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Saeid Eslamian

Fundamentals of Hydrodynamic Modeling in Porous Media

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Fundamentals of Hydrodynamic Modeling in Porous Media

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9.1 Introduction

The vadose zone (VZ) comprised from the unsaturated zone (UZ) and the saturated/unsaturated interface region (SUIR) is an important link between the saturated zone and land surface. The VZ provides storage capacity for both water as one possible fluid and contaminants; a reactor medium for physical, chemical, and biological processes; and a delay time between the release of multicontaminants into the UZ and their transfer by flow of multifluids into the saturated zone. The quantitative relationship between the amount of contaminants released at the soil surface by anthropogenic activities external and/or internal to the VZ, for example, agricultural, industrial, and urban activity, and the resulting concentrations in groundwater is uncertain [6]. The UZ is believed to be with “natural attenuation” potential, which led to consider soil aquifer treatment as an efficient tertiary process for sewage effluents after secondary treatment, a technique that seemed to be a psychological projection of the granular filter methodology [7]. Qualitative decision driven from water scarcity conditions triggered in Israel the directing of rainwater falling on the roofs into the subsurface. Yet, simulations prove that in an urban environment characterized by patchworks of permeable and impervious surfaces, the underground migration of contaminants may be enhanced due to the highly nonuniform recharge of rainwater [1]. In what follows we will specifically refer to the need of accounting for nonhabitual approaches to address the modeling of hydrodynamics in porous media.
9.2 Modeling Approaches for Characterization of Physical Processes

9.2.1 Mathematical Modeling

Let temporal and spatial measurable observations (information) of prime (state) variables made in reference to a tangible system B (tsB). One wishes to establish a virtual system A (vsA) that predicts quantifiable assessments of state variables at a prescribed spatial domain and/or temporal extent of the tsB. If the assessments consistently do not deviate beyond a desired accuracy from the observations, then one follows the premise that the vsA mathematically models the tsB. Thus, further hypotheses can be investigated via the vsA as it is assumed to represent the hydrodynamic essentials of the tsB.

The entire spectrum of temporal and spatial information is always not available. Hence, the vsA structure consists of mathematically formulated physical assumptions referred to as a generic model. Such are, for example, balance equations (conservation laws) of the phase’s extensive quantities (e.g., its volume, mass, linear momentum, angular momentum, and energy), constitutive relations (i.e., state functions), and definitions. The adaptation of an obtained generic model to a subset of prescribed observations (i.e., the inverse problem) is done via estimation of the model sought parameters and the choice of appropriate temporal and spatial conditions (i.e., initial and boundary conditions). The input of the model parameters, initial and boundary conditions, leads to simulation predicting state variables (i.e., the direct problem) that can also be compared against the residual set of the available information. Verification of the calibrated model enables further simulations for predictions resolved from different operation scenarios. The general process of establishing a mathematical model is described in Figure 9.1.

9.2.2 Lumped Parameter Approach

The premise of lumping is that the behavior of a distributed system can be conformed into an interacting set of information characterized by typical, not spatially dependent, entities that approximate the behavior of the original system subject to physical assumptions. As the spatial distribution within each constituent of the set is meaningless, its configuration is irrelevant and can thus be described by a node, or a compartment representing in reality, for example, a cluster of similar information. Implementation of the lumped parameter (LP) approach can be found in different network sets. Figure 9.2 presents two of such LP examples: a mechanical set of mass–spring–damper and an electric set of resistor–capacitor–conductance.

In what follows let us consider a compartment as a region of identifiable physical space characterized by lumped (i.e., not a function of space) quantities. A network section of virtual compartments addressing the hydrodynamic interactions to be modeled by the LP approach for the displacement of fluids and components through a solid matrix is described in Figure 9.3.

We note that as the LP approach is not accounting for spatial dependency, the balance equations conform to ordinary differential equation (ODE) forms. Let us first consider some definitions:

- Phase refers to an identifiable \( \gamma \) body (subject to one’s definition) composed of a sum of \( \alpha (= 1, 2, \ldots, N\alpha) \) components (i.e., species of the \( \gamma \) phase such as ions, molecules, particles). Hence, we write \( \gamma = \sum_{\alpha=1}^{N\alpha} \gamma_{\alpha} \).

- A phase (or component) extensive quantity addresses an additive quantity like mass, volume, momentum, and energy that is bounded by the phase volume.
Assuming that flow directions through the compartmental boundaries are a priori known, we write the mass balance of a $\gamma$ fluid in any compartment $N$ of the compartmental network in the form

$$\frac{d}{dt} (\theta^\gamma_n \rho^\gamma_n V_n) = \sum_{i}^{I_n} \theta^\gamma_i \rho^\gamma_i q^\gamma_{in} - \sum_{j}^{J_n} \theta^\gamma_j \rho^\gamma_j q^\gamma_{jn} + \sum_{d}^{D_n} \theta^\gamma_d J^\gamma_{dn} + \sum_{s}^{S_n} \rho_s^\gamma Q^\gamma_{sn} - \theta^\gamma_n \rho^\gamma_n W^\gamma_n$$

(9.1)

where

$\rho^\gamma_n$ denotes the $\gamma$ fluid density in compartment $N$

$\rho^\gamma_i$ denotes the incoming $\gamma$ fluid density from compartment $I$ to $N$

$q^\gamma_{in}$ denotes the advective flux entering $N$ from the $I$ compartment, through their common boundary

$q^\gamma_{jn}$ denotes the crossing boundary advective flux leaving $N$ into the $J$ compartment

$I_n$ and $J_n$ denote, respectively, the number of incoming and outgoing fluxes across the boundaries of the $N$ compartment

$J^\gamma_{dn}$ denotes the diffusive mass flux of the $\gamma$ fluid crossing the boundary between the $N$ and the $D$ compartment with a total of $D_n$ such compartments

$\rho^\gamma_s$ denotes the $\gamma$ fluid source density injected into $N$ with one of its $s$ ($s \in S_n$) source flux intensity $Q^\gamma_{sn}$

$W^\gamma_n$ denotes all of its sink pumping intensity

$\theta^\gamma_n$ denotes the volume fraction (fluid content) of the $\gamma$ fluid $\left(\sum_{\gamma} \theta^\gamma_n = 1\right)$ occupying the $V_n$ volume of the $N$ compartment

FIGURE 9.1 Processes in enabling a vsA to model a tsB.
Considering the advective flux, say crossing the boundary from the $I$ compartment to the $N$ one, the momentum balance equation for the $\gamma$ fluid that accounts for inertia (rate and quadratic terms of the flux, the latter of which gives rise to vertical motion) and drag (linear flux term) reads

$$\eta_{\text{in}} \frac{dq_{i,n} \gamma}{dt} + \lambda_{in} (q_{i,n} \gamma)^2 + \Psi_{in} q_{i,n} = P_i^\gamma + p_i^\gamma gZ_{i,n}$$  \quad (9.2)$$

where

- $\eta_{\text{in}}$, $\lambda_{in}$, and $\Psi_{in}$ denote, respectively, inductance, transfer, and resistance coefficients across the compartment’s boundary.

