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ABSTRACT

The phenomena of groundwater motion and the recent developments in the Theory of Mixtures are reviewed. Comparisons of these results with those from classical theory are presented. Phenomena of interest that are not well explained are discussed and the potential of the Theory of Mixtures in addressing these phenomena is presented.

1. INTRODUCTION

The flow of groundwater and the physical constraints that affect its behavior have been of interest for centuries. In the past several decades, the availability of groundwater has been affected by excessive withdrawals and the quality of groundwater has been degraded from improper control of contaminants. As a result, social concerns relating to groundwater resources have increased dramatically. Unfortunately, our understanding of groundwater behavior is not sufficient to answer all of the questions related to this valuable natural resource. The Theory of Mixtures provides a means for analyzing groundwater phenomena from a more rigorous point of view than the classical methods applied to groundwater. This paper reviews the Theory of Mixtures as it relates to groundwater phenomena and identifies several issues related to groundwater behavior that may be of interest in future applications of the Theory of Mixtures.

Groundwater abundance is well established, but its presence and physical properties are not easily established as a result of its subsurface location. Most methods of field investigation are intrusive and locally disruptive, and can only provide local information for a domain requiring areal characterization. Furthermore, groundwater is associated with solid geologic materials that are variable in properties and distribution. Given the extraordinary variety of geohydrologic environments, a generalized theory for analyzing groundwater behavior applicable to all aquifers is not available. A large body of descriptive information has evolved to discriminate the many different types of aquifers identified in field studies (Walton 1970). Methods of analysis have evolved for analyzing many different types of groundwater systems utilizing Darcy's Law as the fundamental equation of motion (Freeze and Cherry 1979). Darcy's Law (Darcy 1856) is an empirical rule that states that the flux through a porous medium is proportional to the static pressure gradient. Darcy's Law has been extended to three dimensions and applied to aquifers that are fractured, highly anisotropic or heterogeneous. With an empirical rather than first principle based equation of motion, unanswered questions concerning our understanding of groundwater phenomena are not surprising.

The geologic and physical description of aquifers is typically performed by drilling investigations of a site area. Determining the geohydraulic behavior of the associated aquifer or aquifers beneath the site is often performed using pump test techniques (Bouwer 1978). A variety of methods are available for performing pump tests and recent developments in instrumentation have significantly advanced the precision with which pump tests can be performed. Conceptually, a pump test is performed by injecting or withdrawing water from an aquifer and measuring the change in piezometric head at observation points surrounding the pumped well. Tests can last for days, which is often the case for aquifers with limited transmissivity. with hourly or more frequent observations. The resulting data are then analyzed, using a model of the aquifer, to determine the hydraulic properties of the aquifer. The model of the aquifer is typically based on Darcy's Law and may include much of the descriptive information developed during the drilling program. Implicitly, this method of analysis assumes the behavior of the aquifer under pumping is properly described using Darcy's Law. As will be shown, Darcy's Law does not consider the effects of inertia, viscosity, the motion of the solids, or any local variations in geologic structure about the pumped well. Consequently, an indeterminate source of error can be incorporated into the analysis of field data.

The Theory of Mixtures has been applied to multi–phase systems in recent years. The general theory has been presented by Atkin and Craine (1976a, 1976b), and Bowen (1975). A generalized formulation for groundwater systems utilizing the concepts of rational continuum mechanics that is consistent with the Theory of Mixtures has been developed by Hassanizadeh and Gray (1979a, 1979b, 1980), Gray (1983), and Hassanizadeh (1986a, 1986b). A review of the application of the Theory of Mixtures to soil physics was prepared by Raats (1984). The major emphasis to date has been the theoretical development of the Theory of Mixtures with limited applications of the theory. An application of the Theory of Mixtures that admits the effects of pressure, viscosity and inertia has been performed for a idealized aquifer (Munaf, et al.). However, substantial issues remain to be investigated before a reasoned understanding of the limitations of Darcy's Law is clearly established.

2. WELL HYDRAULICS

Pump tests are analyzed by combining Darcy's Law with the equation of continuity. The resulting partial differential equation in cylindrical coordinates is;

$$\frac{\partial^2 h}{\partial r^2} + \frac{1}{r}\frac{\partial h}{\partial r} = \frac{S}{T}\frac{\partial h}{\partial t} \quad , \qquad [1]$$

where S is the aquifer storativity, T is the aquifer transmissivity, and h is the piezometric head. Assumptions related to the derivation of this equation are that the equation of state for the aquifer is;

$$\rho = \rho_0 e^{\beta p} \quad , \qquad [2]$$

where β is the compressibility of water, ρ is the density of water, and p is the fluid pressure. Additionally, the stresses associated with the solid displacement can be approximated as;

