

MATH 5490 - Mathematics of Flow in Porous Media Lecture Notes

Libao Jin (ljin1@uwo.edu)

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Contents

1	Basic Mechanics	1
1.1	Kinematics (Description of Motion)	1
1.1.1	Balance laws	2
1.1.2	Local momentum balance	2
1.1.3	Constitutive Laws	3
1.1.4	Hagen-Poiseuille flow	5
1.1.5	Stokes problem	5
1.2	Mechanics of mixtures	6
1.2.1	Constituents	6
1.2.2	Densities and volume fractions	6
1.2.3	Categorites of mixtures	7
1.2.4	Balance Laws	8
1.2.5	Momemntum Balance	8
2	Modles of Single-Phase Fluid FLOW in a Porous Medium	9
2.1	Darcy's Law	9
2.1.1	Derivation from momentum balance	9
2.2	Permeability	11
2.3	Flow equation for single-phase fluids	11
2.4	Non-Darcy Flows	12
2.4.1	Brinknum law (1947)	12
2.4.2	Forchkeimer law (1901)	13
2.5	Potential formulation	13
2.6	Reformulation of flow equation	15
2.7	Areal flows	16
2.8	Well hydraulics	17
2.8.1	Dirac- δ model	17
2.8.2	Thiem model (1906)	19
2.8.3	Theis model (1935)	20
2.9	Tensor-valued permeability	20
2.9.1	Properties attributed to $\tilde{\mathcal{K}}$ and $\tilde{\mathbf{k}}$	22
3	Transport in Porous Media	23
3.1	Trasnport equation	23
3.2	Hydrodynamic dispersion	24
3.3	1-D nonreacting transport	25
3.4	Tranport with adsorption	27
3.5	Linear adsorption isotherms and retardation	27

4	Multiphase Flows in Porous Media	28
4.1	Porous-medium equation	28
5	Multiphase Flows in Porous Media	30
5.1	Capillary pressure	30
5.2	Wettability	31
5.3	Macroscopic picture	32
5.4	Multiphase flow equations	32
5.4.1	Classification	33
5.5	The Buckley-Leverett Problem (1942)	33
5.6	Welge tangent construction (1952)	34
5.7	Variably saturated flow	35
5.8	Observations	35
5.9	Alternative formulations	36
6	Flows with interphase mass transfer	36
6.1	Compositional models (in general)	36
6.2	Equation-of-state methods	39

Disclaimer: there might be some typo, use this notes with caution. Also please feel free to let me know if there is anything wrong.

1 Basic Mechanics

Goal: Develop balance laws

1.1 Kinematics (Description of Motion)

Definition 1.1. A *body* \mathcal{B} is a set of *particles* (material points) X .

Definition 1.2. A *configuration* is a mapping $\tilde{\chi} : \mathcal{B} \rightarrow \mathbb{E}$, where $\mathbb{E} \subset \mathbb{R}^3$, that is, 1-1, C^1 (continuous differentiable), with C^1 inverse $\tilde{\chi}^{-1} : \tilde{\chi}(\mathcal{B}) \rightarrow \mathcal{B}$. Let $\tilde{\chi}(X) = \mathbf{X}$ be the position of X in the configuration.

Fix a *reference configuration*, $\tilde{\kappa} : \mathcal{B} \rightarrow \mathbb{E}$. Let $\mathbf{X} = \tilde{\chi}(X)$ = new label for X = referential or Lagrangian coordinates of X (like the home address). Associate with any body \mathcal{B} to a 1-parameter family of configurations $\tilde{\chi}_k(\cdot, t) : \tilde{\kappa}(\mathcal{B}) \rightarrow \mathbb{E}$ such that

1. At each time t , $\tilde{\chi}_k(\cdot, t)$ is 1-1, C^1 with C^1 inverse.
2. $\tilde{\chi}_k(\mathbf{X}, t)$ = position of particle X at time t .

where $\tilde{\chi}_k$ is the deformation of \mathcal{B} , $\tilde{\chi}_k(\mathbf{X}, t)$ = spatial or Eulerian coordinates of X at time t . By invertibility, $\mathbf{X} = \tilde{\chi}^{-1}(\mathbf{x}, t)$ gives (the referential coordinates of) the particle that is occupying \mathbf{x} at time t .

Definition 1.3. The *referential* (or *Lagrangian*) *velocity* is $\frac{\partial \tilde{\chi}_k}{\partial t}(\mathbf{X}, t)$. (velocity of particle \mathbf{X} , where it is.)

To find velocity at prescribed position \mathbf{x} (whatever particle is there)

1. Find $X = \tilde{\chi}^{-1}(\mathbf{x}, t)$.
2. Compute $\mathbf{v}(\mathbf{x}, t) = \frac{\partial \tilde{\chi}_k}{\partial t}(\tilde{\chi}_k^{-1}(\mathbf{x}, t), t)$, which is called the *spatial* or *Eulerian velocity*.

Proposition 1.1. $\mathbf{v}(\mathbf{x}, t)$ is independent of κ .

Definition 1.4. The *material derivative* of a function $f(\mathbf{X}, t)$ is

$$\frac{Df}{Dt}(\mathbf{X}, t) = \frac{\partial f}{\partial t}(\mathbf{X}, t) \quad \text{hold } \mathbf{X} \text{ fixed.}$$

Theorem 1.1. For a function $f(\mathbf{x}, t)$ (spatial description)

$$\frac{Df}{Dt}(\mathbf{x}, t) = \frac{\partial f}{\partial t}(\mathbf{x}, t) + \mathbf{v}(\mathbf{x}, t) \cdot \nabla f(\mathbf{x}, t),$$

where $\nabla f = \sum_{i=1}^3 \frac{\partial f}{\partial x_i} \mathbf{e}_i$ = gradient of f .

Proof. By chain rule,

$$\begin{aligned} \frac{Df}{Dt}(\mathbf{x}, t) &= \frac{\partial f}{\partial t}(\tilde{\chi}_k(\mathbf{X}, t), t). \\ &= \partial_1 f(\tilde{\chi}_k(\mathbf{X}, t), t) \frac{\partial \tilde{\chi}_k}{\partial t}(\mathbf{X}, t) + \partial_2 f(\tilde{\chi}_k(\mathbf{X}, t), t) \cdot 1 \\ &= \partial_1 f(\tilde{\chi}_k(\mathbf{X}, t), t) \mathbf{v}(\mathbf{x}, t) + \partial_2 f(\tilde{\chi}_k(\mathbf{X}, t), t). \\ &= \partial_1 f(\mathbf{x}, t) \mathbf{v}(\mathbf{x}, t) + \partial_2 f(\mathbf{x}, t). \\ &= \nabla f(\mathbf{x}, t) \cdot \mathbf{v}(\mathbf{x}, t) + \frac{\partial f}{\partial t}(\mathbf{x}, t). \end{aligned}$$

□

1.1.1 Balance laws

Associate with \mathcal{B} a mass density $\rho(\mathbf{x}, t)$ such that $\forall \mathcal{P} \subset \mathcal{B}$

$$\text{mass in } \mathcal{P} = \int_{\mathcal{R}(t)} \rho(\mathbf{x}, t) dV,$$

where $\mathcal{R}(t) \subset \mathbb{E}$ is the region occupied by \mathcal{P} at time t .

Local (differential) mass balance:

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{v} = 0.$$

where $\nabla \cdot \mathbf{v} = \sum_{i=1}^3 \frac{\partial v_i}{\partial x_i}$ = divergence of \mathbf{v} . Equivalent form:

$$\frac{\partial \rho}{\partial t} + \mathbf{v} \cdot \nabla \rho + \rho \nabla \cdot \mathbf{v} = 0 \iff \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0.$$

Interpretation: for fixed region $\mathcal{R} \subset \mathbb{E}$, integrate and use divergence theorem, we have

$$\begin{aligned} \int_{\mathcal{R}} \frac{\partial \rho}{\partial t} dV &= \frac{d}{dt} \underbrace{\int_{\mathcal{R}} \rho dV}_{\text{total mass in } \mathcal{R}} \\ &= - \int_{\mathcal{R}} \nabla \cdot (\rho \mathbf{v}) dV \\ &= \underbrace{- \int_{\partial \mathcal{R}} \rho \mathbf{v} \cdot \mathbf{n} d\sigma}_{\text{total inward flux of mass across } \partial \mathcal{R}} \end{aligned}$$

where \mathbf{n} is the normal unit vector pointing outward of the region \mathcal{R} .

Special case: $\frac{D\rho}{Dt} = 0 \implies \nabla \cdot \mathbf{v} = 0$. The interpretation would be

1. \mathbf{v} is *solenoidal*.
2. Flow is *incompressible*.

1.1.2 Local momentum balance

We have a vector-valued equation:

$$\frac{D}{Dt}(\rho \mathbf{v}) + \rho(\mathbf{v} \cdot \nabla) \mathbf{v} - \nabla \cdot \mathcal{T} - \rho \mathbf{b} = \mathbf{0}.$$

where $\mathbf{v} \cdot \nabla = \sum_{j=1}^3 v_j \frac{\partial}{\partial x_j}$, so $(\mathbf{v} \cdot \nabla) \mathbf{v} = \sum_{i=1}^3 \sum_{j=1}^3 v_j \frac{\partial v_i}{\partial x_j} \mathbf{e}_i$, $\mathbf{b}(\mathbf{x}, t)$ is the body force per unit mass (gravitational acceleration). The total body force acting on $\mathcal{P} \subset \mathcal{B}$ is

$$\int_{\mathcal{R}(t)} \rho \mathbf{b} dV,$$

where $\mathcal{R}(t)$ is the region occupied by \mathcal{P} . And \mathcal{T} is the stress tensor. Gives force/area (traction) acting on $\partial \mathcal{R}(t)$ as

$$\int_{\partial \mathcal{R}(t)} \mathcal{T} \mathbf{t} d\sigma.$$

Remark 1.1 (Remark about \mathcal{T}).

1. In Cartesian coordinates, \mathcal{T} has matrix representation

$$\begin{bmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{bmatrix}, T_{ij} = \mathbf{e}_i \cdot \mathcal{T} \mathbf{e}_j.$$

It is a linear transformation acting on vectors.

2. T_{ij} gives the i -th component of force/area acting on surfaces that is perpendicular to \mathbf{e}_j . T_{jj} is the *compressible* or *tensile* stresses (e.g. pressure), and T_{ij} ($i \neq j$) are the shear stresses.

3. Possible to show $T_{ij} = T_{ji}$ (symmetric), i.e., $\mathcal{T}^T = \mathcal{T}$.

$$\nabla \cdot \mathcal{T} = \sum_{j=1}^3 \begin{bmatrix} \partial T_{1j} / \partial x_j \\ \partial T_{2j} / \partial x_j \\ \partial T_{3j} / \partial x_j \end{bmatrix}$$

Example 1.1. Multiply mass balance by \mathbf{v} and subtract from momentum balance to get

$$\underbrace{\rho \frac{D\mathbf{v}}{Dt}}_{\text{mass / vol} \cdot \text{accel}} = \underbrace{\nabla \cdot \mathcal{T} + \rho \mathbf{b}}_{\text{total force / volume}} = \underbrace{\rho \frac{\partial \mathbf{v}}{\partial t} + \rho (\mathbf{v} \cdot \nabla) \mathbf{v}}_{\text{inertial terms}}$$

1.1.3 Constitutive Laws

Motivation: We have four scalar PDEs:

$$\begin{aligned} \frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{v} &= 0, \\ \rho \frac{D\mathbf{v}}{Dt} &= \nabla \cdot \tilde{\mathcal{T}} + \rho \mathbf{b}, \end{aligned} \tag{1.1}$$

for $\rho, \mathbf{v}, \tilde{\mathcal{T}}, \mathbf{b}$ (16 scalar unknowns), 13 if we use $(\tilde{\mathcal{T}})^T = \tilde{\mathcal{T}}$, then we need 9 additional equations to close system.

Regard (1.1) as governing ρ, \mathbf{v} . Need constitutive relations to give $T_{11}, T_{12}, T_{13}, T_{22}, T_{23}, T_{33}, b_1, b_2, b_3$ possibly in terms of ρ, \mathbf{v} .

Example 1.2. $\mathbf{b} = -g\mathbf{e}_3$ is the gravity, where $g \approx 9.8\text{m/s}^2$ is gravitational acceleration. And $z(\mathbf{x})$ is the depth of \mathbf{x} below some datum. That implies

$$\nabla z = \sum_{i=1}^3 \frac{\partial z}{\partial x_i} \mathbf{e}_i = -\mathbf{e}_3.$$

Example 1.3 (ideal fluids). Let $\tilde{\mathcal{T}} = -p\tilde{\mathcal{I}}$, where $p = p(\mathbf{x}, t)$ is the mechanical pressure (force/area), which is not homogenous,

$$\tilde{\mathcal{I}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

Thus,

$$\tilde{\mathcal{T}} = - \begin{bmatrix} p & 0 & 0 \\ 0 & p & 0 \\ 0 & 0 & p \end{bmatrix}$$

is called *normal* (meaning $T_{ij} = 0$ for $i \neq j$) and *isotropic* ($T_{11} = T_{22} = T_{33}$). Momentum balance for ideal fluid with gravity:

$$\rho \frac{\partial \mathbf{v}}{\partial t} + \rho(\mathbf{v} \cdot \nabla) \mathbf{v} = -\nabla p + \rho g \nabla z.$$

Quasi-steady: inertial terms (acceleration) negligible.

$$\begin{aligned} \nabla p &= \rho g \nabla z, \\ \frac{\partial p}{\partial x_3} &= \rho g \frac{\partial z}{\partial x_3} \implies p \Big|_{x_3=-z} = p \Big|_{x_3=0} + \rho g z. \end{aligned}$$

The second equation is called hydrostatic equation.

Example 1.4 (Incompressible Newtonian fluids).

$$\tilde{\mathcal{T}} = -p\tilde{\mathcal{I}} + 2\mu\tilde{\mathcal{D}},$$

where $\tilde{\mathcal{D}} = \frac{1}{2}[\nabla \mathbf{v} + (\nabla \mathbf{v})^T]$ is the stretching tensor, $(\nabla \mathbf{v})_{ij} = \frac{\partial v_i}{\partial x_j}$, μ is the coefficients of dynamic viscosity. And the dimension of $\mu : \rho L^2 T^{-1} = ML^{-1} T^{-1}$, common unit: centipoise (Poiseville) (H_2O at $20C$, latin)

Shallow, horizontal flow: neglect body force (gravity), we have the Naviers-Stokes equation

$$\rho \frac{D\mathbf{v}}{Dt} = \rho \frac{\partial \mathbf{v}}{\partial t} + \rho(\cdot \nabla) \mathbf{v} = -\nabla p + \mu \Delta \mathbf{v}$$

where $\Delta \mathbf{v} = \sum_{i=1}^3 \begin{bmatrix} \partial^2 v_1 / \partial x_i^2 \\ \partial^2 v_2 / \partial x_i^2 \\ \partial^2 v_3 / \partial x_i^2 \end{bmatrix}$.

Dimensionless Form: Rewrite N-S in a form independent of units. Dimensionless variables: $\xi = \mathbf{x}/R, \tau = v_\infty t/R, \mathbf{v}^* = \mathbf{v}/v_\infty, p^* = p/(\rho v_\infty^2)$.