If the flux rate is negligible, then (9.2) conforms to the LP form of Forchheimer's law. If inertia terms are assumed negligible, then (9.2) conforms to the LP form equivalent to Darcy’s law.
A flow model addresses (9.1) for all network compartments with (9.2), which is assigned to the common compartmental boundaries. Removing the assumption of knowing a priori the flux direction, we rewrite (9.1), for the fluid mass balance equation, in the form

\[
\frac{d}{dt} V_n = \sum_i^{\text{In}} \left( \theta_n^i \rho_n^i \frac{q_n^i + q_n^i}{2} + \theta_n^i \rho_n^i \frac{q_n^i - q_n^i}{2} \right) + \sum_d^{\text{Dn}} \theta_n^d J_{dn}^\gamma + \sum_s \tilde{\rho}_n^s Q_n^s - \theta_n^\gamma \rho_n^\gamma W_n
\]

where In denotes the total number of compartment boundaries through which flux \( q_n \) is entering or leaving compartment \( N \). Instead of (9.2), we now rewrite the fluid momentum balance equation assigned to each of the \( \text{In} \) boundaries of compartment \( N \) to read

\[
\eta_n \left[ \frac{d}{dt} \left( \frac{q_n^i + q_n^i}{2} \right) + \frac{d}{dt} \left( \frac{q_n^i - q_n^i}{2} \right) + \lambda_n \left( \frac{q_n^i + q_n^i}{2} \right)^2 - \left( \frac{q_n^i - q_n^i}{2} \right)^2 \right] + \Psi_n \left[ \left( \frac{q_n^i + q_n^i}{2} \right)^2 + \left( \frac{q_n^i - q_n^i}{2} \right)^2 \right] = P_{i,n}^\gamma + \rho_n^\gamma g Z_{i,n}
\]

We note that (9.3) and (9.4) represent the LP flow model for the compartmental network when the flow direction is not assumed to be known a priori.

Referring to the \( \gamma \) fluid diffusive mass flux \( J_{dn}^\gamma \) across the (membrane) boundary between the \( N \) and \( D \) compartments in (9.1), we write

\[
J_{dn}^\gamma = D_{dn} P_{d,n}^\gamma - \chi_{dn} \Pi_{d,n}^\gamma
\]

where at the \( dn \) boundary of all \( Dn \) diffusive boundaries \((dn \in Dn)\) of the \( N \) compartment, \( D_{dn} \) denotes the diffusion coefficient due to the partial pressure difference \( P_{d,n}^\gamma \) across it, and \( \chi_{dn} \) denotes the diffusion coefficient due to the osmotic pressure difference \( \Pi_{d,n}^\gamma \) across it.

Note that the diffusive flux associated with the osmotic pressure \( \Pi_{dn}^\gamma \) is in contrary direction to the one generated by the hydrodynamic pressure difference. The osmotic pressure depends linearly on the concentration difference (i.e., follows the notion of a potential flow law) of all \( \alpha \) components associated with the \( \gamma \) fluid within the \( D \left( \text{C}_{\alpha,D}^\gamma \right) \) and \( N \left( \text{C}_{\alpha,N}^\gamma \right) \) compartments:

\[
\Pi_{dn}^\gamma = \sum_\alpha \sigma_{\alpha,\text{dn}} \left( \text{C}_{\alpha,D}^\gamma - \xi_{\alpha} \text{C}_{\alpha,N}^\gamma \right)
\]

in which \( \xi_{\alpha} \) denotes a chemical equilibrium (partition) coefficient and \( \sigma_{\alpha,\text{dn}} \) denotes a reflection coefficient across a \( dn(\in Dn) \) boundary so that (1) \( \sigma_{\alpha,\text{dn}} = 1 \), when the boundary is permeable to the
solvent (fluid) and not to the solute, and (2) \( \sigma_{\alpha,\text{dn}} = 0 \), when the boundary is permeable to both the fluid and the solute.

We assume that the storage capacity addressed by the occupied volume can change, resulting from deflection of the compartment boundaries. This is similar to the change in a specific yield due to fluctuation of the unsaturated–saturated interface. In reference to (9.3), we associate changes in \( V_n \) of the \( N \) compartment with the sum of all \( \gamma \) fluid partial pressure difference change \( \{P_{\gamma,\text{dn}}^{\prime} \} \) across its \( ne \) (\( \in \) \( En \)) boundary:

\[
dV_n = \sum_{\alpha} E_n \sum_{\gamma} n_{\alpha,\text{dn}} \sum_{\gamma} dP_{\text{n,}e}^{\gamma}
\]

in which \( e_{\alpha} \) denotes a compliance factor of the \( ne \) wall. We note that (9.7) is similar to Hook’s constitutive law for an elastic deformation with \( V_n/e_{\alpha} \) as its measure of stiffness (i.e., Young’s modulus) and \( dV_n/V_n \) associated with dilatation (i.e., skeleton strain).

Accounting for the assumption of not a priori determined flow direction, following (9.3), we write the mass balance equation for an \( \alpha \) solute being a species of a \( \gamma \) fluid occupying an \( N \) compartment:

\[
\frac{d}{dt}\left(\theta_n\, C_{\alpha,n}^\gamma \, V_n\right) = \sum_{\alpha} \left( \theta_{\alpha}^\gamma C_{\alpha,n}^\gamma \, q_{\alpha,\text{in}}^\gamma + \theta_{\alpha}^\gamma C_{\alpha,n}^\gamma \, \frac{q_{\alpha,\text{dn}}^\gamma}{2} + \theta_{\alpha}^\gamma C_{\alpha,n}^\gamma \, \frac{q_{\alpha,\text{dn}}^\gamma}{2} \right)
\]

\[
+ \sum_{\alpha} \theta_{\alpha}^\gamma J_{\alpha,\text{dn}}^\gamma + R_{\alpha,\text{in}}^\gamma + \sum_{s} \tilde{C}_{\alpha,sn}^\gamma Q_{\alpha,sn} - \theta_{\alpha}^\gamma C_{\alpha,n}^\gamma W_n
\]

in which \( \tilde{C}_{\alpha,sn}^\gamma \) denotes the \( \alpha \) solute external \( sn \) (\( \in Sn \)) source concentration injected with the \( \gamma \) fluid and \( R_{\alpha,\text{in}}^\gamma = R_{\alpha,\text{in}}^\gamma \left( C_{\alpha,\text{a-1}}, C_{\alpha,\text{a-2}},..., C_{\alpha,\text{a-N}} \right) \) denotes the generation rate of the \( \alpha \) solute in the \( \gamma \) fluid, occupying the \( N \) compartment, by chemical reactions with other solutes, with their corresponding concentrations, of that fluid. We note that summation of (9.8) over the \( \alpha \) solutes, based on \( \sum_{\alpha} C_{\alpha,\text{in}}^\gamma = \rho_{\alpha}^\gamma, \sum_{\alpha} J_{\alpha,\text{dn}}^\gamma = J_{\text{dn}}, \sum_{\alpha} R_{\alpha,\text{in}} = 0 \), yields the \( \gamma \) fluid mass balance equation in the form of (9.3). For concentration-dependent fluid density, we address the mass fraction \( f_{\alpha,\text{in}}^\gamma \) of the \( \alpha \) solute in the \( \gamma \) fluid (i.e., \( \sum_{\alpha} f_{\alpha,\text{dn}}^\gamma = 1 \)) and assign \( C_{\alpha,\gamma}^\gamma = \rho_{\alpha}^\gamma f_{\alpha,\text{in}}^\gamma. \) Further, by mathematical manipulation between (9.3) and (9.8), we can rewrite the latter without terms of mass efflux through the \( N \) compartmental boundaries and via a sink term. In (9.8), we refer to the diffusive flux \( J_{\alpha,\text{dn}}^\gamma = J_{\alpha,\text{dn}}^\gamma \left( C_{\alpha,\text{D,}N}^\gamma \right) \) of the \( \alpha \) solute associated with the \( \gamma \) fluid across the \( \text{dn} \) boundary as a function of the concentration difference of that solute in the \( D \) and \( N \) compartments. This mass diffusion of the \( \alpha \) solute assuming to be uncharged and with no account for chemical reactions reads

