Numerical Simulation of Multi-Phase Flows

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Outline

- Fundamentals of multiphase, nonisothermal flows
  occurrence, physics, mathematical model
- Numerical simulation
  general approach: space and time discretization,
  TOUGH2: methods, architecture, input data
- Hands-on use of TOUGH2
  illustrative applications and sample problems,
  problem variations

Phases and Components

Phases

- Homogeneous continuum
- Thermophysical properties (density, viscosity, specific enthalpy) vary slowly and continuously with position
- May consist of one or more chemical components
- Examples: aqueous phase, non-aqueous (oil) phase, gas, solid
- In a closed system, amount of different phases present may change
- Phase change usually involves substantial heat effects

Components

- Chemical species
- Can be present in several different phases
- Examples: H_2O, NaCl, CO_2, C_nH_{2n+2},...
- Distribution of components among phases is determined by chemical potential, kinetics
- All components in a phase flow together
- In a closed system, components are conserved (except for chemical reactions)

Gibbs' phase rule: $f = NK + 2 - NPH$

In a system with NPH phases, have NPH-1 phase saturations: $\sum_{\beta=1}^{NPH} S_\beta = 1$

Number of degrees of freedom is then f+NPH-1 = NK+1

Multiphase Flow Systems

Flow System	Phases	Components
groundwater aquifer	aqueous	water, solutes
vadose zone	aqueous gas NAPL	water, solutes air, vapor, CO_2, ... VOCs, water, air
gas reservoir	gas aqueous	CH_4, CO_2, water vapor water, solutes
oil reservoir	oil gas aqueous	alkanes, aromatics, solutes CH_4, ... water, solutes

Storage: the amount of mass present in a unit volume of the flow system

Pore volume: ϕ
Volume of phase β: ϕS_β

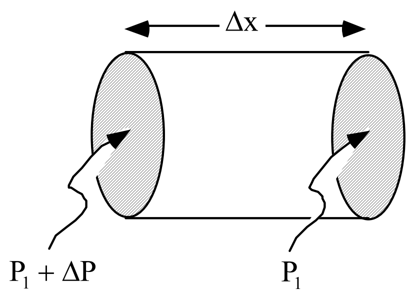
Mass of a single phase: $M = \phi\rho$
Mass of component κ in that phase: $M^\kappa = \phi\rho X^\kappa$

Mass of phase β: $M_\beta = \phi S_\beta \rho_\beta$
Mass of component κ in phase β: $M_\beta^\kappa = \phi S_\beta \rho_\beta X_\beta^\kappa$

Total mass of component κ in all phases: $M^\kappa = \phi \sum_\beta S_\beta \rho_\beta X_\beta^\kappa$

Total mass of component κ in volume V: $\int_V M^\kappa \, dV$

Darcy's Law (Henri Darcy, 1856)



$$F = -k\frac{\rho}{\mu}\frac{\Delta P}{\Delta x} = u\rho$$

k - permeability (m^2), 1 darcy ≈ 10^{-12} m^2

Analogy to Ohm's law: $I = \frac{\Delta U}{R}$

$I \equiv F$ $\quad \Delta U \equiv \Delta P$ $\quad R \equiv \frac{\Delta x}{k(\rho/\mu)}$

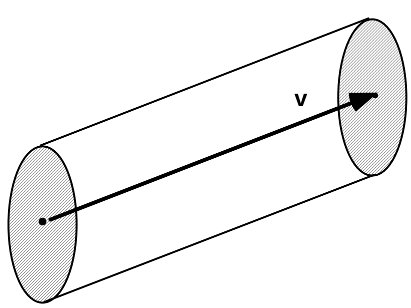
Fluid Flux in 3-D

$$\begin{pmatrix} F_x \\ F_y \\ F_z \end{pmatrix} = -k\frac{\rho}{\mu}\begin{pmatrix} \Delta P/\Delta x \\ \Delta P/\Delta y \\ \Delta P/\Delta z + \rho g \end{pmatrix}$$