$$\nabla \cdot \vec{v}_s = \frac{\partial}{\partial_z} \left[\frac{Du_z}{Dt} \right] = \alpha \frac{Dp}{Dt} \quad , \qquad [3]$$

where v_s is the velocity of the solid, u_z is the vertical displacement of the solid, and α is the compressibility of the aquifer. Theis (1935) provided the classical analytical solution applied to the analysis of data generated by pump tests. He assumed a homogeneous aquifer of infinite areal extent that is fully confined with uniform thickness and properties. The initial condition was;

$$h(r, 0) = h_0 \quad . \qquad [4]$$

The boundary conditions were;

$$h(\infty, t) = h_0 \quad ,$$

$$\lim_{r \to 0} \left[r \frac{\partial h}{\partial r} \right] = \frac{Q}{2 \pi T} \quad \text{for } t>0 \quad , \qquad [5]$$

where Q is the constant pump rate. Using Laplace transforms, the resulting solution in terms of the drawdown is;

$$h_0 - h = \frac{Q}{4\pi T} W(u) \quad , \qquad [6]$$

where $W(u)$, which is called the well function, is the exponential integral;

$$W(u) = \int_u^\infty \frac{e^{-u} du}{u} \quad , \qquad [7]$$

with u expressed as;

$$u = \frac{r^2 S}{4Tt} \quad . \qquad [8]$$

Other analytical solutions have been developed with varying boundary conditions to provide an analyst with a wide variety of alternatives for evaluating pump test data. Equation 1 has also been utilized as the fundamental governing equation for a wide variety of numerical solvers. It is important to note that the presumption of groundwater flow being driven solely by a pressure gradient is at the basis of all the available solutions. The extensive use of this solution over the past several decades and its wide acceptance underscores its utility and value in attempting to understand the behavior of groundwater. However, few aquifers have the characteristics assumed by Theis and the relationship of the governing equation to first principles is less than clear. By applying mixture theory, some insight into the implicit assumptions of Theis and Darcy is gained.

3. MIXTURE THEORY

Consider the solid and fluid materials as ideal continua mutually occupying a spatial point with properties of each material averaged over a small volume containing the point. The volume contains material of both the solid and the fluid with superscripts (1) and (2) indicating the solid and fluid, respectively.

If an elastic solid is considered, the deformation gradient can be expressed as;

$$F_{ij} = \partial x_i^{(1)} / \partial X_j^{(1)} \quad , \qquad [9]$$

with x_i referring to the time varying coordinates and X_j referring to the reference coordinates. For a Newtonian fluid, the deformation gradient can be expressed as;

$$d_{ij}^{(2)} = \frac{1}{2} (\partial v_i^{(2)} / \partial x_j + \partial v_j^{(2)} / \partial x_i) \quad , \qquad [10]$$

where v_i is the fluid velocity in the time varying coordinates.

The density of the mixture, which is the total mass per time–varying volume, is expressed as the sum of the solid and fluid densities without interconversion of mass or chemical reactions. The conservation of mass for the solid is expressed as;

$$\rho_1 \det |F_{ij}| = \rho_{10} \quad , \qquad [11]$$

with ρ_1 referring to the density in the mixed state and ρ_{10} referring to the density in the unmixed state. The conservation of mass for the fluid is expressed as;

$$\frac{\partial \rho_2}{\partial t} + \frac{\partial}{\partial x_i}\left[\rho_2 v_i^{(2)}\right] = 0 \quad , \qquad [12]$$

with ρ_2 referring to the density in the mixed state.

The laws of motion for the mixture arise from the partial stresses for the solid and the fluid. Each constituent is subjected to an external body force and an interactive force. The equations of motion for the solid and the fluid have the form;

$$\frac{\partial \sigma_{ij}^{(1)}}{\partial x_j} + \Pi_i + \rho_1 b_i^{(1)} = \rho_1 a_i^{(1)} \quad , \qquad [13]$$

$$\frac{\partial \sigma_{ij}^{(2)}}{\partial x_j} - \Pi_i + \rho_2 b_i^{(2)} = \rho_2 a_i^{(2)} \quad , \qquad [14]$$

σ_{ij} represents the partial stresses on the fluid and solid, Π_i represents the body force of the fluid on the solid per unit current volume, b_i represents the external body force (i.e., gravity), and a_i represents the acceleration in the time varying coordinates. The total stress of the mixture is the sum of the partial stresses of the solid and the fluid. Conservation of angular momentum requires that the total stress be symmetric, although the partial stresses need not be symmetric.

Equations 13 and 14 can be reduced to Darcy's Law by invoking the following assumptions;

- The solid motion can be ignored. Hence, ignore equation 13.
- The inertia of the fluid can be neglected. Hence, the right hand side of equation 14 can be neglected.