\[
J_{\alpha,\text{dn}}^\gamma = \omega_{\alpha,\text{dn}} \left( C_{\alpha,\text{D}}^\gamma - C_{\alpha,\text{N}}^\gamma \right) + J_{\text{dn}}^\gamma (1 - \sigma_{\alpha,\text{dn}}) C_{\alpha,\text{dn}}^\gamma
\]

in which \( \omega_{\alpha,\text{dn}} \) denotes the \( \alpha \) solute diffusion coefficient and \( C_{\alpha,\text{dn}}^\gamma \) denotes a concentration subject to conditions associated with the \( \text{dn} \) boundary:

\[
C_{\alpha,\text{dn}}^\gamma = \begin{cases} 
\frac{C_{\alpha,\text{N}} - C_{\alpha,\text{D}}}{\ln \left( \frac{C_{\alpha,\text{N}}}{C_{\alpha,\text{D}}} \right)} & \text{When concentration varies on membrane surface} \\
C_{\alpha,\text{D}} & \text{When } J_{\alpha,\text{dn}}^\gamma \text{ from } D \text{ to } N \\
C_{\alpha,\text{N}} & \text{When } J_{\alpha,\text{dn}}^\gamma \text{ from } N \text{ to } D
\end{cases}
\]
As a concluding example, let us consider modeling the problem of a one fluid flow through a “Pin Forest” (e.g., urban landscape) carrying one solute, as described in Figure 9.4. We note that the layout of virtual compartments is identifiable throughout the investigated domain, and moreover, these are chosen to cover certain geometrical characterizations that will be reflected by a volume ratio associated with each subdomain. The actual “Pin Forest” reality (Figure 9.4) is replaced by a virtual compartmental layout (Figure 9.5), which will be our modeling premises.

In view of Figure 9.5 we note that compartments 0 and 5 represent the environment surrounding the assigned 1–4 compartments. Thus, we consider \( P_0, P_5, \rho_0, \rho_5, C_0, \) and \( C_5 \) as known constant quantities, \( V_0 \) and \( V_5 \) are constant volumes, and \( \theta_0 = \theta_5 = 1 \). For the single fluid for which we prescribed its flow direction through the “Pin Forest,” let us assume that its compressible density state function \( (\rho = \rho(P_{\text{in}})) \) is given for which the compressibility \( \beta \equiv (1/\rho)(d\rho/dP_{\text{in}}) \) is constant, assign \( \theta_2 < \theta_3 < \theta_1 < \theta_4 = 1 \) as the fluid volume ratio distribution, and neglect its diffusive flux through any boundary. By virtue of (9.1), we can now write the fluid mass balance equations. For the surrounding environment, we obtain \( Q_0 = q_{01} + q_{02} \) for compartment 0 and \( \rho_5 = \rho_1, q_{35} = \rho_4 q_{45} \) for compartment 5. Four additional fluid mass balance equations will be written for compartments 1–4. This, for example, for the fluid-occupying compartment 2, by virtue of (9.1) accounting for (9.7), will read

\[
\theta_2 \rho_2 \left[ (\beta V_2 + \epsilon_{20}) \frac{dP_2}{dt} + (\beta V_2 + \epsilon_{21}) \frac{dP_{2,1}}{dt} + (\beta V_2 + \epsilon_{24}) \frac{dP_{2,4}}{dt} \right] = \rho_0 q_{02} + \theta_1 \rho_1 q_{12} - \theta_4 \rho_2 q_{24}
\]

FIGURE 9.4 Inflow \((Q_0)\) and outflow \((Q_5)\) through a “Pin Forest” configuration, for which a subdivision into four virtual compartments is chosen.

FIGURE 9.5 Compartmental setup chosen to represent the “Pin Forest” system depicted in Figure 9.4. Compartmental cross boundary flow directions and mutual interactions are ascribed a priori.
We note that the left-hand side (LHS) of the fluid mass balance equation in compartment 2 is associated with storage factors due to its compressibility and the fluctuation of some of its boundaries. To complete the flow model, we need to write the fluid momentum balance equation for any common compartmental boundary with a crossing flux. For the eight such common boundaries (Figure 9.5), let us assume that inertia due to temporal and spatial changes together with friction between the fluid and the solid interface are contributors to the momentum fluxes; hence, in view of (9.2), for example, for boundary 12 we write

\[ \eta_{12} \frac{dq_{12}}{dt} + \lambda_{12} q_{12} + \Psi_{12} q_{12} = P_{12} + \rho_{1} g Z_{12} \]

The flow model is well posed as for the prescribed values of \( P_{0}, P_{5}, \rho_{0}, \rho_{5}, \eta_{ij}, \lambda_{ij}, \psi_{ij} \), and the 14 unknowns \( Q_{0}, q_{01}, q_{02}, q_{13}, q_{24}, q_{35}, Q_{5}, P_{1}, P_{2}, P_{3}, P_{4} \) can be solved by eight momentum balance equations and six mass balance equations.

Considering the one solute carried by the fluid, we suppose that mass generation by chemical reactions is negligible, and in addition to the previous assumptions, we propose that its diffusive mass fluxes cannot be neglected in comparison to its advective fluxes. In view of (9.8), when addressing flow direction and accounting for (9.9), we write four solute mass balance equations addressing compartments 1–4. Hence, this, for example, for compartment 2, reads

\[ \frac{d}{dt} \left( \theta_{2} V_{2} C_{2} \right) = C_{0} q_{02} + \theta_{1} C_{1} q_{12} - \theta_{3} C_{3} q_{32} - \omega_{2} (C_{0} - \xi C_{2}) \theta_{2} + \omega_{12} (C_{1} - \xi C_{2}) \theta_{2} + \omega_{24} (C_{4} - \xi C_{2}) \theta_{2} \]

We note that after solving for the flow problem, the various across-boundary fluxes were resolved and the compartmental volumes can be evaluated by virtue of (9.7). Hence, with prescribed values for \( C_{0}, C_{3}, \omega_{ij}, \xi \), the four unknowns \( C_{1}, C_{2}, C_{3}, C_{4} \) can be solved using the four solute mass balance equations.

### 9.2.3 Microscopic Continuum Approach

The continuum approach applies if average, measurable manifestations associated with the smallest typical length of the problem structure are significantly greater than a typical lattice constant (e.g., mean free path of the molecules). Mathematically, this represents a phase body as a region bounded by a surface (Figure 9.6), assuming that process relevant state quantities and properties are homogeneous within that region and can be assigned to every point within it. This spatial domain is thus referred to behave as a continuum, and the level of description of phenomena within the phase is addressed as description at the microscopic level.

![FIGURE 9.6](image_url)  
A phase extensive quantity bound within some continuum domain.
With reference to the continuum approach, let $E$ denote an extensive quantity of any $\gamma$ phase ($m$ mass, $V$ volume, $M$ momentum vector, $e$ energy) bounded by $U$, the phase volume; $e \equiv dE/dU$ denotes the intensive quantity (i.e., specific $E$ value); $X^E$ denotes a position vector of a particle moving along a trajectory (Lagrangian concept) carrying $E$; and $\phi^E \equiv \partial X^E / \partial t \mid_{E = \text{Const.}}$ denotes a velocity vector of $E$ with reference to a $\xi^E$ location at an initial time relative to a fixed frame of reference. We note that this velocity can be measurable only for $E \equiv V$, $J^E \equiv e \phi^E$ denotes the flux vector of $E$, $\Gamma^E$ denotes the rate of generating $E$ (source of $E$) per unit mass of the phase, and $D_\gamma / Dt \equiv (\partial / \partial t) + \mathbf{v} \cdot \nabla$ denotes the material (hydrodynamic or Lagrangian) time derivative that addresses the rate at a fixed frame of reference and the rate due to travel with a velocity $\mathbf{v}$ tangent to a track of spatial change.