Chain rule:

$$\nabla = \sum_{i=1}^3 \mathbf{e}_i \frac{\partial}{\partial x_i} = \sum_{i=1}^3 \mathbf{e}_i \frac{d\xi_i}{dx_i} \frac{\partial}{\partial \xi_i} = \frac{1}{R} \sum_{i=1}^3 \mathbf{e}_i \frac{\partial}{\partial \xi_i} = \frac{1}{R} \nabla_\xi$$

Therefore,

$$\Delta = \sum_{i=1}^3 \frac{\partial^2}{\partial x_i^2} = \frac{1}{R^2} \Delta_\xi.$$

And

$$\frac{D}{Dt} = \frac{d\tau}{dt} \frac{D}{D\tau} = \frac{v_\infty}{R} \frac{D}{D\tau}.$$

Exercise 1.1. Substitute and simplify get

$$\frac{D\mathbf{v}^*}{D\tau} = -\nabla_\xi p^* + \frac{1}{\text{Re}} \Delta_\xi \mathbf{v}^*,$$

where $\text{Re} = \rho R v_\infty / \mu$ is the *Reynolds number*, which is dimensionless. When $\text{Re} < 1$, it represents the slow, noninertial flows.

1.1.4 Hagen-Poiseuille flow

Steady, axisymmetric flow in cylindrical pipe, ρ and μ are constant. Seek solutions in which $\mathbf{v} = [v(r) \ 0 \ 0]$, where $r = \sqrt{x_2^2 + x_3^2}$ and $p = p(x_1)$. Then

$$\underbrace{\frac{D\mathbf{v}}{Dt}}_0 = -\nabla p + \frac{1}{\text{Re}} \nabla^2 \mathbf{v}.$$

Need only solve first coordinate,

$$0 = \frac{\partial p}{\partial x_1} + \underbrace{\frac{1}{\text{Re}} \left(\frac{\partial^2 v}{\partial x_2^2} + \frac{\partial^2 v}{\partial x_3^2} \right)}_{\text{independent of } x_1}.$$

So $\partial p / \partial x_1 = \text{constant}$, in other words, independent of x_1 . Convert to cylindrical coordinate:

$$\frac{1}{r} \left(\frac{d}{dr} r \frac{dv}{dr} \right) = \text{Re} \frac{\partial p}{\partial x_1}.$$

General solution:

$$v = \frac{\text{Re}}{4} (r^2 + C_1 \log r + C_2).$$

Determine C_1 and C_2 using boundary conditions:

$$\lim_{r \rightarrow 0} |v(r)| < \infty \implies C_1 = 0.$$

No-slip boundary condition: $v(R) = 0$. Then we have the parabolic velocity profile:

$$v(r) = \frac{\text{Re}}{4} \frac{\partial p}{\partial x_1} (R^2 - r^2).$$

1.1.5 Stokes problem

Slow flow around a solid sphere assuming inertial terms negligible

$$\underbrace{\mu \Delta \mathbf{v} = \nabla p}_{\text{momentum balance}}, \quad \nabla \cdot \underbrace{\mathbf{v} = 0}_{\text{mass balance}}.$$

And we have

$$\lim_{\|\mathbf{x}\| \rightarrow \infty} \mathbf{v} = v_\infty \mathbf{e}_1, \quad \mathbf{v}(\mathbf{x}) = 0, \quad \|\mathbf{x}\| = R.$$

Use dimensional analysis to analyze

$$\mathbf{F}_{\text{drag}} = F \mathbf{e}_1, \quad (\text{drag force on sphere}).$$

Then we have Stokes drag

$$F = F(\mu, v_\infty, R) = C \mu^{\alpha_1} v_\infty^{\alpha_2} R^{\alpha_3},$$

where $\alpha_1, \alpha_2, \alpha_3$ to be determined. Both sides have same dimensions:

$$MLT^{-2} = (ML^{-1}T^{-1})^{\alpha_1} (LT^{-1})^{\alpha_2} L^{\alpha_3} = M^{\alpha_1} L^{-\alpha_1 - \alpha_2 + \alpha_3} T^{-\alpha_1 - \alpha_2}$$

Then solving the following the linear system

$$\begin{bmatrix} 1 & 0 & 0 \\ -1 & -1 & 0 \\ -1 & 1 & 1 \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{bmatrix} = \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix} \implies \alpha_1 = \alpha_2 = \alpha_3 = 1.$$

Remark 1.2. Stokes (1856) found that

$$F = 6\pi\mu Rv_\infty$$

where 6π is the shape factor - expect something different for other shapes.

1.2 Mechanics of mixtures

1.2.1 Constituents

N bodies $\mathcal{B}_\alpha, \alpha = 1, \dots, N$ called *constituents*. Overlapping continua: each point $x \in \mathbb{E}$ can be occupied by particles X from every constituent. For each \mathcal{B}_α , fix a reference configuration $\tilde{\kappa}_\alpha : \mathcal{B}_\alpha \rightarrow \mathbb{E}, \mathbf{X}_\alpha = \tilde{\kappa}(X_\alpha)$ is the position of X_α in reference configuration. Associated with each \mathcal{B}_α is a 1-parameter family of mappings $\tilde{\chi}_{\kappa,\alpha}(\cdot, t)$ such that

- (a) At each time t , $\tilde{\chi}_{\kappa,\alpha}(\cdot, t)$ is 1-1, C^1 , with C^1 inverse.
- (b) $\mathbf{x} = \tilde{\chi}_{\kappa,\alpha}(\mathbf{X}_\alpha, t)$ is spatial position of \mathbf{X}_α at time t , where $\tilde{\chi}_{\kappa,\alpha}$ is the deformation of \mathcal{B}_α .

The *referential (Lagrangian)* velocity of \mathcal{B}_α is

$$\frac{\partial \tilde{\chi}_{\kappa,\alpha}(\mathbf{X}_\alpha, t)}{\partial t}.$$

To find the velocity of α at fixed $\mathbf{x} \in \mathbb{E}$ (whatever particle from \mathcal{B}_α is there).

1. Find $\mathbf{X}_\alpha = \tilde{\chi}_{\kappa,\alpha}^{-1}(\mathbf{x}, t)$.
2. Compute $\frac{\partial \tilde{\chi}_{\kappa,\alpha}}{\partial t}(\tilde{\chi}_{\kappa,\alpha}^{-1}(\mathbf{x}, t), t) = \mathbf{v}_\alpha(\mathbf{x}, t)$ is the spatial or Eulerian velocity.

Definition 1.5. The *material derivative* associated \mathcal{B}_α is

$$\frac{D^\alpha f}{Dt}(\mathbf{X}_\alpha, t) = \frac{\partial}{\partial t} f(\mathbf{X}_\alpha, t).$$

Then applying chain rule to

$$\frac{D^\alpha f}{Dt}(\mathbf{x}, t) = \frac{D^\alpha f}{Dt}(\tilde{\chi}_{\kappa,\alpha}(\mathbf{X}_\alpha), t) = \frac{\partial f}{\partial t}(\mathbf{x}, t) + \mathbf{v}_\alpha(\mathbf{x}, t) \cdot \nabla f(\mathbf{x}, t).$$

1.2.2 Densities and volume fractions

Associate with each \mathcal{B}_α a *mass density* $\rho_\alpha(\mathbf{x}, t)$ such that for any $\mathcal{P}_\alpha \subset \mathcal{B}_\alpha$, the mass of α in the region $\mathcal{R}(t)$ occupied by \mathcal{P}_α is

$$\int_{\mathcal{R}(t)} \rho_\alpha(\mathbf{x}, t) dv,$$

where $\rho_\alpha(\mathbf{x}, t) = \frac{\text{mass of } \alpha}{\text{total volume of mixture}}$.

1.2.3 Categorites of mixtures

- *Multiphase* or *immiscible* mixtures: Microscopic geometry interfaces between constituents
- Volume fraction of fluid vs. radius of avergaing window: the ratio would decrease from 1 to a smaller quantity, then fluctuates in a range until the radius is big enough, then the it will stablize at some fraction.
- Interfaces affect physics called the constituents phases
- *Multispecies* or *miscible* mixtures: Segregation among constituents observable only at molecular scales. Constituents are *species*. Example: $Na^+ + Cl^- + H_2O$.
- Associate with each phase α in a multiphase mixture a *volume fraction* $\varphi(\mathbf{x}, t)$ such that volume occupied by α in any region $\mathcal{R}(t)$ is

$$\int_{\mathcal{R}(t)} \varphi_{\alpha}(\mathbf{x}, t) dv.$$

Remark 1.3.

(1) φ_{α} has dimensions $\frac{\text{volume of } \alpha}{\text{total volume}}$.

$$(2) \sum_{\alpha=1}^N \phi_{\alpha} = 1.$$

(3) *True density* of α : $\gamma_{\alpha} = \frac{\rho_{\alpha}}{\varphi_{\alpha}} = \frac{\text{mass of } \alpha}{\text{volume of } \alpha}$.

(4) *Mixture density*: $\sum_{\alpha=1}^N \rho_{\alpha} = \rho$.

Note: $\rho = \sum_{\alpha=1}^N \varphi_{\alpha} \gamma_{\alpha}$ for multiphase mixtures.

Definition 1.6. The barycentric velocity of the mixture is

$$\mathbf{v} = \frac{1}{\rho} \sum_{\alpha=1}^N \rho_{\alpha} \mathbf{v}_{\alpha},$$

and the *diffusion velocity* of α is

$$\tilde{\mathbf{v}}_{\alpha} = \mathbf{v}_{\alpha} - \mathbf{v}.$$

Exercise 1.2. Show that

$$\sum_{\alpha=1}^N \rho_{\alpha} \tilde{\mathbf{v}}_{\alpha} = 0.$$

Also, we have the barycentric derivative of mixture

$$\frac{Df}{Dt}(\mathbf{x}, t) = \frac{\partial f}{\partial t}(\mathbf{x}, t) + \mathbf{v}(\mathbf{x}, t) \cdot \nabla f(\mathbf{x}, t).$$

And

$$\frac{D^{\alpha} f}{Dt}(\mathbf{x}, t) = \frac{\partial f}{\partial t}(\mathbf{x}, t) + \mathbf{v}_{\alpha}(\mathbf{x}, t) \cdot \nabla f(\mathbf{x}, t).$$

1.2.4 Balance Laws

Mass balance:

$$\sum_{\alpha=1}^N \left(\frac{D^\alpha \rho_\alpha}{Dt} + \rho_\alpha \nabla \cdot \mathbf{v}_\alpha \right) = 0.$$

Allos for mass exchange among constituents. We can rewrite the balance law as follows

$$\frac{D^\alpha \rho_\alpha}{Dt} + \rho_\alpha \nabla \cdot \mathbf{v}_\alpha = r_\alpha, \alpha = 1, \dots, N, \text{ where } \sum_{\alpha=1}^N r_\alpha = 0.$$

Note that r_α is the rate of prodcution of α by

- phase chagnes
- interphase mass transfer
- chemical reactions

For multiphase mixtures,

$$\frac{D^\alpha}{Dt}(\varphi_\alpha \gamma_\alpha) + \varphi_\alpha \gamma_\alpha \nabla \cdot \mathbf{v}_\alpha = r_\alpha, \alpha = 1, \dots, N.$$

Define *mass fraction* of α by

$$\omega_\alpha = \frac{\rho_\alpha \text{ mass of } \alpha}{\rho \text{ total mass}}.$$

Equivalent form:

$$\frac{D^\alpha}{Dt} + \rho \omega_\alpha \nabla \cdot \mathbf{v}_\alpha = r_\alpha.$$

By product rule we have

$$\frac{\partial}{\partial t}(\rho \omega_\alpha) + \nabla \cdot (\rho \omega_\alpha \mathbf{v}_\alpha) = r_\alpha.$$

Then

$$\underbrace{\frac{\partial}{\partial t}(\rho \omega_\alpha)}_{\text{accumulation}} + \underbrace{\nabla \cdot (\rho \omega_\alpha \mathbf{v})}_{\text{advection}} + \underbrace{\nabla \cdot \mathbf{j}_\alpha}_{\text{diffusion}} = \underbrace{r_\alpha}_{\text{reaction}},$$

where $\mathbf{j}_\alpha = \rho \omega_\alpha \tilde{\mathbf{v}}_\alpha$ is the diffusive flux.

Exercise 1.3. Show that

$$\sum_{\alpha=1}^N \left(\frac{D^\alpha \rho_\alpha}{Dt} + \rho_\alpha \nabla \cdot \mathbf{v}_\alpha \right) = 0 \iff \frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{v} = 0.$$

1.2.5 Momemntum Balance

$$\frac{D^\alpha(\rho_\alpha \mathbf{v}_\alpha)}{Dt}(\rho_\alpha \mathbf{v}_\alpha) + \rho_\alpha (\mathbf{v}_\alpha \cdot \nabla) \mathbf{v}_\alpha - \nabla \cdot \tilde{\mathbf{T}}_\alpha - \rho_\alpha \mathbf{b}_\alpha = \mathbf{m}_\alpha, \quad \alpha = 1, \dots, N, \text{ where } \sum_{\alpha=1}^N \mathbf{m}_\alpha = 0.$$

Note that \mathbf{m}_α is the momentum exchange into constituents α .

Exercise 1.4. Multiply mass balance by \mathbf{v}_α and subtract to get

$$\rho_\alpha \frac{D\mathbf{v}_\alpha}{Dt} - \nabla \cdot \tilde{\mathcal{T}}_\alpha - \rho_\alpha \mathbf{b}_\alpha = \mathbf{m}_\alpha - \mathbf{v}_\alpha r_\alpha, \quad \alpha = 1, \dots, N,$$

where $-\mathbf{v}_\alpha r_\alpha$ is the rate of momentum transfer into α via mass exchange from other constituents.

Exercise 1.5. Sum α from 1 to N to get

$$\rho \frac{D\mathbf{v}}{Dt} - \nabla \cdot \tilde{\mathcal{T}} - \rho \mathbf{b} = \mathbf{0}.$$

where $\mathbf{b} = \frac{1}{\rho} \sum_{\alpha=1}^N \rho_\alpha \mathbf{b}_\alpha$, $\tilde{\mathcal{T}} = \sum_{\alpha=1}^N (\tilde{\mathcal{T}}_\alpha - \underbrace{\rho \tilde{\nu}_\alpha \otimes \rho \tilde{\nu}_\alpha}_{\text{Reynolds stresses}})$ is the mixture stress.

Remark 1.4.

(1) $\sum_{\alpha=1}^N \tilde{\mathcal{T}}_\alpha = \tilde{\mathcal{T}}_I$ is the inner stress.

(2) For two vectors \mathbf{a} and \mathbf{b} , $\mathbf{a} \otimes \mathbf{b}$ is a tensor having action.

$$(\mathbf{a} \otimes \mathbf{b})\mathbf{u} := \mathbf{a}(\mathbf{b} \cdot \mathbf{u}).$$

In Cartesian coordinates,

$$\tilde{\nu} \otimes \tilde{\nu} = \begin{bmatrix} \tilde{\nu}_1 \\ \tilde{\nu}_2 \\ \tilde{\nu}_3 \end{bmatrix} \begin{bmatrix} \tilde{\nu}_1 & \tilde{\nu}_2 & \tilde{\nu}_3 \end{bmatrix} = \begin{bmatrix} \tilde{\nu}_1 \tilde{\nu}_1 & \tilde{\nu}_1 \tilde{\nu}_2 & \tilde{\nu}_1 \tilde{\nu}_3 \\ \tilde{\nu}_2 \tilde{\nu}_1 & \tilde{\nu}_2 \tilde{\nu}_2 & \tilde{\nu}_2 \tilde{\nu}_3 \\ \tilde{\nu}_3 \tilde{\nu}_1 & \tilde{\nu}_3 \tilde{\nu}_2 & \tilde{\nu}_3 \tilde{\nu}_3 \end{bmatrix},$$

which has rank 1.

2 Modles of Single-Phase Fluid Flow in a Porous Medium

2.1 Darcy's Law

Darcy's experiment (1856)

Flow rate in steady state:

$$Q = KA \frac{h_1 - h_2}{l},$$

where K is constant for any choice of sand (m/s), A is the area of the tank.