$$\mathbf{F} = -k\frac{\rho}{\mu}\left(\nabla P - \rho\mathbf{g}\right)$$

$$\mathbf{u} = -\frac{k}{\mu}\left(\nabla P - \rho\mathbf{g}\right)$$

Pore Velocity



$$\mathbf{u} = \phi\mathbf{v}$$

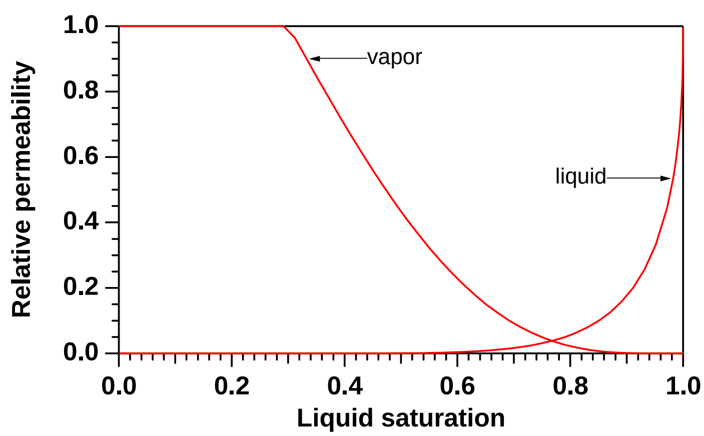
$$\mathbf{v} = \mathbf{u}/\phi$$

Multiphase Flow

$$\mathbf{F}_\beta = -k \frac{k_{r\beta}\rho_\beta}{\mu_\beta}\left(\nabla P_\beta - \rho_\beta \mathbf{g}\right)$$

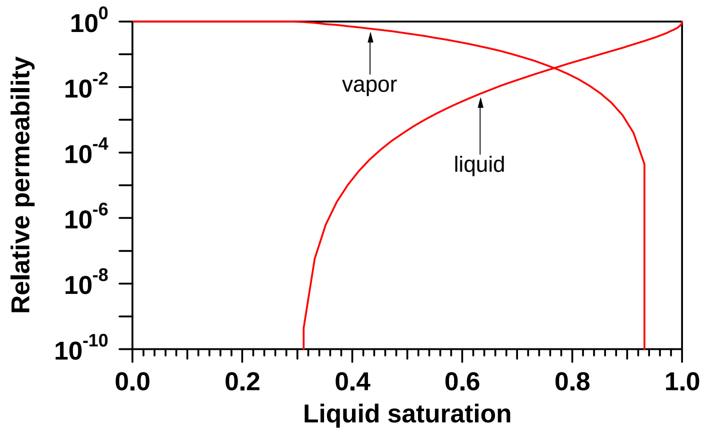
- phases: β = liquid, gas
- relative permeability: $k_{r\beta}$
- phase pressure: $P_\beta = P_{ref} - P_{cap}$
- capillary pressure: $P_{cap} = P_{gas} - P_{liq}$

Relative Permeability

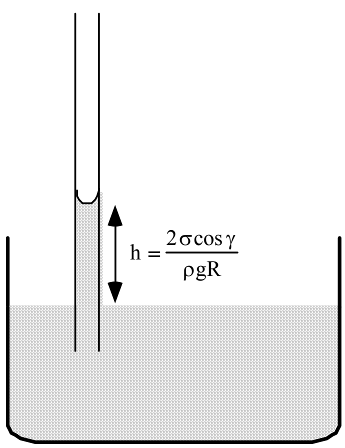


Relative Permeability

(log scale)



Capillary Pressure



$$P_{cap} = \rho g h = \frac{2\sigma\cos\gamma}{R}$$

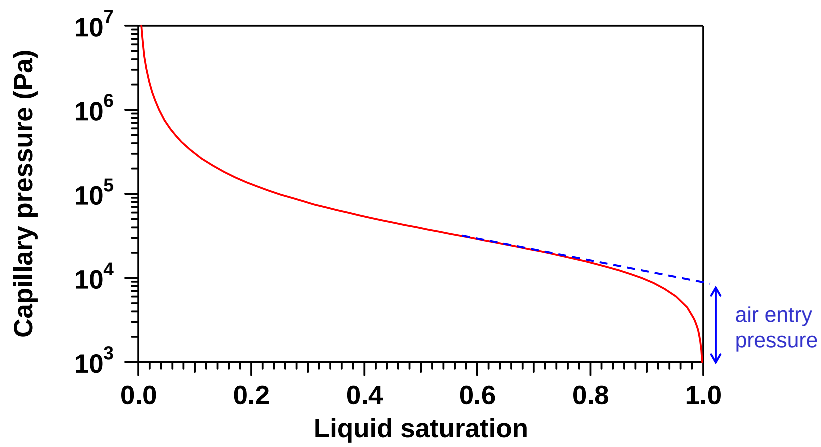
water

$\sigma(T = 20\ ^\circ C) \approx 0.073$ N/m; $\cos\gamma \approx 1$

for $R = 1\ \mu m = 10^{-6}$ m have
$P_{cap} \approx 1.46 \times 10^{5}$ Pa = 1.46 bar