In view of the Reynolds transport theorem, we write

$$
\frac{D_\gamma}{Dt} \left( \int_U e dU \right) = \int_U \frac{\partial e}{\partial t} dU + \int_s e \mathbf{v} \cdot \mathbf{\zeta} ds
$$

(9.11)

where on the left hand side (LHS) of (9.11), we account for the material derivative over the total extensive quantity within the phase volume. As we may want to account for this derivative addressing $\phi^E$, we add and subtract $\int_s e \phi^E \cdot \mathbf{\zeta} ds$, and thus, (9.11) conforms to

$$
\frac{D_\gamma}{Dt} \left( \int_U e dU \right) = \int_U \frac{\partial e}{\partial t} dU + \int_s e \phi^E \cdot \mathbf{\zeta} ds - \int_s e (\phi^E - \mathbf{v}) \cdot \mathbf{\zeta} ds
$$

(9.12)

The conservation of $E$ in $U$ expressing the balance equation for $E$ reads

$$
\frac{D_\gamma^E}{Dt} \left( \int_U e dU \right) = \int_U \rho \Gamma^E dU
$$

(9.13)

By virtue of (9.12) and (9.13), the integral form for the balance equation for $E$ becomes

$$
\frac{D_\gamma^E}{Dt} \left( \int_U e dU \right) + \int_s e (\phi^E - \mathbf{v}) \cdot \mathbf{\zeta} ds = \int_U \rho \Gamma^E dU
$$

(9.14)

We note that (9.14) is mostly suitable when the investigated domain is of a known spatial configuration. Using the relation of (9.11), the divergence theorem, and in view of (9.13), for infinitesimal phase volume (i.e., $U \rightarrow 0$), the partial differential equation (PDE) form of the balance equation for $E$, per unit volume of the phase, reads

$$
\frac{\partial e}{\partial t} + \nabla \cdot (e \phi^E) - \rho \Gamma^E = 0
$$

(9.15)

As $\phi^E$ in (9.15) is not a measurable quantity (unless for $E \equiv U$), we replace it for the $\gamma$ phase by an $E$-weighted velocity, using the first moment notion (i.e., balancing $E_i \phi_i = \sum_a E^a \phi^a, E_i = \sum_a E^a$ between $E$ fluxes). Hence, the mass-weighted velocity $\phi$ for the $\gamma$ phase will be obtained from the summation over
its $\alpha$ components $m^a = \sum m^a$ and its mass $m = \sum m^a$. To circumvent the inability to measure the $E$ flux $J^E \equiv e \vartheta$, we add and subtract the $e \vartheta$ flux and obtain $J^E = e \vartheta + e(\vartheta - \vartheta^a)$ in which $e \vartheta$ refers to the advective flux of $E$ with respect to $\vartheta$ the phase mass-weighted velocity, and $J^{E^m} \equiv e(\vartheta^a - \vartheta)$ refers to the diffusive flux of $E$ relative to that velocity. We note that $J^{E^m}$ vanishes for the phase mass-weighted velocity and, as it refers to the nonmeasurable $\vartheta^a$, its form is habitually proposed to follow a potential flow pattern and is empirically (state function or constitutive law) adopted.

The Eulerian form of the balance equation for $E$ reads

$$\frac{\partial e}{\partial t} + \nabla \cdot (e \vartheta + J^{E^m}) - \rho \Gamma^E = 0$$  \hspace{1cm} (9.16)$$

The Lagrangian form of the balance equation for $E$ reads

$$\frac{D \vartheta}{Dt} = -e \nabla \cdot \nabla J^{E^m} + \rho \Gamma^E$$  \hspace{1cm} (9.17)$$

We note that both (9.16) and (9.17) are PDEs constructed of specific flux terms (i.e., per unit volume of the phase). The divergent terms in (9.16) and (9.17) address fluxes perpendicular crossing the enclosing boundaries for which boundary conditions need to be assigned. The general form of conditions that balance between ascribed fluxes at an $\Omega$ boundary segment reads

$$(e \vartheta + J^{E^m}) \cdot \zeta + \alpha \rho \Gamma^E |_{\Omega} = 0$$  \hspace{1cm} (9.18)$$

in which the fluxes in (9.18) are per plan square length units for a 3D problem, per curve length units for a 2D problem, and at a point for a 1D problem; $\zeta$ denotes an outward-directed unit vector perpendicular to the $\Omega$ boundary segment; and $\alpha, e, \rho \Gamma^E |_{\Omega}$ are prescribed at the $\Omega$ boundary segment. The dimensional parameter $\alpha$ serves as a variable controlling the type of boundary conditions resulting from (9.18). These are (1) Dirichlet’s (1st kind) condition $e = e_0$ for $\alpha \to \infty$, (2) Neumann’s (2nd kind) condition $(e \vartheta + J^{E^m}) \cdot \zeta = \rho \Gamma^E |_{\Omega}$ for $\alpha = 0$, and (3) the mixed Cauchy’s (3rd kind) condition $(e \vartheta + J^{E^m}) \cdot \zeta + B(e - e_0) = \rho \Gamma^E |_{\Omega}$ for $\infty > \alpha = B > 0$.

We note that (9.16) or (9.17) describes a general “cookbook” formula to which one assigns the specific ingredients to construct the balance equation of the phase (or component) extensive quantity. Let us, for example, construct the mass balance equation of component $\alpha$ within any phase. We assign $E \equiv m^a \Rightarrow e \equiv e^a$, $J^{E^m} \equiv e^a \left( \vartheta^a - \vartheta \right) = -D^a \cdot \nabla e^a$, using Fick’s constitutive law for which $D^a$ denotes the diffusion tensor. By virtue of (9.16) and the aforementioned ingredients, Eulerian form of the mass balance equation of component $\alpha$ reads

$$\frac{\partial C^a}{\partial t} = -\nabla \cdot \left( \nabla C^a \left( \vartheta^a - D^a \cdot \nabla C^a \right) \right) + \rho \Gamma^m$$

Upon summing over all $\alpha$ components and noting that $\sum C^a = \rho$, $\sum J^{m^a} = 0$, $\sum \Gamma^m = 0$, we obtain the phase mass balance that reads

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \vartheta)$$

For constructing a phase momentum equation, we assign $E$ and $\vartheta$ with $F$ denoting a specific (i.e., per phase mass, e.g., $-g \nabla Z$) body force being the momentum source flux, and the diffusive
momentum flux is given by \( J^M = \rho \mathbf{M} - \mathbf{9} \) where \( \mathbf{M} \) denotes a stress tensor that follows a constitutive relation (e.g., \( \tau = \mu (\nabla \mathbf{9} + (\nabla \mathbf{9})^T) + \lambda' \nabla \cdot \mathbf{9} \mathbf{I} \), the Newtonian fluid shear stress with \( \mu \) and \( \lambda' \) denoting, respectively, the first and second viscosities and \( \mathbf{I} \) denoting the unit tensor). Moreover, in case of a fluid phase, we have \( \mathbf{M} = \tau - \rho \mathbf{I} \). By virtue of (9.16) and the aforementioned ingredients, Eulerian form of the momentum balance equation of any phase reads \( \frac{\partial}{\partial t} (\rho \mathbf{9}) = - \nabla \cdot (\rho \mathbf{9} - \mathbf{M}) \). From which after subtracting the phase mass balance equation, we can write the Lagrangian form of the momentum balance equation of any phase:

\[
\frac{D \mathbf{9}}{D t} = \nabla \cdot \mathbf{M} + \rho \mathbf{F}
\]

To conclude let us note that any continuum-defined microscopic balance PDE can be transformed into its LP counterpart ODE. As an example, let us consider the 2D, Cartesian coordinates, mass balance PDE for a component carried by a fluid, which reads

\[
\frac{\partial c}{\partial t} = \nabla \cdot (\mathbf{D} \nabla c - \mathbf{9} \mathbf{c})
\]

This PDE is to be solved addressing a 2D plan, discretized into a map of virtual compartments, each of which with a prescribed pole point where we seek the estimation of the state variable \( C \) (Figure 9.7).

