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EDITORIAL

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Preface to the John M. Prausnitz Festschrift

This special issue of the *Journal of Chemical and Engineering Data* (JCED) honors John M. Prausnitz for his manifold scholarly and personal contributions of knowledge, thought, processes, and inspiration about the fundamentals and applications of thermodynamics. He is most noted for the creating the discipline of *molecular thermodynamics* and extending it to modeling of the property behaviors of an incredible range of chemical systems.

John Prausnitz was born in Berlin on January 7, 1928. He came to the U.S. in 1937 and attended elementary and high school in Forest Hills, NY. In 1950, he received a (five-year) B.Ch.E. degree from Cornell University, which was followed by an M.S. in chemical engineering at the University of Rochester in 1951. At these universities, John developed a strong interest in physical chemistry and chemical thermodynamics. Special faculty at Cornell also stirred an interest in the history of science, engendered a lifelong love for German poetry, and fostered skills in technical writing. John then began Ph.D. studies at Princeton University, joining the research group of Professor R. H. Wilhelm; his thesis was on rapid mixing and chemical reaction in fixed-bed reactors. He also gained some practical research experience by working for two summers at the Brookhaven National Laboratory.

As an instructor at Princeton, John was introduced to the teaching of chemical engineering thermodynamics, taught a course in chemical engineering for non-chemical-engineering students, and supervised several undergraduate bachelor theses. He also was "thrilled by magnificent choral music at the Princeton Chapel, inspired by sermons from numerous outstanding theologians including Reinhold Niebuhr and Paul Tillich", and engaged in philosophy seminars with Martin Buber.

Upon graduation, John moved in 1955 to the University of California, Berkeley, where chemical engineering was a division of the Chemistry Department. The program was small, with only 15 graduate students. While he was hired to do research and teaching in chemical-reaction design and supervised three Ph.D. theses in that area, John soon found he was more interested in chemical thermodynamics and, in particular, phase equilibria. His 30 publications between 1955 and 1961 are nearly equally split between the area of transport and reaction and the field of thermodynamics. Thereafter, the content was strictly physical properties and thermodynamics. The development of John's ultimate program was much inspired by chemistry professors Joel Hildebrand, Ken Pitzer, and Leo Brewer as well as by Bernie Alder at Livermore National Laboratory. Although John retired in 2004 after nearly 50 years in the Department of Chemical Engineering at the University of California, he is still active daily in research and correspondence.

Over many years, John Prausnitz has been remarkably productive in regard to insights, techniques, and results from molecular thermodynamics (this name first appeared in a 1967 paper with C.A. Eckert and H. Renon). This title signifies the combination of molecular theory with strategic data and appropriate computation to uncover and describe patterns of property behavior in chemical systems. His work has covered substances ranging from noble gases to hydrocarbons, petrochemicals, polymers, electrolytes, and proteins. The structures and mixtures include gases, liquids, solids, hydrates, colloids, gels, hydrogels, zeolites, fluid−fluid and fluid−solid interfaces, and critical regions. The content has thermodynamic and statistical-mechanics formalisms, consistency tests, formulation of phenomenological models based on physical chemistry, parameter estimation, and equation solving. The research has new data measurements, extensions of theories, and/or computation. Many in the field are unaware of John's extensive contributions of new data; he published 27 papers in JCED from 1971 to 2011, and many other journals show data from his laboratory.

To illustrate the incredible range and amount of John's output, CAS now lists John as an author of over 760 articles in 134 journals. His rate of publication has increased with every decade of work: in the year 2000, 35 papers had his name on them. John's international impact for personally engaging others is indicated by the fact that he has had 421 different coauthors from 67 different academic, industrial, and governmental organizations in more than 20 countries. The importance of his work is shown by

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the ISI Citation Index, which lists over 90 papers after 1970 having 50 or more citations. The 1975 article on the UNIQUAC excess Gibbs energy model coauthored with Denis Abrams has been cited nearly 2100 times.