$\sigma(T = 250\ ^\circ C) \approx 0.026$ N/m

Capillary Pressure in Porous Media



Mass Transport

- fluid mixtures: solutes, non-condensible gases (water, NaCl, CO_2, other solutes and NCGs)
- advective mass flux in two-phase system

$$\mathbf{F}^{\kappa} = X_g^{\kappa}\mathbf{F}_g + X_l^{\kappa}\mathbf{F}_l$$

- diffusion

$$\mathbf{f}_{\beta}^{\kappa} = -\phi\,\tau_0\,\tau_{\beta}\,\rho_{\beta}\,d_{\beta}^{\kappa}\nabla X_{\beta}^{\kappa}$$

- hydrodynamic dispersion

<u>Mass conservation</u> (mass balance)

change of fluid mass in volume V	=	mass of fluid entering V	-	mass of fluid leaving V

Mass Balance

change in fluid mass in volume V = net fluid inflow across surface of V + net gain of fluid from sinks and sources

$$\frac{d}{dt}\int_V M^\kappa \, dV = \int_\Gamma \mathbf{F}^\kappa \bullet \mathbf{n} \, d\Gamma + \int_V q^\kappa dV$$

M - "accumulation term" **F** - "flow (or flux) term" q - "sink/source term"

Gauss' (divergence) theorem

$$\int_\Gamma \mathbf{F}^\kappa \bullet \mathbf{n} \, d\Gamma = -\int_V \mathrm{div}\mathbf{F}^\kappa \, dV$$

$$\Longrightarrow \int_V \left\{ \frac{\partial}{\partial t} M^\kappa + \mathrm{div}\mathbf{F}^\kappa \right\} dV = 0 \quad \Longrightarrow \frac{\partial}{\partial t} M^\kappa + \mathrm{div}\mathbf{F}^\kappa = 0$$

single-phase, single component

$$\boxed{\frac{\partial}{\partial t} M = -\mathrm{div}\mathbf{F}} \quad M = \phi\rho \quad \mathbf{F} = -k\frac{\rho}{\mu}\nabla P \Longrightarrow \mathrm{div}\mathbf{F} \approx -k\frac{\rho}{\mu}\Delta P$$

$$\frac{\partial}{\partial t}(\phi\rho) = \rho\frac{\partial\phi}{\partial t} + \phi\frac{\partial\rho}{\partial t} = \left[\rho\frac{d\phi}{dP} + \phi\frac{d\rho}{dP}\right]\frac{\partial P}{\partial t}$$

$$= \phi\rho\left[\frac{1}{\phi}\frac{d\phi}{dP} + \frac{1}{\rho}\frac{d\rho}{dP}\right]\frac{\partial P}{\partial t} = \phi\rho\left(c_\phi + c_\rho\right)\frac{\partial P}{\partial t} = \phi\rho c\frac{\partial P}{\partial t}$$

$$\boxed{\frac{\partial P}{\partial t} = \frac{k}{\phi c \mu}\Delta P}$$ diffusion equation with diffusivity $$\boxed{D = \frac{k}{\phi c \mu}}$$

"partial differential equation" (PDE)

single-phase, two component

$$\frac{\partial}{\partial t} M^\kappa = -\mathrm{div}\,\mathbf{F}^\kappa \qquad M^\kappa = \phi\rho X^\kappa \qquad \mathbf{F}^\kappa = -k\frac{\rho}{\mu} X^\kappa \nabla P = \mathbf{u}\rho X^\kappa$$

change notation: $X^\kappa \equiv C$ solute concentration

$$\frac{\partial}{\partial t}(\phi\rho C) \approx \phi\rho\frac{\partial C}{\partial t} \qquad \mathrm{div}\,\mathbf{F}^\kappa = \rho\,\mathbf{u}\bullet\nabla C$$

$$==> \quad \boxed{\frac{\partial C}{\partial t} + \mathbf{v}\bullet\nabla C = 0} \qquad \text{with} \quad \mathbf{v} = \mathbf{u}/\phi$$

Variably Saturated Flow

- water flow in the vadose zone
- consider air a passive bystander at constant pressure
- neglect air dissolution in water, water evaporation into air
- neglect variations in liquid density and viscosity

$$\frac{\partial}{\partial t} M = -\mathrm{div}\,\mathbf{F}$$

mass balance just for water

$$\frac{\partial}{\partial t}\phi S_l \rho_l = \mathrm{div}\left[k\frac{k_{rl}}{\mu_l}\rho_l\nabla(P_l + \rho_l g z)\right]$$

$$\rho_l \frac{\partial}{\partial t}\phi S_l = \rho_l\,\mathrm{div}\left[k\frac{k_{rl}}{\mu_l}\rho_l g\nabla\left(\frac{P_l}{\rho_l g} + z\right)\right]$$

Richards' equation (1931) $\boxed{\frac{\partial}{\partial t}\theta = \mathrm{div}[K\nabla h]}$