2.1.1 Derivation from momentum balance

$$\begin{aligned} \varphi_R \gamma_R \frac{D^R \mathbf{v}_R}{Dt} - \nabla \cdot \tilde{\mathcal{T}}_R - \varphi_R \gamma_R \mathbf{b}_R &= \mathbf{m}_R - \mathbf{v}_R r_R \quad (\text{rock}), \\ \varphi_w \gamma_w \frac{D^w \mathbf{v}_w}{Dt} - \nabla \cdot \tilde{\mathcal{T}}_w - \varphi_w \gamma_w \mathbf{b}_w &= \mathbf{m}_w - \mathbf{v}_w r_w \quad (\text{water}). \end{aligned}$$

Assumptions about physical setting:

- rock is chemically inert, $r_R = 0 \implies r_w = 0$ (mass balance).
- rock forms a rigid matrix: there's a coordinate system in which $\mathbf{v}_R = \mathbf{0}$.
- fluid flow is slow, i.e., flow acceleration is negligible compared with other terms.

Non-inertial flow:

$$\frac{D^F \mathbf{v}_F}{Dt} \approx \mathbf{0}.$$

No need to solve for \mathbf{v}_R . For fluid

$$-\nabla \cdot \tilde{\mathcal{T}}_F - \varphi_F \gamma_F F = \mathbf{m}_F.$$

Drop subscript F , we have φ is the porosity of rock, and $\gamma_F = \rho$ is the density of water.

Constitutive laws

1. Fluid is Newtonian

$$\tilde{\mathcal{T}} = -\varphi p \tilde{\mathcal{I}} + \underbrace{\mu[\nabla \mathbf{v} + (\nabla \mathbf{v})^T]}_{\text{viscous stress}}.$$

Momentum transfer "down" the velocity gradient. Assume momentum transfer via velocity effects is small compared with momentum losses to rock. Hence

$$\tilde{\mathcal{T}} = -\varphi p \tilde{\mathcal{I}}.$$

Fluid-fluid traction across only across part of consisting of water. So far

$$-\nabla \tilde{\mathcal{T}} = \nabla \cdot (\varphi p \tilde{\mathcal{I}}) = \varphi \nabla p + p \nabla \varphi = \varphi p \mathbf{b} + \mathbf{m}, \quad (2.1)$$

where $\varphi \nabla p$ is the flow in response to pressure gradients, $p \nabla \varphi$ is the flow in response to porosity

gradients (not observed), $\tilde{\mathcal{I}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$.

Momentum exchange: Has a Stokes-drag component $\mathbf{m} = -\Lambda^{-1} \mathbf{v} + p \nabla \varphi$, where $-\Lambda^{-1} \mathbf{v}$ is the resembles Stokes drag $C \mu R \mathbf{v}_\infty$, resistivity $\Lambda^{-1} > 0$, expect $\Lambda^{-1} \propto \mu$. $p \nabla \varphi$ exactly cancels that in (2.1). Arises from thermodynamic argument: flow in response to porosity gradients violates second law of thermo.

Gravity is the only body force $\varphi \rho \mathbf{b} = \varphi \rho g \nabla z$, where z is the depth below datum (datum can be sea level height, etc., in other words, it is arbitrary). Subtract all constitutive relations into momentum balance:

$$\varphi \nabla p - \varphi \rho g \nabla z = -\Lambda^{-1} \mathbf{v} \implies \mathbf{v} = -\Lambda \varphi (\nabla p - \rho g \nabla z),$$

where the second equation is Darcy's law.

Remark 2.1.

- Possible to relax some assumptions (e.g., $\mathbf{v}_R = \mathbf{0}$) and still derive Darcy's law.
- Common to define *filtration velocity* $\varphi \mathbf{v}$. Todd (*Groundwater Hydrology*) calls \mathbf{v} the *average interstitial velocity*. Note interstitial derives from interstices, which means "spaces between". $\|\mathbf{v}\| > \|\varphi \mathbf{v}\|$, where $\varphi \mathbf{v} = -\Lambda \varphi^2 (\nabla p - \rho g \nabla z)$.

Further reading: [Darcy's law](#), [Darcy's law](#)

2.2 Permeability

Nutting (1930) and Wyckoff (1934) proposed

$$\varphi \mathbf{v} = -\frac{k}{\mu}(\nabla p - \rho g \nabla z),$$

where $k > 0$ is the permeability, which depends only on rock properties. Dimensions:

$$LT^{-1} = \frac{[k]}{ML^{-1}T^{-1}} \cdot \frac{ML^{-1}T^{-2}}{L} \implies [k] = L^2.$$

Discharge rate: $Q = \|\mathbf{v}\| \cdot A (L^3T^{-1})$, $dp/dx = 1 \text{ atm/cm}$, $\mu = 1 \text{ cp}$, $\|\|\| = 1 \text{ cm/s}$.

$$k = \frac{\|\mathbf{v}\| \mu}{|dp/dx|} = 1 \text{ darcy} = 0.987 \times 10^{-12} \text{ m}^2.$$

Typical “clean” sandstones: $10^{-3} \text{ darcies} < k < 1 \text{ darcy}$.

2.3 Flow equation for single-phase fluids

Idea: Substitute Darcy’s law (1st order PDE) into mass balance (1st order PDE) to get 2nd order PDE governing flow. Then we have the mass balance for fluid:

$$\frac{\partial}{\partial t}(\varphi \rho \mathbf{v}) + \nabla \cdot (\varphi \rho \mathbf{v}) = 0. \iff \varphi \frac{D^F \rho}{Dt} + \rho \frac{\partial \varphi}{\partial t} + \rho \nabla \cdot (\varphi \mathbf{v}) = 0. \quad (2.2)$$

Similar for rock:

$$\varphi \frac{D^R \gamma_R}{Dt} + \gamma_R \frac{\partial}{\partial t}(1 - \varphi) + \gamma_R \nabla \cdot ((1 - \varphi) \mathbf{v}_R) = 0.$$

Rock grains incompressible:

$$\frac{D^R \gamma_R}{Dt} = 0 \implies \frac{\partial \varphi}{\partial t} = \nabla \cdot ((1 - \varphi) \mathbf{v}_R). \quad (2.3)$$

Decompose $\mathbf{v} = \mathbf{v}_R + \mathbf{v}_\Delta$ and rewrite (2.2)

$$\varphi \frac{D^F \rho}{Dt} + \rho \nabla \cdot ((1 - \varphi) \mathbf{v}_R) + \rho \nabla \cdot [\varphi (\mathbf{v}_R + \mathbf{v}_\Delta)] = \varphi \frac{D^F \rho}{Dt} + \rho \nabla \cdot \mathbf{v}_R + \rho \nabla \cdot (\varphi \mathbf{v}_\Delta) = 0. \quad (2.4)$$

Exercise 2.1. Using product rule and (2.3)

$$(1 - \varphi) \rho \nabla \cdot \mathbf{v}_R = \rho \frac{D^R \varphi}{Dt}.$$

Substitute into (2.4) and use $\varphi \neq 1$:

$$\varphi \frac{D^F \rho}{Dt} + \frac{\rho}{1 - \varphi} \frac{D^R \varphi}{Dt} + \rho \nabla \cdot (\varphi \mathbf{v}_\Delta) = 0. \quad (2.5)$$

Constitutive assumptions:

1. Fluid obeys an equations of state: $\rho = \rho(p)$.

$$\begin{cases} \frac{D^F \rho}{Dt} = \rho'(p) \frac{D^F p}{Dt} = \beta \rho \frac{D^F p}{Dt}, \\ \nabla \rho = \beta \rho \nabla p, \end{cases}$$

where $\beta = \rho'/\rho$ is the fluid compressibility. $[\beta] = [1/p] = M^{-1}LT^2$.

2. Rock matrix is compressible: $\varphi(p)$.

$$\implies \frac{D^R \varphi}{Dt} = \varphi'(p) \frac{D^R p}{Dt} = (1 - \varphi) \alpha \frac{D^R p}{Dt},$$

where $\alpha = \varphi'(p)/(1 - \varphi)$, $[\alpha] = M^{-1} L T^2$. Substitute into (2.5) and divide by ρ :

$$\varphi \beta \frac{D^F p}{Dt} + \alpha \frac{D^R p}{Dt} + \nabla \cdot (\varphi \mathbf{v}_\Delta) = 0.$$

If velocities and pressure gradient are small (e.g. most groundwater flows)

$$\mathbf{v}_R \cdot \nabla p \approx 0 \approx \mathbf{v} \cdot \nabla p.$$

Hence,

$$(\varphi \beta + \alpha) \frac{\partial p}{\partial t} + \nabla \cdot (\varphi \mathbf{v}_\Delta) = 0, \quad (2.6)$$

where $\varphi \beta + \alpha = S_p$ is the compressibility effects which has dimension $1/p$. Substitute Darcy's law, we have

$$\varphi \mathbf{v}_\Delta = -\frac{k}{\mu} (\nabla p - \rho g \nabla z).$$

Then (2.6) becomes the single-phase flow equation,

$$S_p \frac{\partial p}{\partial t} - \nabla \cdot \left[\frac{k}{\mu} (\nabla p - \rho g \nabla z) \right] = 0.$$

2.4 Non-Darcy Flows

Darcy's law fails when

- (a) pores are large enough for momentum transfer by viscosity to be significant.
- (b) inertial effects are significant

$$\text{Re}_{\text{pore}} = \frac{\rho \|\mathbf{v}\| d}{\mu} \gtrsim 40,$$

where d is the grain diameter.

2.4.1 Brinknum law (1947)

Keep viscous terms. $\tilde{\mathcal{T}} = -\varphi p \tilde{\mathcal{L}} + \mu [\nabla \mathbf{v} + (\nabla \mathbf{v})^T]$, where μ is uniform.

Exercise 2.2. Show that

$$\nabla \cdot \tilde{\mathcal{T}} = -\nabla(\varphi p) + \mu \nabla \cdot (\nabla \mathbf{v}) = -\nabla(\varphi p) + \mu \Delta \mathbf{v}.$$

Retain other assumptions:

- (i) inertial terms negligible.
- (ii) $\mathbf{m} = -\frac{\mu}{k} \mathbf{v} + p \nabla \varphi$ (Stokes drag).
- (iii) $\mathbf{b} = g \nabla z$.

Substitute into momentum balance for fluid:

$$-\nabla p - \mu \Delta \mathbf{v} + \rho g \nabla z = \frac{\mu}{k} \varphi \mathbf{v}.$$

2.4.2 Forchheimer law (1901)

Turbulence in pores.

$$\frac{p_2 - p_1}{x_2 - x_1} = \frac{\mu}{k} \varphi v + \beta \rho (\varphi v)^2,$$

where β is the Non-Darcy coefficient. Reconcile with momentum balance:

$$\mathbf{m} = F(\|\varphi \mathbf{v}\|) \varphi \mathbf{v} + p \nabla \varphi,$$

where we can expand $F(\|\varphi \mathbf{v}\|)$ using Taylor expansion.

$$F(\|\varphi \mathbf{v}\|) = \frac{\mu}{k} + \beta \rho \|\varphi \mathbf{v}\| + O(\|\varphi \mathbf{v}\|^2).$$

Neglect $O(\|\varphi \mathbf{v}\|^2)$ and retain assumptions (i) and (iii), we have

$$-(\nabla p - \rho g \nabla z) = \left(\frac{\mu}{k} + \beta \rho \|\varphi \mathbf{v}\| \right) \varphi \mathbf{v}.$$

2.5 Potential formulation

Hubbert (1956). Write Darcy's law as

$$\varphi \mathbf{v} = -\frac{k}{\mu} (\nabla p - \rho g \nabla z) = \frac{pk}{\mu} \mathbf{E},$$

where \mathbf{v} is the average interstitial velocity, $\mathbf{E} = g \nabla z - \frac{1}{\rho} \nabla p$ is force/mass acting on fluid. Objective: determine conditions under which $\mathbf{E} = -\nabla \Phi$, Φ is the scalar potential. Necessary condition: the curl of potential \mathbf{E} :

$$\nabla \times \mathbf{E} = \begin{bmatrix} \frac{\partial E_3}{\partial x_2} - \frac{\partial E_2}{\partial x_3} & \frac{\partial E_1}{\partial x_3} - \frac{\partial E_3}{\partial x_1} & \frac{\partial E_2}{\partial x_1} - \frac{\partial E_1}{\partial x_2} \end{bmatrix} = \mathbf{0},$$

that is, \mathbf{E} is irrotational.

Exercise 2.3. Review sufficient conditions under which

$$\nabla \times \mathbf{E} = \mathbf{0} \implies \mathbf{E} = -\nabla \Phi.$$

When is $\nabla \mathbf{E} = \mathbf{0}$? Assuming g is constant,

$$\begin{aligned} \nabla \times \mathbf{E} &= g \nabla \times \nabla z - \nabla \times [1/\rho \nabla p] \\ &= \mathbf{0} - \nabla \times [1/\rho \nabla p] \\ &= -\nabla(1/\rho) \times \nabla p - (1/\rho) \nabla \times \nabla p \\ &= -\nabla(1/\rho) \times \nabla p - (1/\rho) \mathbf{0}. \end{aligned}$$

So $\nabla \times \mathbf{E} = \mathbf{0}$ when

$$\begin{cases} \nabla p = \mathbf{0}, \\ \rho = \text{constant}, \\ \nabla(1/\rho) \parallel \nabla p. \end{cases}$$

For the last two cases, level sets of p are level sets of $1/\rho$ (hence ρ). Conclusion $\mathbf{E} = -\nabla \Phi$ only if $\rho = \rho(p)$ (including the case $\rho = \text{constant}$) This condition excludes:

- $\rho = \rho(p, T)$ (nonisothermal flows).
- $\rho = \rho(p, \text{chemical composition})$.

Terminology: when $\rho = \rho(p)$, fluid is barotropic. Next, what is Φ ? ($\mathbf{E} = -\nabla\Phi$, so expect Φ to be defined up to an arbitrary constant.) Pick \mathbf{x}_{ref} such that $z(\mathbf{x}_{\text{ref}}) = -\mathbf{x}_{\text{ref}} \cdot \mathbf{e}_3 = 0$. To define $\Phi(\mathbf{x})$, pick $\tilde{\zeta} : [0, 1] \rightarrow \mathbb{E}$ to be a C^1 arc in \mathbb{E} such that $\tilde{\zeta}(0) = \mathbf{x}_{\text{ref}}$, $\tilde{\zeta}(1) = \mathbf{x}$. By Fundamental Theorem of Calculus, we have

$$\begin{aligned}
 \Phi(\mathbf{x}) &= \Phi(\mathbf{x}_{\text{ref}}) + \int_{\tilde{\zeta}} \nabla\Phi \cdot d\mathbf{x} \\
 &= \Phi(\mathbf{x}_{\text{ref}}) - \int_0^1 \mathbf{E}(\tilde{\zeta}(s)) \cdot \tilde{\zeta}'(s) ds \\
 &= \Phi(\mathbf{x}_{\text{ref}}) - g \int_0^1 \nabla z(\tilde{\zeta}(s)) \cdot \tilde{\zeta}'(s) ds - \int_0^1 \frac{\nabla p(\tilde{\zeta}(s))}{\rho(p(\tilde{\zeta}(s)))} \cdot \tilde{\zeta}'(s) ds \\
 &= \Phi(\mathbf{x}_{\text{ref}}) - g \int_0^1 \frac{d}{ds} z(\tilde{\zeta}(s)) ds - \int_{p(\mathbf{x}_{\text{ref}})}^{p(\mathbf{x})} \frac{du}{\rho(u)} \\
 &= \Phi(\mathbf{x}_{\text{ref}}) - g[z(\mathbf{x}) - z(\mathbf{x}_{\text{ref}})] - \int_{p(\mathbf{x}_{\text{ref}})}^{p(\mathbf{x})} \frac{du}{\rho(u)} \\
 &= \Phi(\mathbf{x}_{\text{ref}}) - gz(\mathbf{x}) - \int_{p(\mathbf{x}_{\text{ref}})}^{p(\mathbf{x})} \frac{du}{\rho(u)}.
 \end{aligned}$$

Can set $\Phi(\mathbf{x}_{\text{ref}})$ as any constant, say 0. In this case,

$$\Phi(\mathbf{x}) = -gz(\mathbf{x}) + \int_{p(\mathbf{x}_{\text{ref}})}^{p(\mathbf{x})} \frac{du}{\rho(u)}$$

which is called Hubbert potential, which has unit (energy/mass = L^2T^{-2}). Special case: $\rho = \text{constant}$, then

$$\Phi(\mathbf{x}) = -gz(\mathbf{x}) + \frac{p(\mathbf{x}_{\text{ref}}) - p(\mathbf{x})}{\rho(u)}.$$

Rearrange the following

$$\mathbf{E} = \frac{\mu}{\rho k} \varphi = -\Phi \implies \varphi = -\frac{\rho k}{\mu} \Phi.$$

Common to define *piezometric head* (which has dimension L)

$$H(\mathbf{x}) = \frac{\Phi(\mathbf{x})}{g} = -z(\mathbf{x}) + \int_{p(\mathbf{x}_{\text{ref}})}^{p(\mathbf{x})} \frac{du}{\rho(u)g},$$

which is the height (above $z = 0$) to which fluid rises in a piezometer tapped into porous medium at \mathbf{x} . Again, we have the special case, when $\rho = \text{constant}$,

$$H = -z + \frac{p(\mathbf{x}_{\text{ref}}) - p(\mathbf{x})}{\rho(u)g}.$$

2.6 Reformulation of flow equation

Goal: rewrite mass balance and Darcy's law

$$\begin{aligned} S_s \frac{\partial p}{\partial t} + \nabla \cdot (\varphi \mathbf{v}) &= 0, \\ \varphi \mathbf{v} + \frac{k}{\mu} (\nabla p - \rho g \nabla z) &= 0. \end{aligned}$$

in terms of piezometric head $H(\mathbf{x}, t)$.

