GRUNDVANDSMODELLER:
ET HISTORISK PERSPEKTIV PÅ DEN FREMTIDIGE UDVIKLING

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GRUNDVANDSMODELLER FOR MODELFOLK

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ABSTRACT

Ground water modeling has a rich history with four parallel streams of development. Ground water theory and analytical models have evolved simultaneously over the last 200 years. Numerical models arose in response to the availability of scientific computing facilities from the 1950s onward, and user friendly commercial and public domain models followed the arrival of personal computers in the early 1980’s. The arrival of user friendly software does not reflect a maturation or stagnation of the discipline. Important new developments in ground water modelling include a movement away from programming, toward using higher level PDE solvers, with more focus on the problems and less on the development of new numerical methods. New types of data, and integration of that data into models will continue to be a focus area. Finally, the boundaries of the discipline of ground water will continue to be extended and blurred as it becomes important to integrate groundwater into other dynamic systems.

INTRODUCTION

In 2001 Schwartz and Ibaraki published a very provocative discussion paper in which they hypothesized the maturation of the discipline of hydrogeology where most of the major discoveries have been made and the number of impactful publications is dwindling /1/. His analysis was based on trends in citation and publications databases. This paper was followed by a strong rebuttal by Miller and Gray /2/, who provided a list of unresolved challenges in ground water - a list worthy of the attention of a whole new generation of hydrogeologists.

In this context it is worth reviewing the history and future perspectives for ground water modeling. Is it a mature discipline or one that is vibrant and growing? Where are the challenges in ground water modeling? There has been an explosion in the number of publications in groundwater over the last 2 centuries. Has the discipline reached a saturation point, or does there continue to be fundamental advances? What will our future groundwater models look like?

Methodologically, this review presents considerable challenges. References and citations are provided to important events in the history of the discipline. However, in the interest of maintaining a compact presentation, not all key authors and their papers are presented. The review attempts to identify some important issues and trends in the discipline without attempting to provide a comprehensive overview of the subject.

HISTORY

The development of ground water modeling is occurring in four parallel streams, development of new theory, analytical solutions, solutions using numerical methods, and application in user friendly modeling systems. Ground water theory has steadily developed over the last two centuries (Table 1). New breakthroughs in our conceptual understanding have occurred regularly during that period and continue up to the present. Analytical modeling has occurred parallel to the theoretical development and continues to be important today. The potential of numerical models for ground water was recognized very early in the development of computing with foundations of numerical modeling being laid in the 1950’s to 1970’s. With
the advent of desktop computers in the 1980’s widespread application of user friendly groundwater models became possible. The theoretical developments of previous decades are now becoming widely available in the form of commercial or public domain software.

It is commonly believed that the first groundwater theory was that of Darcy /3/. However, a much earlier publication was an analysis of the salt water intrusion problem published by Du Commun in 1828 /4/ (cited in /5/). These two papers were then followed by the development of the basic theory of groundwater in the period from 1900 up to the 1950s. The theory of contaminant transport followed in the years from the 1960’s to the present. Two centuries of research has been punctuated by regular major advances in our understanding. While it is beyond the scope of this article to comprehensively review current developments, two recent breakthroughs are highlighted to show that research in ground water is far from reaching a conclusion. The first is the development of the groundwater age equation by Goode /6/ which allows the direct interpretation of environmental tracer data. The age equation is having a significant impact, for example it is now being applied in the calibration of groundwater models /7/. The second is the development by Gray and Hassanizadeh of a thermodynamically based theory for the multiphase flow equations /8/. This theory is necessary because the empirically based multiphase extension of Darcy’s law, the multiphase flow equations and associated constitutive relations, has repeatedly been shown to be inadequate for the description of real multiphase systems. This work is far from concluded as researchers struggle to come to terms with the implications of the new theory, but it has spurred a great deal of new research activity, for example in the classical area of pore network models /9/.