Let \( S_I \) denote the area of the \( I \) compartment and \( L_{IJ} \) denote the distance between two poles at the \( I \) and \( J \) compartments, perpendicular to their common boundary, which its length is denoted by \( \Lambda_{IJ} \). Following the notion of lumping the aforementioned PDE, we write \( \int_S \frac{\partial c}{\partial t} dS = \int \nabla \cdot (\mathbf{D} \nabla c - \mathbf{9} \mathbf{c}) dS \) and conform it to \( \frac{\partial c}{\partial t} \int_L d\Lambda = \int_L \nabla \cdot (\mathbf{D} \nabla c - \mathbf{9} \mathbf{c}) \cdot \mathbf{\zeta} d\Lambda \) as \( \frac{\partial c}{\partial t} \) is assumed to be not space dependent. Using a first-order

![FIGURE 9.7](image-url)

**FIGURE 9.7** A 2D domain discretized into virtual compartments, each of which depicts a pole where concentration estimation will be obtained, after conforming its microscopic mass balance PDE into its LP counterpart ODE.

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difference, the aforementioned relation is approximated to
\[
\frac{\partial C_I}{\partial t} S_I = \sum_A \Lambda_{ij} \left( D_{ij} \left( C_I - C_I - C_I + \frac{9_{ij}}{2} \right) - C_I \frac{9_{ij} - 9_{ij}}{2} \right)
\]
for any I compartment with no a priori presumption of the flux direction. Finally, the mass balance PDE conforms to its ODE equivalent in the form
\[
\frac{dc_I}{dt} = \sum_A \omega_{ij} (c_I - c_I) - \lambda_{ij} \left( C_I \frac{q_{ij} + q_{ij}}{2} + C_I \frac{q_{ij} - q_{ij}}{2} \right) ; \omega_{ij} = \frac{\Lambda_{ij} D_{ij}}{S_i L_{ij}} ; \lambda_{ij} = \frac{\Lambda_{ij}}{(S_j)^2}
\]
which can be referred as an elaboration of the previously introduced LP approach, as the location of the sought state variable inside each compartment directly dictates the apparent diffusion coefficient \(\omega_{ij}\).

A similar procedure is applicable to any E balance PDE, using, for example (9.16).

### 9.2.4 Macroscopic, Volume-Averaged, and Continuum Approach

The basic notions of obtaining the macroscopic continuum based on spatial averaging over a representative elementary volume (REV), and from its macroscopic balance equations of phase (or components) extensive quantities, can be found in [2]. Figure 9.8 describes some of the essences addressing the REV concept, intensive quantities (\(e_\alpha, e_\beta, \ldots\)) associated with interacting phases (\(\alpha, \beta, \ldots\)) in it, and their spatial averaging over their respective volumes within the REV. On top of the fundamental definitions appearing in Figure 9.8, we also find in [2] the relations
\[
e_1 + e_2 = e_1 - e_2 \quad e_\alpha = e_1 - e_2 \quad e_\alpha = e_1 - e_2
\]

![FIGURE 9.8](image-url)

**FIGURE 9.8** Fundamental notions concerning the REV and spatial fundamental notions concerning the representative elementary volume and spatial averaging over intensive quantities associated with interacting phases in it.
where \( \bar{\varepsilon}_i^\alpha \) (\( \equiv \int e_i dU / U_{0\alpha} \)) denotes the intensity of the macroscopic quantity associated with the \( \alpha \) phase spatially averaged over the volume it occupies within the REV. Actually the notion of \( e^\alpha \equiv e_i^\alpha \) in (9.19) can, for example, refer to the microscopic phase extensive quantity being the momentum (\( \varepsilon^\alpha \equiv \mathbf{M} \)) vector for which \( e = \rho \mathbf{\Phi} \); \( e_i^\alpha = \rho_i \); \( e_i^\alpha = \mathbf{\Phi} \) (see second example in Section 9.3). Following [8], we note that phase motion is not of a Brownian type, as the vanishing of its macroscopic intensive quantity will cause the disappearance of the deviation from that intensive quantity (i.e., \( e = 0 \Leftrightarrow \varepsilon^\alpha = 0 \Rightarrow e^\alpha = 0 \)). Hence, adding to the definition in (9.19), we write

\[
\dot{e} = \Lambda_e e
\]  

(9.20)

in which \( \Lambda_e \) denotes a factor (e.g., obtained empirically) that can be a scalar or an element of a vector or of a tensor. Following [2], we write the averaging over the REV a spatial derivative that represents the macroscopic spatial derivative of \( G_{\alpha\beta} \) element (scalar, vector, or tensor associated with \( \alpha \)) of \( e^\alpha \):

\[
\frac{\partial}{\partial x_i} G_{\alpha\beta} = \frac{\partial}{\partial x_i} \overline{G_{\alpha\beta}} + \frac{1}{U_0} \int G_{\alpha\beta} \xi_i ds
\]  

(9.21)

The modified rule for the macroscopic spatial derivative reads

\[
\frac{\partial e^\alpha}{\partial x_i} \equiv \frac{\partial e^\alpha}{\partial x_j} T_{\alpha ij} \equiv \frac{1}{\theta_\alpha U_0} \int_{\alpha\beta} \left[ e_i \xi_j dS \right]
\]  

(9.22)

where \( T_{\alpha ij} \) denotes the \( \alpha \) phase tortuosity tensor summing over the \( \alpha \)–\( \alpha \) part of the REV enclosing interface of the tortuous passage length along the interface of two adjacent phases.

The REV average time derivative, representing the macroscopic time derivative, reads

\[
\frac{D}{Dt} \left( e^\alpha \right) = \frac{\partial e^\alpha}{\partial t} + \frac{1}{U_0} \int e_i \mathbf{v} \cdot \xi_i ds
\]  

(9.23)

We note in (9.23) that \( 1 \ll St^e \Leftrightarrow \frac{D}{Dt} \left( e^\alpha \right) \equiv \frac{\partial e^\alpha}{\partial t} \) denotes the Strouhal number, for which \( L^e, t^e, \mathbf{\Phi} \) denote characteristic values of length, time, and velocity, respectively, of the phase intensive quantity.