Exercise 2.4. Use chain rule and fundamental theorem of calculus to prove Leibnize rule:

$$\int_{a(\xi)}^{b(\xi)} f(\xi, \eta) d\eta = \int_{a(\xi)}^{b(\xi)} \frac{\partial f(\xi, \eta)}{\partial \xi} d\eta + f(\xi, b(\xi)) \frac{d}{d\xi} b(\xi) - f(\xi, a(\xi)) \frac{d}{d\xi} a(\xi).$$

Use to calculate derivatives of H . Assume that $\rho = \text{constant}$, and $p(\mathbf{x}_{\text{ref}})$ to be atomespheric pressure. Then

$$\begin{aligned} \frac{\partial}{\partial t} H(\mathbf{x}, t) &= -\frac{\partial}{\partial t} z(\mathbf{x}) + \int_{p(\mathbf{x}_{\text{ref}})}^{p(\mathbf{x})} \frac{\partial}{\partial t} \frac{1}{\rho(u)g} du + \frac{1}{\rho g} \frac{\partial p}{\partial t}(\mathbf{x}, t) - \frac{1}{\rho g} \frac{\partial p}{\partial t}(\mathbf{x}_{\text{ref}}, t) \\ &= \int_{p(\mathbf{x}_{\text{ref}})}^{p(\mathbf{x})} \frac{\partial}{\partial t} \frac{1}{\rho(u)g} du + \frac{1}{\rho g} \frac{\partial p}{\partial t}(\mathbf{x}_{\text{ref}}). \end{aligned}$$

Then

$$\nabla H(\mathbf{x}, t) = -\nabla z(\mathbf{x}) + \int_{p(\mathbf{x}_{\text{ref}})}^{p(\mathbf{x})} \nabla \frac{1}{\rho(u)g} du + \frac{1}{\rho g} \nabla p - \frac{1}{\rho g} \nabla p(\mathbf{x}_{\text{ref}}) = -\nabla z(\mathbf{x}) + \frac{1}{\rho g} \nabla p.$$

Then

$$\frac{\partial p}{\partial t} = \rho g \frac{\partial H}{\partial t}, \nabla p - \rho g \nabla z = \rho g \nabla H.$$

So we get

- Mass balance:

$$S_s \frac{\partial H}{\partial t} + \nabla \cdot (\varphi \mathbf{v}) = 0, \quad (2.7)$$

where $S_s = \rho g S_p$ is the specific storage.

- Darcy's law:

$$\varphi \mathbf{v} + K \nabla H = 0, \quad (2.8)$$

where $K = k \rho g / \mu$ is the hydraulic conductiuity, which has dimension LT^{-1} .

- Flow equation:

$$S_s \frac{\partial H}{\partial t} - \nabla \cdot (K \nabla H) = 0.$$

2.7 Areal flows

Goal: rewrite flow equation in 2-D form, useful when aquifer thickness is small compared with areal extent and

$$\frac{\partial \varphi}{\partial x_3} = \frac{\partial K}{\partial x_3} = \frac{\partial S_s}{\partial x_3} = \mathbf{v} \cdot \mathbf{e}_3 = 0.$$

Definition 2.1. The *vertical average* of a generic function $\Psi(x_1, x_2, x_3)$ is

$$\frac{1}{l} \int_a^b \Psi(\mathbf{x}) dx_3 = \bar{\Psi}(x_1, x_2),$$

where $l = b(\mathbf{x}) - a(\mathbf{x})$.

For mass balance, apply to (2.7), we have

$$\int_a^b \left[S_s \frac{\partial H}{\partial t} + \nabla \cdot (\varphi \mathbf{v}) \right] dx_3 = 0.$$

Use $\partial S_s / \partial x_3 = 0$, apply Leibniz rule

$$\int_a^b S_s \frac{\partial H}{\partial t} dx_3 = S_s \int_a^b \frac{\partial H}{\partial t} dx_3 = S_s \left[\frac{\partial}{\partial t} \int_a^b H dx_3 - H \Big|_{x_3=b} \frac{b}{t} + H \Big|_{x_3=a} \frac{a}{t} \right] = S_s \frac{\partial}{\partial t} (l \bar{H}).$$

Exercise 2.5. Show that

$$\begin{aligned} \int_a^b \nabla \cdot (\varphi \mathbf{v}) dx_3 &= \nabla_2 \cdot \int_a^b \varphi \mathbf{v} dx_3 - \varphi \mathbf{v} \Big|_{x_3=b} \cdot \nabla b + \varphi \mathbf{v} \Big|_{x_3=a} \cdot \nabla a, \\ &= \nabla_2 \cdot l \varphi \mathbf{v} - \varphi \mathbf{v} \Big|_{x_3=b} \cdot \nabla b + \varphi \mathbf{v} \Big|_{x_3=a} \cdot \nabla a, \end{aligned}$$

where $\nabla_2 = \mathbf{e}_1 \frac{\partial}{\partial x_1} + \mathbf{e}_2 \frac{\partial}{\partial x_2}$

Therefore, the vertical averaged mass balance is

$$S_s \frac{\partial}{\partial t} (l \bar{H}) + \nabla_2 \cdot (l \varphi \mathbf{v}) + \varphi \mathbf{v} \Big|_{x_3=b} \cdot \nabla (x_3 - b) - \varphi \mathbf{v} \Big|_{x_3=a} \cdot \nabla (x_3 - a) = S \frac{\partial \bar{H}}{\partial t} + \nabla_2 \cdot (l \varphi \mathbf{v}) + q_{\text{top}} - q_{\text{bottom}} = 0,$$

where $q_{\text{top}} = \varphi \mathbf{v} \Big|_{x_3=b} \cdot \nabla (x_3 - b)$ and $q_{\text{bottom}} = \varphi \mathbf{v} \Big|_{x_3=a} \cdot \nabla (x_3 - a)$. Interpret q_{top} as the flux across upper boundary $x_3 = b(x_1, x_2)$. Similar to q_{bottom} . And $q_{\text{top}} - q_{\text{bottom}}$ is the leakage and $S = l S_s$ is the storativity.

For Darcy's law (2.8), apply the vertical average and recall $\partial K / \partial x_3 = 0$ and assume $\bar{H} = H \Big|_{x_3=a} = H \Big|_{x_3=b}$, we have

$$\begin{aligned} \int_a^b (\varphi \mathbf{v} + K \nabla H) dx_3 &= \int_a^b \varphi \mathbf{v} dx_3 + \int_a^b K \nabla H dx_3 \\ &= l \bar{\varphi} \mathbf{v} + K \left(\nabla \int_a^b H dx_3 - \bar{H} \nabla b + \bar{H} \nabla a \right) \\ &= l \bar{\varphi} \mathbf{v} + K (\nabla (l \bar{H}) - \bar{H} \Delta l) \\ &= l \bar{\varphi} \mathbf{v} + K l \nabla \bar{H} \\ &= l \bar{\varphi} \mathbf{v} + T \nabla \bar{H} \\ &= 0, \end{aligned}$$

where $T = Kl$ is the transmissivity. Flow equation substitute Darcy's law into mass balance:

$$S \frac{\partial \bar{H}}{\partial t} - \nabla_2 \cdot (T \nabla_2 \bar{H}) = q_{\text{bottom}} - q_{\text{top}}.$$

2.8 Well hydraulics

2.8.1 Dirac- δ model

In the absence of leakage, areal mass balance

$$S \frac{\partial \bar{H}}{\partial t} + \nabla_2 \cdot (l\bar{\varphi}\bar{\mathbf{v}}) = 0.$$

Consider any region Ω having a well as an internal boundary $\partial\Omega_w$. Global mass balance and then apply divergence theorem:

$$\int_{\Omega} S \frac{\partial \bar{H}}{\partial t} dv = - \int_{\Omega} \nabla_2 \cdot (l\bar{\varphi}\bar{\mathbf{v}}) dv = - \int_{\partial\Omega} l\bar{\varphi}\bar{\mathbf{v}} \cdot \mathbf{n} d\sigma = - \int_{\partial\Omega_e} l\bar{\varphi}\bar{\mathbf{v}} \cdot \mathbf{n} d\sigma - \underbrace{\int_{\partial\Omega_w} l\bar{\varphi}\bar{\mathbf{v}} \cdot \mathbf{n} d\sigma}_{Q_w < 0 \text{ for withdrawal}}.$$

where the left hand side is the rate of change of fluid mass in Ω . Simplification: replace Ω by Ω_e the interior of region bounded by $\partial\Omega_e$. Replace mass balance by

$$S \frac{\partial \bar{H}}{\partial t} + \nabla_2 \cdot (l\bar{\varphi}\bar{\mathbf{v}}) = Q_w \delta(\mathbf{x} - \mathbf{x}_w),$$

where

$$\int_R \varphi(\mathbf{x}) \delta(\mathbf{x} - \mathbf{x}_w) dv = \begin{cases} \varphi(\mathbf{x}_w) & \mathbf{x}_w \in R, \\ 0 & \mathbf{x}_w \notin R, \end{cases}$$

where $\delta(\mathbf{x})$ is the Dirac δ -distribution, φ is any C^∞ function. Global mass balance remains unchanged: in any region Ω_e containing the well bore at \mathbf{x}_w .

$$\int_{\Omega_e} S \frac{\partial \bar{H}}{\partial t} dv = - \int_{\partial\Omega_e} l\bar{\varphi}\bar{\mathbf{v}} dv + \int_{\Omega_e} Q_w \delta(\mathbf{x} - \mathbf{x}_w) dv.$$

Sample problem: steady, areal flow in an ∞ aquifer with well at \mathbf{x}_w .

$$-\nabla_2 \cdot (T \nabla_2 \bar{H}) = Q \delta(\mathbf{x} - \mathbf{x}_w).$$

For polar coordinates, $\mathbf{x} - \mathbf{x}_w = \begin{bmatrix} r \cos \theta \\ r \sin \theta \end{bmatrix} = \Psi \left(\begin{bmatrix} r \\ \theta \end{bmatrix} \right)$. Let $\varphi = \varphi((\mathbf{x} - \mathbf{x}_w)(r, \theta))$, then we have the chain rule:

$$\begin{bmatrix} \frac{\partial \varphi}{\partial r} & \frac{\partial \varphi}{\partial \theta} \end{bmatrix} = \begin{bmatrix} \frac{\partial \varphi}{\partial x_1} & \frac{\partial \varphi}{\partial x_2} \end{bmatrix} \begin{bmatrix} \frac{\partial x_1}{\partial r} & \frac{\partial x_1}{\partial \theta} \\ \frac{\partial x_2}{\partial r} & \frac{\partial x_2}{\partial \theta} \end{bmatrix} \implies \begin{bmatrix} \frac{\partial \varphi}{\partial x_1} & \frac{\partial \varphi}{\partial x_2} \end{bmatrix} = \begin{bmatrix} \frac{\partial \varphi}{\partial r} & \frac{\partial \varphi}{\partial \theta} \end{bmatrix} \begin{bmatrix} \frac{\partial x_1}{\partial r} & \frac{\partial x_1}{\partial \theta} \\ \frac{\partial x_2}{\partial r} & \frac{\partial x_2}{\partial \theta} \end{bmatrix}^{-1}$$

Exercise 2.6.

$$\nabla_2 \varphi = \left[\cos \theta \frac{\partial \varphi}{\partial r} - \frac{\sin \theta}{r} \quad \sin \theta \frac{\partial \varphi}{\partial r} + \frac{\cos \theta}{r} \frac{\partial \varphi}{\partial \theta} \right].$$

and

$$\Delta_2 \varphi = \nabla_2 \cdot \nabla_2 \varphi = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \varphi}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 \varphi}{\partial \theta^2}.$$

Remark 2.2. $\int_{\partial D(r)} f = \int_a^b f(\zeta(s)) \|\zeta'(s)\| ds.$

If T is constant

$$-\Delta_2 \bar{H} = \frac{Q_w}{T} \delta(\mathbf{x} - \mathbf{x}_w),$$

where $\Delta_2 = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} = \frac{1}{r} \frac{\partial}{\partial r} (r \frac{\partial}{\partial r}) + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2}$. By symmetry, $\bar{H} = \bar{H}(r)$, so

$$\frac{1}{r} \frac{d}{dr} \left(r \frac{d\bar{H}}{dr} \right) = 0, 0 < r.$$

Then

$$\lim_{r \rightarrow 0} \iint_{D(r)} \Delta_2 \bar{H} dx_1 dx_2 = \lim_{r \rightarrow 0} \int_{\partial D(r)} \nabla_2 \bar{H} \cdot \mathbf{n} \quad (2.9)$$

General solution: $\bar{H}(r) = C_1 \log r + C_2$. Parameterize $\partial D(r)$ by $\zeta(\theta) = (r \cos \theta, r \sin \theta)$, $\theta \in [0, 2\pi]$, and $\mathbf{n} = (\cos \theta, \sin \theta)$. Then (2.9) becomes

$$\begin{aligned} \lim_{r \rightarrow 0} \int_{\partial D(r)} \nabla_2 \bar{H} \cdot \mathbf{n} &= \lim_{r \rightarrow 0} \int_0^{2\pi} \left(\cos \theta \frac{d\bar{H}}{dr}, \sin \theta \frac{d\bar{H}}{dr} \right) \cdot (\cos \theta, \sin \theta) r d\theta \\ &= \lim_{r \rightarrow 0} r \frac{d\bar{H}}{dr} \int_0^{2\pi} 1 d\theta \\ &= \lim_{r \rightarrow 0} 2\pi r \frac{d\bar{H}}{dr} \\ &= -\frac{Q_w}{T}. \end{aligned}$$

That implies

$$C_1 = r \frac{d\bar{H}}{dr} = -\frac{Q_w}{2\pi T}.$$

Exercise 2.7. Also, $C_2 = \bar{H}(1)$.