Analytical models are a natural adjunct to theoretical developments because they allow a direct analysis of processes and the relationship between parameters. An outstanding example of this use of analytical models is the work of Toth /10/, which lead to an understanding of regional hydrogeology. The discipline of hydrogeology would be much poorer without indispensable analytical solutions like the Theis equation /11/. A hasty analysis might conclude that the era of analytical model is over, given easy access to numerical solutions. Two recent analytical models serve to illustrate that the impetus for development of analytical models is as large today as it always has been. The first is a solution derived by Sudicky and Frind /12/ for the transport of contaminants in fractures. It is one amongst the most cited papers published in the 1980’s. A second example is the analytical solution for CO2 leakage recently developed by Norbotten and Celia /13/. This solution is important because the large scale simulation of well fields being considered for CO2 sequestration is beyond the capability of current numerical models.

Numerical models have revolutionized our ability to analyse ground water systems because they allow the simulation of far more complex systems than is possible with analytical approaches. The first to develop numerical models for groundwater systems were petroleum engineers /14/. But hydrogeologists were quick to recognize the potential of the approach, and a hectic period in the 1960s and 1970s saw the development of the first numerical models for many of the most pressing problems in groundwater. The timeline shown in Table 1 might suggest that with the publication of the first papers, the problems were solved, but this is not the case. For example, 20 years after the publication of the first numerical solution of Richards equation, Celia and Bouloutas published a new numerical solution that solved the mass balance problems occurring in previous models /15/. A review of the literature shows
that new numerical methods for the solution of Richards equation continue to be regularly published. Similar developments have occurred in all areas of numerical modeling.

The advent of cheap and powerful personal computers has meant that research models are now becoming widely available to practitioners. The 1980’s and 90’s have seen an explosion in the availability of commercial and public domain groundwater models. Such a development could be interpreted as a sign of the maturity of the field of ground water research, with a long era of development in theory and solution techniques, now culminating in an array of commercial and public domain products. But, this is a misleading analysis. Rather, the appearance of widely available models reflects easy access to technology. As demonstrated above, groundwater continues to be a very active area of research. With societal pressure for scientists to demonstrate applicability, it is likely that developments of new theory and numerical models will continue to be closely followed by the release of commercial software.
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Table 1. Overview of the history of groundwater modeling.
WHERE TO FROM HERE?

Our groundwater models are already very sophisticated and it could be argued that the theoretical foundations of the most popular groundwater models, like MODFLOW were laid many years ago. However, that would be a naïve argument, which does not reflect the continued improvement groundwater models have experienced with time. Two current trends in groundwater research are highlighted to illustrate the importance of continuing and recent research.

The first trend is a fundamental one because it reflects the way that ground water scientists work. Up until quite recently, if you wanted to set up a new numerical model of a groundwater system, then you had to have specialized knowledge in programming and a lot of time to do the programming. Conferences on groundwater modeling featured sessions that considered both developments in numerical methods and new developments in theory and practice. But now, commercial ground water modeling software has become available with good user interfaces. This means that the bulk of users do not need to be able to construct complex input files and debug software problems as they have done in the past.

For new theoretical development, commercial software is of limited use because it cannot be modified to accommodate new features. These users will increasingly be drawn to powerful generic PDE solvers, like MULTIPHYSICS /44/. This software allows researchers to develop new mathematical models, quickly find their solution and present results graphically. The availability of such software will greatly speed up research because it reduces the need for major research programs devoted to numerical solutions and model programming. The advent of this type of software also means that developments in numerical methods will increasingly be done by the applied mathematicians who maintain and develop such codes. While these developments will reduce the number of ‘hard core’ researchers in numerical methods for groundwater, there will still be some need for them. Generic PDE solvers cut development times, but can have poorer performance resulting in longer run times. They are also not designed to handle specialist input data, for example information on geology. This means that for large problems and specialist data input, specialist software will still be important.

