REVIEW OF MATHEMATICAL MODELS OF FLOW AND CONTAMINANT TRANSPORT IN SATURATED POROUS MEDIA

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Summary

This brief review contains a number of the most typical conceptual and mathematical models that describe the flow of a single fluid phase and the transport of a single chemical species ($\equiv$ a contaminant) in saturated two- and three-dimensional porous medium domains. The emphasis is on flow and contaminant transport in ground water domains. All models are based on the *continuum approach* and are written at the *macroscopic level*. The material covered in this review can be found in numerous texts. Bear *et al* (1968), Bear (1979) and Bear and Verruijt (1987, or later editions) may serve as examples. Hence, no effort has been made to support the presentation by an extensive list of references.

1. Introduction

1.1. Model Definition

A *model* may be defined as a *selected simplified version of a real system, and phenomena that take place within it that approximately simulates the system's excitation-response relationships that are of interest.* For example, a ground water system may be 'excited' by pumping, by artificial recharge, or by changing boundary condition. Its 'response' takes the form of spatial and temporal changes in water levels and in contaminant concentrations.

With the above definition, all that a model can do is to *predict* the future behavior of an investigated system. Nevertheless, modeling activities may be conducted to achieve any of the following objectives:

- To predict the behavior of a considered system, in response to excitations that stem from the implementation of management decisions.
- To obtain a better understanding of a considered system from the geological, hydrological, and chemical points of view.
- To provide information required in order to comply with regulations.
- To provide information for the design of a monitoring network, by predicting the system's future behavior.
- To provide information for the design of field experiments.

Although a model is eventually expressed in mathematical terms, the mathematical notation is used merely as a compact way of describing the physical and chemical

phenomena that are relevant to the considered problem. However, the mathematical formulation is needed if we wish predict the system's future behavior.

The first step in any modeling process is the establishment of the conceptual model of the considered problem and problem domain.

1.2. Conceptual Model

The *conceptual model* of a problem and a problem domain consists of a set of assumptions that reduce the real problem and the real domain to simplified versions that are satisfactory in view of the modeling objectives, the information that the model is expected to provide, and the associated management problem. Determining the conceptual model is the first, perhaps the most important, step in the modeling process. Once a conceptual model has been selected, it is translated into a mathematical one.

The following is a list of typical aspects that require assumptions:

- Geometry of the surface that bounds the domain of interest.
- The dimensionality of the model (one, two, or three dimensions).
- Steady-state or time dependent behavior.
- The kind of soil and rock materials comprising the domain, and the inhomogeneity, anisotropy, and deformability of these materials.
- The number and kinds of fluid phases and the relevant chemical species involved.
- The extensive quantities transported within the domain.
- The relevant material properties of the fluid phases (density, viscosity, compressibility, Newtonian or non-Newtonian behavior).
- The relevant transport mechanisms within the domain.
- The possibility of phase change and exchange of chemical species between adjacent phases.
- The relevant chemical, physical, and biological processes that take place in the domain.
- The fluid flow regime involved (e.g., laminar or non-laminar).
- The existence of isothermal or non-isothermal conditions (and their effect on fluid phase properties and on chemical–biological processes).
- The presence of assumed sharp macroscopic fluid-fluid boundaries, such as a phreatic surface.
- The relevant state variables, and the areas or volumes over which averages of such variables are taken.
- The presence of sources and sinks of fluids and chemical species within the domain, and their nature.
- The conditions on the domain's boundaries.
- The initial conditions within the domain.

In this chapter, unless otherwise specified, we shall assume that the flow regime is *laminar*, and that the considered fluid phase – water – is *Newtonian*. We shall also assume that the considered porous medium domain is such that it can be described at the

macroscopic or continuum level. At this level all variables are averages of their respective *microscopic* values over a Representative Elementary Volume (REV).

Intrinsic phase average. The intrinsic phase average of e_α, taken over the domain of the REV of volume $\mathcal{U}_o$, centered at the point **x**, is defined as

$$\overline{e_\alpha}^\alpha(\mathbf{x},t) = \frac{1}{\mathcal{U}_{o\alpha}(\mathbf{x},t)} \int_{\mathcal{U}_{o\alpha}(\mathbf{x},t)} e_\alpha(\mathbf{x}',t;\mathbf{x})\,d\mathcal{U}_\alpha(\mathbf{x}'), \qquad (1.1)$$

where $\mathcal{U}_{o\alpha}$ is the volume of the α-phase within $\mathcal{U}_o$, and $\mathbf{x}'$ is a point in the REV centered at **x**. The *intrinsic phase average* is, thus, an average of E_α per unit volume of the considered phase.

1.3. Mathematical Model

The conceptual model is "translated" into a mathematical model, the solution of which, subject to specified initial and boundary conditions, provides the information required for making management decisions.

