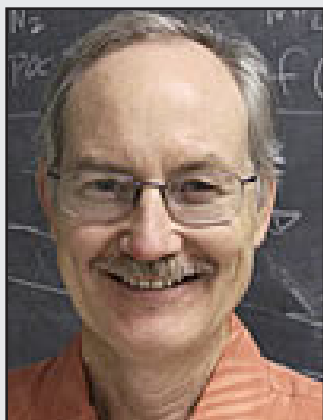## O.E. MEINZER AWARD

Presented to
David L. Parkhurst

David L. Parkhurst
U.S. Geological Survey, Denver

Citation By Pierre D. Glynn

I am honored to introduce David L. Parkhurst as the recipient of the 2012 O.E. Meinzer Award of the Hydrogeology Division of the Geological Society of America. This award is presented to David in recognition of his outstanding contributions to groundwater studies and geochemical modeling.

David's development and application of PHREEQE, NETPATH, PHREEQC, PHAST and related programs for geochemical modeling has changed the way that hydrologists and geochemists calculate, interpret, and predict geochemical reactions and subsurface reactive transport. David's mathematical, programming, and geochemical skills have produced software that is user-friendly, fast, robust, and widely accepted. As a result, geochemical calculations of exceptional theoretical and computational sophistication have now become standard techniques. In addition to his development of a wide diversity of geochemical codes, David Parkhurst has demonstrated the practical application of these highly sophisticated numerical tools in the hydrologic sciences.

David began his career at the U.S. Geological Survey (USGS) in 1969 when he was hired by Blair Jones as a student directly out of high school. David worked part time and during the summers at USGS Headquarters in Rosslyn, Virginia, and later in Reston, for Blair Jones and Niel Plummer, conducting research on many topics, including ion exchange, brines, and calcite dissolution kinetics (Plummer, Wigley and Parkhurst, 1978, American Journal of Science, v. 72). After completing his Bachelor of Arts in Mathematics from Davidson College in 1974, David briefly left the USGS in 1976 to work for the Federal Emergency Management Administration (FEMA) in Charlottesville, VA. Fortunately, David returned to the USGS in 1977 to work on the Potomac Estuary Project. This was a major gain for the USGS—and a loss for FEMA. This was when David began working on development of geochemical modeling software.

David wrote and published the geochemical code PHREEQE (Parkhurst, Thorstenson, and Plummer, 1980, U.S. Geological Survey Water-Resources Investigations Report 80-96) in 1980, a reaction-path model that enabled calculation of mineral equilibrium reactions, ion exchange reactions, and electron-balance calculation of redox reactions, as well as the simulation of solution mixing and simple irreversible reactions. PHREEQE was a highly innovative program at the time it was published. It was widely used for at least 15 years, and it also served as the basis for several other codes: including PHRQPITZ, a version of PHREEQE that incorporated the Pitzer equations to model high-ionic-strength brines (Plummer, Parkhurst, Fleming, and Dunkle, 1988, Water-Resources Investigations Report 88-4153), and PHREEQM (Appelo and Willemson, 1987, Journal of Hydrology, v. 94), another revolutionary code that allowed the simulation of 1D reactive transport.

David also wrote and published the inverse geochemical modeling code BALANCE (Parkhurst and others, 1982). Inverse geochemical modeling was a major conceptual breakthrough, in that it provided a mathematical technique that could help geochemists deduce the reactions responsible for the geochemical evolution of waters, including in environments undergoing oxidation-reduction reactions. The BALANCE code provided a foundation for the subsequent development of several other inverse modeling codes, notably the NETPATH codes published in 1991 and 1994 by Plummer, Prestemon, and Parkhurst. David recognized an essential limitation of the codes based on BALANCE, namely the fact that the calculations did not consider the uncertainties in chemical and isotopic measurements and in sample variability. David addressed this problem (Parkhurst, 1997, Water Resources Research, v. 33, no. 8) through an elegant derivation that allowed mole-balance models to be tested in such a way that every possible adjustment to the analytical measurement results within specified uncertainties was considered. He implemented this approach as one of the new capabilities of the general geochemical modeling code PHREEQC, a code based on PHREEQE but written entirely in the C programming language.