Pick datum so that $\bar{H}(1) = 0$. Result $\bar{H}(r) = -\frac{Q_w}{2\pi T} \log r$, where $-\frac{Q_w}{2\pi T} > 0$ is for fluid withdrawal. Logarithm singularity at well bore. Practical application:

$$-\nabla_2 \cdot [T(\mathbf{x}) \nabla_2 \bar{H}] = Q_w \delta(\mathbf{x} - \mathbf{x}_w).$$

Finite difference and finite element methods lose accuracy and near singularities. Decompose

$$\bar{H} = \bar{H}_r + \bar{H}_s,$$

where \bar{H}_r and \bar{H}_s are regular and singular solution, respectively. Pick \bar{H}_s as solution to

$$-\Delta_2 \bar{H}_s = \frac{Q_w}{T} \delta(\mathbf{x} - \delta x_w),$$

where

$$\bar{T} = \frac{1}{\pi R^2} \int_0^{2\pi} \int_0^R T(r, \theta) dr d\theta.$$

R is the radius of the region where T is representative.

$$\bar{H}_s(r) = -\frac{Q_w}{2\pi \bar{T}} \log r.$$

Substitute into the equation

$$-\nabla_2 \cdot [T(\mathbf{x}) \nabla_2 \bar{H}_r] = \nabla_2 \cdot [(T - \bar{T}) \nabla_2 \bar{H}_s].$$

2.8.2 Thiem model (1906)

$$S \frac{\partial \bar{H}}{\partial t} - \nabla_2 \cdot (T \nabla_2 \bar{H}) = q_{\text{bottom}} - q_{\text{top}}.$$

Assumptions

(a) Areal flow, steady, with incompressible confining layers.

(b) T is spatially uniform, we have a 2-D Laplace equation

$$\nabla_2 \cdot \nabla_2 \bar{H} = \Delta_2 \bar{H} = 0.$$

(c) Flow is axisymmetric: $\bar{H} = \bar{H}(r)$.

$$\frac{1}{r} \frac{d}{dr} \left(r \frac{d\bar{H}}{dr} \right) = 0, \quad r_w < r < r_e.$$

(d) Sufficiently far from well, $\bar{H}_e = \bar{H}_\infty$.

(e) Discharge rate at well is prescribed. Then we have Darcy's law integrated over face of well bore.

$$2\pi r_w T \bar{H}'(r_w) = Q \iff 2\pi r_w l K \bar{H}'(r_w) = Q',$$

where Q has dimension $L^3 T^{-1}$.

Then the boundary-value problem:

$$\frac{d}{dr} \left(r \frac{d\bar{H}}{dr} \right) = 0, \quad r_w < r < r_e, \bar{H}(r_e) = H_\infty, \bar{H}(r) = \frac{Q}{2\pi r_w T}.$$

It is known that the general solution is

$$\bar{H}(r) = C_1 \log r + C_2.$$

Exercise 2.8.

(a) $\bar{H}(r) = H_\infty + \frac{Q}{2\pi T} \log(r/r_e)$.

(b) For $r_1, r_2 \in (r_w, r_e)$, show the Thiem equation

$$\bar{H}(r_1) - \bar{H}(r_2) = \frac{Q}{2\pi T} \log(r_1/r_2).$$

Reformulate in terms of *drawdown*. Let $s(r) = H_\infty - \bar{H}(r)$. Then

$$s(r_2) - s(r_1) = \frac{Q}{2\pi T} \log(r_1/r_2).$$

Thiem's method:

(a) Pump active well to steady state.

(b) Measure drawdown at () wells.

(c) Plot $s(r)$ vs. $\log(r)$.

$$T = \frac{Q}{2\pi \Delta s} (\log r_1 - \log r_2).$$

2.8.3 Theis model (1935)

Single well, areal aquifer, axisymmetric, S , T spatially uniform and constant in time. We have the radial heat equation

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \bar{H}}{\partial r} \right) = \frac{S}{T} \frac{\partial \bar{H}}{\partial t}, \bar{H}(r, 0) = H_0, \lim_{r \rightarrow \infty} \bar{H}(r, t) = H_\infty, \lim_{r \rightarrow \infty} 2\pi r T \frac{\partial \bar{H}}{\partial r}(r, t) = Q,$$

where H_0 is obtained by spatially uniformity and Q is a constant. The solution of the equation is

$$\bar{H}(r, t) = H_0 - \frac{Q}{4\pi t} E_i \left(-\frac{Sr^2}{4Tt} \right),$$

where $E_i(-\xi) = \int_\xi^\infty \frac{e^{-u}}{u} du$. In terms of drawdown $s(r, t)$, we have

$$s(r, t) = H_0 - \bar{H}(r, t) = \frac{Q}{4\pi t} E_i \left(-\frac{Sr^2}{4Tt} \right).$$

Observations

- (a) $s(r, t)$ has continuous derivatives.
- (b) For $t > 0$, $s(r, t) \neq 0, \forall r > 0$ "Infinite propagation spread".

The approximate solution (Coopers & Jacob, 1946). Use asymptotic expansion:

$$E_i(-\xi) = -\gamma - \log \xi + \xi - \frac{1}{2} \frac{\xi^2}{2!} + \frac{\xi^3}{3!} - \dots \approx -0.5772 - \log \xi,$$

where $\gamma = 0.5772$ is the Euler's constant, for $\xi = \frac{Sr^2}{4Tt} < 0.01$ (small r and large t). Then

$$s(r, t) \approx \frac{Q}{4\pi T} \left(-0.5772 - \log \frac{r^2 S}{4Tt} \right) = \frac{Q}{4\pi T} \log \frac{2.25Tt}{r^2 S} = \frac{Q}{4\pi T} \log t + \frac{Q}{4\pi T} \log \frac{2.25T}{r^2 S}.$$

2.9 Tensor-valued permeability

Write Darcy's law as $\varphi \mathbf{v} = k \mathbf{q}$, where $\mathbf{q} = -\frac{1}{\mu} (\nabla p - \rho g \nabla z) \implies \mathbf{v} \parallel \mathbf{q}$. Rock texture can alter this relationship. Accomodate by writing $\varphi \mathbf{v} = \tilde{\mathbf{k}} \mathbf{q}$, where $\tilde{\mathbf{k}}$ is tensor-valued function of \mathbf{x} . At each $\mathbf{x} \in E$, $\tilde{\mathbf{k}}(\mathbf{x}) : \mathbb{E} \rightarrow \mathbb{E}$ is a linear transformation.

Remark 2.3.

1. Geometric action of any tensor is independent of coordinate system.
2. Given on orthogonal coordinate system defined by orthonormal basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$, $\tilde{\mathbf{k}}$ has matrix representation.

$$\begin{bmatrix} k_{11} & k_{12} & k_{13} \\ k_{21} & k_{22} & k_{23} \\ k_{31} & k_{32} & k_{33} \end{bmatrix}, \mathbf{e}_i \cdot \tilde{\mathbf{e}}_j = k_{ij}.$$

3. With respect to this basis,

$$\mathbf{q} = \sum_{i=1}^3 q_i \mathbf{e}_i, \quad q_i = \mathbf{e}_i \cdot \mathbf{q}.$$

In this basis, calculate a representation of $\tilde{\mathbf{k}}\mathbf{q}$ as

$$\begin{bmatrix} k_{11} & k_{12} & k_{13} \\ k_{21} & k_{22} & k_{23} \\ k_{31} & k_{32} & k_{33} \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \\ q_3 \end{bmatrix}.$$

4. Changing basis from $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ to $\{\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3\}$ (orthonormal) changes these representations:

$$\mathbf{q} = \sum_{i=1}^3 q_i \mathbf{e}_i = \sum_{i=1}^3 \hat{q}_i \hat{\mathbf{e}}_i.$$

Exercise 2.9. Show that

$$\hat{q}_i = \sum_{j=1}^3 Q_{ij} q_j,$$

where Q_{ij} is the (i, j) th direction cosine. Also,

$$q_i = \sum_{l=1}^3 Q_{lj}^T \hat{q}_j,$$

where $Q_{lj}^T = Q_{jl}$.

Exercise 2.10. If $k_{ij} = \mathbf{e}_i \cdot \tilde{\mathbf{e}}_j$ and $\hat{k}_{ij} = \tilde{\mathbf{e}}_i \cdot \hat{\mathbf{e}}_j$, show that

$$k_{ij} = \sum_{l=1}^3 \sum_{m=1}^3 Q_{il}^T \hat{k}_{lm} Q_{mj},$$

$$\hat{k}_{lm} = \sum_{i=1}^3 \sum_{j=1}^3 Q_{li} k_{ij} Q_{jm}^T.$$

Hint: Look at $\mathbf{p} = \tilde{\mathbf{k}}\mathbf{q} = \sum_{i=1}^3 p_i \mathbf{e}_i = \sum_{i=1}^3 \hat{p}_i \hat{\mathbf{e}}_i$.

Tensor version of Darcy's law:

$$\varphi \mathbf{v} = \tilde{\mathbf{k}}\mathbf{q} = -\frac{\tilde{\mathbf{k}}}{\mu} (\nabla p - \rho g \nabla z).$$

Accomodate scalar k by setting any orthonormal basis.

$$\tilde{\mathcal{K}} = k\tilde{\mathcal{I}} = k \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Definition 2.2. If $\tilde{\mathbf{k}}(\mathbf{x})\tilde{\mathcal{I}}$, the permeability is *isotropic*. Observation: every nonzero vector in \mathbb{E} is an eigenvector of $k\tilde{\mathcal{I}}$ with eigenvalue k . No preferred coordinate system.

In terms of hydraulic conductivity and piezometric head,

$$\varphi \mathbf{v} = -\tilde{\mathcal{K}}\nabla H, \quad \tilde{\mathcal{K}} = \frac{\rho g}{\mu} \tilde{\mathbf{k}}.$$

2.9.1 Properties attributed to $\tilde{\mathcal{K}}$ and $\tilde{\mathbf{k}}$

(a) $\tilde{\mathcal{K}}$ is *positive definite*:

$$\mathbf{q} \cdot \tilde{\mathcal{K}}\mathbf{q} \geq 0, \forall \mathbf{q} \in \mathbb{E}, \mathbf{q} \cdot \tilde{\mathcal{K}}\mathbf{q} = 0 \iff \mathbf{q} = \mathbf{0}.$$

Rationale: fluid doesn't flow up the head gradient

$$0 \geq \nabla H \cdot \varphi \mathbf{v} = -\nabla H \cdot \tilde{\mathcal{K}}\nabla H.$$

$\nabla H \cdot \varphi \mathbf{v} = 0$ corresponds to the impermeable medium.

(b) $\tilde{\mathcal{K}}$ is symmetric.

$$\mathbf{p} \cdot \tilde{\mathcal{K}}\mathbf{q} = \tilde{\mathcal{K}}\mathbf{p} \cdot \mathbf{q}, \forall \mathbf{p}, \mathbf{q} \in \mathbb{E} \implies K_{ij} = K_{ji} \text{ with respect to any orthonormal basis.}$$

Rationale is less clear.

Observation:

(a) Several justifications use thermodynamic principles beyond standard balance laws and entropy inequality.

(b) Can decompose

$$\tilde{\mathcal{K}} = \underbrace{\frac{1}{2}(\tilde{\mathcal{K}} + \tilde{\mathcal{K}}^T)}_{\tilde{\mathcal{K}}_{\text{symm}}} + \underbrace{\frac{1}{2}(\tilde{\mathcal{K}} - \tilde{\mathcal{K}}^T)}_{\tilde{\mathcal{K}}_{\text{extskew}}},$$

where $\tilde{\mathcal{K}}_{\text{skew}}^T = -\tilde{\mathcal{K}}_{\text{skew}}$, $\tilde{\mathcal{K}}^T$ is defined by $\mathbf{p} \cdot \tilde{\mathcal{K}}^T \mathbf{q} = \tilde{\mathcal{K}}\mathbf{p} \cdot \mathbf{q}$.

(c) A PDE similar to the flow equation g* heat transfer:

$$c\rho \frac{\partial \theta}{\partial t} - \nabla \cdot (\tilde{\mathbf{k}}\nabla \theta) = 0,$$

where $\tilde{\mathbf{k}}$ is thermal cardinality. C.. Weng (1984) showed material finite diff indifference, $\tilde{\mathbf{k}} = \tilde{\mathbf{k}}^T$ in seven of thirteen symmetry classes of materials.

(d) Some upscaling methods yield nonsymmetric $\mathbf{K}_{\text{macro}}$ even if $\tilde{\mathbf{k}}$ is symmetric (King 1995). Consequence: if $\tilde{\mathbf{k}}$ is symmetric and positive definite, then we can find an orthormal basis $\{\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3\}$ consisting of eigenvectors of $\tilde{\mathcal{K}}$ and the eigenvalues k_1, k_2, k_3 are positive:

$$\tilde{\mathcal{K}}\mathbf{p}_j = k_j\mathbf{p}_j, \quad k_j > 0.$$

Exercise 2.11. If $\tilde{\mathcal{K}}$ is uniform ($\tilde{\mathcal{K}} \neq \tilde{\mathcal{K}}(\mathbf{x})$), then

$$\nabla \cdot (\tilde{\mathcal{K}}\nabla H) = \nabla \cdot (\tilde{\mathcal{K}}_{\text{symm}}\nabla H),$$

even when $\tilde{\mathcal{K}}_{\text{skew}} = \tilde{\mathcal{O}}$.

Remark 2.4. In general, $-\tilde{\mathcal{K}}_{\text{skew}}\nabla H \neq \tilde{\mathcal{O}}$.

Remark 2.5. $\tilde{\mathcal{K}} = \tilde{\mathcal{K}}(\mathbf{x}) \implies \mathbf{p}_j = \mathbf{p}_j(\mathbf{x})$ and $k_j = k_j(\mathbf{x})$. When $k_1(\mathbf{x}) = k_2(\mathbf{x}) = k_3(\mathbf{x})$, $\tilde{\mathbf{k}}$ is isotropic. Otherwise, *anisotropic*.

When $\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3$ are independent of spatial position, use them to define a Cartesian coordinate system.

$$K_{ij} = \mathbf{p}_i \cdot \tilde{\mathbf{K}} \mathbf{p}_j = \mathbf{p}_i \cdot k_j \mathbf{p}_j = \begin{cases} 0 & i \neq j, \\ k_j & i = j. \end{cases}$$

Then we have the matrix representation for $\tilde{\mathcal{K}}$ as follows

$$\begin{bmatrix} k_1 & 0 & 0 \\ 0 & k_2 & 0 \\ 0 & 0 & k_3 \end{bmatrix}.$$

Then

$$\nabla \cdot (\tilde{\mathcal{K}} \nabla H) = \nabla \cdot \begin{bmatrix} k_1 & 0 & 0 \\ 0 & k_2 & 0 \\ 0 & 0 & k_3 \end{bmatrix} \begin{bmatrix} \partial H / \partial x_1 \\ \partial H / \partial x_2 \\ \partial H / \partial x_3 \end{bmatrix} = \nabla \cdot \begin{bmatrix} k_1 \partial H / \partial x_1 \\ k_2 \partial H / \partial x_2 \\ k_3 \partial H / \partial x_3 \end{bmatrix} = \sum_{i=1}^3 \frac{\partial}{\partial x_i} \left(k_i \frac{\partial H}{\partial x_i} \right). \quad (2.10)$$

Call $\{\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3\}$ the *principal directions* of $\tilde{\mathcal{K}}$, k_1, k_2, k_3 the *principal conductivities*.

Remark 2.6. (2.10) will not work if $\{\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3\}$ vary in space.

Definition 2.3. If $\tilde{\mathcal{K}} = \tilde{\mathcal{K}}(\mathbf{x})$, $\tilde{\mathcal{K}}$ is *heterogeneous*. Otherwise, *homogeneous*.

	Homogeneous	Heterogeneous
Isotropic	$k\tilde{\mathcal{I}}$	$k(\mathbf{x})\tilde{\mathcal{I}}$
Anisotropic	$\tilde{\mathcal{K}}$	$\tilde{\mathcal{K}}(\mathbf{x})$

3 Transport in Porous Media

3.1 Transport equation

Given species $i = 1, \dots, N$ distributed in several phases (e.g., $\alpha = R, F$), regard each (i, α) as a constituent.