$\theta = \phi S_l$ specific volumetric moisture content

$K = k\frac{k_{rl}}{\mu_l}\rho_l g$ hydraulic conductivity

$h = \frac{P_l}{\rho_l g} + z$ hydraulic head

Two Phases, two Components

(Buckley-Leverett Problem)

- consider flow of two immiscible fluids (oil-water)
- assume fluids are incompressible
- neglect capillary pressure effects
- neglect gravity
- specialize to 1-D

basic mass balances

$$\frac{\partial}{\partial t}\phi S_i \rho_i = -\mathrm{div}\mathbf{F}_i = -\frac{\partial F_i}{\partial x}$$

mass fluxes

$$F_i = -k\frac{k_{ri}}{\mu_i}\rho_i\frac{\partial P}{\partial x} = u_i\rho_i$$

$$\frac{\partial}{\partial t}\phi S_i = -\frac{\partial u_i}{\partial x} \qquad \Longrightarrow \qquad \frac{\partial}{\partial t}\phi(S_1+S_2) = 0 = -\frac{\partial(u_1+u_2)}{\partial x}$$

==> total volumetric flux $u = u_1 + u_2$ is constant

$$u_i = \frac{k_{ri}/\mu_i}{k_{r1}/\mu_1 + k_{r2}/\mu_2}u = f_i u \qquad \frac{\partial}{\partial t}S_i = -\frac{u}{\phi}\frac{\partial f_i}{\partial x} = -v\frac{df_i}{dS_i}\frac{\partial S_i}{\partial x}$$

"fractional flow" f_i

Buckley-Leverett Problem (cont'd)

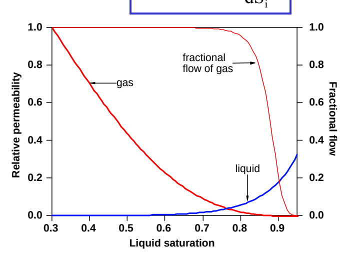
$$dS_l = \frac{\partial S_l}{\partial t}dt + \frac{\partial S_l}{\partial x}dx$$

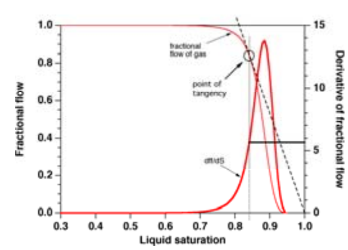
Consider a fixed saturation value; then $dS_l = 0$, and we get:

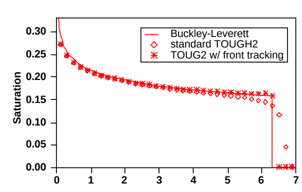
$$\frac{dx}{dt} = -\frac{\partial S_l/\partial t}{\partial S_l/\partial x} = v\frac{df_i}{dS_i}$$

$$\left(\frac{\partial S_i}{\partial t} = -v\frac{df_i}{dS_i}\frac{\partial S_i}{\partial x}\right)$$

$$\Longrightarrow \qquad x = x_0 + v\frac{df_i}{dS_i}t$$







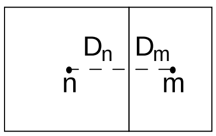
Diffusion

$$\mathbf{f} = -d\nabla C$$
$$\mathbf{f}_\beta^\kappa = -\phi\,\tau_0\,\tau_\beta\,\rho_\beta\,d_\beta^\kappa\nabla X_\beta^\kappa$$

$$\mathbf{f}^\kappa = -\Sigma_l^\kappa\,\nabla X_l^\kappa - \Sigma_g^\kappa\,\nabla X_g^\kappa$$
$$\Sigma_\beta^\kappa = \phi\,\tau_0\,\tau_\beta\,\rho_\beta\,d_\beta^\kappa$$

$$\left(f^\kappa\right)_{nm} = -\left(\Sigma_l^\kappa\right)_{nm}\frac{\left(X_l^\kappa\right)_m - \left(X_l^\kappa\right)_n}{D_{nm}} - \left(\Sigma_g^\kappa\right)_{nm}\frac{\left(X_g^\kappa\right)_m - \left(X_g^\kappa\right)_n}{D_{nm}}$$

Space discretization for single-phase conditions



$$\mathbf{f} = -\Sigma\nabla X$$

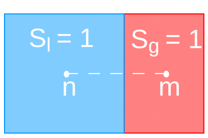
$$f_{nm} = \Sigma_{nm}\frac{X_m - X_n}{D_n + D_m} = \Sigma_n\frac{X_{nm} - X_n}{D_n} = \Sigma_m\frac{X_m - X_{nm}}{D_m}$$

Harmonic weighting

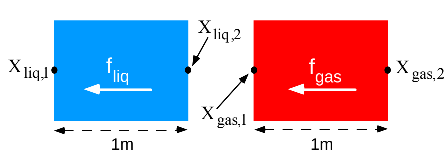
$$\frac{D_n + D_m}{\Sigma_{nm}} = \frac{D_n}{\Sigma_n} + \frac{D_m}{\Sigma_m}$$

