Groundwater

Historical Note/ History Editor/David Deming

The Amazingly Rapid Birth, Growth, and Maturing of Digital Computer Modeling in Hydrogeology

by Fred J. Molz III

The Early Years

The roots of digital computer modeling in hydrogeology are found within the fields of Petroleum Engineering, Soil Physics, and Water Resources Engineering. Prior to the 1960s, digital computers were not sufficiently large or fast to solve most groundwater problems of interest, so many organizations, such as the U.S. Geological Survey (USGS) and the Illinois State Water Survey, developed electric analog models. Prominent names from that era include Gordon Bennett, Tom Prickett, Herb Skibitzke, Robert Stallman, and William Walton (Robinove 1962; Walton and Prickett 1963). Wealthy oil companies, such as Humble Oil and Refining in Houston, TX, anticipated the digital computer revolution, and in the mid-1950s Peaceman and Rachford (1955) and Douglas and Rachford (1956) developed numerical procedures for solving the linear, two-dimensional (2D), heat-flow equation, and related equations of the parabolic and elliptic types, which includes groundwater flow equations. At about the same time, a soil physicist at the CSIRO in Australia, John Philip, was studying nonlinear diffusion and heat flow—a more complex problem. Philip (1955) developed a combined analytical/numerical solution to the nonlinear diffusion equation with the diffusivity concentration-dependent. This laid the foundation for moving into unsaturated soil water problems, and Philip became a prolific contributor by developing his theory of infiltration.

By the end of the 1950s, the main mathematical basis for applied numerical analysis was established, but the required knowledge was not widespread. Also, the computational demands were ahead of the available computer power in most places. During the 1960s, however, computer power began to surge, and by mid-decade several groups were going strong—often without knowing about each other. Many of the now prominent journals, such as *Groundwater* and *Water Resources Research* were just beginning publication. So how did the petroleum engineering and soil-physics-based numerical methods move into hydrogeology?

Figure 1. Photograph of Irwin Remson at a graduation ceremony.

Across the world, many people contributed to the computer modeling surge, but in the United States two prominent individuals were the late Irwin Remson and late Paul Witherspoon; both were visionary researchers and truly outstanding educators (Figures 1 and 2). Irwin Remson worked at the USGS, Drexel Institute of Technology (now Drexel University), and then Stanford University, while Paul Witherspoon worked at the University of California Berkeley and the Berkeley Lab.

In a USGS Water Supply paper, Remson et al. (1961) presented a numerical analysis of water flow to a well in an unconfined aquifer based on the Dupuit assumptions. The resulting equation was a form of the radial heat-flow equation, so the procedure developed by Philip (1955) could be used. This was followed by a series of three papers published in the *ASCE Journal of the Hydraulics Division* (McNeary et al. 1962; Remson et al. 1965a, 1965b) that dealt with various aspects of soil water and

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Figure 2. Photograph of Paul Witherspoon.

groundwater flow. Numerical results were compared with previous field experiments (Remson et al. 1960). Remson et al. (1965a) paper entitled, "Ground Water Models Solved by Digital Computer" anticipated the next two decades of computer modeling in hydrogeology. Quotes from that paper include: (1) "The program in Table 3 may be applied to any aquifer—described by Equation (6)." (2) "It is believed that most groundwater data will eventually be stored on magnetic tapes and punched cards." (3) "It will be possible to analyze such data with the aid of readily available (computer) programs." Remson followed his own advice, and by 1970 he and his Ph.D. candidates at that time completed a textbook entitled, *Numerical Methods in Subsurface Hydrology* (Remson et al. 1971). Due to the influence of John Philip and his own consulting work at Seabrook Farms in New Jersey, Remson, and colleagues were interested in soil water flow as well as groundwater flow, and this stimulated my own early interests in transpiration, water flow to plant roots, and transport processes in plant tissue. Professor Remson never discouraged interdisciplinary interests.

