

THE VORTEX

AMERICAN CHEMICAL SOCIETY
VOLUME LXXIV NUMBER 7

CALIFORNIA SECTION
September 2013



Rollie Meyers receiving the ACS 70 year member certificate from Attila Pavlath

Table of Contents

CHAIR'S MESSAGE	PAGE 3
SEPTEMBER SECTION MEETING	PAGE 4
CALIFORNIA SECTION ELECTION INFORMATION	PAGE 4
WESTERN REGIONAL MEETING	PAGE 5
OCTOBER SECTION MEETING	PAGE 5
SCIENCE CAFE	PAGE 5
DIRT ON DRY CLEANING PART 4 (W. MOTZER)	PAGE 6
INTERNATIONAL OLYMPIAD	PAGE 7
VOLUNTEERS NEEDED	PAGE 7
FAMILY SCIENCE NIGHT (POETRY CONTEST)	PAGE 8
FUN WITH FOOD MEETING REPORT	PAGE 8
PRESIDENT-ELECT 2014 CANDIDATE STATEMENTS	PAGE 9
BUSINESS DIRECTORY	PAGE 11
INDEX OF ADVERTISERS	PAGE 11



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THE VORTEX

Published monthly except July & August by the California Section, American Chemical Society. Opinions expressed by the editors or contributors to THE VORTEX do not necessarily reflect the official position of the Section. The publisher reserves the right to reject copy submitted. Subscription included in \$13 annual dues payment. Nonmember subscription \$15.

MAGAZINE OF THE CALIFORNIA SECTION, AMERICAN CHEMICAL SOCIETY

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Quantity Postcards
255 4th Street #101 Oakland CA 94607
Printed in USA on recycled paper

510-268-9933

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Chair's Message

Wally Yokoyama

Summer was hectic for me, and I am sure it was for you too. Every year I look forward to catching up on projects during summer. And because I saved up projects for the summer and take on student interns, summer becomes even busier. I am looking forward to Fall, and thank goodness it is September.

If you have not already done so please register for WRM! The registration website is www.wrm2013.org. The 44th Western Regional Meeting will be held in Santa Clara, CA, October 3-6. This is a great opportunity for students to present their research results and for all of us to learn about what is going on at some of our local but great chemical research institutions. Often I don't get a chance to talk to my peers, even though they may be local, unless we attend the same meeting somewhere in the world other than at our own institutions. The Hyatt Regency Santa Clara will host the conference and offers the conference rate of \$139. There will be some enlightening and entertaining talks such as UC Davis brewing Professor Charlie Bamforth's talk on beer. Some of you may remember him from the documentary, "How Beer Saved the World". The Bay Area is also the home of many

chemical instrument companies. This is a great opportunity to see the new instruments and learn more about them from local sales representatives.

The California section will have or have had a booth at the 39th Solano Stroll in Albany, CA. I hope that you will stop by (or have stopped by) to see us or, better yet, volunteered to man the booth. If you are looking for other volunteer activities please go to our website: CALACS.org. A small amount of your time can make a big difference in the community, especially to kids.

Speaking of kids, the U.S. Chem Olympiad team including a couple of Californians did extremely well this year. The results: Saaket Agrawal, Mira Loma High School, CA, silver medal, David Liang, Carmel High School, IN, gold medal, Rungpeng Liu, Ladue Horton Watkins High School, MO, gold medal, and Stephen Ting, Monta Vista High School, CA, silver medal. Congratulations to these students and their teachers.

I also want to congratulate the institution I work for: USDA, Western Regional Research Center, Albany, CA. WRRC was awarded an ACS Historic Chemical Landmark Award on August 29. The presentation of the award was made by Dr. Marinda Wu, President, ACS and California Section member.

Summer was busy and a lot was accomplished.



September Section Meeting *Understanding Detonations at the Atomic Scale*

Topic: Understanding detonations at the atomic scale: a grand computational and experimental challenge

Speaker: Laurence E. Fried, Group Leader for Chemistry at Extreme Conditions, Lawrence Livermore National Laboratory, Livermore, CA

Date: Thursday, September 26th, Social Hour Snacks: 6:00-7:00pm, Talk: 7:00pm

Place: Chevron Auditorium, 100 Chevron Way, Richmond, CA

RSVP: office@calacs.org (510-351-9922). \$10 for Members and Guests, \$5.00 for Students. Pay at door.