In view of (9.16), (9.19), (9.21), and (9.23), the macroscopic form of the general balance equation for the \( \alpha \) phase \( E \) quantity reads

\[
\frac{D}{Dt} \left( e^\alpha \right) = \mathbf{\nabla} \cdot \left[ \theta_\alpha \left( e^\alpha \mathbf{\Phi}^\alpha + e^\alpha \mathbf{\Phi}^\alpha + \mathbf{\Phi}^{\alpha m} \right) + \theta_\alpha \rho_a \Gamma^\alpha \right] - \frac{1}{U_0} \int e_i \left( \mathbf{\Phi}_a - \mathbf{v} \right) \cdot \xi_i ds
\]  

(9.24)

in which \( e^\alpha \mathbf{\Phi}^\alpha \) is referred to as the macroscopic dispersive flux, which is an artifact of the spatial averaging procedure. The combined \( e^\alpha \mathbf{\Phi}^\alpha + \mathbf{\Phi}^{\alpha m} \) macroscopic dispersive and diffusive flux in (9.24) is referred as the macroscopic hydrodynamic dispersive flux. Assuming that (1) a material \( \alpha \)–\( \beta \) interface,
that is, \( \mathbf{v} \cdot \mathbf{q} = \mathbf{9}_a^\alpha \cdot \mathbf{q} \Rightarrow [e_a(\mathbf{9}_a - \mathbf{v}) + \mathbf{J}_a^m] \cdot \mathbf{q} = 0 \), and (2) \( 1 \ll St \Rightarrow \frac{D_a}{Dt}(e_a) \equiv \frac{\partial}{\partial t}e_a \), we rewrite (9.24) the general \( \alpha \) phase balance equation for its \( E \) quantity to read

\[
\frac{\partial}{\partial t} \left( \theta_a e_a^\alpha \right) = -\nabla \left[ \theta_a e_a^\alpha \mathbf{9}_a^\alpha + \theta_a \left( \mathbf{c}_a \mathbf{9}_a + \mathbf{J}_a^m \right) \right] + \theta_a \rho_d \Gamma E_a^\alpha
\]

(9.25)

As an example let us consider the macroscopic mass balance of a \( \delta \) component in \( \alpha \) phase, considering \( \mathbf{v} \) its volume-weighted velocity. Hence, considering \( E = m^\delta \Rightarrow e = \rho_d^\delta (\equiv C^\delta) \); \( \mathbf{J}^m \) (\( \equiv \mathbf{I} \)); \( \Gamma^m \) (\( \equiv \Gamma^\delta \)) and assigning Fick’s law as the potential flow pattern defining the hydrodynamic dispersion flux

\[
\mathbf{J} = -D_h^\delta \nabla C^\delta
\]

then in view of (9.25) we write

\[
\frac{\partial}{\partial t} \left( \theta_a C^\delta_a^\alpha \right) = -\nabla \cdot \left( \theta_a C^\delta_a^\alpha \mathbf{9}^\delta - \theta_a D_h^\delta \nabla C^\delta_a^\alpha \right) + \theta_a \rho \Gamma^\delta
\]

in which \( q = \theta_a \mathbf{9}^\delta \) can be referred to as Darcy’s specific flux, for negligible solid phase velocity.

### 9.2.5 Spatial Scale–Dependent Macroscopic Balance Equations

Accounting for the possibility that \( \mathbf{9}^\delta \) and by virtue of (9.19), we note that the advective flux can become

\[
e \mathbf{9}^\delta = e \mathbf{9}^\delta + \mathbf{e} \mathbf{9} = \left( e_1 e_2 + e_1 e_2 \right) \mathbf{9}^\delta + e \mathbf{9}
\]

in which \( d^\delta \equiv e \mathbf{9} \) accounts for macroscopic deviations from the intensive macroscopic quantity \( e^\delta \) of \( \alpha \) phase and \( e \mathbf{9} \) presents deviation from the advective flux. When substituting this into (9.25), we obtain the \( \alpha \) phase balance equation of its \( E \) quantity that reads

\[
\frac{\partial}{\partial t} \left[ \theta_a \left( e_1 e_2 + d^\delta \right) \right] = -\nabla \cdot \left[ \theta_a \left( e_1 e_2 + d^\delta \right) \mathbf{9}^\delta + \theta_a \left( \mathbf{e} \mathbf{9} + \mathbf{J}^\delta \right) \right] + \theta_a \rho \Gamma^\delta
\]

(9.26)

Hereinafter, for the sake of reducing the overload of notations, we will refer to macroscopic quantities without the \( \mathbf{1} \) designator. By virtue of (9.20) we can relate the dispersive flux in (9.26) to the advective flux and the deviation from the intensive quantity, reading

\[
e \mathbf{9} = \mathbf{A} \cdot \mathbf{9}, \mathbf{A} \equiv \Lambda_2 \Lambda_3, \mathbf{9} = \Lambda_3 \cdot \mathbf{9}; d^\delta \equiv e \mathbf{9} = \Lambda_{c12} e_1 e_2, \Lambda_{c12} \equiv e \mathbf{9} = \Lambda_2
\]

(9.27)

where \( \Lambda_a \) denotes a tensor quantity. Referring to (9.26) and in view of (9.27), we chose to make the following assumptions:

\[
[A.1] \ e_2 \gg |d^\delta| \Rightarrow |d^\delta| \equiv |\Lambda_{c12} e_2| \Rightarrow e_2 \equiv |\Lambda_{c12}| \ll 1 \Rightarrow \Lambda_{c12} = e_2 \delta_
u \Rightarrow |\delta_\nu| = 1;

[A.2] \ |\mathbf{e} \mathbf{9}| \gg |e \mathbf{9}| \equiv |\mathbf{e} \mathbf{A} \mathbf{9}| \ll 1 \Rightarrow \mathbf{A} = \mathbf{e} \mathbf{B} \Rightarrow |\mathbf{B}| = 1.
\]
By virtue of [A.1] we rewrite (9.26) to read

\[
\frac{\partial}{\partial t} (e_1 \epsilon) + e_\alpha \frac{\partial}{\partial t} (\theta B_\epsilon \epsilon e_2) = -\nabla \left[ \theta \left( e_1 \epsilon \epsilon + \epsilon \epsilon + J^E \right) \right] + \theta \rho \Gamma^E - e_\alpha \nabla \left( \theta e_1 \epsilon \epsilon \epsilon \epsilon \right)
\]  

(9.28)

which accounts for the advective and the hydrodynamic dispersive fluxes. The latter is habitually adopting a potential flow pattern fitting an empirical relation.

By virtue of [A.1] and [A.2], we rewrite (9.26) to read

\[
\frac{\partial}{\partial t} (e_1 \epsilon) + e_\alpha \frac{\partial}{\partial t} (\theta B_\epsilon \epsilon e_2) = -\nabla \left[ \theta \left( e_1 \epsilon \epsilon + J^E \right) \right] + \theta \rho \Gamma^E - \nabla \left[ \theta \left( e_\alpha B_1 + eB \right) \epsilon \epsilon \right]
\]  

(9.29)

which addresses the advective and diffusive fluxes.