The areas of John Prausnitz' attention have evolved over the years, demonstrating his fearless ambition to lead and prod others into new areas while filling in gaps in well-studied subjects. The thermodynamics work of his first decade focused on modeling and analysis, from the molecular to the macroscopic, of well-defined petroleum and chemical systems. The goal was to extend existing concepts such as intermolecular pair potentials, virial coefficients, and local composition models for activity coefficients for practical purposes. In the next decade, John took on polymers, chromatography, liquid adsorption, hydrates, and more complex chemical systems as well as group-contribution methods (notably UNIFAC) and more sophisticated molecular theories, such as models for statistical-mechanical partition functions. During the 1960s and 1970s, the Prausnitz laboratory produced work covering a range of traditional substances and systems that may have been wider than any in the world. Data and modeling dealt with vapor—liquid equilibria (VLE) and liquid—liquid equilibria (LLE) at high and low pressures, including some at cryogenic temperatures. Also measured were gas solubility, cryogenic surface tension, adsorption of gases on solids, aqueous vapor solubility and diffusivity, UV spectroscopy of solvating systems, and heats of mixing. Modeling included intermolecular potential models for virial coefficients and transport properties, statistical-mechanical partition functions, equations of state, excess Gibbs energy models, phase behavior of gas hydrates, specific chemical-theory models for complexing substances, and generalized corresponding-states property models for normal fluids and adsorption systems. Multiphase systems included solids in liquids and gases, gases in liquids and hydrates, and liquids in liquids.

In John's next decade, work in some prior areas continued, and new investigations examined electrolytes as well as complex mixtures such as petroleum fractions, waxes, asphaltenes, coal liquids, and polymers, mainly within the framework of continuous thermodynamics. After 1985, John began an exceptionally fruitful collaboration with Harvey Blanch on biochemical systems; CAS reports that they have coauthored 140 publications. The subjects were mostly related to proteins and their properties but also included electrolytes, surfactants, colloids, phase behavior, and partitioning. The works report experiments, modeling, and molecular simulation.

By the early 1990s, John had attacked essentially the whole panoply of fundamental and model systems that molecular thermodynamics could straightforwardly address. Since then, while he has continued to fill in gaps, his orientation has been toward systems applications, such as contact lenses and silicon wafers (mainly with Clay Radke), protein separations, and hydrogels.

In addition to being the ideal role model for advancing areas and renewing oneself, John has described opportunities for others to make a difference in addresses such as "Some New Frontiers in Chemical Engineering Thermodynamics" (1995) and "Athena, Hercules and Nausica: Three Dimensions of Chemical Engineering in the 21st Century" (2007), both of which were keynote lectures at the Triennial International Conferences on Properties and Phase Equilibria for Product and Process Design that were published in *Fluid Phase Equilibria*. Still at it in 2011, he cowrote an article entitled "Opportunities for Chemical Engineering Thermodynamics in Biotechnology: Some Examples" that appeared in *Industrial & Engineering Chemistry Research*.

Along the way, John produced the widely adopted graduate textbook *Molecular Thermodynamics of Fluid-Phase Equilibria*, which is currently in its third edition with coauthors R. N. Lichtenthaler and E. G. de Azevedo. He also has been involved with five monographs. The first, *Computer Calculations of Vapor—Liquid Equilibria* in 1967, was written with graduate students Eckert, Orye, and O'Connell to supplement an earlier work by Donald Hanson on computer calculations for the design of staged multicomponent distillation and extraction processes. Hanson assumed that the required phase equilibrium information could be found "somewhere", although there were no reliable public sources of data or models for petrochemical systems because the Van Laar and Margules models were unsuitable for many binaries and essentially all multicomponent systems. John recognized the power of the local composition approach of Grant Wilson and guided the development of that model as well as techniques for parameter regression and solving multicomponent VLE relations for low to moderate pressures. These were collected together with computer code in the book. It was revised and extended to LLE in 1980 with additional coauthors. A similar monograph for high-pressure VLE systems was written with Ping Chueh in 1968. Thus, the Prausnitz books and their computer codes became the principal public sources for the design program calculations. In a similar vein, John (with Aage Fredenslund) developed the UNIFAC group-contribution method to provide an accessible formulation of the solution-of-groups method for estimation of excess Gibbs energies of solutions.

In other dimensions, John joined Hildebrand and Scott in a later edition of their landmark book to publish *Regular and Related Solutions.* He also became involved in the third through fifth editions of *The Properties of Gases and Liquids*, the principal handbook of property data and modeling for fluid properties. The two first editions were authored in 1957 and 1967 by Robert Reid and Tom Sherwood. John joined them in 1977 to add content on phase equilibria; he continued to contribute to the later editions of 1987 and 2000 with Bruce Poling. Still at it, he now is the editor of *Annual Review of Chemical and Biomolecular Engineering*, whose inaugural volume was published in 2010.