Directions: From SF Bay Bridge Take 80 North (Towards Sacramento), Exit Right on 580 at 80/580 Split. Continue about 6 mi from the split and take Richmond Pkwy/Pt Richmond Exit. Chevron parking is directly across from the offramp.

Biography

A high explosive (HE) releases chemical energy in an extremely short period of time. The release of energy is so fast that it creates a shock wave, called detonation, which travels at typical speeds of 8 km/sec, or 18,000 m/h. Detonating HEs reach enormous pressures and temperatures. When a typical HE detonates, it achieves pressures as high as 400,000 atmospheres (i.e., 6 million pounds per square inch), and temperatures reach more than 3,000 degrees Celsius. Under these extreme conditions, the nature of chemistry is fundamentally changed due to strong overlap of electrons and fast atomic motion.

LLNL scientists are investigating the chemical mechanisms of energy release in HEs. These investigations promise to enable the ever more precise predictions of the behavior of explosive materials across a wide range of conditions, and improvements in the safety of high explosives. Advances in computer power, coupled with advanced algorithms have allowed us to simulate detonations on the scale of atoms. Computer simulations predict very unusual chemical behavior during detonation. For instance, we have found that water can act as a catalyst in accelerating HE decomposition, and that nitromethane can take on metallic character for picosecond time scales. In order to validate and better understand these predictions, ultrafast shock wave experiments are being

performed that can measure shock waves in samples with thicknesses of only 10 μm , with a time resolution of 10 ps.

Although both experiments and simulations currently have shortcomings, we are making significant progress in understanding the chemistry of detonation. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Biography

Dr. Fried is a computational chemist specializing in chemical processes at extreme temperatures and pressures. His research activities include the first principles simulation of shock waves and detonations, the development of advanced equations of state for reactive materials, and chemical equilibrium modeling at extreme conditions.

Dr. Fried has a MS in Physical Chemistry and a PhD in Theoretical Chemistry from Cornell University in Ithaca. His undergraduate degree is a BA (Biochemistry) from Brown University, Providence, RI.

He is a member of both the American Chemical and American Physical Societies and recognized as a Fellow by the American Physical Society. In 2001 Dr. Fried was awarded the DOE Defense Programs Award of Excellence for development of the Cheeta thermochemical code.



44th Western Regional Meeting
October 3-6, 2013
Santa Clara, CA
www.wrm2013.com

Register now and pay a discounted early registration fee (before September 12) and save. This will be a great meeting with more than 400 technical papers and poster sessions, a Symposium on Nuclear Chemistry honoring Darleane Hoffman and a number of special events on the Chemistry of Beer and the Chemistry of Flavors. Visit the website for the complete program. A website is now available to book your hotel rooms. Reservations can be made at this web address: <https://resweb.passkey.com/go/ACSWRegion> There are reduced registration fees for students and pre-college instructors, retired, and unemployed member.

Exhibitors

Registration for exhibit space is still open. With the large number of papers being presented, there will be subjects pertinent to your company. The topics are timely: Fracking, stem cell; and the special programs will be entertaining. Abstracts of all papers and the name of speakers will be on the website by mid September. Visit and register online, **www.wrm2013.org** or send an email to vendorchair@wrm2013.org. Mention this meeting to your associates and colleagues.

Sponsorship

We are grateful to those companies who are providing additional support for this meeting by their contribution to one of the following programs.

The levels are:

Platinum \$10,000 Registration for 20, full page ad in program

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These represent an excellent opportunity to have your company's name and logo prominently displayed at the meeting, in publicity materials and on our website. Contact the general chairs at chair@wrm2013.org for more information. We are a 501(c) organization. Make your plans now to exhibit at a great meeting. We look forward to hearing from you soon.