As both solutions of (9.28) and (9.29), when \( \epsilon \approx 0 \) (\( \epsilon_\alpha \)) are functions of \( \epsilon \ll 1 \), we can expand their dependent variables using terms associated with a polynomial of \( \epsilon \) powers. Approximate solutions to (9.28) and (9.29) can thus be obtained by solving an infinite set of the corresponding balance equations of descending order magnitudes. While the first (i.e., when \( \epsilon = 0 \)) balance equation may be nonlinear and of the highest order of magnitude, the others are linear balance equations as they are combined with variables obtained from the solution of equations that are of higher-order magnitude. By virtue of [A.1] and in view of (9.28), we obtain the set of general macroscopic balance equations for any \( \alpha \) phase of its \( E \) extensive quantity:

The primary (dominant) one corresponding to the REV (larger) length scale reads

\[
\frac{\partial}{\partial t} (e_1 \epsilon) = -\nabla \left[ \theta \epsilon \epsilon \epsilon + \theta \left( e_1 \epsilon \epsilon + J^E \right) \right] + \theta \rho \Gamma^E
\]  

(9.30)

Concurrently, the secondary one that corresponds to a length span much smaller than that of (9.30) reads

\[
\frac{\partial}{\partial t} (0 d^E) = -\nabla \left( 0 d^E \epsilon \epsilon \epsilon \right)
\]  

(9.31)

We note that (9.30) and (9.31) are based on a different premise and thus can represent different characteristics. At the REV (larger) spatial scale and subject to different assumptions, the governing balance equation (9.30) can accommodate pure advection (hyperbolic PDE), advection–dispersion (hyperbolic or parabolic PDE, respectively), or pure dispersion (elliptic PDE) fluxes. The secondary governing balance equation (9.31) describes the concurrent pure advection (i.e., hyperbolic PDE characterized by a sharp front migration of the state variable) of the deviation \( d^E \) from the intensive quantity, at a spatial scale much smaller than that of the REV. The solution for \( d^E \) of (9.31) also on \( \epsilon \) obtained from the solution of (9.30). Moreover, one can seek further resolution modes of \( d^E \) and \( \epsilon \), via an iterative process between (9.31) and the combined form of (9.30) and (9.31), which is the form expressed in (9.28).

By virtue of [A.1] and [A.2] and in view of (9.29), another possible set of general macroscopic balance equations of the \( E \) extensive quantity for any \( \alpha \) phase:

The primary (dominant) one valid at the REV (larger) length scale reads

\[
\frac{\partial}{\partial t} (e_1 \epsilon) = -\nabla \left( e_1 \epsilon \epsilon \epsilon + \theta \epsilon \epsilon \epsilon + J^E \right) + \theta \rho \Gamma^E
\]  

(9.32)

Concurrently, the secondary one that corresponds to a length span much smaller than that of (9.32) reads

\[
\frac{\partial}{\partial t} (0 d^E) = -\nabla \left( 0 d^E \epsilon \epsilon \epsilon \right)
\]  

(9.33)
in which the dispersive flux \( \phi \) is also addressed. The discussion and procedure referring to (9.28), (9.30), and (9.31) correspond, respectively, also to (9.29), (9.32), and (9.33).

On the premises of sets (9.30) and (9.31), let us exemplify the construction of a spatial-scaled component mass balance equations in a fluid. In [5], we consider a \( \gamma \) component for which \( m= \) denotes its mass so its extensive quantity is with the intensive quantity \( \rho \) related to its mass fraction (\( \omega \)), and let us account for the specific component source

\[
\Gamma_m(\gamma) = \Gamma_m \rho \omega.
\]

Let us consider a saturated domain, and following Fick’s law based on a potential flow pattern, we combine the component diffusive flux vector \( \nabla \cdot \nabla = \nabla \cdot (D \cdot \nabla) \) and its dispersive flux vector \( \nabla \cdot \nabla = \nabla \cdot (C \cdot \nabla) \) for which \( D \) denotes the component constant hydrodynamic dispersion tensor. In view of (9.30), for the REV length scale, we obtain the primary component mass balance equation in the form

\[
\frac{\partial}{\partial t} \left( \phi C \right) = -\nabla \cdot (\phi (C - D \cdot \nabla C)) + \phi \Gamma_m
\]

that describes the transport of a component subject to advective and dispersive flux mechanisms, interpreted by hyperbolic and parabolic PDE characteristics, respectively.

In view of (9.31), at the smaller scale, the secondary component mass balance equation becomes

\[
\frac{\partial}{\partial t} \left( \phi \cdot d_m \right) = -\nabla \cdot (\phi \cdot d_m \cdot \delta) \quad ; \quad d_m = \omega \rho
\]

that governs transport at the pore scale by pure advection (hyperbolic PDE) and in which \( d_m \) denotes the deviation from the component concentration.

In reference to sets (9.32) and (9.33), let us exemplify the construction of the spatial-scaled momentum balance equations of a phase. Following [4] and [5], here the phase extensive quantity is its momentum (i.e., \( E=M \)), for which its macroscopic quantities are \( e=M \) (i.e., \( e_1=M \), \( e_2=M \) denote the deviation from the intensive quantity, and \( \delta \) represents the momentum dispersive flux tensor), the momentum diffusive flux \( J_m=\sigma \) (\( \sigma \)-phase stress tensor), and \( \Gamma_m=F \) (\( F \)-specific body force acting on the phase) refers to the momentum source flux vector. In view of (9.32) for the REV length scale, we obtain the primary phase momentum balance equation in the form

\[
\frac{\partial}{\partial t} (\theta \delta) = -\nabla \cdot (\theta (\theta \delta - \theta \sigma)) + \theta \rho F
\]

In view of (9.33), at a scale much smaller than the REV length scale, the secondary phase momentum balance equation becomes

\[
\frac{\partial}{\partial t} (\theta d^M) = -\nabla \cdot (\theta \cdot (1 + \Lambda) \cdot d^M \cdot \delta) \quad ; \quad \Omega = (L_{\rho}, L_V)^{-1} L_{\rho V} L_V
\]

Letting the \( \alpha \) phase represent a Newtonian fluid, then the macroscopic Navier–Stokes equation resulting from the aforementioned primary momentum balance equation can govern the propagation of shock waves through porous media [3] and conform to Forchheimer’s law accounting for the transfer of fluid inertia through the microscopic solid–fluid interface or to Darcy’s law when friction at that interface is dominant [4]. At the much smaller scale, the hyperbolic PDE addressing the secondary phase
momentum balance equation describes an inertia momentum balance equation in the form of a wave equation that governs the concurrent propagation of the $d^{th}$ quantity.

9.2.6 Modeling of Multiphase Multicomponent Transport Phenomena

We maintain that the modeling of the temporal and spatial distribution of contaminants in the unsaturated and saturated zones is best demonstrated via an example [1]. This will thus be developed through the case of three $l=q, n, g$ interacting mobile phases: $q$ denoting the aqueous fluid, $n$ denoting the nonaqueous phase liquids (NAPL), and $g$ denoting the gas fluid. The described model accounts for $p=w, a, c_m$ three components, $w$ denoting water, $a$ denoting air, and $c_m$ denoting a contaminant (e.g., trichloroethylene (TCE)), undergoing equilibrium or nonequilibrium partitioning between the three mobile phases as well as sorption into the solid matrix. Schematization of the interactions between the phases and the components is depicted in Figure 9.9.

Let us thus consider the case of equilibrium partitioning of components between phases under isothermal conditions; we then write the following:

The mass balance equation of the contaminant, $c_m$, in the three phases, $q, g, n$, reads

$$\frac{\partial}{\partial t} \left[ \phi \left( S_q M_q X_{q-m} + S_n M_n X_{n-m} + \rho_b K_d M_q X_{n-m} \right) \right] = \nabla \cdot \left( \phi S_q D_{iq}^{\\text{eq}} \cdot M_q \nabla X_{q-m} - M_q X_{q-m} \phi \right)$$

$$+ \nabla \cdot \left( \phi S_g D_{ig}^{\\text{eq}} \cdot M_g \nabla X_{g-q} - M_g X_{g-q} \phi \right) + q_{m}$$

(9.34)

The mass balance equation of the water component, $w$, in the two phases, $q, g$, reads

$$\frac{\partial}{\partial t} \left[ \phi \left( S_q M_q X_{q-w} + S_g M_g X_{g-w} \right) \right] = \nabla \cdot \left( \phi S_q D_{iq}^{\\text{eq}} \cdot M_q \nabla X_{w-q} - M_q X_{w-q} \phi \right)$$

$$+ \nabla \cdot \left( \phi S_g D_{ig}^{\\text{eq}} \cdot M_g \nabla X_{g-w} - M_g X_{g-w} \phi \right) + q_{w}$$

(9.35)

Multiphase and multicomponent interactions through the unsaturated/saturated zone

Consider three, $l=(n)—\text{NAPL}; q—\text{aqueous}; g—\text{gaseous})$ fluid phases and three, $p=(w)—\text{water}; a—\text{air}; c_m—\text{contaminants}$) components.