The range of gas/water/mineral/surface reactions that could be simulated In PHREEQC was greatly expanded beyond the capabilities that had been available in PHREEQE; additionally, the new code allowed both forward and inverse geochemical modeling. Subsequent work with C.A.J. Appelo led to publication of PHREEQC Version 2 (Parkhurst and Appelo, 1999, U.S. Geological Survey Water-Resources Investigations Report 99-4259). This version added capabilities to simulate dispersion (or diffusion) and stagnant zones in 1D-transport calculations; to model kinetic reactions with user-defined rate expressions; to model the formation or dissolution of ideal, multicomponent, or non-ideal, binary solid solutions; to model fixed-volume and fixed-pressure gas phases; to allow the number of surface or exchange sites to vary with the dissolution or precipitation of minerals or kinetic reactants; and to include isotope balances in inverse modeling calculations.

PHREEQC has continued to evolve since then. For example, it now includes a thermodynamic approach to isotopic fractionation processes that treats each isotope as a separate component (Thorstenson and Parkhurst, 2004, Geochimica et Cosmochimica Acta, v. 68). High-ionic strength activity coefficients and the Pitzer specific ion interaction approach have also been added, and the CDMUSIC (Charge Distribution-Multisite Ion Complexation) surface complexation model has been implemented.

While continuing to improve general geochemical modeling capabilities through his development of PHREEQC and associated codes, David recognized the need to couple forward geochemical modeling with groundwater flow and transport modeling. The 3D reactive-transport simulator PHAST (Parkhurst, Kipp, and Charlton, 2010, U.S. Geological Survey Techniques and Methods: 6–A35) was developed by David Parkhurst in collaboration with Ken Kipp, Peter Engesgaard, and Scott Charlton. PHAST combines the solute-transport simulator HST3D (Kipp, 1997, U.S. Geological Survey Water-Resources Investigations Report 97-4157) with PHREEQC. The simplicity of the model design and the ability to model

flow, solute transport, and a full array of chemical reactions make PHAST a widely used 3D reactive-transport code that has very impressive and useful simulation capabilities.

These contributions are all remarkable by themselves. They have advanced the understanding of groundwater geochemistry and more generally the application of aqueous geochemistry around the world. It is important, however, to recognize that David's achievements also stem from his deep practical understanding of the application of his codes, and from his constant willingness to help scientists and resource managers with their research or application problems.

David's practical understanding of geochemistry and hydrogeology developed during his career. He was awarded participation in the USGS graduate school program which led to a Master's degree in Applied Hydrogeology from Stanford University in 1983, and exposed David to highly advanced analytical techniques for the characterization of mineral surfaces. In turn, this led to David's assignment from 1983 to 1989 to the Oklahoma Water Science Center where he was the lead geochemist on a USGS National Water-Quality Assessment pilot project investigating abandoned lead and zinc mines. This experience gave David firsthand knowledge of the need for practical tools in groundwater studies. He returned to the USGS National Research Program in Lakewood, Colorado, in 1989 to lead a research project in geochemical model development.

Through his career, David has applied his expertise to a wide diversity of problems and settings, such as for example, laboratory studies of calcite reaction kinetics, the distribution of arsenic in Oklahoma groundwaters, the transport of phosphate in Cape Cod sewage plume, and studies of Aquifer Storage and Recovery in South Carolina. David is also recognized for his commitment and leadership in teaching groundwater geochemistry and geochemical modeling in the USGS and around the world. Teaching gave David broad exposure to many different types of problems, case studies and applications of groundwater geochemistry. In return, many scientists have greatly benefited from David's courses, and even more often from his advice and expertise; there are few people as selfless as David in helping other scientists.

In summary, David Parkhurst's work on chemical and reaction-transport modeling, and on the theory of inverse geochemical modeling, has greatly advanced hydrogeology and many other areas of science. It is not possible today to work in the field of aqueous geochemistry without being aware of, and needing to use, the products of David's research. David's scientific expertise and his sense of service and practicality reflect well on the scientific tradition set by O.E. Meinzer.

Please join me in congratulating David L. Parkhurst, recipient of this year's O.E. Meinzer award, for his outstanding contributions to the science of hydrogeology.