Two-Phase System

$$\left(f^\kappa\right)_{nm} = -\left(\Sigma_l^\kappa\right)_{nm}\frac{\left(X_l^\kappa\right)_m - \left(X_l^\kappa\right)_n}{D_{nm}} - \left(\Sigma_g^\kappa\right)_{nm}\frac{\left(X_g^\kappa\right)_m - \left(X_g^\kappa\right)_n}{D_{nm}}$$

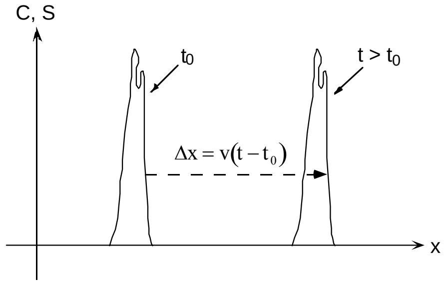


$$\left(\Sigma_g\right)_n = 0; \Rightarrow \left(\Sigma_g\right)_{nm} = 0$$
$$\left(\Sigma_l\right)_m = 0; \Rightarrow \left(\Sigma_l\right)_{nm} = 0$$



$$\left(f^\kappa\right)_{nm} = -\left\{\Sigma_l^\kappa + \Sigma_g^\kappa\frac{\left(X_g^\kappa\right)_m - \left(X_g^\kappa\right)_n}{\left(X_l^\kappa\right)_m - \left(X_l^\kappa\right)_n}\right\}_{nm}\frac{\left(X_l^\kappa\right)_m - \left(X_l^\kappa\right)_n}{D_{nm}}$$

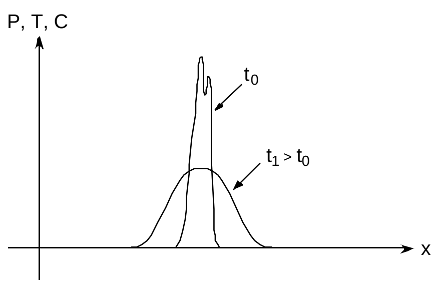
advection



$$\frac{\partial C}{\partial t} + v\frac{\partial C}{\partial x} = 0$$

$$\boxed{C(x,t) = C_0(x - v[t - t_0])}$$

diffusion



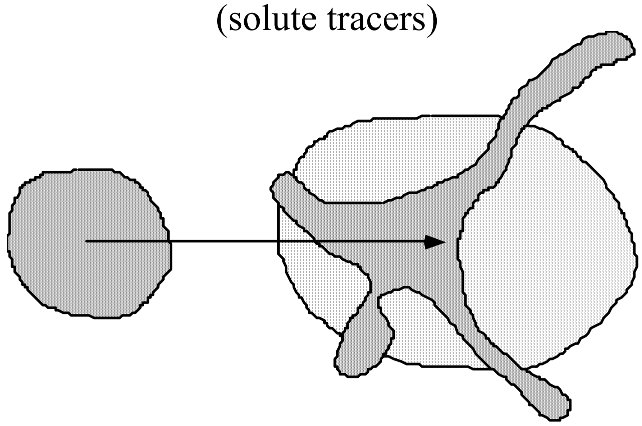
$$\frac{\partial P}{\partial t} - D\frac{\partial^2 P}{\partial x^2} = 0$$

$$\boxed{P(x,t) = \frac{\exp\left(-x^2/4Dt\right)}{\sqrt{t}}}$$

penetration depth $x = 2\sqrt{Dt}$

Hydrodynamic Dispersion

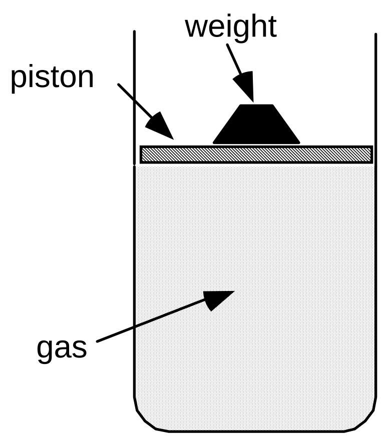
(solute tracers)



diffusive analogue (Scheidegger, 1952; Bear, 1972)

$D \approx \alpha v; \quad x = \sqrt{\alpha v t} = \sqrt{\alpha L}$

Energy Balance



First Law of Thermodynamics

$$\Delta U = G + W$$

work W = force x distance

$$W = -PA\Delta z = -P\Delta V$$

$$\Delta U = G - P\Delta V$$

enthalpy $H = U + PV$ (J)