Natalie McClure, Santa Clara Valley Section
Lee Latimer, California Section

General Co-Chairs
chair@wrm2013.org

Save the Date October Meeting

"First in a series – Innovative Companies in the Bay area." October Meeting Thursday, October 10th. No-host social time from 6-6:30pm, dinner from 6:30-7:30pm, and talk from 7:30-8:30pm. Venue will be determined.

Science Cafe Lafayette Library
Wed., Sept. 25th

7:00pm - 8:00pm, LLLC Community Hall, Reserve@LLLCF.org or (925) 283-6513 x.103 COST: \$ 5.00 per adult, free for youth

Join Pixar's Director of Photography for Lighting, Danielle Feinberg, as she demonstrates the process and varying stages in making an animated movie.

Complete information at www.calacs.org



The Dirt on Dry Cleaning Part 4

Bill Motzer

In Parts 1 and 2, I described the history of dry cleaning from Greco-Roman times until the Industrial Revolution.

In Part 3, I described the history of organic solvents as dry cleaning agents noting that by World War II, tetrachloroethene (PCE) had become the most popular solvent for cleaning and by 1962, it became the leading cleaning solvent of choice in the U.S. The unique chemical characteristics that made this solvent so useful and popular and its environmental impacts are described in this article.

General Characteristics

PCE (C_2Cl_4) (aka perchloroethylene and perc) belongs to a chemical group known as the aliphatic chlorinated hydrocarbons; these are largely synthetically produced volatile organic compounds (VOCs). However, PCE can occur naturally as it is produced by several temperate and subtropical marine macroalgae.

In general, chlorinated VOCs display very similar properties when released into the environment. PCE is a rather mobile VOC with a low boiling point (121 °C), moderate water solubility (~150 mg/L @ 25 °C), and low vapor pressure ($V_p = \sim 14$ mm Hg @ 20 °C). In its pure solvent state, PCE is heavier and less viscous than water; therefore, when released to surface water or a subsurface aquifer, it will sink through the water column: hence these solvents are called dense non aqueous phase liquids (DNAPLs). Its relatively low viscosity is also important. Because it is more fluid than water, PCE readily penetrates fractures and even micro fractures, such as those in cement/concrete, clay layers in sediment, soil, and rock. In the dissolved phase, however, its relative density (specific gravity or s.g.) is not significant; therefore, dissolved PCE does not sink through the water column.

Transport/Fate Processes

Air Transport:

Approximately 80-90% of PCE used annually in the U.S. is released to the

atmosphere, largely from dry cleaning use because PCE is a relatively volatile solvent. Fate: When released as a gas it degrades photochemically to phosgene and chloroacetyl chlorides with half lives ($t_{1/2}$) ranging from 96 to 251 days. Some PCE is subject to precipitation washout because of its solubility.

Soil Transport:

Because its density is greater than water, when released pure PCE will percolate through most soils, particularly sand and gravels. Dissolved PCE generally has lower percolation rates because its density is modified by being dissolved in water; the ultimate density of solubilized PCE is dependent on water concentrations. PCE movement may be somewhat retarded by very silty and clay-rich soil because it tends to sorb to the clay fraction. Based on its organic carbon coefficient (Koc), it is only moderately sorbed to most soils. But pure PCE can be relatively mobile in soils with low organic fractions (e.g., 0.1 to 4.9%) because it has a rather low soil partition coefficient (K_d) ranging from 0.05 to 0.5. PCE's mobility therefore depends on a soil's mineral and organic content; the general order for sorption of PCE in some natural materials is:

peat moss > clay > dolomitic sandstone > sand. Peat moss has the greatest sorption and sand virtually none.

Fate: PCE does not readily degrade in soil under aerobic conditions. Even though laboratory experiments show that PCE has an aerobic $t_{1/2}$ ranging from 6 months to one year, under actual conditions it may persist for decades.

Surface Water and Groundwater Transport: When spilled to surface water (i.e., lakes, rivers, and streams), PCE readily dissolves because of its high solubility. Because PCE has a low Henry's Law Constant ($K_H = \sim 1.5 \times 10^{-2}$ atm-m³/mol), it readily volatilizes from surface water, particularly if agitated or turbulent, and from groundwater.