**FIGURE 9.9** Schematization of four interacting phases (three mobile fluids) with three components. A possible transport phenomenon in an urban area aquifer.
The mass balance equation of the air component, \( a \), in the \( g \) phase reads

\[
\frac{\partial}{\partial t} \left[ \phi_S g M_g X_{ag} \right] = \nabla \cdot \left( \phi_S g D_{ng}^g M_g \nabla X_{ag} - M_g X_{ag} \mathbf{g} \right) + q_a
\]  

(9.36)

In (9.34) through (9.36), \( X_{pl} = n_{pl}/n_l \) \( \sum p X_{pl} = 1, \forall l \) denotes the mole fraction of component \( p \) in fluid \( l \); porosity is denoted by \( \phi \), fluid content by \( \phi S \); in which \( \sum_i S_i = 1 \) denotes saturation of the \( l \) fluid; the relation between the \( l \) fluid mass density \( \rho_l \) and its molar density \( M_l \) is defined by

\[
\rho_l = \frac{\sum_p m_{pl}}{n_l} \Rightarrow \rho_l = M_l \left( \sum_p m_{pl} \right) / \sum_p n_{pl} = M_l \sum_p W_p \frac{n_{pl}}{n_l} / \sum_p \frac{n_{pl}}{n_l} = M_l \sum_p W_p X_{pl}
\]

where

- \( m_l = \sum_p m_{pl} \) denotes the \( l \) fluid mass in [mole/volume]
- \( n_l \approx \sum_p n_{pl} \) denotes a quantity of substance of phase \( l \) in [mole]
- \( W_p = m_p/n_p \) denotes the molecular weight of the \( p \) component
- \( \rho_p \) denotes the solid mass density
- \( K_d \) denotes the sorption coefficient onto the solid phase
- \( q_p \) denotes a source/sink mass flux of the \( p \) component

Using the fluid linear momentum balance equations given by Darcy’s law (friction dominant between fluid and solid phases, at their common microscopic interface), we obtain \( \mathbf{g}_l \) the \( l \) fluid velocity vectors (Darcy’s specific flux) in the form

\[
\mathbf{g}_l = -K \frac{k_{rl}}{\mu_l} \left( \nabla P_l + \rho_l g \nabla Z \right); \forall l
\]  

(9.37)

where

- \( K \) is the absolute permeability tensor
- \( k_{rl} \) denotes the relative permeability of the \( l \) fluid
- \( \mu_l \) denotes its viscosity

A typical graph for \( k_{rl} \) is depicted in Figure 9.10.

The \( l \) fluid partial pressure \( P_l \) in (9.37) is given by constitutive relations in the form

\[
P_l = P_n + \alpha P_{c,g} (S_g) + (1 - \alpha) \left[ P_{c,q} (S_q) - P_{c,n,q} (S_q = 1) \right]; \quad \alpha = \min \left( 1, S_n/S_n^* \right)
\]  

(9.38)

where

- \( P_{c,k/l} \) denotes the capillary pressure between the \( l \) and \( k \) fluids
- \( S_n^* \) denotes a blending parameter
The $ij$ element of the hydrodynamic dispersion tensor $D_{ll}^{ij}$ for component $p$ in the $l$ fluid is defined by

$$
\phi S_l D_{ll}^{ij} = \left( \phi S_l D_{ll}^p + \alpha_{ll} \right) \delta_{ij} + \left( \alpha_{ll} - \alpha_{ll} \right) \frac{S_l}{|S_l|} \delta_{ij}; \quad \forall l
$$

(9.39)

where

- $\alpha_{ll}$ and $\alpha_{ll}$ denote, respectively, the transverse and longitudinal dispersivities of the $l$ fluid
- $D_{ll}^p$ denotes the diffusion coefficient of component $p$ in the $l$ fluid
- $\delta$ denotes the Kronecker delta tensor

Equilibrium partitioning coefficients between the gas, $g$, and the nonaqueous fluids, $n$, as well as the gas, $g$, and the aqueous fluids, $q$. In these cases we have state functions in the form

$$
X_{cm} = \frac{X_{cm}^* P_g^*}{P_g} X_{cm}^*; \quad X_{cm} = \frac{X_{cm}^* P_g}{X_{cm}^* P_g^*} X_{cm}^*; \quad X_{wg} = \frac{\beta_{wg}}{P_g} X_{wg}
$$

(9.40)

where

- $X_{cm}^*$, $X_{cm}^*$ denote the mole fractions of contaminant in equilibrium with nonaqueous fluids
- $P_g^*$ denotes a reference pressure for the $l$ fluid
- $\beta_{wg}$ denotes the partial pressure of water in gas fluid in equilibrium with the aqueous fluid

The state functions associated with the fluid molar densities $M_g$, $M_n$, $M_g$ are expressed in the form

$$
M_l = 1 + \beta_l \left( P_l - P_l^* \right), \quad l \equiv q, n; \quad M_g = \frac{P_g}{RT_l^*}
$$

(9.41)
where

\( M^* \) denotes the fluid molar density at \( P = P^* \)
the fluid compressibility is denoted by \( \beta \)
the ideal gas constant is denoted by \( R \)
\( T^* \) denotes a reference temperature

Finally, for the case of need to accommodate the point-to-point variability in a heterogeneous permeability field, the capillary pressure \( P_{c,ij} \) curves associated with the \( i \) and \( j \) fluids are scaled using \( P_{c,ij}^D \) the dimensionless capillary pressure between these fluids in the form

\[
P_{c,ij}^D = \frac{P_{c,ij}}{\sigma_{ij}} \left( \frac{|K|}{\phi} \right)^{\frac{1}{\alpha}} \sim 0.5; \quad l_i, l_j \equiv \text{gn, gg, nq}
\]  

where \( \sigma_{ij} \) denotes the interfacial tension between the \( i \) and \( j \) fluids.

### 9.3 Summary and Conclusions

Fundamental formulation was addressed for modeling the transport of multiphase and multicomponent through heterogeneous media. Although beyond the scope of the current interest, in the case of nonequilibrium dissolution, separate mass balance equations for the contaminant will need to be prescribed. Moreover, as simulations may be consuming significant computational time, seeking for the possibility of studying small-scale (spatial span and evolution periods) examples can yield qualitative and quantitative assessments on trends for larger-scale examples. This scale-up process can be achieved by using nondimensional analysis of the involved balance equations.

### References

5. Sorek, S. and Ronen, D., 2006, Scale dependent fluid momentum and solute mass macroscopic balance equations: Theory and observations, CMWR XVI, Copenhagen, Denmark, http://proceedings.cmwr-xvi.org/getFile.py/access?contribId=801&amp;sessionId=11&amp;resId=0&amp;materialId=paper&amp;confId=a051