Example 3.1. Salt (species) in water (fluid).

Mass balance for constituent (i, α)

$$\frac{\partial}{\partial t} (\varphi_\alpha \gamma_{(i,\alpha)}) + \nabla \cdot (\varphi_\alpha \gamma_{(i,\alpha)} \mathbf{v}_{(i,\alpha)}) = r_{(i,\alpha)}, \quad i = 1, \dots, N, \alpha = F, R, \dots$$

And the global balance is

$$\sum_{i=1}^N \sum_{\alpha} r_{(i,\alpha)} = 0.$$

Rewrite using mass fractions:

$$\omega_{(i,\alpha)} = \frac{\gamma_{(i,\alpha)}}{\gamma_\alpha}, \quad \sum_{i=1}^N \omega_{(i,\alpha)} = 1, \quad \sum_{i=1}^N \omega_{(i,\alpha)} \mathbf{v}_{(i,\alpha)} = \mathbf{v}_\alpha.$$

Then

$$\frac{\partial}{\partial t} (\varphi_\alpha \omega_{(i,\alpha)} \gamma_\alpha) + \nabla \cdot (\varphi_\alpha \omega_{(i,\alpha)} \gamma_\alpha \mathbf{v}_{(i,\alpha)}) = r_{(i,\alpha)}, i = 1, \dots, N, \alpha = F, R, \dots$$

Taking sum gives mass balance for phase α :

$$\frac{\partial}{\partial t} (\varphi_\alpha \gamma_\alpha) + \nabla \cdot (\varphi_\alpha \gamma_\alpha \mathbf{v}_\alpha) = \sum_{i=1}^N r_{(i,\alpha)} = r_\alpha, \quad \alpha = F, R, \dots$$

Denote the concentration of i in α : $c_{(i,\alpha)} = \gamma_\alpha \omega_{(i,\alpha)}$, dimension: mass of (i, α) / volume of α .

Let the diffusion velocity of species i in phase α : $\tilde{\mathbf{v}}_{(i,\alpha)} = \mathbf{v}_{(i,\alpha)} - \mathbf{v}_\alpha$. Then

$$\frac{\partial}{\partial t} (\varphi_\alpha c_{(i,\alpha)}) + \nabla \cdot (\varphi_\alpha \mathbf{v}_\alpha c_{(i,\alpha)}) + \nabla \cdot \mathbf{j}_{(i,\alpha)} = r_{(i,\alpha)},$$

where $\mathbf{j}_{(i,\alpha)} = \varphi_\alpha c_{(i,\alpha)} \tilde{\mathbf{v}}_{(i,\alpha)}$, $\frac{\partial}{\partial t} (\varphi_\alpha c_{(i,\alpha)})$ accumulation term, $\nabla \cdot (\varphi_\alpha \mathbf{v}_\alpha c_{(i,\alpha)})$ is advection term, $\nabla \cdot \mathbf{j}_{(i,\alpha)}$ is diffusion term, and $r_{(i,\alpha)}$ is the reaction term. Special case: track a single species i in a fluid F flowing through a porous medium, the advection-diffusion-reaction equation is

$$\frac{\partial}{\partial t} (\varphi c) + \nabla \cdot (\bar{\mathbf{v}} c) + \nabla \cdot \mathbf{j} = r,$$

where $\varphi = \varphi_F$, $\bar{\mathbf{v}} = \varphi \mathbf{v}$, $\mathbf{j} = \mathbf{j}_{(i,F)}$ and $r = r_{i,F}$.

3.2 Hydrodynamic dispersion

Common to decompose $\mathbf{j} = \mathbf{j}_{\text{mol}} + \mathbf{j}_{\text{mech}}$, where \mathbf{j}_{mol} is called the molecular diffusion and \mathbf{j}_{mech} is called the mechanical diffusion. Fick's law stated as follows,

$$\mathbf{j}_{\text{mol}} = -\varphi D_m \nabla c,$$

where D_m is molecular diffusion coefficient whose dimension is $L^2 T^{-1}$, and φ is rearding effect of rock. Contributions to \mathbf{j}_{mech} :

- (a) Taylor diffusion. Lateral spreading in thin tubes driven by parabolic velocity profile. Longitudinal spreading.
- (b) Stream splitting.
- (c) Variable path lengths.

Standard model:

$$\mathbf{j} = -\tilde{\mathcal{D}} \nabla c,$$

where $\tilde{\mathcal{D}}$ is hydrodynamic dispersion tensor, to be more exact,

$$\tilde{\mathcal{D}} = \varphi D_{\text{mol}} \tilde{\mathcal{I}} + \alpha_L \|\bar{\mathbf{v}}\| \tilde{\mathcal{W}} + \alpha_T \|\bar{\mathbf{v}}\| (\tilde{\mathcal{I}} - \tilde{\mathcal{W}}),$$

where

$$\tilde{\mathcal{W}} = \frac{1}{\|\bar{\mathbf{v}}\|^2} \bar{\mathbf{v}} \otimes \bar{\mathbf{v}} = \frac{1}{\|\bar{\mathbf{v}}\|^2} \begin{bmatrix} \bar{v}_1 \bar{v}_1 & \bar{v}_1 \bar{v}_2 & \bar{v}_1 \bar{v}_3 \\ \bar{v}_2 \bar{v}_1 & \bar{v}_2 \bar{v}_2 & \bar{v}_2 \bar{v}_3 \\ \bar{v}_3 \bar{v}_1 & \bar{v}_3 \bar{v}_2 & \bar{v}_3 \bar{v}_3 \end{bmatrix}.$$

In effect,

$$\begin{aligned}\mathbf{j}_{\text{mech}} &= \mathbf{j}_{\text{long}} + \mathbf{j}_{\text{trans}}, \\ \|\mathbf{j}_{\text{long}}\| &= \alpha_L \|\bar{\mathbf{v}}\| \|\nabla c\|, \\ \|\mathbf{j}_{\text{trans}}\| &= \alpha_T \|\bar{\mathbf{v}}\| \|\nabla c\|,\end{aligned}$$

where α_L and α_T are longitudinal dispersivity and transverse dispersivity, both have dimension L and positive.

Remark 3.1.

- (a) $D_{\text{mol}} \ll \alpha_T \|\bar{\mathbf{v}}\| < \alpha_L \|\bar{\mathbf{v}}\|$.
- (b) α_T, α_L are properties of the rock matrix. Both of them increase as the scale of observation increases.

3.3 1-D nonreacting transport

Governing equation (assuming φ is constant)

$$\frac{\partial c}{\partial t} + v \frac{\partial c}{\partial x} - \frac{D}{\varphi} \frac{\partial^2 c}{\partial x^2} = 0,$$

where $\partial c / \partial t$ is accumulation term, $v \partial c / \partial x$ is the advection term, and $\frac{D}{\varphi} \frac{\partial^2 c}{\partial x^2}$ is the diffusion term. Dimensionless form: given length scale L , define

$$\xi = \frac{x}{L}, \tau = \frac{t\varphi v L}{D} = \frac{t\bar{v}L}{D}.$$

Exercise 3.1. Use chain rule to show

$$\frac{\partial c}{\partial \tau} + \frac{\partial c}{\partial \xi} + \frac{1}{\text{Pe}} \frac{\partial^2 c}{\partial \xi^2} = 0,$$

where $\text{Pe} = \frac{\varphi v L}{D}$ is the Péclet number (advection / diffusion). When $\text{Pe} \gg 1$, advection dominates.

One extreme: examine IVP.

$$\begin{aligned}\frac{\partial c}{\partial t} + v \frac{\partial c}{\partial x} &= 0, \quad -\infty < x < \infty, \\ c(x, 0) &= \begin{cases} 1 & x \in [0, 1], \\ 0 & \text{otherwise.} \end{cases}\end{aligned}$$

Consider a path $(t(s), x(s))$ in the (t, x) -plane ($\sigma : [a, b] \rightarrow \mathbb{R}^2$).

$$\begin{aligned}\frac{dt}{ds} \frac{\partial c}{\partial t} + \frac{dx}{ds} \frac{\partial c}{\partial x} &= \frac{dc}{ds}, \\ \frac{\partial c}{\partial t} + v \frac{\partial c}{\partial x} &= 0.\end{aligned}$$

Consistency along any path $(t(s), x(s))$ for which

$$\frac{dt}{ds} = 1, \frac{dx}{ds} = v,$$

which is called the *characteristic curve*, we must have

$$\frac{dc}{ds} = 0 \implies c = \text{const.},$$

which is called the *characteristic equation*.

Exercise 3.2. Show that $c(x, t) = c(x - vt, 0)$. Sketch this solution at several values of t .

Solve the same IVP for the advection-diffusion-reaction equation

$$\frac{\partial c}{\partial t} + v \frac{\partial c}{\partial x} = -kc,$$

where $k > 0$ is the decay coefficient.

Exercise 3.3. Introduce moving coordinates $\hat{\xi} = \xi - \tau, \hat{\tau} = \tau$ to get a diffusion equation,

$$\frac{c}{\partial \hat{\tau}} - \frac{1}{\text{Pe}} \frac{\partial^2 c}{\partial \hat{\xi}^2} = 0.$$

Problem 1. Moving plume.

$$c_1(\hat{\xi}, \hat{0}) = \sigma(\hat{\xi}),$$

where $c_1(\hat{\xi}, \hat{\tau})$ is bounded. We have the fundamental solution to the diffusion (heat) equation:

$$c_1(\hat{\xi}, \hat{\tau}) = \frac{1}{\sqrt{4\pi\hat{\tau}/\text{Pe}}} \exp\left(\frac{-\text{Pe}\hat{\xi}^2}{4\hat{\tau}^2}\right).$$

Problem 2. Moving front.

$$c_2(\hat{\xi}, \hat{0}) = c_I(\hat{\xi}) = \begin{cases} 1 & \hat{\xi} < 0, \\ 0 & \hat{\xi} \geq 0. \end{cases}$$

Solution is a superposition of responses to point sources:

$$\begin{aligned} c_2(\hat{\xi}, \hat{\tau}) &= \int_{-\infty}^{\infty} c_I(\hat{\xi}), c_1(\zeta - \hat{\xi}, \hat{\tau}) d\zeta \\ &= \int_{-\infty}^0 c_1(\zeta - \hat{\xi}, \hat{\tau}) d\zeta \\ &= \int_{\hat{\xi}}^{\infty} c_1(\eta, \hat{\tau}) d\eta \\ &= \frac{1}{2} - \int_0^{\hat{\xi}} c_1(\eta, \hat{\tau}) d\eta \\ &= \frac{1}{2} - \int_0^{\hat{\xi}} \frac{1}{\sqrt{4\pi\hat{\tau}/\text{Pe}}} \exp\left(\frac{-\text{Pe}\eta^2}{4\hat{\tau}^2}\right) d\eta \\ &= \frac{1}{2} - \int_0^{\hat{\xi}/\sqrt{4\hat{\tau}/\text{Pe}}} \frac{1}{\sqrt{\pi}} e^{-s^2} ds \\ &= \frac{1}{2} - \frac{1}{2} \text{erf} \frac{\hat{\xi}}{\sqrt{4\hat{\tau}/\text{Pe}}}, \end{aligned}$$

where $c_I(\hat{\xi})$ is the weighting factor, $c_1(\zeta - \hat{\xi}, \hat{\tau})$ is the response at time $\hat{\tau}$ to unit phase $\delta(\hat{\xi} - \zeta)$, $\text{erf}(u) = \frac{2}{\sqrt{\pi}} \int_0^u e^{-s^2} ds$.

3.4 Transport with adsorption

Solute transport in fluid F , solute can adsorb onto rock R . Denote:

$$c = c_{(i,F)}, a = c_{(i,R)},$$

and we have mass balance in F and R as follows

$$\begin{aligned} \frac{\partial}{\partial t}(\varphi c) &= -\nabla \cdot (\bar{\mathbf{v}}c) + \nabla \cdot (\tilde{\mathcal{D}}\nabla c) + r_{(i,F)}, \\ \frac{\partial}{\partial t}[(1 - \varphi)a] &= r_{(i,R)}. \end{aligned}$$

If no chemical reactions convert species i to other species, $r_{(i,F)} + r_{(i,R)} = 0$:

$$\frac{\partial}{\partial t}[\varphi c + (1 - \varphi)a] = -\nabla \cdot (\bar{\mathbf{v}}c) + \nabla \cdot (\tilde{\mathcal{D}}\nabla c). \quad (3.1)$$

Assume adsorption is fast. Neglect reaction kinetics and write adsorption isotherm $a = a(c)$, then (3.1) becomes

$$\frac{\partial}{\partial t}[\varphi c + (1 - \varphi)a(c)] = -\nabla \cdot (\bar{\mathbf{v}}c) + \nabla \cdot (\tilde{\mathcal{D}}\nabla c).$$

Common isotherms:

- linear isotherm (may be valid for small c)

$$a(c) = \kappa c, \kappa > 0.$$

- Freundlich $a(c) = \kappa c^n, \kappa > 0$.
- Langmuir isotherm $a(c) = \frac{\kappa_1 c}{1 + \kappa_2 c^2}, \kappa_i > 1, i = 1, 2$.

3.5 Linear adsorption isotherms and retardation

Adsorption slows transport. If flow is incompressible, $\nabla \cdot \bar{\mathbf{v}} = 0$.

$$\frac{\partial}{\partial t}[\varphi + \kappa(1 - \varphi)c] = -\bar{\mathbf{v}} \cdot \nabla c + \nabla \cdot (\tilde{\mathcal{D}}\nabla c).$$

When φ, κ are constant, define

$$R = 1 + \frac{\kappa(1 - \varphi)}{\varphi} > 1.$$

Then we have

$$\varphi \frac{\partial c}{\partial t} + \frac{\bar{\mathbf{v}}}{R} \nabla c - \nabla \cdot \left(\frac{\tilde{\mathcal{D}}}{R} \nabla c \right) = 0,$$

where $\bar{\mathbf{v}}/R, \tilde{\mathcal{D}}/R$ are effective transport coefficients. Apparent advection and hydrodynamic dispersion are slower. Langmuir (concave down) isotherms and front sharpening. Simple version of mass balance for solute:

$$[\varphi + (1 - \varphi)a'(c)] \frac{c}{\partial t} + \bar{\mathbf{v}} \frac{\partial c}{\partial x} = 0.$$

Neglect hydrodynamic dispersion, and φ is constant. Examine path $(x(s), t(s))$ in the (x, t) -plane. By chain rule, $c(x(s), t(s))$ obeys

$$\frac{dt}{ds} \frac{\partial c}{\partial t} + \frac{dx}{ds} \frac{\partial c}{\partial x} = \frac{dc}{ds}.$$

Consistency requires

$$\frac{dc}{ds} = 0$$

along any path for which

$$\frac{dx}{dt} = \frac{\bar{v}}{\varphi + (1 - \varphi)a'(c)}.$$

Consider the initial condition $c(x, 0)$. Downward concavity of $a(c) \implies a''(c) < 0 \implies a'(c)$ decreasing. That implies $v(c)$ increasing function of c .

4 Multiphase Flows in Porous Media

4.1 Porous-medium equation

Simple model of nonlinear diffusion

$$\frac{\partial u}{\partial t} - \Delta u^{n+1} = 0, n \geq 1, u \geq 0.$$

Equivalent:

$$\frac{\partial u}{\partial t} - \nabla \cdot [(n+1)u^n \nabla u] = 0,$$

where $(n+1)u^n$ is called the diffusion coefficient (non-linear).

Exercise 4.1. Derive it from the mass balance

$$\varphi \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \varphi \mathbf{v}) = 0,$$

and Darcy's law

$$\varphi \mathbf{v} = -\frac{k}{\mu} \nabla p,$$

polytopic equation of state:

$$p = p_0 \rho^n, n \geq 1,$$

when $n = 1$ it is ideal gas law.