Response by David L. Parkhurst

I am deeply honored to receive the O.E. Meinzer Award from the Hydrogeology Division of GSA. I know that the scientists and scientific environment that so shaped my career can be directly traced to the work of O.E. Meinzer, who established the groundwater discipline in the USGS. So I offer my thanks to Pierre for his kind words, the Hydrogeology Division and the Awards Committee, and my friends and colleagues inside and outside the USGS who have made this Award possible. I also take a moment to thank my mother, who is here today. I have received a fraction of her intelligence and a fraction of my father's persistence, which have served me well. I thank them and my wife Renee for all of their support.

I was fortunate to begin my career just as computers were coming into wide use. It was inevitable that the field of geochemistry would be transformed by the possibilities presented by computing, and I was able to participate in that transformation. Computer programming suited me perfectly. I loved that you can take just a few programming commands and build complicated programs that could calculate such things as the amount of salt that dissolves in water, the chemical composition of a limestone groundwater, the migration of radionuclides from disposal sites, or the reactions necessary to account for the chemistry of a groundwater sample. It is extremely satisfying that computer codes that I and my coworkers Tony Appelo and Ken Kipp have written, particularly PHREEQC and PHAST, have been used by researchers, students, government agencies, consultants, and industry throughout the world.

I have spent nearly my entire career with the USGS starting as a high school volunteer, who had only a little chemistry and math, but an ability and willingness to learn. And I had great teachers. At any time, I could ask Blair Jones about clay mineralogy, Niel Plummer about carbonate chemistry and kinetics, Don Thorstenson about sulfate reduction and redox processes, and I could rely on all three when it came to the emerging field of geochemical modeling. In addition, the USGS sent me to graduate school for a year and I learned surface chemistry from George Parks, mineralogy from Gordon Brown, and dipped into the world of high energy physics at the Stanford Synchrotron Radiation Laboratory to study zinc ions at the atomic scale. So I was fortunate to learn my trade from some of the best in their fields.

I also learned the practical side of geochemistry through several major studies. In the laboratory, I helped to run experiments on the kinetics of calcite dissolution. In the field, we investigated the flux of nutrients from sediments in the Potomac River, sampled mine and stream water from abandoned lead and zinc mines in Oklahoma, made regional groundwater assessment of the Roubidoux Aquifer, and worked on a pilot National Water Quality Assessment (NAWQA) study of natural and anthropogenic contaminants in the Central Oklahoma aquifer. This experience taught me the realities of field studies, the limitations of data, and the opportunities for geochemical modeling.

From very early in my career, I developed geochemical models. However, I think the motivation to continually improve the models derived from teaching geochemical modeling to other scientists. I have taught dozens of short courses over the last three decades in the USGS and at outside institutions. Teaching is the quickest way to learn what works for users of a computer program and what does not. I always wanted to focus on the geochemical principals, but too often the mechanics of modeling got in the way. I hated trying to explain to a struggling student why an index needed to be a 2 instead of a 1, or that the input was in the wrong order. I wanted modeling to be easy; it should be like "back-of-the-envelope" calculations, where you can easily see the ramifications of selected chemical reactions. Accordingly, we have worked to make the modeling process more intuitive, so that models are more a source of insight from modeling results and less a source of frustration with modeling mechanics. And here, I must acknowledge the work of Scott Charlton, who is responsible for the simplicity of the graphical user interfaces for PHREEQC and PHAST.

Over the years, I have tried to answer all of the inquiries I have received about geochemical modeling. I have sent thousands of emails to scientists, consultants, professors, and graduate students. In part it was because I wanted my models to be used, but it was also an effort to do my part in extending the groundwater science of the USGS as envisioned by O.E. Meinzer. I also recognize that I have worked to develop tools for

studying problems, but, by communicating with other scientists, I can help begin the real work, which is to provide scientific solutions for the major environmental issues we face today, such as carbon capture and storage, radioactive waste disposal, mining for resources, aquifer storage recovery, and mitigation of groundwater contamination. So, if you have a geochemical modeling problem, especially you younger scientists, who will do the hard work on these issues in your careers, drop me an email and I will try to help.

It is a great honor to accept the Meinzer Award, and I thank you all.