Dissolved PCE and its degradation products tend to move with groundwater; this process is known as advective transport or advection. PCE tends to sorb onto individual soil particles, particularly the silt, clay, and

(Continued on page 7)

(continued from page 6)

organic fractions that slow or retard a VOC's movement. In most soils, groundwater traveling by itself has a retardation factor (R_f) of 1.0, particularly if soil is largely composed of sand; e.g., in sandy water-saturated soil, with total organic carbon (TOC) content between 0.001 and 0.1%, PCE's calculated R_f is from 1.01 to 1.66. However, for consolidated silty-clay, water-saturated soil with TOCs ranging from 0.001 to 0.1%, PCE R_f s are somewhat higher ranging from 1.01 to 1.50. Therefore, in such soils, PCE would be expected to move slower than groundwater advection rates.

Fate:

PCE does not degrade by hydrolysis. Most of PCE's degradation occurs by reactions or processes known as reductive dechlorination. This occurs largely from natural anaerobic or methanogenic bacteria secreting enzymes that catalyze the hydrocarbon molecule's chlorine, stripping and replacing it with a hydrogen ion. Therefore, molecular degradation or "decay" occurs by sequential dechlorination of the chlorinated hydrocarbon. The actual degradation process by such anaerobic bacteria is known as dehydrohalogenation with a generalized decay path of PCE as follows:

(1) PCE degrades to trichloroethene (TCE: C_2HCl_3).

(2) TCE degrades to cis-1,2 and trans-1,2-dichloroethene (cis 1,2-DCE and trans 1,2-DCE: $C_2H_2Cl_2$) with cis 1,2-DCE generated at approximately 30 times the concentration of trans 1,2-DCE and by a factor of 25:1.

(3) Cis 1,2-DCE, trans 1,2-DCE degrades to vinyl chloride (VC: C_2H_3Cl). VC degrades to ethene (ETE: C_2H_4) and carbon dioxide (CO_2) and water (H_2O).

A simplified anaerobic degradation pathway is:



VC is a known human carcinogen and in 2012, after years of extensive scientific study, the U.S. EPA changed PCE's classification from a "probable" carcinogen to a "likely" carcinogen.

Under experimental anaerobic conditions, PCE's $t_{1/2}$ range from 98 days to 4.5 years. In actual groundwater environments, anaerobic decay occurs at much slower rates, probably on the order of 5 to 10 years, which is why we find groundwater plumes with the different decomposition products many years after spills or releases. In a subsequent paper, I will describe how we are able to remediate this recalcitrant chemical.



International Chemistry Olympiad.

Team USA was awarded gold and silver at the 45th International Chemistry Olympiad. The U.S. National Chemistry Olympiad program would like to proudly announce the success of the Alpha Zeta Team at the 45th International Chemistry Olympiad competition, which concluded July 23, 2013 in Moscow, Russia.

U.S. Team students:

Saaket Agrawal, Mira Loma High School, CA, won silver medal

David Liang, Carmel High School, IN, won gold medal

Runpeng Liu, Ladue Horton Watkins High School, MO, won gold medal

Stephen Ting, Monta Vista High School, CA, won silver medal

The USA Team students competed against 291 students from 73 countries.

Congratulations to Team USA for this great achievement!

Volunteers Needed

Volunteers are needed to work on many aspects of the WRM meeting, please contact chair@wrm2013.org.

Family Math & Science Night October 23rd, 2013

National Chemistry Week is the leading ACS outreach program and a tribute to the vision of the late George Pimentel who launched the first celebration in 1987. It is where we tell the public how chemistry has improved our lives, and spark the curiosity that will encourage kids to study science. This year's NCW theme is, "Energy – Now and Forever!"

Our signature NCW event is Family Science Night, a tradition that goes back to 1997. We are looking forward to celebrating chemistry with Thornton Junior High School in Fremont who is hosting on Wednesday, October 23rd, 2013, 6:30 to 8:30 PM. Even if you've never participated before, consider joining our volunteer team for a memorable evening of entertainment and hands-on fun. The Scientific Jam Band will open the show, which will also include some spectacular demonstrations by Bryan Balazs. The Thornton staff is eager to help us fill the gym and a dozen classrooms with demonstrations and hands-on activities. Whether you have an idea for an activity, or just want to help out at one of the stations, we would love to hear from you.