1-D NP with $n = 1$.

$$\begin{cases} \frac{\partial u}{\partial t} - \frac{\partial}{\partial x} (2u \frac{\partial u}{\partial x}) = 0, -\infty < x < \infty, \\ u(x, 0) = \delta(x) \quad \text{point source.} \end{cases}$$

Since

$$\int_{-\infty}^{\infty} \delta(x) dx = 1,$$

expect

$$\int_{-\infty}^{\infty} u(x, t) dx = 1, \forall t > 0 \text{ and } u(x, t) \geq 0.$$

Idea: look for *self-similar* solutions. Find *stretching transformation*

$$\xi = \varepsilon x, \tau = \varepsilon^a t, \eta = \eta^b u,$$

any scaling parameter $\varepsilon > 0$ such that

$$u(x, t) = \eta(\xi, \eta) = \varepsilon^b u(\varepsilon x, \varepsilon^a t).$$

If such a transformation exists, then choosing $\varepsilon = t^{-1/a}$ gives

$$u(x, t) = t^{-b/a} u(xt^{-1/a}, 1) = t^{-b/a} U(\zeta),$$

where $\zeta = xt^{-1/a}$. In this case, we can replace the PDE for $u(x, t)$ by an ODE for $U(\zeta)$.

Exercise 4.2. Show

$$\begin{cases} \frac{\partial \eta}{\partial \tau} = \varepsilon^{b-a} \frac{\partial u}{\partial t}, \\ \frac{\partial \eta}{\partial \xi} = \varepsilon^{b-1} \frac{\partial u}{\partial x}. \end{cases}$$

So

$$\frac{\partial \eta}{\partial \tau} - \frac{\partial}{\partial \eta} \left(\tau \eta \frac{\partial \eta}{\partial \xi} \right) = \varepsilon^{b-a} \frac{\partial u}{\partial t} - \varepsilon^{2b-2} \frac{\partial}{\partial x} \left(2u \frac{\partial u}{\partial x} \right).$$

Invariance condition requires

$$\varepsilon^{b-a} = \varepsilon^{2b-2} \forall \varepsilon > 0 \implies a = 2 - b.$$

Conclude that

$$u(x, t) = \varepsilon^{-b} \eta(\xi, \tau),$$

Special choice $\varepsilon = t^{-1/(2-b)}$ gives

$$u(x, t) = t^{b/(2-b)} \eta(xt^{-1/(2-b)}, 1) = t^{b/(2-b)} U(xt^{-1/(2-b)}).$$

Determine b using mass conservation: For $t > 0$,

$$1 = \int_{-\infty}^{\infty} u(x, t) dx = t^{b/(2-b)} \int_{-\infty}^{\infty} U(xt^{-1/(2-b)}) dx = t^{1/(2-b)} t^{b/(2-b)} \int_{-\infty}^{\infty} U(y) dy \quad (\text{change of variables}).$$

RHS independent of t , then

$$b = -1, a = 3 \implies \zeta = xt^{-1/3}, u(x, t) = t^{-1/3} U(\zeta).$$

Step 2: Find the ODE for $U(\zeta)$. Substitute $u(x, t)$ into the PDE to get

$$3(U^2)'' = -U - \zeta U' = -(\zeta U')' \implies (U^2)' = -\frac{1}{3} \zeta U + C_1. \quad (4.1)$$

Determine C , using symmetry about $x = 0$ (i.e., about $\zeta = xt^{-1/3}$ for $t > 0$).

$$0 = \frac{\partial u}{\partial x}(0, t) = t^{-2/3} U'(0).$$

Exercise 4.3. Apply this condition to (4.1) to show $C_1 = 0$. (Symmetry about $x = 0$)

Exercise 4.4. Show that $U = 0$, $U = C_2 - \frac{1}{12} \zeta^2$ are solutions.

The following solution respects $U \geq 0$ and $\int_{-\infty}^{\infty} U(\zeta) d\zeta = 1$:

$$U(\zeta) = \begin{cases} \frac{\sqrt[3]{3}}{4} - \frac{1}{12} \zeta^2 & \frac{\zeta^2}{12} < \frac{\sqrt[3]{3}}{4}, \\ 0 & \text{otherwise.} \end{cases}$$

Barenblatt solution, in terms of $u(x, t)$,

$$u(x, t) = \begin{cases} t^{-1/3} \left(\frac{\sqrt[3]{3}}{4} - \frac{1}{12} x^2 t^{-2/3} \right) & x < (9t)^{1/3}, \\ 0 & \text{otherwise.} \end{cases}$$

Interesting properties:

- (a) Self-similar (shape of $u(x, t)$ preserved except for scaling).
- (b) Compact support (not zero only on finite interval).
- (c) Front moves with finite speed.

$$\frac{dx_0}{dt} = 3^{-1/3} t^{-2/3}.$$

5 Multiphase Flows in Porous Media

Characteristic feature: fluid-fluid interfaces observable at microscopic scale.

Example 5.1.

- (a) air + water in soils.
- (b) oil + water.
- (c) oil + gas + water
- (d) CO_2 + water.

5.1 Capillary pressure

Microscopic picture: look at energy with the interface.

Definition 5.1. The *interface tension* between two fluids is the energy/area in the interface that separates them.

Dimensions:

$$\frac{\text{energy}}{\text{area}} = MT^{-2} = \frac{\text{force}}{\text{distance}}.$$

Notation: IFT = σ .

Example 5.2. Pieces of smooth surface Σ . Parametrize $\partial\Sigma$ as a closed arc $\tilde{\gamma} : [a, b] \rightarrow \mathbb{E}$. Assume that

- (a) Σ is a well-defined unit normed vector field \mathbf{n} .
- (b) $\tilde{\gamma}$ is positively oriented with respect to \mathbf{n} , and $\|\tilde{\gamma}'\| = 1$ (Always possible.)

Force on

$$\partial\Sigma = \int_{\tilde{\gamma}} \sigma \mathbf{n} \times \mathbf{t} da = \int_a^b \sigma \mathbf{n}(\tilde{\gamma}(s)) \times \tilde{\gamma}'(s) ds.$$

Force on $\partial\Sigma = \int_{\tilde{\gamma}} \sigma \mathbf{n} \times \mathbf{t} ds /$

Claim 5.1. If Σ is curved, $p_1 \neq p_2$. Force balance on Σ :

$$\int_{\Sigma} [p_1 \mathbf{n} + p_2 (-\mathbf{n})] da - \int_{\tilde{\gamma}} \sigma \mathbf{n} \times \mathbf{t} ds = 0.$$

By corollary to Stokes theorem with $\mathbf{f} = \sigma \mathbf{n}$,

$$\begin{aligned} \int_{\tilde{\gamma}} \sigma \mathbf{n} \times \mathbf{t} \, ds &= \int_{\Sigma} \sigma [(\nabla \cdot \mathbf{n})\mathbf{n} - (\nabla \mathbf{n})\mathbf{n}] \, da. \\ &= \int_{\Sigma} \sigma [(\nabla \cdot \mathbf{n})\mathbf{n} - \frac{1}{2} \nabla(\mathbf{n} \cdot \mathbf{n})] \, da. \\ &= \int_{\Sigma} \sigma [(\nabla \cdot \mathbf{n})\mathbf{n} - \frac{1}{2} \nabla 1] \, da. \\ &= \int_{\Sigma} \sigma (\nabla \cdot \mathbf{n})\mathbf{n} \, da. \end{aligned}$$

Therefore,

$$\int_{\Sigma} [p_1 - p_2 - \sigma (\nabla \cdot \mathbf{n})]\mathbf{n} \, da = 0.$$

Holds for all pieces of smooth interface, $p_1 - p_2 - \sigma \nabla \cdot \mathbf{n} = 0$ at all points. Then we have Young-Laplace equation:

$$p_1 - p_2 = \sigma \nabla \cdot \mathbf{n}.$$

Remark 5.1. $\frac{1}{2} \nabla \cdot \mathbf{n}$ is the *mean curvature* of Σ . Given a representation of Σ as a level set of some function $F : \mathbb{E} \rightarrow \mathbb{R}$:

$$F(x_1, x_2, x_3) = 0 \text{ on } \Sigma,$$

such that $\nabla F(x_1, x_2, x_3) \neq 0$ everywhere.

$$\mathbf{n}(\mathbf{x}) = \frac{\nabla F(\mathbf{x})}{\|\nabla F(\mathbf{x})\|}.$$

Exercise 5.1. Show the mean curvature of

- A circular cylinder of radius R is $\frac{1}{2R}$.
- A sphere of radius R is $\frac{1}{R}$.

Notation: Denote the *mean radius of curvature* by $\frac{1}{2} \nabla \cdot \mathbf{n} = \frac{1}{\bar{r}}$. Then rewrite the Young-Laplace equation as

$$\underbrace{p_c}_{\text{capillary pressure}} = \underbrace{p_1 - p_2}_{\text{pressure higher on concave side}} = \frac{2\sigma}{\bar{r}}.$$

5.2 Wettability

Solid wall has greater affinity for wetting fluid W than the nonwetting fluid N . Convention $p_c = p_N - P_W$, contact angle is less than $\pi/2$.

Example 5.3.

(a) Capillary rise in a tube of radius a . At equilibrium,

$$p_{\text{air}} = p_{\text{water}} + \gamma_{\text{water}} g l.$$

Substitute $p_c = 2\sigma/\bar{r} = 2\sigma \cos \theta/a$. Solve

$$l = \frac{2\sigma \cos \theta}{\gamma_{\text{water}} g} \cdot \frac{1}{a}.$$

Therefore, we can get the relation that the capillary rise is $l \propto \frac{1}{a}$.

(b) Bundle of tubes, random radii. Capillary rise has a distinction of values.

5.3 Macroscopic picture

3-phase mixture.

$$\alpha = \begin{cases} R & \text{rock,} \\ W & \text{wetting fluid,} \\ N & \text{nonwetting fluid.} \end{cases}$$

For $\alpha = W, N$,

$$\text{saturation} = \frac{\varphi_\alpha}{\varphi} = S_\alpha.$$

Simple hypothesis:

$$p_c = p_N - p_W = p_c(S_w)$$

Reality: p_c also depends on history.

5.4 Multiphase flow equations

Muskat and Meres (1937):

$$\varphi_\alpha \mathbf{v}_\alpha = -\frac{k_\alpha}{\mu_\alpha} (\nabla p_\alpha - \gamma_\alpha g \nabla z), \quad \alpha = N, W, \quad (5.1)$$

where $k_\alpha < k$ is *effective permeability* (because other fluids interfere). Common Decomposition: $k_\alpha = k k_{r\alpha}$, where $k_{r\alpha} = k_{r\alpha}(S_W)$ is relative permeability of fluid α .

Remark 5.2.

(a) $k_{r\alpha}$ must be measured.

(b) They exhibit hysteresis.

Substitute (5.1) into mass balance,

$$\frac{\partial}{\partial t} (\varphi_\alpha \gamma_\alpha) + \nabla \cdot (\varphi_\alpha \gamma_\alpha \mathbf{v}_\alpha) = r_\alpha, \quad \alpha = N, W,$$

where $\varphi_\alpha = \varphi S_\alpha$. Assume no interphase mass transfer ($r_\alpha = 0$).

$$\frac{\partial}{\partial t} (\varphi S_\alpha \gamma_\alpha) = \nabla \cdot \left[\frac{\gamma_\alpha k k_{r\alpha}}{\mu_\alpha} (\nabla p_\alpha - \gamma_\alpha g \nabla z) \right], \quad \alpha = N, W.$$

We have 2 PDEs for p_N, p_W, S_N, S_W . For closure, need 2 more equations

$$S_N + S_W = 1, \quad p_N - p_W = p_c(S_W).$$

Also require constitutive relations for $\varphi, \gamma_\alpha, k, k_{r\alpha}(S_W), \mu_\alpha$ and g and ∇z . Because of $k_{r\alpha}(S_W)$ and $p_c(S_W)$ systems is nonlinear.

5.4.1 Classification

Assume that

- (a) $\gamma_N, \gamma_W, \varphi$ constant.
- (b) gravity effects are negligible (horizontal flow $\implies \nabla z = \mathbf{0}$).

Flow equations simplify:

$$\begin{cases} \varphi \frac{\partial S_W}{\partial t} &= \nabla \cdot (\lambda_W \nabla p_W), \\ \varphi \frac{\partial}{\partial t} (1 - S_W) &= -\varphi \frac{\partial S_W}{\partial t} = \nabla \cdot (\lambda_N \nabla p_N), \end{cases} \quad (5.2)$$

where $\lambda_\alpha = \frac{k k_{r\alpha}}{\mu_\alpha}$ fluid mobilities. Adding gives the total fluid flux:

$$\nabla \cdot \mathbf{Q} = 0, \quad \mathbf{Q} = -(\lambda_W \nabla p_W + \lambda_N \nabla p_N).$$

Exercise 5.2. Show that the above equation is equivalent to pressure equation (an elliptic equation for p):

$$\nabla \cdot (\lambda \nabla p) = \nabla \cdot \left(\frac{\lambda_W - \lambda_N}{2} \nabla p_c \right),$$

where $\lambda = \lambda_N + \lambda_W, p = \frac{1}{2}(p_N + p_W)$.

Leaves 1 independent equation from (5.2).

Exercise 5.3. Show (5.2) is equivalent to

$$\varphi \frac{\partial S_W}{\partial t} = -\nabla \cdot [f(S_W) \mathbf{Q}] - \nabla \cdot \underbrace{[f(S_W) \lambda_N(S_W) p'_c(S_W)]}_{\text{nonlinear "diffusion"}},$$

where the fraction flow function $f(S_W) = \frac{\lambda_W}{\lambda_N + \lambda_W} = \frac{\lambda_W(S_W)}{\lambda_N(S_W) + \lambda_W(S_W)}$, which is the fraction of flowing fluid that is water. Saturation equation is parabolic for S_W (hyperbolic if capillary term is negligible).

5.5 The Buckley-Leverett Problem (1942)

Simplifying assumptions:

- Flow is horizontal (1D), so $\nabla z = \mathbf{0}, \mathbf{v} = (v, 0, 0)$.
- Uniform geometry in x_2, x_3 -dimensions.
- $\varphi, \gamma_N, \gamma_W$ constant.
- $\nabla p_c(S_W)$ is negligible (high flow rate \mathbf{Q}).

Exercise 5.4. Integrate saturation over cross section to get Buckley-Leverett saturation equation (dropping subscript W , 1st-order hyperbolic)

$$\frac{\partial S}{\partial t} + \frac{Q}{\varphi} \frac{\partial f}{\partial x}(S) = 0.$$

Initial-value problem:

$$\frac{\partial S}{\partial t} + \frac{Q}{\varphi} \frac{\partial f(S)}{\partial x} = 0, x, t > 0,$$

with the initial condition

$$S(x, 0) = \begin{cases} 1 - S_{Nr} - \frac{x}{L}(1 - S_{Nr} - S_{Wr}) & 0 \leq x < L, \\ S_{Wr} & x \geq L, \end{cases}$$

$$S(0, t) = 1 - S_{Nr}, t \geq 0.$$

Method of characteristics, the PDE becomes

$$\frac{\partial S}{\partial t} + \frac{Q}{\varphi} f'(S) \frac{\partial S}{\partial x} = 0.$$

Chain rule gives

$$\frac{\partial S}{\partial t} + \frac{dx}{dt} \frac{\partial S}{\partial x} = \frac{dS}{dt}.$$

Consistency requires

$$\frac{dS}{dt} = 0$$

along smooth paths obeying the characteristic curves

$$\frac{dx}{dt} = \frac{Q}{\varphi} f'(S).$$

Intersecting charat. curve, multi-valued $S(x, t)$ impossible. Resolution: discontinuous solution.

