Variable density groundwater flow: From current challenges to future possibilities

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Introduction

Over the last decade or two, there has been an explosion in the field of variable density flow because of worldwide concern about the future of energy and water resources and environmental pollution. Recent exhaustive review articles on this topic by Diersch and Kolditz (2002) and Simmons et al. (2001) clearly illustrate the widespread importance, diversity and interest in applications of variable density flow phenomena in groundwater hydrology. These include seawater intrusion, fresh-saline water interfaces and salt-water upconing in coastal aquifers, subterranean groundwater discharge, dense contaminant plume migration, DNAPL studies, density driven transport in the vadose zone, flow through salt formations in high level radioactive waste disposal sites, heat and fluid flow in geothermal systems, palaeohydrogeology of sedimentary basins, sedimentary basin mass and heat transport and diagenesis, processes beneath sabkhas and salt lakes and buoyant plume effects in applied tracer tests. A number of interesting but yet implicit points also emerge from these recent reviews that set the scene for this essay and it is useful to examine the ancestry of this field briefly. Firstly, the field evolved from traditional fluid mechanics and its evolutionary timeline appears to contain four major stages. Earliest work was carried out in the early 1900s in heated fluids only with a move to combined heat and porous media studies in the 1940s, then to solute and porous media studies in the 1950s and 1960s and finally combined thermohaline studies in porous media in the 1960s. Whilst these studies provide the necessary foundations for the study of variable density flow in groundwater, there are numerous implicit and explicit assumptions, simplifications and fundamental differences that make the direct application of traditional fluid mechanics to groundwater hydrology challenging. Secondly, as groundwater hydrologists, our interest in energy and solute transport is relatively recent (post-1950s in general) so that there is only a small amount of overlap between the timelines for the developments made in traditional fluid mechanics and their somewhat immediate applications in groundwater hydrology. These points are of fundamental importance because it is often in the underlying subtle and not so subtle differences between groundwater applications and their fluid mechanics ancestry that currently identified challenges and shorter-term future research needs in the field of variable density flow are found. The number of unresolved issues in this field of research leaves little room for speculation on this point and it appears that in comparison to some other areas of hydrogeology, our understanding of variable density flow in real field scale applications is in its infancy. For the safe of brevity, this essay does not repeat the exhaustive reviews of Diersch and Kolditz (2002) and Simmons et al. (2001) and is therefore not a detailed bibliographic review. The reader is referred to those reviews for extensive reference lists. The intention here is to draw upon those cited reviews as well as a current literature investigation to highlight key emerging research challenges and to conclude by speculating on what appears to be enormous range of future possibilities for this field of hydrogeology.

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Variable density flow is important

By equating a very modest density gradient with a typical head gradient encountered in the field, the potential importance of variable density flow is revealed. Consider a typical groundwater hydraulic gradient of say a 1-m hydraulic head drop over a lateral distance of a kilometre. The equivalent "driving force" in density terms is a density difference of 1 kg/m^3 relative to a reference density of freshwater of 1,000 kg/m^3. This is equivalent to a seawater solution diluted to a concentration of about 2 g/l (only about 5% of seawater!), which is quite dilute in comparison to some plumes encountered in groundwater. This calculation shows that only very small concentration differences are required to achieve density driven flow gradients equivalent to typical field scale hydraulic head gradients. However, whether density driven flow is the dominant process involves a complex interplay between fluid properties, the competing demands of both flow driven purely by density differences (free convection) and that driven by hydraulic gradients (forced convection or advection), the properties of the porous medium and, very importantly, dispersion that dissipates density driven flow. The critical point to be made here is that a significant number of current studies on, for example, leachate plumes from landfills or tracer tests, should consider variable density effects but do not do so. This is because they assume, whether implicitly or explicitly, that density effects are small in comparison to other competing factors with little or no supporting justification.