The ACS also sponsors an NCW Illustrated

Poem contest for K – 12 students. Illustrations must be hand-drawn, and the poem should pertain to the NCW theme, "Energy Now and Forever!" Entries must be received at the California Section office no later than Friday, October 25th, 2013. The Section will award prizes for the best entries in the following categories: grades K -2, 3 -5, 6 -8, 9 -12, and the winning entries will compete in the national contest for cash prizes. Help make this contest a success by encouraging your local teachers or school to participate. Please contact the California Section office for details, including the required entry form. If you would like to help with judging the contest entries, please contact the NCW Coordinator.

Is your school or community group looking for resources to celebrate NCW? The California Section can supply NCW stickers, temporary tattoos, and other souvenirs, as well as copies of the Celebrating Chemistry publication, with a variety of articles and activities aimed at younger students. This publication and many other resources can also be found on-line at www.acs.org/ncw.

Alex Madonik
Councilor and NCW Coordinator
California Section, ACS

"Fun with Food" Meeting Report at the San Leandro Public Library

The San Leandro Public Library invited the California Section to present demonstrations and hands-on activities as part of their summer reading program. On Saturday afternoon, July 13th, we soon welcomed over 100 beginning readers and their parents who were delighted by Eileen Nottoli and Paul Vartanian's demonstrations-- a colorful demonstration of acid indigestion and the transformation of balloons frozen in liquid nitrogen – twenty large balloons were packed flat into one small cooler box, only to resume their fully inflated shape when taken out and warmed up again.

After the show, just about everyone seems to have tried the strawberry DNA extraction (supervised by Nicki Davis), as well as building some molecular models of plant scent compounds (guided by Charlie Gluchowski), and, of course, tasting the

liquid nitrogen ice cream. We were aided by over a dozen enthusiastic library volunteers from San Leandro's high schools. Special thanks to children's librarian Kelly Keefer, who arranged our visit, and to Chris Ota, our host. We are also grateful to AirGas of San Leandro for their generous donation of liquid nitrogen.

Many participants were ready to continue the discovery activities at home and took copies of Celebrating Chemistry with them, as well as Earth Day souvenirs and Periodic Table wallet cards. Celebrating Chemistry is published twice a year, in connection with the ACS celebrations of Earth Day and National Chemistry Week. If your local library would like to help us distribute them, please contact the California Section office and we will get them to you.

Alex Madonik

Statements from President-Elect 2014 Candidates

National ACS elections this fall will have three candidates for president-elect. An abbreviated statement from each of the Candidates is provided for your review.

Bryan Balazs

It's a great time to be a chemist!

The California Section has over a century of astounding contributions to chemistry, to our members, and to advocacy for science and education, and I am proud to have been an active section member for over twenty years. As Chair of the section in 2011, the International Year of Chemistry, I saw first hand our exciting wealth of programs and events, successes that were recognized with a record four ChemLuminary awards!

Against a backdrop of ever accelerating scientific advances, the ACS is in a position to continue to advocate for global investments in science, education, and policy. As ACS President I would be your ambassador for chemistry and our profession, and these are my priorities:

Education

Education is at the foundation of everything we strive to achieve through the ACS. I support advocacy for early exposure to science, especially for those where access is lacking. We also need to reposition ACS programs to address educational pipeline and student retention issues, along with defining the impact of, and our role in, educational changes as we continue to transition into a digital era.

(continued on page 10)

Charles Kolb

It's an honor to ask for your support as a candidate for ACS president. ACS is a vibrant and vital organization, successfully serving many members' professional needs. It is also a very important source of scientific information and insight for members and the planet's policymakers.