Each mathematical model consists of:

- A definition of the *geometry* of the surface that bounds the considered domain.
- *Partial differential equations* that express the *balances* of the considered extensive quantities (e.g., mass of fluids, mass of chemical species, energy) .(Momentum, as an extensive quantity, is not mentioned, as in the models considered here, the momentum balance is introduced in its degenerated form of Darcy's law)
- *Flux equations* that relate the fluxes of the considered extensive quantities to the relevant state variables of the problem.
- *Constitutive equations,* that define the behavior of the particular phases and the chemical species involved (e.g., dependence of density and viscosity on pressure, temperature, and solute concentration).
- *Sources and sinks* of the relevant extensive quantities.
- *Initial conditions* that describe the *known* state of the considered system at some initial time.
- *Boundary conditions* that describe the interaction of the considered domain with its environment (i.e., outside the delineated domain) across their common boundaries.

1.4. General Macroscopic Balance Equation

The core of any mathematical model that describes the transport of an *extensive quantity* is a partial differential equation (p.d.e.) that expresses the balance of that quantity, per unit volume of porous medium. This approach, of taking a balance of an extensive quantity over a small volume centered at a point, and then letting this volume be gradually reduced to zero, is referred to as the *Lagrangian approach*.

The general microscopic balance equation for any extensive property of a fluid phase, E, having a density e, can be expressed in the form

$$\frac{\partial e}{\partial t} = -\nabla \cdot (e\mathbf{V} + \mathbf{j}^E) + \rho \Gamma^E, \tag{1.2}$$

where $\mathbf{j}^E$ is the *diffusive flux* of E, relative to the fluid phase *mass weighted velocity*, $\mathbf{V}$, ρ denotes the phase mass density, and Γ^E denotes the source of E, expressed as E per unit mass of the phase per unit time. The diffusive flux of E is related to the velocity of E by: $\mathbf{j}^E = e(\mathbf{V}^E - \mathbf{V})$.

By averaging the above equation over the considered α-phase within the REV, we obtain the general macroscopic balance equation for E in the form (Bear and Bachmat, 1990)

$$\frac{\partial \theta \overline{e}^{\alpha}}{\partial t} = -\nabla \cdot \theta (\overline{e}^{\alpha} \overline{\mathbf{V}}^{\alpha} + \overline{\overset{\circ}{e}\overset{\circ}{\mathbf{V}}}^{\alpha} + \overline{\mathbf{j}^E}^{\alpha})$$

$$- \frac{1}{\mathcal{U}_o} \int_{\mathcal{S}_{\alpha\beta}} [e(\mathbf{V} - \mathbf{u}) + \mathbf{j}^E] \cdot \mathbf{n} \, d\mathcal{S} + \theta \overline{\rho \Gamma^E}^{\alpha}, \tag{1.3}$$

where θ and $\overline{\mathbf{V}}^{\alpha}$ denote the volumetric fraction and the (mass averaged) velocity, respectively, of the considered phase, $\mathbf{n}$ denotes the outward unit vector normal to the (microscopic) surface $\mathcal{S}_{\alpha\beta}$, between the α-phase and all other (β-)phases within an REV, and we have made use of the decomposition of the (intrinsic phase) averaged advective flux of E within the α-phase, $\overline{e\mathbf{V}}^{\alpha}$, into two fluxes: a macroscopic advective flux $\overline{e}^{\alpha} \overline{\mathbf{V}}^{\alpha}$, and another macroscopic flux, $\overline{\overset{\circ}{e}\overset{\circ}{\mathbf{V}}}^{\alpha}$. In this equation:

- The flux, $\overline{\overset{\circ}{e}\overset{\circ}{\mathbf{V}}}^{\alpha}$, which is the flux of E in excess of the average advection of E carried by the phase, is the *dispersive flux* of E.
- The term

$$\frac{1}{\mathcal{U}_o} \int_{\mathcal{S}_{\alpha\beta}} [e(\mathbf{V} - \mathbf{u}) + \mathbf{j}^E] \cdot \mathbf{n} \, d\mathcal{S} \equiv f_{\alpha \to \beta}^E$$

expresses the flux of E from the α to all β-phases, across the $\mathcal{S}_{\alpha\beta}$-surface, which separates the α-phase from all other β-phases within $\mathcal{U}_o$, by advection relative to the possibly moving $\mathcal{S}_{\alpha\beta}$-surface, that moves at a velocity $\mathbf{u}$, and by diffusion.

More about the diffusive and dispersive fluxes is presented in Section 4.

1.5. Boundary Surface

The considered porous medium domain is delineated by boundary surfaces. Let $F(\mathbf{x}, t) = 0$ represent the equation of a possibly moving (macroscopic) boundary surface. The speed of displacement of this boundary, $\mathbf{u}$, should not be mixed up with the velocities of the fluids present on both sides of the surface. As the surface moves, its shape may change, but its equation, $F(\mathbf{x}, t) = 0$, remains unchanged. The quantity F is, thus, a conservative property of the points on the surface, for which the total derivative vanishes, i.e.

$$\frac{DF}{Dt} \equiv \frac{\partial F}{\partial t} + \mathbf{u} \cdot \nabla F = 0. \tag{1.4}$$

By definition,

$$\mathbf{n} = \frac{\nabla F}{|\nabla F|}, \tag{1.5}$$

where $\mathbf{n}$ denotes the unit vector normal to the surface $F = 0$.