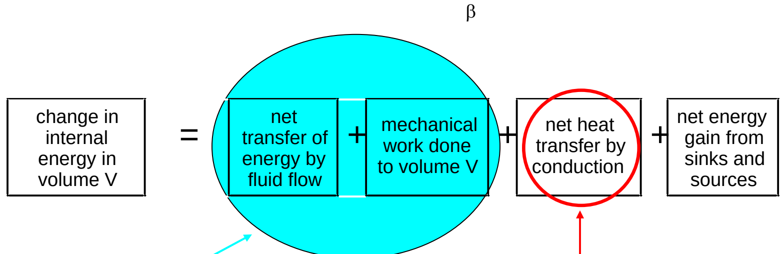
specific enthalpy

$$h = u + Pv = u + \frac{P}{\rho} \quad \text{(J/kg)}$$

Energy Balance

internal energy of rock-fluid mixture

$$M^h = (1-\phi)\rho_R C_R T + \phi \sum_\beta S_\beta \rho_\beta u_\beta$$



$$\mathbf{F}^h = \sum_\beta h_\beta \mathbf{F}_\beta$$

$$G = -K \nabla T$$

(Fourier's Law)

Energy Balance for Isotropic Solid

Accumulation term (heat content, internal energy per unit volume) $M = \rho c T$

Conductive heat flux (Fourier's Law) $\mathbf{G} = -K \nabla T$

Heat balance equation $\frac{d}{dt}\int_V M\,dV = \int_\Gamma \mathbf{G}\bullet\mathbf{n}\,d\Gamma$

$$\int_V \rho c \frac{\partial T}{\partial t} dV = -\int_V \mathrm{div}\mathbf{G}\,dV = \int_V K\Delta T\,dV$$

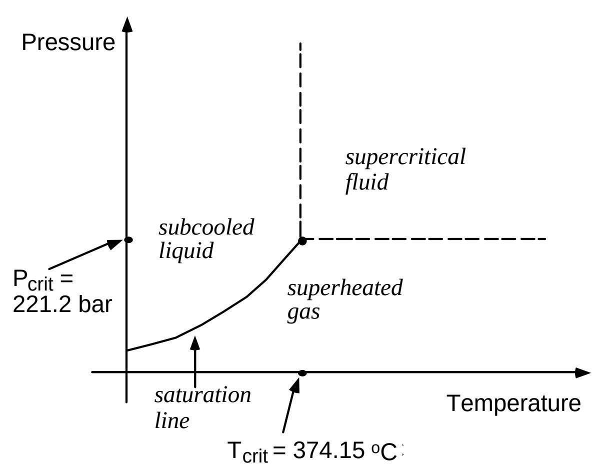
$$===> \int_V \left(\frac{\partial T}{\partial t} - \frac{K}{\rho c}\Delta T\right) dV = 0$$

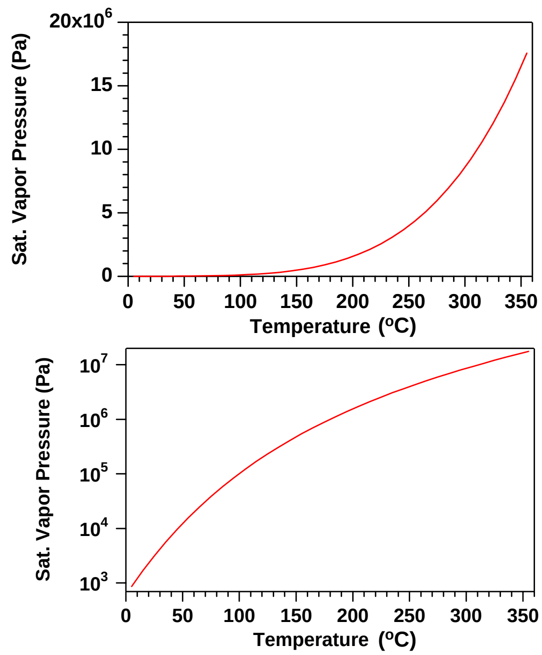
$\frac{K}{\rho c} = D = \text{diffusivity}$

$$===> \frac{\partial T}{\partial t} = \frac{K}{\rho c}\Delta T = \frac{K}{\rho c}\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2}\right)$$

partial differential equation (PDE)

Phase States of Water





Vapor Pressure Lowering (VPL)