Paul Witherspoon was a petroleum/geological engineer, who came to Berkeley in 1957, so it was natural for the previous numerical modeling capability developed by the Oil Industry to enter groundwater through the Berkeley conduit. While maintaining an interest in the oil/energy/geothermal areas, Professor Witherspoon and his colleagues produced a stream of world-class students and papers devoted to computer modeling in hydrogeology. Motivated by the earlier analytical work of Toth (1963), a distinguished Canadian hydrogeologist, Freeze and Witherspoom (1966) published a landmark paper developing a steady-state solution to the three-dimensional (3D), nonhomogeneous, groundwater flow equation. A 2D version was also solved, and it compared favorably with an analytical solution. Finite-difference equations were solved by successive over-relaxation and Gauss-Seidel iteration. Cited previous work included Forsythe and Wasow (1960), McCraken and Dorn (1964), and Remson et al. (1965a). Two other noteworthy papers followed. In many ways, Alan Freeze may be viewed as the first of the next generation of groundwater modelers, and he went on to have a very distinguished career in groundwater modeling and analysis (Freeze & Cherry, 1979). He stayed at the forefront of computer processing capability by working initially at the IBM Thomas J. Watson Research Center. In later life he received numerous awards from virtually all areas of hydrogeology, served as president of the American Geophysical Union (AGU) Hydrology section, and he is now a foreign member of the National Academy of Engineering (NAE).

Several of the graduate students of Remson and Witherspoon in the hydrogeology area made early contributions in various areas of applied numerical analysis. Javandel and Witherspoon (1969) along with Neuman and Witherspoon (1970) introduced the finite element method for solving groundwater problems and free-surface seepage problems, while Hornberger et al. (1969) published the first paper dealing with combined saturated/unsaturated flow. Hornberger, also the recipient of numerous awards, went on to serve as editor of *Water Resources Research* and the *Journal of Hydrologic Processes*. In 1996, he was elected to the NAE. Neuman's distinguished career also included many awards and NAE membership.

It is hard to overestimate the contributions of George Pinder and John Bredehoeft. Guided into hydrogeology by John Cherry and Robert Farvolen, Pinder, also a member of the NAE, received his Ph.D. in geology in 1968 with a minor in civil engineering and statistics from the University of Illinois. Taking leave from the USGS, Bredehoeft came to the University of Illinois as a visiting professor and began working with Pinder. They taught themselves numerical methods based on the petroleum literature. Pinder and Bredehoeft (1968) published a famous paper on aquifer evaluation using the digital computer. They dealt specifically with the 2D transient, heterogeneous, groundwater flow equation, and then with multiaquifer systems (Bredehoeft and Pinder 1970). Bredehoeft and Pinder (1973) extended their work to coupled flow and transport in groundwater, an indication of how fast the field was progressing. This model development was a precursor to MODFLOW. In 1972, Pinder and Frind introduced the Galerkin Finite Element method to the groundwater area.

It would be a real oversight to not review the contributions of the late Tom Prickett, a unique individual and lifelong learner. Prickett sought employment at the Illinois State Water Survey (ISWS) in 1960 with a B.S. degree in general engineering, and he was hired by Bill Walton. Prickett and Walton worked together on electric analog models applied to groundwater flow problems (Figure 3), but he made the transition to finite differences and digital flow models in the late 1960s, self-learning the equivalent of a Ph.D. in groundwater modeling. Prickett

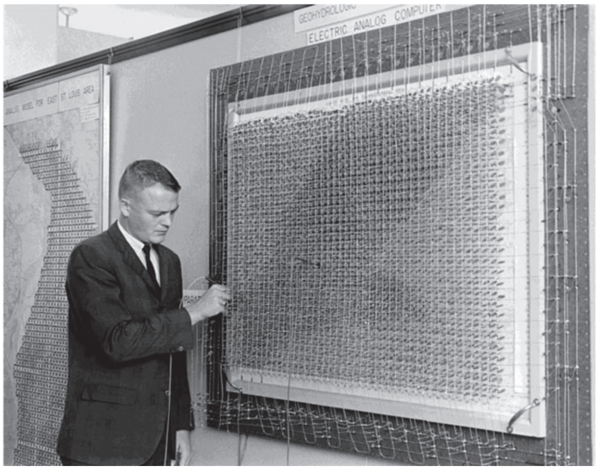

Figure 3. Photograph of a young Tom Prickett working on an aquifer electric analog.

and Lonnquist (1971) published an ISWS bulletin entitled, *Selected Digital Computer Techniques for Ground Water Resource Evaluation*. They developed one of the earliest, documented, general-purpose models called, "Prickett Lonnquist Aquifer Simulation Model (PLASM)" that was also a precursor to MODFLOW. Immediately there was a solid demand for Prickett's model-based consulting services, so in 1977 he left the ISWS to become a full-time consultant at Camp Dresser & McKee. In 1981, he opened his own office (Prickett and Associates), and some of Irwin Remson's former students worked there. Tom participated in many short courses on computer modeling, one of which I attended at the University of Wisconsin in 1972. There he argued good-naturedly with Jacob Bear about how to best derive finite-difference approximations to partial differential equations. (It turned out both were correct.)