A second trend has to do with the data that we use to drive and calibrate our models. Historically groundwater models have been calibrated using data on heads. However, new data is becoming available that can supplement head data, and parameter estimation techniques have improved so that it is now possible to conduct multiconstrained optimization, where the objective function is formulated to fit multiple constraints imposed by several types of data.

New data that can drive groundwater models includes radar measurement of precipitation, remote sensing of evapotranspiration and crop development, global climate model data to drive long term simulations, and geophysics. To illustrate the possibilities arising from new types of data, developments in gravimetric measurement are briefly reviewed. The basis of the technique is that the amount of water in groundwater storage affects the earth’s gravitational field. This observation dates back to the early 1970’s when Montgomery used changes in the earth’s gravitational field to estimate specific yield /48/. However, instrument sensitivity has until recently limited widespread adoption of the method. The recent literature suggests that
these barriers are increasingly being overcome /49/. The launch of the Grace satellite means that sensitive gravimetric readings are now also available via remote sensing. The Grace satellite has a bigger footprint (~300km) than earth based instruments, but is being used to calibrate hydrological models at cm vertical resolution on the continental scale /50/. This is but one example of the considerable advances that are being made in techniques for characterizing ground water systems.

Parallel to improvements in data that can be used to calibrate groundwater models are improvements to model calibration methods. Calibration tools are now available that can be coupled to any model /51/ and techniques for evaluating model uncertainty are becoming more sophisticated /52/. Statistical methods are being developed to assist in model choice /53/ and data assimilation techniques developed in meteorology allow for the dynamic calibration of ground water models /54/. All these developments will enhance our ability to analyse and identify new avenues of ground water research.

WHERE ARE THE BOUNDARIES OF THE DISCIPLINE OF GROUND WATER?

If a narrow view of groundwater is taken, for example, that the “groundwater hydrologist is primarily concerned with the water contained in the zone of saturation” /55/, then it could be argued that ground water is a mature discipline, with the most important developments having occurred long ago. But as Freeze and Cherry /56/ so succinctly stated “We shall retain this classical definition, but we do so in full recognition that the study of groundwater must rest on an understanding of the subsurface water regime in a broader sense”. This viewpoint continues to be as relevant today as it was 30 years ago. Much of the development of the discipline is occurring at its fringes, where groundwater interfaces with other physical, chemical and biological systems. These could be new work on ecohydrology, theoretical advances in multiphase flow, applications to carbon dioxide sequestration, interfaces to climate models and global carbon balances, or the coupling of groundwater into human management systems, to name a few areas of current research interest.

Amongst the most important trends in the development of new numerical models is a trend toward integration. In this regard, the development of groundwater models has an interesting parallel with climate models. Climate models have gradually increased in complexity, with increasing numbers of processes and more sophisticated coupling between them (e.g. figure 1.2, page 99 /57/). One of the challenges with this type of modeling is that it is highly interdisciplinary and requires huge resources. Hence some of this development is occurring in collaboration with institutions like the USGS /58/, or in commercial software concerns like DHI, with their MIKE series of products /38/. Researchers play an active role in these developments. One example of an integrated model that illustrated this trend is the development of a snow/ice/groundwater model designed to simulate hydrogeological systems over geological time scales to study climatic impacts on groundwater /59/.

CONCLUSION

Is groundwater research dead? No! It is looking up! Upward toward the land surface where there is intensive research being conducted on the interaction of the groundwater system with other components of the hydrological system. Future groundwater models will allow
increasing integration with other components of the hydrologic cycle. Contaminant mass balances and water quality will be part of this trend toward increased model integration. The future promises new measurement methods, and techniques to integrate these measurements into models of increasing complexity. At the same time, our understanding of classical groundwater will continue to be challenged, for example as we come to grips with new theories on multiphase flow. Our modeling tools will increasingly be built using advanced PDE solvers and commercial software as we move away from user designed and programmed software solutions. The gap between research and practical products will become even smaller, as technology allows the transfer of the latest research into new or improved user friendly modeling systems.

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