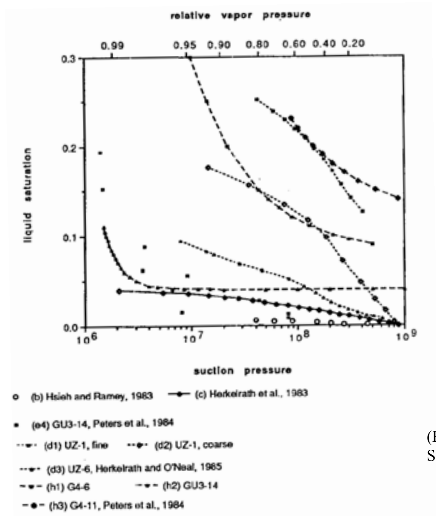
- in porous media, liquid water can be held by capillary force, and by adsorption on hydrophilic mineral surfaces
- the interaction between water and rock alters the physical properties of water
- an important effect is vapor pressure lowering (VPL)

$$P_v(T,S_l) = f_{VPL}(T,S_l) \cdot P_{sat}(T)$$

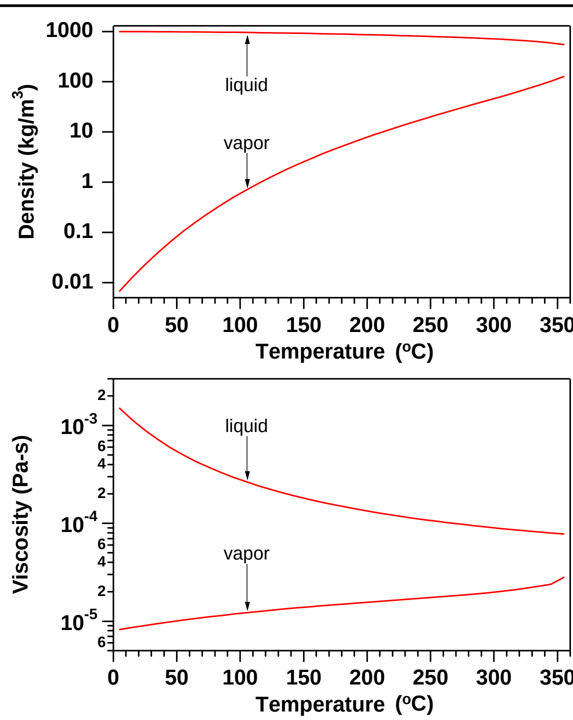
$$f_{VPL} = \exp\left[\frac{M_w\, P_{suc}(S_l)}{\rho_l\, R\,(T+273.15)}\right] \qquad \text{“Kelvin’s equation”}$$

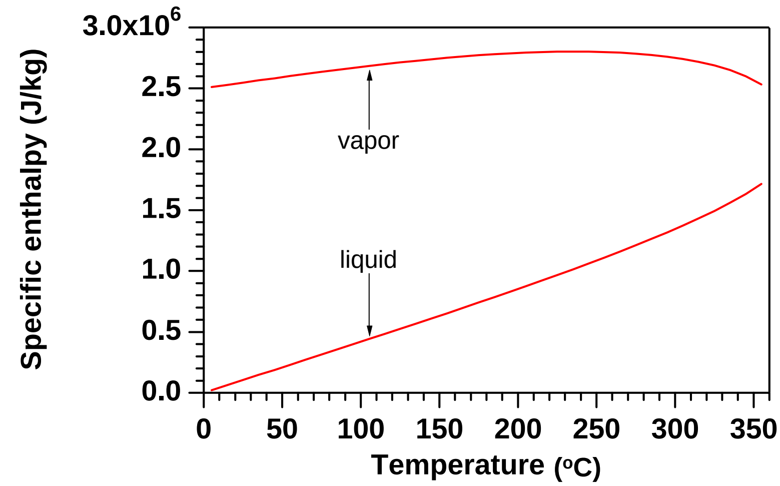
- P_{suc} is suction pressure
- the upshot is that liquid water can be present when $P < P_{sat}$
- important for vapor-dominated reservoirs

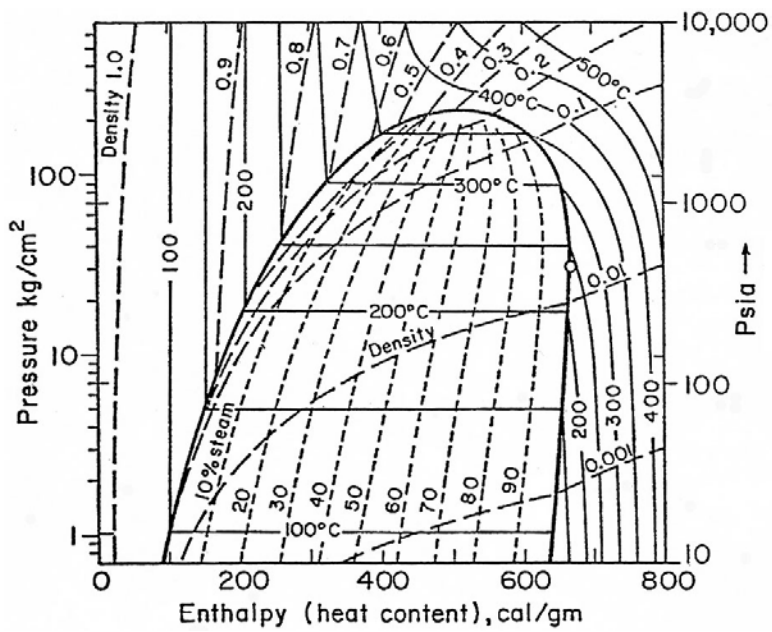
Suction Pressure Characteristics for Different Geologic Media