5.6 Welge tangent construction (1952)

Resolution to multivalued saturation solution: solution with jumpy discontinuity. Derive jump condition from integral form of mass balance: over any interval $[x_L, x_R]$ containing $\Sigma(t)$.

$$\begin{aligned} \frac{d}{dt} \int_{x_L}^{x_R} S dx &= \frac{Q}{\varphi} f(S(x_L, t)) - \frac{Q}{\varphi} f(S(x_R, t)) \\ &= \frac{d}{dt} \int_{x_L}^{\Sigma(t)} S dx + \frac{d}{dt} \int_{\Sigma(t)}^{x_R} S dx \\ &= \left(\int_{x_L}^{\Sigma(t)} + \int_{\Sigma(t)}^{x_R} \right) \frac{\partial S}{\partial t} dx + S(\Sigma(t)-, t) \frac{d\Sigma}{dt} - S(\Sigma(t)+, t) \frac{d\Sigma}{dt} \\ &= \int_{x_L}^{x_R} \frac{\partial S}{\partial t} dx - [S] \frac{d\Sigma}{dt}, \end{aligned} \tag{5.3}$$

where $[\cdot] = \lim_{x \rightarrow \Sigma+} (\cdot) - \lim_{x \rightarrow \Sigma-} (\cdot) =$ jump across Σ . Substitute into (5.3) and take $\lim_{x_L \rightarrow \Sigma-}, \lim_{x_R \rightarrow \Sigma+}$ to get Rankine-Hugniot condition,

$$\frac{d\Sigma}{dt} = \frac{Q}{\varphi} \frac{[f]}{[S]}.$$

Application:

- Downstream of $\Sigma(t)$, $(\Sigma+, t) = S_{Wr}$ (signal from left hasn't reached $\Sigma(t)+$.)

- Upstream of $\Sigma(t)$, $S(\Sigma-, t) = S^*$, where

$$\underbrace{\frac{Q}{\varphi} f'(S^*) = \frac{dx}{dt}}_{\text{method of characteristics}} = \underbrace{\frac{d\Sigma}{dt} = \frac{Q [f]}{\varphi [S]}}_{\text{jump condition}}.$$

Remark 5.3.

- Jump eliminates characteristic curve crossings.
- von Neumann showed tangent \iff mass balance.

Wedge solution is a *weak solution* to the PDE, satisfying

$$\int_0^\infty \int_0^\infty \left(S \frac{\partial \varphi}{\partial t} + \frac{Q}{\varphi} f \frac{\partial \varphi}{\partial x} \right) dx dt = 0, \quad (5.4)$$

$\forall \varphi(x, t)$ (test function) such that φ all derivatives tend to 0 as $x, t \rightarrow \infty$. (5.4) doesn't guarantee uniqueness. The correct weak solution is the limit, as $D_{\text{cap}}(S) \rightarrow 0$, of

$$\frac{\partial S}{\partial t} + \frac{Q}{\varphi} \frac{\partial}{\partial x} f(S) + \frac{1}{\varphi} \frac{\partial}{\partial x} \left[\underbrace{f(S) \lambda_W(S) p'_c(S)}_{-D_{\text{cap}}(S)} \frac{\partial S}{\partial x} \right] = 0,$$

which is a parabolic PDE. Numerically implement this condition using upstream weighting.

5.7 Variably saturated flow

Soils near Earth's surface saturated with air (A) and water (W). L.A. Richards (1931):

$$p_A = p_{\text{atm}} = 0 (\text{gauge pressure}).$$

Typically W is the wetting fluid

$$p_C = p_A - p_W = -p_W > 0.$$

Define *pressure head*

$$\psi = \frac{p_W}{\gamma_W g} = \frac{-p_C}{\gamma_W g},$$

which has the dimension $[L]$. And *water content*,

$$\Theta = \varphi S_W = \frac{\text{volume water}}{\text{total volume}}.$$

5.8 Observations

(a) $p_C = p_C(S_W) \implies \psi = \psi(\Theta)$, assume invertible (neglecting hysteresis).

(b) Darcy's law for W :

$$\varphi \mathbf{v}_W = -\frac{k k_{rW}}{\mu_W} (\nabla p_W - \gamma_W g \nabla z) = -K(\Theta) (\nabla \psi + \mathbf{e}_3),$$

where the *unsaturated hydraulic conductivity* $K(\Theta) = \frac{k k_W \gamma_W g}{\mu_W}$ (assuming γ_W is constant).

(c) Mass balance has the form:

$$\frac{\partial}{\partial t}(\gamma_W \Theta) + \nabla \cdot (\gamma_W \varphi \mathbf{v}_W) = 0.$$

Substitute for $\varphi \mathbf{v}_W$:

$$\frac{\partial \Theta}{\partial t} - \nabla \cdot [K(\Theta) \nabla \psi(\Theta) + K(\Theta) \mathbf{e}_3] = 0.$$

Special cases: purely vertical flow:

$$\frac{\partial \Theta}{\partial t} - \frac{\partial}{\partial x_3} \left[K(\Theta) \left(\frac{\partial \psi}{\partial x_3} + 1 \right) \right] = 0.$$

Purely horizontal flow:

$$\frac{\partial \Theta}{\partial t} - \frac{\partial}{\partial x_1} \left[K(\Theta) \frac{\partial \psi}{\partial x_1} \right] = 0.$$

5.9 Alternative formulations

(a) ψ -based: write $\Theta = \Theta(\psi)$, so $K(\Theta) = K(\Theta(\psi))$.

$$\Theta'(\psi) \frac{\partial \psi}{\partial t} - \nabla [K(\Theta(\psi))(\nabla \psi + \mathbf{e}_3)] = 0,$$

where $\Theta'(\psi)$ is the specific moisture capacity (positive).

(b) Θ -based: write $\nabla \psi(\Theta) = \psi'(\Theta) \nabla \Theta$. Then

$$\frac{\partial \Theta}{\partial t} - \nabla \cdot [D_W(\Theta) \nabla \Theta + K(\Theta) \mathbf{e}_3] = 0, \quad (5.5)$$

where soil-moisture diffusivity $D_W(\Theta) = K(\Theta) \psi'(\Theta) \geq 0$ (dimension: $L^2 T^{-1}$, useful for horizontal flow). *Observation:* (5.5) is a nonlinear heat equation with $D(\Theta) = 0$ at endpoints.

6 Flows with interphase mass transfer

6.1 Compositional models (in general)

Multiple fluid phases, multiple chemical species transferring among phases via evaporation dissolution. Four phases:

- (a) Rock (R)
- (b) Water (W)
- (c) Oil (O)
- (d) Gas (G)

$N + 1$ species: $i = 1, \dots, N$ in fluids (e.g., H_2O, CO_2, CH_4, \dots), $i = N + 1$ (rock). Each pair (i, α) is a constituent. Examples of constituents:

$$(CH_4, G), (CH_4, W), (CH_4, O), (n - C_4H_{10}, O).$$

Each has true density $\gamma_{(i,\alpha)} \left[\frac{\text{mass of } i \text{ in } \alpha}{\text{volume of } \alpha} \right]$, velocity $\mathbf{v}_{(i,\alpha)}$. Each phase α has a volume fraction φ_α . Define $\varphi = 1 - \varphi_R$, and the saturation of fluid phase α : $S_\alpha = \varphi_\alpha / \varphi$. Derived quantities:

$$\begin{aligned} \text{true density of fluid phase } \alpha : \gamma_\alpha &= \sum_{i=1}^N \gamma_{(i,\alpha)}, \\ \text{mass fraction of species } i \text{ in phase } \alpha : \omega_{(i,\alpha)} &= \frac{\gamma_{(i,\alpha)}}{\gamma_\alpha}, \\ \text{bulk density of fluids: } \rho &= \varphi \sum_{\alpha \neq R} S_\alpha \gamma_\alpha, \left[\frac{\text{mass fluid}}{\text{total volume}} \right], \\ \text{total mass fraction of } i \text{ in fluids } \left[\frac{\text{mass } i}{\text{mass of fluids}} \right] : \omega_i &= \frac{\varphi}{\rho} \sum_{\alpha \neq R} S_\alpha \gamma_\alpha \omega_{(i,\alpha)}, \\ \text{barycentric velocity of fluid phase } \alpha : \mathbf{v}_\alpha &= \frac{1}{\gamma_\alpha} \sum_{i=1}^N \gamma_{(i,\alpha)} \mathbf{v}_{(i,\alpha)}, \\ \text{diffusion velocity: } \tilde{\mathbf{v}}_{(i,\alpha)} &= \mathbf{v}_{(i,\alpha)} - \mathbf{v}_\alpha. \end{aligned}$$

Restrictions:

$$\sum_{i=1}^N \omega_{i,\alpha} = \sum_{i=1}^N \omega_i = \sum_{\alpha} \varphi_\alpha = \sum_{\alpha \neq R} S_\alpha = 1, \quad \sum_{i=1}^N \tilde{\mathbf{v}}_{i,\alpha} = 0.$$

Mass balance for fluid constituent (i, α) :

$$\frac{\partial}{\partial t} (\varphi S_\alpha \gamma_{(i,\alpha)}) + \nabla \cdot (\varphi S_\alpha \gamma_{(i,\alpha)} \mathbf{v}_{(i,\alpha)}) = r_{(i,\alpha)}, \quad i = 1, \dots, N, \alpha = W, O, G, \quad \text{subject to } \sum_{i=1}^N \sum_{\alpha \neq R} r_{(i,\alpha)} = 0. \quad (6.1)$$

Assume no intraphase (“homogeneous”) chemical reactions:

$$\sum_{\alpha \neq R} r_{(i,\alpha)} = 0, \quad i = 1, \dots, N.$$

Exercise 6.1.

$$\begin{aligned} \frac{\partial}{\partial t} (\rho \omega_i) + \nabla \cdot [(S_G \gamma_G \omega_{(i,G)} \mathbf{v}_G + S_O \gamma_O \omega_{(i,O)} \mathbf{v}_O + S_W \gamma_W \omega_{(i,W)} \mathbf{v}_W)] \\ + \nabla \cdot (\mathbf{j}_{(i,G)} + \mathbf{j}_{(i,O)} + \mathbf{j}_{(i,W)}) = 0, \quad i = 1, \dots, N, \end{aligned}$$

which has N chemical species (or pseudo species), the diffusive flux of i in α $\mathbf{j}_{(i,\alpha)} = \varphi S_\alpha \gamma_\alpha \omega_{(i,\alpha)} \tilde{\mathbf{v}}_{(i,\alpha)}$.

Phase velocities: Darcy’s law.

$$\mathbf{v}_\alpha = -\frac{\lambda_\alpha}{\varphi S_\alpha} (\nabla p_\alpha - \gamma_\alpha g \nabla z).$$

Define $p_{COW} = p_O - p_W$, $p_{CGW} = p_G - p_W$. Diffusive fluxes: Petroleum reservoir simulator: $\mathbf{j}_{(i,\alpha)} = \mathbf{0}$. Graduate contamination simulator: not so realistic. Transport equation for each species:

$$\begin{aligned} \frac{\partial}{\partial t} [\varphi (S_G \gamma_G \omega_{(i,G)} + S_O \gamma_O \omega_{(i,O)} + S_W \gamma_W \omega_{(i,W)})] \\ - \nabla \cdot [\lambda_G \gamma_G \omega_{(i,G)} (\nabla p_G - \gamma_G g \nabla z) + \text{flux}_O + \text{flux}_W] = 0, \quad i = 1, \dots, N. \end{aligned}$$

Closure: Zhou (2013) proposed

$$\begin{aligned} p_O &= p_W + p_{COW}(S_W), \\ p_G &= p_O + p_{COG}(S_G, S_O). \end{aligned}$$

Relative permeabilities: Coreg et al. (1956) put forward

$$\begin{aligned} k_{rG} &= k_{rG}(S_G), \\ k_{rO} &= k_{rO}(S_W, S_G), \\ k_{rW} &= k_{rW}(S_W). \end{aligned}$$

Restrictions:

$$\begin{aligned} \sum_{i=1}^N \omega_{(i,\alpha)} &= 1, \quad (\alpha = W, O, G) \\ \sum_{i=1}^N \omega_i &= 1 = S_O + S_W + S_G. \end{aligned}$$

Assume fluids are in local thermodynamic equilibrium

$$\begin{aligned} \gamma_\alpha &= \gamma_\alpha(\tilde{\omega}_\alpha, p_\alpha), \omega_\alpha = (\omega_{(1,\alpha)}, \omega_{(2,\alpha)}, \dots, \omega_{(N-1,\alpha)}), \alpha = G, O, W, \\ \tilde{\omega}_\alpha &= \tilde{\omega}_\alpha(\tilde{\omega}, p), \tilde{\omega} = (\omega_1, \omega_2, \dots, \omega_{N-1}), p = p_G, \\ S_\alpha &= S_\alpha(\tilde{\omega}, p), \alpha = G, O, W. \end{aligned}$$

These functions are typically implicit.

$$\tilde{\omega}, p \rightarrow \boxed{\text{“flash” calculation}} \rightarrow \tilde{\omega}_\alpha, S_\alpha, \alpha = G, O, W \rightarrow \boxed{\text{equations of state}} \rightarrow \gamma_\alpha, \alpha = G, O, W.$$

Transport equation for H_2O ($i = N$):

$$\frac{\partial}{\partial t}(\varphi S_W \gamma_W) - \nabla \cdot [\lambda_W \gamma_W (\nabla p_O - \nabla p_{COW} - \gamma_W g \nabla z)] = 0.$$

Transport equations for hydrocarbons:

$$\frac{\partial}{\partial t}(\rho_H \omega_i) - \nabla \cdot [\text{flux}_O + \text{flux}_G] = 0, i = 1, \dots, N-1, \rho_H = S_O \gamma_O + S_G \gamma_G. \quad (6.2)$$

Taking $\sum_{i=1}^{N-1}$ (6.2) gives

$$\frac{\partial \rho_H}{\partial t} + \nabla \cdot [(\lambda_O \gamma_O + \lambda_G \gamma_G) \nabla p_O + \lambda_G \gamma_G \nabla p_{CGO} - (\lambda - O \gamma_O + \lambda_G \gamma_G) \nabla z] = 0,$$

which is regarded as pressure equation. Leaves $N-2$ independent transparent equations (6.2).

$$\text{overall mole fractions} \rightarrow \tilde{\omega}, p \rightarrow \boxed{\text{flash}} \rightarrow \tilde{\omega}_G, \tilde{\omega}_O, Y_O, Y_G,$$

where $\tilde{\omega} = (\omega_1, \dots, \omega_{N-1})$, Y_O and Y_G are mole fractions of phases. System of $2N+2$ nonlinear equations:

$$f_{(i,O)}(\tilde{\omega}_{(1,O)}, \dots, \tilde{\omega}_{(N,O)}, p) = f_{(i,G)}(\tilde{\omega}_{(1,G)}, \dots, \tilde{\omega}_{(N,G)}, p), i = 1, \dots, N.$$

where $f_{(i,\alpha)}$ is the *fugacity* of species i in phase α (generalizes partial pressures).

$$Y_O \tilde{\omega}_{(i,O)} + Y_G \tilde{\omega}_{(i,G)} = \tilde{\omega}_i, i = 1, \dots, N - 1.$$

Then

$$\begin{aligned} Y_O + Y_G &= 1, \\ \sum_{i=1}^N \tilde{\omega}_{(i,O)} &= 1, \\ \sum_{i=1}^N \tilde{\omega}_{(i,G)} &= 1. \end{aligned}$$

6.2 Equation-of-state methods

Cubic equations of state (Redlich-Kwong, Peng-Robinson)

$$Z^3 + c_2 Z^2 + c_1 Z + c_0 = 0,$$

where the compressibility factor $Z = \frac{p}{\rho RT}$ ($= 1$ for ideal gas), c_0, c_1, c_2 depends on fluid composition and pressure.

$$f_{(i,\alpha)} = \rho \exp \left[\int_0^p \frac{Z_{(i,\alpha)} - 1}{\eta} d\eta \right]$$