However, we live in a very challenging and rapidly changing world. Venerable institutions can become outmoded and irrelevant surprisingly quickly. It's vitally important that we ensure ACS's future relevance and effectiveness. We need ACS to help our current members deal with today's scientific and economic challenges. We also need an ACS prepared to meet the needs of our youngest members over their 50-year professional lives.

To ensure ACS's continued success I believe we must achieve three long-term goals:

First, we need a **robust, innovative and sustainable industrial base.**

ACS must work much harder to help develop the strategies required for faster evolution of an agile and sustainable chemistry-enabled industrial sector, where ACS members can innovate, produce and thrive. I believe that ACS can serve as a catalyst, bringing industrial leaders together to determine how to overcome

(continued on page 10)

Diane Grob Schmidt

BUILDING BRIDGES TO A BRIGHTER FUTURE

our world today is volatile, uncertain, complex and ambiguous. We face a global "reset" from many changes – after effects of the great recession; unemployment issues; a competitive global workforce and economy; universal, networked communication; racing technological change; heightened awareness of limited resources.

To assure a bright future for our members, let's marshal resources to bridge gaps and solve problems. Here's where to concentrate:

Employment: Our major concern! We need an atmosphere that encourages growth and increased employment.

Education. ACS can provide leadership toward an education that prepares future chemical professionals for gainful employment.

Scientific Information. Access to trusted scientific information anywhere/ anytime, a core member need.

Advocacy. Advocating strengthened funding of the Chemical Enterprise is critical to re-ignite America's commitment to science and technology, and to drive sustainable growth.

Collaboration. We must expand our strategic interactions with sister societies worldwide to

(continued on page 10)

(Balazs from page 9)

Careers

An education in science remains a great investment, and employers want the analytical thinking and advanced skills that result from hiring chemistry graduates. I pledge to help enable job-seekers to identify a broader set of opportunities including non-traditional employers of chemists and to provide more tools to address the dynamic nature of the job search environment. The ACS must also do more to nurture entrepreneurship, both within start up companies and small businesses as well as in educational institutions.

Public Outreach

Engaging the public is crucial to promoting the role of chemistry in a global context. To do this, we can partner with public figures to promote the value of science and science education, and we can better engage our connected and enthusiastic Student Members. We must also capitalize on ACS influence to connect science advocacy groups and unite them in our common mission.

For more information, see www.bryanbalazs.com. I would appreciate your vote – together let's lead the ACS into an exciting future!



(Kolb from page 9)

both technical and non-technical barriers blocking more efficient, cost-effective and environmentally acceptable processes and products.

Second, our members and students need **expanded understanding of chemistry's role in the world.**

ACS needs to help educators at all levels to help effectively present the beauty of fundamental chemistry. But we also need to help them convey the critical role chemistry can and must play to sustain and enhance our economy, security, health and environment.

Third, we need **members prepared to seize the future.**

Nearly all the critical challenges we face have significant chemical components. ACS must help members better understand how their vision and skills can contribute to a more prosperous and sustainable future.

Let's work together to achieve these three goals.



(Schmidt from page 9)

address issues of mutual and global interest.

What can the President do? Lead the way to initiate and support actions for solutions! The President can work with the grassroots to envision directions, to energize and engage the members. "Nothing great was ever achieved without enthusiasm".

What do I bring?

Experience in active leadership of ACS, energy for our shared vision, dedication to the Society and its members. I bring diversity and balance from industrial, national laboratory, and academic experience. I bring an open mind to our issues.

My Pledge: I will work with all in Council, Divisions and Local Sections to hear your concerns and suggestions, to communicate continuously with you. I offer determination, diligence, commitment and enthusiasm for our goals. My long, effective involvement in ACS governance at all levels from the Local Sections to the Board of Directors can give you this assurance. For more information, please visit my website at www.dianegschmidt.org.



BUSINESS DIRECTORY

SEARCHING FOR THAT SPECIAL JOB?

There are many companies and organizations searching for chemical and biochemical personnel to fill important jobs in their organizations.

- Companies for laboratory and management positions
- Universities & Colleges for teaching positions and laboratory personnel
- Hospitals for technical and research personnel

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- www.mboservices.net
- <http://www.calacs.org/page.asp?id=22>

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