Another prolific individual who followed a path of his own making was Gour-Tsyh (George) Yeh. George received his Ph.D. in hydrology at Cornell University in 1969 under Wilfried Brutsaert. He started publishing in 1968, and during the next 45 years he developed a huge number of documented general-purpose numerical models. Included were FEMWATER, FEMWASTE, and HYDROGEOCHEM. Yeh was a dedicated researcher dealing with the fluid mechanics of natural systems; he was a PI or Co-PI on 76 research projects and also coauthored 4 books. He worked as a consultant, an employee at the Oak Ridge National Lab, and as a professor at Penn State University and then the University of Central Florida. I'm sure that many of his programming techniques using the finite element method live on in a number of contemporary models. This is true for many of the early contributors, because most of the early programs were made freely available to anyone who was interested.

From the late 1960s and on, the programs at Berkeley, Stanford, the USGS, and Princeton (under George Pinder) graduated or mentored many of the early individuals with a modeling bent who went on to make major contributions to hydrogeology. Those from *Berkeley* included Alan Freeze (NAE member), Shlomo Neuman (NAE member), Iraj Javandel, T.N. Narisimhan, Karsten Pruess (NAE member), Ron Falta, Stefan Finsterlie, and others. *Princeton* produced Jim Mercer, Peter Huyakorn, Clifford Voss, Allen Shapiro, Linda Abriola (NAE member), and Mary Hill. *Stanford* yielded George Hornberger (NAE member), Fred Molz, Mary Anderson (NAE member), Steve Gorelick, Jean Behr, and Jim Butler, among others. Numerous famous groundwater names are associated with the *USGS*, both before and after the rise of groundwater modeling, and their constructive roles were vital. Those during the main period of interest include John Bredehoeft (NAE member), Stavros Papadopulos, George Pinder (NAE member), Peter Trescott, S.P. Larson, Arlen Harbaugh, Michael McDonald, Jim Mercer, Len Konikow, and Mary Hill. Over the years I've always been impressed with USGS leadership and productivity in the water resources area (Appel and Bredehoeft 1976).

The Rise of MODFLOW and Associated Models

According to McDonald and Harbaugh (2003), the immediate motivation for MODFLOW was that by 1981, there were approximately 500 separate flow models on the USGS mainframe computer, an indication of the rapid proliferation of groundwater modeling. The objective was to get most people dealing with practical problems working with the same highly flexible model, so a modular programming structure was utilized that would make it easy to add future model capabilities. This type of model structure became common, and the first version of MODFLOW was published in 1984.

As the modeling of groundwater flow began to mature in the 1980s, interest focused more on mass transport in groundwater. As a result, many specialized transport models were developed. Then in 1990, Chunmiao Zheng at the University of Alabama developed a model called Mass Transport in 3 Dimensions (MT3D) that interfaced with MODFLOW. By 1998 the model had been generalized to MT3DMS, with the "MS" standing for "multiple species." MT3DMS was then combined with MODFLOW and generalized to produce the public domain model called SEAWAT. This USGS-supplied model is designed to simulate 3D, variable density groundwater flow coupled with multispecies solute and heat transport. Zheng was an academic descendent of Irwin Remson through Mary Anderson. Both coauthored noteworthy books on modeling, with extensive reference lists (Anderson and Woessner 1992; Zheng and Bennett 2002).

Multiphase Flow at the Lawrence Berkeley Lab

In 1976, Narisimhan and Witherspoon published a paper in *Water Resources Research* describing the "integrated finite-difference method" for solving partial differential equations. This became the numerical basis for the TOUGH family of nonisothermal, multiphase

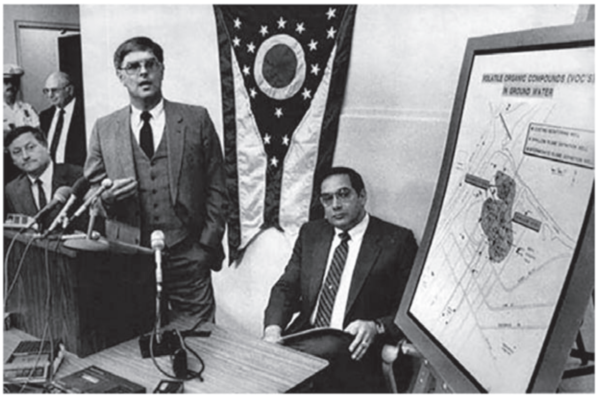

Figure 4. Photograph of Jim Mercer explaining problems at the Chem-Dyne superfund site.