From (1.4), we obtain

$$\mathbf{u} \cdot \nabla F = -\frac{\partial F}{\partial t}. \tag{1.6}$$

The component of $\mathbf{u}$ normal to the surface is then given by

$$u_n \equiv \mathbf{u} \cdot \mathbf{n} = -\frac{\partial F / \partial t}{|\nabla F|} = -\frac{\partial F / \partial t}{\partial F / \partial s_n}, \tag{1.7}$$

where s_n is a distance measured along $\mathbf{n}$.

1.6. Phases and Components

A *chemical species* is defined as an identifiable homogeneous chemical compound (element, ion or molecule) that participates as an entity (whether as a reactant or as a product) in a chemical reaction that takes place within a phase.

The term refers to the actual form which a molecule or an ion is present in a solution, or a phase. For example, *iodine* in an aqueous solution may exist in the form of one or more of the species: I_2, I^-, HIO, IO^-, IO_3^-. The same compound in solution and as an adsorbate on a solid are considered as two different species. Similarly, the same compound present in different phases are considered different species.

A *phase* may be defined as a portion of space occupied by a material such that a single set of constitutive relations describes the behavior everywhere within that material. This definition enables us to refer to disjoint portions of space occupied by the same liquid as a single phase.

Another way, not rigorous, but more descriptive, is to define a phase as a homogeneous portion of space that is separated from other such portions by a well defined observable sharp physical boundary (*interphase boundary*, or *interface*).

There can be only one gaseous phase in the void space of a porous medium domain, as all gaseous phases are completely *miscible*, and a distinct boundary cannot be maintained between them. Two *miscible liquids* also constitute a single phase. We may, however, have more than one liquid phase occupying the void space. The term *immiscible* is sometimes used to describe distinct liquid phases.

Often, a chemical species, initially present in one fluid phase, will cross an interfacial boundary and diffuse into an adjacent fluid phase. Nevertheless, as long as a sharp interface is maintained between the two fluids, we regard them as separate phases, albeit *not* as completely *immiscible* ones.

A phase may be composed of a large number of chemical species. However, under conditions of *chemical equilibrium*, the number of independent chemical species necessary to completely describe the composition of a given phase may be much smaller. We use the term *component* to denote a chemical species that belongs to the smallest set of such species that is required in order to completely define the chemical composition of the phase under equilibrium conditions. When chemical equilibrium **is not** assumed, all species are defined to be components.

For the sake of simplicity, we shall often use the term 'component' also to denote a mixture of a number of independent chemical species in a liquid or a gas. The selection of components is not unique, in the sense that different chemical species, or assembly of species, may be selected as components of a given phase.

2. Modeling Flow in a Three-Dimensional Domain

The model will be written at the macroscopic level. All variables are averages of their respective values at the microscopic level. However, we shall not use any symbol to indicate this fact.

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Biographical Sketch

Jacob Bear is a Professor Emeritus in the Department of Civil Engineering at the Technion--Israel Institute of Technology in Haifa, Israel. He received his Ph.D. in Civil Engineering from the University of California at Berkeley (1960), and Honorary Doctorates from Delft University of Technology, The Netherlands, and from ETH, Zurich, Switzerland. He is a Fellow of AGU and first recipient of the Brisdall Distinguished Lectureship in Hydrogeology awarded by the Geological Society of America, Hydrogeological Div., Washington, D.C., as well as the M. K. Hubbert Award by the National Ground Water Association (USA). In 1998, he was awarded in Israel the prestigious Rothschild Prize in Engineering. He received the 2003 Excellence in Geophysical Education Award from the American Geophysical Union (AGU). His teaching, research and consulting cover the areas of groundwater hydrology, management of water resources, water policy, groundwater contamination and remediation, and the theory of transport phenomena in porous media. Prof. Bear has been acting as consultant on groundwater hydrology, and management of water resources to the Ministry of Agriculture, Israel, to Lawrence Livermore National Laboratory and to government and to private companies in Israel and abroad. His well known books include Dynamics of Fluids in Porous Materials (Elsevier, 1972; Dover, 1988), Hydraulics of Groundwater (McGraw-Hill, 1979), Modeling Groundwater Flow and Pollution (co-author A. Verruijt; Reidel, 1987), and Introduction to Modeling Transport Phenomena in Porous Media (co-author Y. Bachmat; Kluwer, 1990). These books are used by students and practitioners all over the world. Prof. Bear is the editor of the international journal Transport in Porous Media (TIPM). He has been teaching short courses for engineers and scientists on Groundwater Hydrology, Management of Water Resources, and Modeling Flow and Pollution In the Subsurface at many universities around the world.