Emerging research challenges

The complexity of variable density problems generally increases as one moves from situations where light fluid overlies dense fluid to potentially unstable situations where dense fluid overlies less dense fluid. The nature of the concomitant research questions generally grows in the same way and for this reason there is a natural bias in

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this essay towards unstable situations of variable density flow because these are, in general, the more scientifically challenging situations at present. In unstable cases, transport can be characterised by rapid instability development where finger instabilities sink under gravitational influence enhancing solute transport and mixing. On the basis of a review of current literature, a number of immediate challenges emerge for shorter-term future research. These include:

i. Spatial and temporal scales.
Whilst it is inevitable that some variable density processes will continue to require study at the laboratory scale where the controlling factors can be described better, field scale water resource management is necessarily one major practical driver for research. In moving from small scale laboratory experimentation to field scale applications, problems arise in defining appropriate conceptual models (e.g., heterogeneous vs. homogeneous) as well as understanding how critical features in that system change over longer time scales (e.g., sea-level rise in seawater intrusion problems). The difficulty lies less in the large scales as such, but more in the fact that variable density flow phenomena may be triggered, grow and decay over a very large mix of different spatial and temporal scales. The important consequence is that information on very small spatial scales and short time scales is needed to feed into long time and large spatial scale processes and simulations. Measuring field scale parameters across this large range of spatial and temporal scales also poses major technical challenges.

ii. Heterogeneity and dispersion.
Only recently has heterogeneity been considered in the study of dense plume migration. Studies show that heterogeneity in hydraulic properties can perturb flow over many length scales (from slight differences in pore geometry to larger heterogeneities at the regional scale), triggering instabilities in density-stratified systems and also enhancing dispersion in stable systems. Heterogeneity is a critical feature controlling the onset, growth and/or decay in variable density flow processes and dense plume migration is therefore not easily amenable to prediction. Understanding the role that variable density flow plays in enhancing dispersion is an area that requires further investigation since it will add to mixing, due to fingering, and is not covered by the current theoretical notion of dispersion. There is also a need to explore how more complex and realistic heterogeneity geometries affect variable density flow processes in sedimentary and fractured rock aquifers.

iii. Transient versus steady state analyses.
Many of the previous analytical research efforts were analyses with inherent steady state assumptions. Whilst many studies have employed a transient analysis with steady state boundary conditions, the use of transient boundary conditions is far more limited and will be very important in understanding the behaviour of variable density systems. For example, the source of dense plumes migrating from a landfill is often represented by simplified constant head, flux or concentration boundary conditions and yet the temporal loading is expected to be important. In general, the boundary conditions used in variable density flow analyses are far too simple and it is not yet clear what the implications of this simplification are.

iv. Nature of fluids, solutes and fluid–solute–matrix interaction.
Previous studies have typically been limited to single species conservative transport but a few have examined heat and solute transport simultaneously within thermohaline convection regimes. This may be important in understanding processes including mineralisation and ore formation in sedimentary basins, geothermal extraction processes and flow near salt domes. Complexity is exemplified where multiple species with differing diffusivities interact. Current research suggests that a more accurate depiction of fluid–solute–matrix interactions can be critical. It has pointed to the importance of (i) coupling chemical reactions with density dependent mass transport, (ii) incorporating precipitation and dissolution reactions, (iii) errors that may arise in ignoring viscosity variation, and (iv) effects that variable saturation of the matrix can have on variable density processes.

v. Analytical and numerical modeling approaches.
Whilst variable density flow problems do not lend themselves easily to analytical study except under simplified conditions, they may prove useful in addressing some challenges already mentioned e.g., upscaling, heterogeneity and dispersion. In addition, a number of numerical codes exists to simulate variable density flow phenomena. However, there are emerging difficulties and inconsistencies in recent literature that clearly show variable density flow simulation can be problematic at even low to moderate density contrasts. It appears that the nature of fingering and convective cell development are intimately related to choice of spatial discretisation. The important effect is that unlike in usual groundwater modeling, grid convergence cannot currently be achieved for many variable density problems. Future challenges clearly exist in accurately testing the reliability of numerical codes, particularly in unstable situations and in understanding how numerical accuracy, stability and dispersion affect the simulation of these processes. These issues are currently unresolved;.

vi. System complexity and simplification.
Simplification is a necessary step in developing conceptual models of hydrogeologic systems but the extent of permissible simplification and the ramifications of that simplification are not always clear. This is particularly true in variable density flow analyses. In many cases, the supporting science is ambiguous, unresolved or simply ignored and the implications are therefore either not known or not described. Assumptions of homogeneous aquifer properties, spatial dimensionality and the need for 3D simulation, transient versus steady state analyses, fluid–solute–matrix and physiochemical simplifications ignoring reactive transport and natural attenuation are just some examples beginning to emerge in recent literature. It is not clear just how important each is and under what conditions they can safely be ignored. A "mega sensitivity analysis" that includes the vast array of potential controls would be very useful in exploring the nature of the simplifications that are possible but does raise significant computational challenges.