As a reflection of both his discontent with current technical education and his breadth of scholarly vision, John has recently initiated the Bronowski Project to introduce relevant social and humanistic content directly into existing courses in chemistry and chemical engineering. The Project's goal is to prepare and provide a significant number of pertinent case studies that cover a wide range of technology—society interactions as encountered in the chemical and related industries. Science and engineering faculty will be able to use these in their classes to suggest to engineering students that there are alternatives to technology and that there are other ways to attain understanding of our world.

Needless to say, John has received a great number of diverse honors and awards—far too many to list here. The most significant recognitions include the United States Medal of Science (2005) and election to the U.S. National Academy of Sciences (1973), the U.S. National Academy of Engineering (1979), and the American Academy of Arts and Sciences (1988). John has received 12 major awards from the AIChE, ACS, ASEE, IUPAC, and the GPA. He has honorary doctorates from the

University of L'Aquila and the University of Padua (Italy), the Technical University of Berlin, and Princeton University. Twice he received Guggenheim Fellowships, and twice he was chosen for one-year research professorships at Berkeley's Miller Institute. His curriculum vitae lists 35 distinguished and keynote lectureships and 11 visiting professorships and faculty fellowships. He has served on several editorial boards and consulted for many corporations.

All of this productivity and these many honors might make one think that John Prausnitz could be more machine than human. Nothing could be further from the truth. John's positive impacts on people may be even greater than those of his scholarship. For example, it is well-known that John has an amazingly large "academic family"— the coterie of his 84 former graduate students who completed graduate degrees; 12 of these became faculty members, and 58 in succeeding generations went into academics. The family tree that was drawn in 1988 and now hangs in John's office also shows 305 "grandchildren", 104 "great-grandchildren", 42 "great-great-grandchildren" and three "great-great-great-grandchildren". More than 20 years later, there must be an immensely greater number, including many successive generations.

As a research advisor, John has been the perfect combination of counselor, coach, teacher, and banker. He structured his lab's environment to possess an elevated ambience, outstanding graduate students, diverse and able visitors, plenty of equipment, an overload of ideas, and a constant urging to do more and better. The best was that he empowered his colleagues and co-workers to grow and achieve. Thus, everyone benefited from exposure to John's standards of scholarship, learned from his insights and questions, understood his appreciation of all things human, and reflected upon the aspiration to "reach higher than we can grasp."

Those privileged to interact with John up close know he is one of the rare individuals of great capability and depth who is also generous with his attention and time. In addition to the wonderful hospitality he provides to all who visit him in Berkeley for shorter or longer periods, he is constantly uplifting in his manner and interactions, makes time for the many "molecular thermo groupies" who seek him out at many meetings and lectures, and faithfully responds to the vast number correspondences that arrive to ask questions about his work and solicit his wise counsel on personal and professional matters.

Further evidence of John's impact is the fact that nearly 200 papers have been submitted for this issue in his honor. The authors here who have had personal connections with John, as well as those in earlier festschrifts in *Industrial and Engineering Chemistry Research* (1998) and *Fluid Phase Equilibria* (2006), say in various ways and to various extents that he made a significant difference in each of their lives. Some reflect about his influence on them as professionals, while others relate things more personal. Some recall meaningful correspondence; all recall moments of interaction with John that are treasured memories.

Finally, in addition to his humanistic and cultural interests awakened in college, John says, "All my life, I have loved classical music, especially chamber music and opera. But in recent years, I have learned to appreciate popular music thanks to my daughter Stephanie's fiddle in a five-member band (The Stairwell Sisters) and thanks to my wonderful wife Susie of nearly 55 years strumming the ukulele." He is also justifiably proud of his son, Mark, who is Professor, Cherry L. Emerson Faculty Fellow, and Director of the Center for Drug Design, Development, and Delivery at Georgia Institute of Technology.

It is with great satisfaction that JCED presents this unique collection of papers on an exceptionally broad range of subjects to honor John Prausnitz as a profoundly influential person in our discipline. We believe that this Festschrift is in harmony with his positive philosophy, progressive outlook, and supportive attitude. Enjoy!

John P. O'Connell
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