anion Separations San Diego ACS National Meeting, Spring 2001

Abstracts are requested for this symposium featuring anion separations from both fundamental and applied points of view.

Specific subtopics to be covered include:

- *Design and synthesis of novel anion receptors*
- *Selective separation and recovery of anions by ion exchange and solvent extraction*
- *Selective separation and recovery of anions by precipitation methods*
- *Crystallization of metallic anions in hydrometallurgy*
- *Determination of anions by ion chromatography and other analytical methods*
- *Anion-selective inorganic ion exchangers*
- *Environmental remediation and waste treatment*

As interest in new extractants and techniques for the separation of anions continues to expand, a corresponding need is growing for interaction between basic research and end uses. What challenges will have high impact to motivate

basic research? What exciting opportunities are being opened up in basic research that might lead to innovative products and methods? If you have insights to share on such questions, please contact:

Bruce A. Moyer  
Oak Ridge National Laboratory  
Bldg. 4500S, MS-6119  
P. O. Box 2008  
Oak Ridge, TN 37831-6119  
Ph. 423-574-6718 / Fax 423-574-4939  
email moyerba@ornl.gov

Raj P. Singh  
Osram Sylvania  
Chemical and Metallurgical Products Division  
Hawes St.  
Towanda, PA 18848  
Ph. 570-268-5441 / Fax 570-268-5350  
email raj.singh@sylvania.com

---

### 24<sup>th</sup> Actinide Separations Conference May 22–25, 2000

Alexis Park Resort and Spa, Las Vegas NV

#### Deadline for abstracts: Friday April 7, 2000

Suggested topics for this year's conference include:

- Actinide Separations for DOE program needs
- Pyrochemical Separations of Actinides
- Aqueous Separations of Actinides
- Actinide Speciation and Modeling
- Actinide Waste Minimization and Pollution Prevention
- Actinide Stabilization/Immobilization
- Actinides in the Environment, Remediation and Geochemistry
- Actinide Analysis and Characterization
- Special UCNI/Classified Session: any relevant topic

**Nominations for the Glenn T. Seaborg Award**, given annually to a US scientist who has made significant contributions to the laboratory or production scale separation, purification or recovery of actinide elements, are also sought. Deadline is April 7, 2000

**A tour of the Yucca Mountain Facility** on May 22 is planned in conjunction with this meeting. Non-US citizens must return a completed information form for the tour by Monday, March 13, 2000.

#### For abstract and registration information, contact:

Louis D. Schulte  
Phone: (505) 665-1100  
E-mail: lds@lanl.gov

### Gordon Research Conferences

The Gordon Research Conferences promote open discussions and the free exchange of ideas at the research frontiers of the biological, chemical and physical sciences. Scientists with common professional interests come together for a full week of intense discussion and examination of the most advanced aspects of their field.

*Gordon Conferences of Interest to SS&T:*

#### Membranes: Materials & Processes

July 29th - August 3rd, 2000  
Connecticut College, New London, Connecticut  
Chair: Richard D. Noble, University of Colorado  
Vice Chair: Paul Bryan, MIT Practice School

#### Separation and Purification

August 6-11, 2000  
Colby-Sawyer College, New London, NH  
Chair: Rakesh Agrawal, Air Products  
Vice Chair: John Pellegrino, NIST

#### Nuclear Waste and Energy

July 16-21, 2000  
Colby-Sawyer College, New London, NH  
Co-chairs: Ken Mossman, Arizona State University and Jordi Bruno, QuantiSci (Barcelona).  
Vice Chair: Greg Choppin, Florida State University

#### Conference programs and application forms

are available on the web at: <http://www.grc.uri.edu/> or call 401-783-4011.

**Other Symposia of Interest to SS&T**  
*Analytical Chemistry in Nuclear Technology*  
Washington, DC, August 20-24, 2000  
Sponsored by NUCL Division

A session entitled "Separations Chemistry and Radiochemistry" will be part of the symposium on Analytical Chemistry in Nuclear Technology at the Fall 2000 ACS Meeting. This session is an effort to address the traditional subject matter of the Gatlinburg analytical chemistry conference in conjunction with the Washington ACS Meeting. A workshop atmosphere will be encouraged

to allow researchers to communicate more informally and discuss "work-in-progress" results. Approximately one full day of short talks is anticipated, with a few 30-minute presentations where the subject matter warrants. A poster session will also be held if interest warrants. Papers on all aspects of analytical chemistry relating to separations and radiochemistry are solicited. Most talks will be invited, but authors interested in contributing a paper may contact the organizer of the Separations session, David Hobart, NMT-1, Mail Stop G740, Los Alamos National Laboratory, Los Alamos, NM 87544 USA. Phone 505/667-0205. Email dhobart@lanl.gov Hard copy abstracts are due 3/31/00; electronic submissions are due 4/8/00.

---

**New Web Site Makes Searching and Ordering ACS Books Easy and Less Expensive.**

ACS members can now order ACS Books online at a 25% discount and easily search for titles by author, title, keyword, subject, and symposia number by visiting <http://www.oup-usa.org/acs>. The ACS Books home page allows users to search the entire list of ACS Books by author, title, or keyword simply by clicking on the ACS logo. Or click on one of twelve ACS subject classifications and search for titles by subject. On symposia titles for which members qualify for a 40% discount (user is a member of the sponsoring division), orders must be placed using a discount coupon in the division newsletter or emailed to: [ixb@oup-usa.org](mailto:ixb@oup-usa.org). Current additional features include online table of contents for most titles, and an easy-to-use shopping basket for ordering. Future enhancements will include the ability to search and order all OUP chemistry and related titles at the 25% discount and an ACS Books Listserv, so subscribers can quickly learn about just published titles and special offers. For more information about the ACS Books web site contact Mike Seiden at Oxford University Press, 198 Madison Avenue, NY, NY 10016; phone 212-726-6070 or email [mes@oup-usa.org](mailto:mes@oup-usa.org).

---

Rebecca M. Chamberlin  
Editor, SS&T Newsletter  
CST-11, MS J514  
Los Alamos National Laboratory  
Los Alamos, NM 87545

**INSIDE THIS ISSUE...**

Chair's Message: SS&T in Y2K  
SS&T Programming Information  
Other Meetings and Symposia of Interest  
New and Departing Officers  
Electronic Distribution of Newsletter