- The effects of viscosity are wholly expressed in the interaction force and can be ignored as a partial stress. Hence, the partial stress is a result of pressure alone.
- The interactive force is linearly proportional to the relative velocity of the fluid.

These assumptions result in Darcy's Law with the permeability expressed as;

$$K = \frac{\rho g}{\alpha} \quad , \tag{15}$$

where α is the proportional constant for the interactive force, which is not the same as the compressibility of the aquifer.

The pump test can be considered with the Theory of Mixtures to gain additional insight into the consequences of the use of Darcy's Law for addressing groundwater flow. Consider an aquifer with a rigid solid. Assume the materials are isotropic and homogeneous. The equation of motion reduces to equation 14. Consider the density and fluid velocity to be functions of radial position and time only. However, retain the acceleration term on the right hand side of equation 14. Assume the partial stress for the fluid to have the form;

$$\sigma_{ij} = -p\,\delta_{ij} + \lambda\, d_{kk}\,\delta_{ij} + 2\mu\, d_{ij} \quad , \tag{16}$$

where d_{ij} are the components of the rate of deformation tensor, μ is the shear viscosity, and $\lambda + 2/3\,\mu$ is the bulk viscosity. The pressure is the deviation of the density from its value when the fluid is at rest, or;

$$p = k\rho^{+} \quad , \tag{17}$$

where

$$\rho^{+} = \rho - \rho_{20} \quad . \qquad [18]$$

The interaction body force is considered to be linearly proportional to the relative velocity of the fluid. Since the solid is rigid,

$$\Pi_r = \alpha \, v_r \quad , \quad \Pi_\theta = \Pi_z = 0 \quad . \qquad [19]$$

The non–zero components of the deformation tensor are,

$$d_{rr} = \frac{\partial v}{\partial r} \quad , \quad d_{\theta\theta} = \frac{v}{r} \quad . \qquad [20]$$

Combining this into the equation of motion (Eqn. 14) results in,

$$-k \frac{\partial \rho^{+}}{\partial r} + (\lambda + 2\mu)\, D(v) - \alpha v = \rho \left[\frac{\partial v}{\partial t} + \frac{\partial}{\partial r} \left[\frac{v^2}{2}\right]\right] \quad , \qquad [21]$$

where,

$$D(v) = \frac{\partial^2 v}{\partial r^2} + \frac{1}{r}\frac{\partial v}{\partial r} - \frac{v}{r^2} \qquad [22]$$

Equation 22 combined with the continuity equation (Eqn. 12) gives,

$$\frac{\partial \rho^{+}}{\partial t} + \rho_{20} \frac{1}{r}\frac{\partial}{\partial r}(rv) = 0 \quad , \qquad [23]$$

subject to the supplemental boundary condition,

$$\frac{\partial Q}{\partial t}(r,0) = 0 \quad , \quad R_0 \leq r < \infty \quad . \qquad [24]$$

This boundary value problem has been solved by Munaf et al. to examine the effect of inertia and viscosity on the solution for reasonable physical parameters. Rizk (1990) has considered the effect of aquifer anisotropy by allowing the interactive force to have a directional preference. Both investigations have shown that the calculated response obtained by using the Theory of Mixtures was less than the response calculated by the Theis solution.

4. DISCUSSION

The Theory of Mixtures can be applied to improve our understanding of the behavior of groundwater. The initial applications discussed here do more to illustrate the potential utility of the Theory of Mixtures than resolve our lack of understanding. In terms of our understanding of the phenomena of groundwater flow, the determination of aquifer properties and the prediction of transport phenomena that are within an order of magnitude of observed results in field applications is difficult. The differences that have been noted in analyses using the Theory of Mixtures in comparison to similar analyses with Darcy's Law show distinct but relatively small (10 to 20 percent) variations. Several mechanisms remain to be considered. While no single mechanism can be expected to clarify our understanding, a more thorough appreciation of the effects of other mechanisms will allow a reasoned application of Darcy's Law and an understanding of the limitations of Darcy's Law.

Neither Darcy's Law or the Theory of Mixtures, as discussed in this paper, addresses the contribution of the solid on groundwater behavior. Yet, a common phenomena with the construction and operation of wells is the siltation of the well over time. Periodic backwashing of wells, to develop the well, is required in order to maintain well yield. Obviously, the transport of solids is a mechanism that will affect performance but cannot be addressed with the present state of theoretical development. Similarly, as the size of the solid material decreases from gravels to sands and silts, the effect of capillary forces increases. For fine grained silts, capillary forces vastly exceed gravitational forces. However, a means for including the effect of capillarity in the equation of motion is not available. Another recurrent problem in the understanding of groundwater is the heterogeneous nature of subsurface materials in depositional environments that have taken millions of years to evolve. Statistical methods show some promise for addressing these conditions; however, the lack of rigor associated with Darcy's Law may adversely influence the capability of statistical methods to separate the heterogeneous from the phenomenological effects.