flow codes. This included TOUGH, and updated versions, T2VOC, TMVOC, and TOUGHREACT. The ancestor to all of this software was an internal research code called MULCOM that dealt with geothermal energy, nuclear waste, oil, and gas. The person most responsible for this code family is Karsten Pruess, a physicist who received his Ph.D. in 1972 and published early research on nuclear physics. Pruess came to the Lawrence Berkeley Lab in 1977, and his first five papers devoted to geothermal reservoirs were published in 1982. Dr. Ronald Falta, an academic descendent of Paul Witherspoon, and a former student of mine at Auburn University, was the primary author of T2VOC, the first family member aimed mainly at multiphase environmental problems in hydrogeology.

Other creative researchers made many contributions to the environmental aspects of multiphase flow. Notable were the contributions of Hassanizadeh and Gray (1979) and Abriola and Pinder (1985), with many publications following. They built upon earlier work in petroleum engineering to develop theory and procedures better-suited for environmental problems.

The Private Sector Emerges

Following Tom Pricket in 1977, huge private sector contributions came from Starvos Papadopulos, Jim Mercer, and Peter Huyakorn. Papadopulos was an academic descendant of Madhi Hantush, who made prolific contributions to well hydraulics, and the latter two were academic descendants of George Pinder—with Mercer being Pinder's first Ph.D. student at Princeton. Huyakorn and Pinder (1983) published a widely read book entitled, *Computational Methods in Subsurface Flow*.

In the late 1970s, Papadopulos, Mercer, and close colleagues all worked for the USGS in the Washington, DC area. This highly creative group began to disperse, with Papadopulos forming "S.S. Papadopulos and Associates" in 1979. During that same year, the late Jim Mercer along with his colleague Charlie Faust founded "GeoTrans, Inc." (short for geological transport). Mercer and Faust (1981) published a short book through the (then) National Water Well Association attempting to, "... fill the gap between

Figure 5. Photograph of Peter Huyakorn.

those who develop models, and hydrologists, and managers who apply models ..." In 1980, they were joined by Peter Huyakorn who brought expert model development to the growing company. In 1981, Peter Anderson, one of my academic descendants from Auburn University, was hired to provide engineering expertise.

In 1985, GeoTrans was in the national spotlight while working on the Chem-Dyne Superfund Site in Ohio (Figure 4). S.S. Papadopulos and Assoc. also provided services at that site, and several retired USGS personnel joined that company, including Gordon Bennett.

Peter Huyakorn left GeoTrans in 1987, and he joined with another USGS colleague, Jack Robertson, to found their own company called "HydroGeoLogic, Inc." Peter had all the credentials and capabilities to pursue any career that he wanted in the broad fluid mechanics and mathematical modeling areas, but he was also a natural businessman. About four years ago I asked Peter what he thought were the most valuable groundwater-oriented models. His answer was: MODFLOW, MT3DMS, SEAWAT, and his own company code MODHMS. He said "MODHMS is the most comprehensive, MODFLOW-based, integrated, surface water/groundwater flow, and contaminant transport software suite available, and I have no doubt that this was true (Figure 5). In the mid-1980s Peter spent a semester at Auburn University teaching a course on finite-elements and developing simulations of aquifer thermal energy storage data from one of my field projects. He stayed in a double motel room, with one room, the larger one, always covered with computer programs and printout. In those days, mainframe computers were much slower, and there was a lot more paper involved—produced by huge, noisy printers.

The founders of the three companies mentioned are all nearing retirement, in retirement, or passed. The companies, however, are thriving. Hundreds of employees are involved, and each company has national and international offices. GeoTrans is now a subsidiary of the international company "TetraTech." Academic people tend to be devoted to teaching, research, and publishing new knowledge—all noble endeavors. It is easy, however, not to appreciate fully the tremendous contributions of the academically trained entrepreneurs who take the additional step of founding companies and dealing with real-world problems—the types of problems to which the NGWA responds. The origin, proliferation, consolidation, and commercialization of groundwater models define a time period of exceptional creativity in subsurface science. It is a privilege to have been part of that era and to record some of the history. For broad overviews of the past, present, and future of modeling, see volume 50(3) of *Groundwater*.

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