vii. Dimensionless numbers.
In simple settings, dimensionless Rayleigh numbers (Ra) can be used to assess the ratio of buoyancy to dispersive forces and to determine whether a flow system is stable or unstable. However, there are currently problems and assumptions made in applying the Rayleigh number to the analysis of variable density flow problems. These include steady state flow assumptions, averaging of spatially distributed properties for use in dimensionless number computation, an inability to accurately quantify both time-dependent non-dimensionalising length scales and dispersion in plume problems and a limited knowledge of the critical Rayleigh numbers (Ra_c) for the onset of convection in real field settings. In the latter, the critical transition regions in flow and transport behaviour in groundwater systems are rarely known and it cannot be assumed that they are the same as those defined in earlier fluid mechanics for extremely simple boundary and layer conditions (e.g., $Ra_c=4\pi^2$ in an infinite horizontal homogeneous layer with perfect conducting upper and lower boundaries). Will it ever be possible to predict accurately a priori using dimensionless numbers and other generalised criteria?

viii. Field measurement and observations.
Possibly one of the simplest analysis approaches used in variable density flow is the concept of "equivalent freshwater head" but this is often too simple or even erroneous, especially where vertical flow is of interest. Whilst there can be no doubt that some variable density flow processes such as seawater intrusion have been measured in the field for many years, there are limited observations of unstable dense plume phenomena and free convection in field scale settings. Research papers often quote secondary evidence for their existence rather than direct evidence of the processes themselves (e.g., the salt deficit in the salt lake may be accounted for by the slow

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downward convection of dense water; numerical experiments demonstrate the existence of a convection cell; abundant data indicate high fluid fluxes consistent with density driven flow; the system Rayleigh number is greater than the critical value required and, therefore, convection is assumed to exist). But given the issues raised earlier, do these "observations" really support the existence of convective motion in the field?

Speculating on some of the future possibilities

Given the number of emerging challenges already listed, there is little, if any, evidence in current literature that points to the future extinction of this field of hydrogeology. Moreover, in speculating about some of the future possibilities below, there are undoubtedly many more exciting and challenging opportunities ahead that suggest both short-term and long-term prognoses for variable density flow research and its applications are very good. These include:

1. The need to describe and understand these processes better for real large scale aquifers appears to be the key scientific challenge at present. This requires useful tools that can be applied for understanding, predicting and managing both the quantity and quality of our water resources.
2. Variable density flow phenomena will change the way we analyse plumes developing from landfills and radioactive waste disposal sites, particularly in respect to reactive transport and natural attenuation problems. The idea that even a low density difference can affect the flow paths of contaminants is critical but needs wider acceptance.
3. The idea that dispersion, in addition to mixing length scale and porous media structure, is density dependent is largely at a conceptual stage but has important consequences for mixing and transport problems. It is not accounted for in traditional formulations of dispersion.
4. Better geological constraints on variable density flow analyses using lineaments, sedimentary facies data and structural properties of fractured rock aquifers is warranted. Understanding heterogeneity and its impact on variable density processes is very limited and should form a major area of future inquiry since this appears to be one of the most significant limitations at present.
5. Improving the resolution of geophysical, geoprospecting and remote sensing tools for non-invasive characterisation of both dense plumes and the subsurface heterogeneity structure at much finer scales of resolution than is currently possible would provide a wealth of currently unavailable yet necessary data for analyses. Furthermore, the rules for transforming geophysical data into unique quantitative hydrogeological information require clarification.
6. The current fields of tracer hydrogeology and variable density flow appear largely uncoupled. Understanding how environmental tracers used in estimating recharge, groundwater flow speeds and groundwater ages are interpreted in a variable density system is extremely limited. Where circulating and unstable flows exist, substantially different conceptual models for tracer interpretation may be warranted.
7. The development of a new range of artificial tracers for use in characterising dense plume behaviour and subsurface structure such as "smart dust" tracers in nanotechnology, DNA chain-sequence tracers to provide many new tracers with unique codes and benign radioactive tracers are possibilities. One particular feature that must be considered in futuristic tracer design is that of neutral-buoyancy i.e., tracer density relative to the fluid environment in which it is intended for use so as to both minimise floating and sinking of the tracer.
8. There have been a limited number of studies published in geophysical research literature in the 1950s and 1960s on thermally driven free convective mixing in boreholes. They clearly show that free convection can affect the data collected from the groundwater body in the monitoring well and can be a process of significance when interpreting hydrogeochemical log data. This message contained within geophysical literature does not appear to have been translated widely into groundwater studies. Furthermore, the potential for double diffusive convection to occur in monitoring wells has not been investigated but seems at least plausible given that it has been shown to occur in both soil science and oceanography which are respectively more and less "hydraulically constricted" than a well.
9. Artificial recharge "groundwater barriers" using density properties of saline/fresh water may grow in use to protect water resources, particularly in coastal aquifer regions.
10. A detailed analysis of variable density and double diffusive transport in aquifer storage and recovery applications, both for heat and/or fluid storage, is an area that warrants investigation as is the application of these phenomena to hot dry-rock systems.
11. Further understanding how the formation and migration of subsurface mineral energy resources are linked to thermohaline convection requires further elucidation. In particular, conceptual models for sediment diagenesis in low permeability strata require refinement to explain an apparent contradiction that high overburden pressures can be maintained whilst high fluxes through shale or clay layers required for observed levels of diagenesis are permitted. Alternative conceptual models should be explored e.g., a transient model where faults and fractures open and close over long geologic time scales where diagenesis and overburden pressure change are tied in a cyclical, yet possibly out of phase, process.
12. Over the next 100 years, and over substantially longer time scales, many areas of the Earth will undergo major climate changes in temperature, evaporation and precipitation and hence changes in the hydrologic cycle. Importantly, as sea level and coastline positions change, the impact of transgression and/or regression cycles on aquifer salinisation will be critical. The process of top-down reflux salinisation of aquifers by sea level rise is inherently variable density in nature. How to meaningfully couple climate and variable density hydrogeological models together in long-term analyses will be scientifically challenging. Most important are areas where precipitation and evaporation are in a very delicate balance and where a subtle climate change may be sufficient to reverse the dominant climatic process. How this will affect a variety of variable density phenomena is not at all clear.
13. In situ desalinisation within aquifers, particularly in saline environments, is an idea where the more dense stream of bitterns may be locally expelled at the point of desalinisation and sink away from the desalinisation facility in the aquifer. The longevity and environmental impact of such an operation requires a variable density analysis, possibly coupled with a dipole extraction–injection conceptual model.
14. The disposal of greenhouse gases such as carbon dioxide in aquifers has recently been discussed. The gas–liquid phase chemistry of such a process and its efficiency, safety and long-term viability as a storage option will necessarily involve an understanding of variable density transport dynamics with multiple phases.
15. A number of ecohydrological applications and studies are possible. For example, how density stratification affects certain groundwater dependent ecosystems requires further elucidation. The density dependence of baseflow accessions and other surface–groundwater interactions still requires exploration. For example, the efficiency of freshwater flooding and hence recharge across floodplains underlain by saline groundwater is not clear and may be lower than expected when buoyancy effects are properly accounted for. Another ecohydrological application is a density dependent analysis of the chloride "salt-bulge" formation and movement near and below the root zone in both natural and agricultural vegetation settings. In another area, the links between groundwater biology and variable density phenomena could be explored. For example,

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the extent to which the spatiotemporal distribution of stygofauna and biota in subsurface groundwater ecosystems are dependent upon fluid density through concentration and/or temperature is not yet clear. Interestingly, recent studies in oceanography suggest that the spatiotemporal distribution of marine phytoplankton is intimately linked with fluid convection and "phyto-convection" models have been proposed. Are there also links between groundwater biology and variable density phenomena that are currently unthought-of?

16. Some of the above issues point to the need for more accurate coupling of surface water, vadose zone and groundwater models. This is especially true in relation to variable density flow phenomena. There are clear ecohydrological, surface water–groundwater interaction and contaminant transport applications that will require such tools for improving analyses. The latter includes more accurate predictive ability of the fate of LNAPL and DNAPL plumes where processes in the unsaturated zone and at the water table are critical.

References

Diersch HJG, Kolditz O (2002) High-density flow and transport in porous media: approaches and challenges. Adv Water Resour 25(8–12):899–944

Simmons CT, Fenstemaker TR, Sharp JM Jr (2001) Variable-density groundwater flow and solute transport in heterogeneous porous media: approaches, resolutions and future challenges. J Contam Hydrol 52(1–4):245–275

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