In reviewing the application of the Theory of Mixtures to groundwater flow, several important assumptions warrant additional consideration. The nature of the interactive force is prominent among these. A simple linear proportion is a valid first approximation to the nature of the interactive force, but heterogeneous materials and structured layers of material have been shown to have dramatic influences on the transport characteristics of groundwater. While these observations are extremely difficult to quantify and all but impossible to predict, they suggest that more is at work than a simple linear proportion. As noted in the previous paragraph, the consideration of the solid as rigid is simply not consistent with the nature of aquifers. As a next step, an elastic solid would seem appropriate. As more is learned, more elaborate formulations might include elastic–plastic solids and particulate solids with elastic properties. Naturally, the computational efforts for addressing these increasingly difficult problem formulations will be significant.

In spite of what can be learned from theoretical and computational advances, the material properties to be extracted from the subsurface will remain a cause of enormous uncertainty. From single or multiple holes drilled into the ground, we presently attempt to extract material properties information to describe a fundamentally elliptic problem. Since natural settings are rarely, if ever, homogeneous, uniform, and isotropic, the difficulty in characterizing the subsurface will remain an inherent limitation in understanding the behavior of groundwater. Significant advances in the theoretical framework for analyzing the behavior of the subsurface may provide the best hope for guiding the needed advances in subsurface characterization. Without a justifiable understanding of the relevant mechanisms that influence the behavior of groundwater, there is little hope that the mysteries of the subsurface will ever be revealed. The Theory of Mixtures shows every indication of being an effective means towards improving the present understanding and establishing a rational means for analyzing groundwater behavior.

REFERENCES

Atkin, R. J., and Craine, R. E., 1976a, "Continuum Theories of Mixtures: Basic Theory and Historical Development," *Quarterly Journal of Mechanics and Applied Mathematics*, Vol. 29, pp. 209–244.

Atkin, R. J., and Craine, R. E., 1976b, "Continuum Theories of Mixtures: Applications," *Journal of the Institute of Mathematics Applications*, Vol. 17, pp. 153–207.

Bouwer, H., 1978, *Groundwater Hydrology*, McGraw Hill, New York.

Bowen, R. M., 1975, *Continuum Physics*, Vol. III, Academic Press, New York.

Darcy, H., 1856, *Les fontaines publiques de la ville de Dijon*, Victor Dalmont, Paris.

Freeze, R. A., and Cherry, J. A., 1979, *Groundwater*, Prentice Hall, New York.

Gray, W. G., 1983, "General Conservation Equations for Multi–Phase Systems: 4. Constitutive Theory Including Phase Change," *Advances in Water Resources*, Vol. 6, pp. 130–140.

Hassanizadeh, M., and Gray, W. G., 1979a, "General Conservation Equations for Multiphase Systems: 1. Averaging Procedure," *Advances in Water Resources*, Vol. 2, pp. 131–144.

Hassanizadeh, M., and Gray, W. G., 1979b, "General Conservation Equations for Multiphase Systems: 2. Mass, Momenta, Energy and Entropy Equations," *Advances in Water Resources*, Vol. 2, pp. 191–203.

Hassanizadeh, M., and Gray, W. G., 1980, "General Conservation Equations for Multiphase Systems: 3. Constitutive Theory for Porous Media Flow," *Advances in Water Resources*, Vol. 3, pp. 25–40.

Hassanizadeh, M., 1986a, "Derivation of Basic Equations of Mass Transport in Porous Media, Part 1. Macroscopic Balance Laws," *Advances in Water Resources*, Vol. 9, 196–206.

Hassanizadeh, M., 1986b, "Derivation of Basic Equations of Mass Transport in Porous Media, Part 2. Generalized Darcy's and Fick's Laws," *Advances in Water Resources*, Vol. 9, pp. 209–222.

Munaf, D., Wineman, A. S., Rajagopal, K. R., Lee, D. W., "A Boundary Value Problem in Groundwater Motion Analysis – Comparison of Predictions Based on Darcy's Law and the Continuum Theory of Mixtures," (in review).

Raats, P.A.C., 1984, "Application of the Theory of Mixtures in Soil Physics, Appendix 5D," *Rational Thermodynamics* (ed. C. A. Truesdell), 2nd ed., Springer Verlag, New York.

Rizk, T. A., 1990, "Groundwater Flow and Contaminant Transport in Geologic Media" Ph.D. Thesis, North Carolina State University, Raleigh, NC.

Walton, W. C., 1970, *Groundwater Resource Evaluation*, McGraw Hill, New York.

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