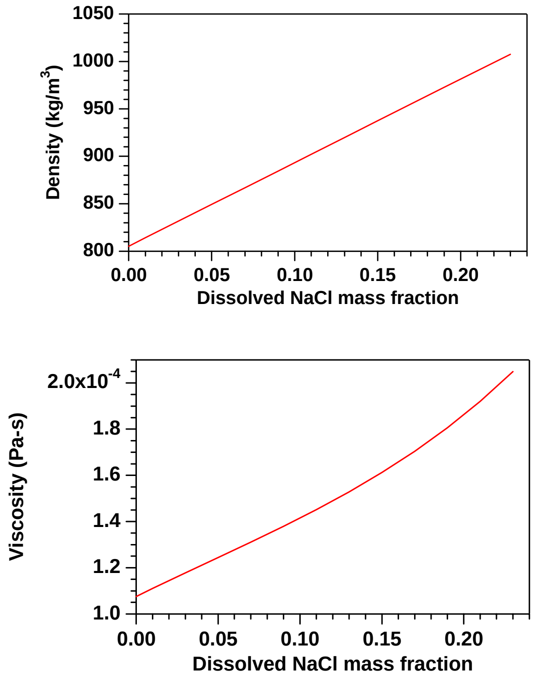


(K. Pruess and M.J. O'Sullivan, Stanford 1992)




3.0x10^6
2.5
2.0
1.5
1.0
0.5
0.0
Specific enthalpy (J/kg)
vapor
liquid
0
50
100
150
200
250
300
350
Temperature (°C)


Density 1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
500°C
400°C
300°C
200°C
100°C
Density
10% steam
20
30
40
50
60
70
80
90
0.01
0.001
100
200
300
400
10,000
1000
100
10
Psia
Pressure kg/cm²
0
200
400
600
800
Enthalpy (heat content), cal/gm



Salinity Effects

(T, P) = (250 ˚C, 100 bar)

Gases

Ideal gas law $PV = nRT$

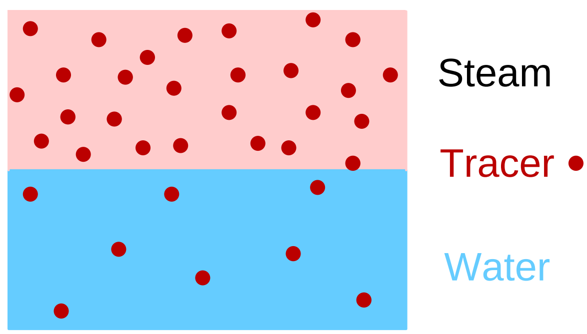
Real gas law $PV = ZnRT$

Z = "real gas compressibility factor"

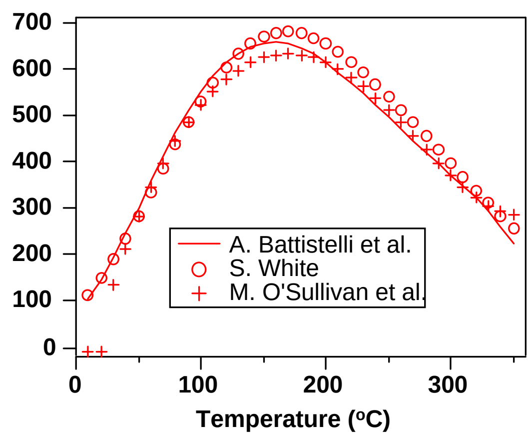
Compressibility $c_T = -\frac{1}{V}\frac{\Delta V}{\Delta P} = \frac{1}{P}$

Phase Partitioning

Henry's Law $P_{NCG} = K_h \, x_{aq}^{NCG}$

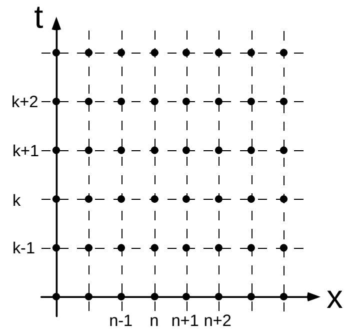


Henry's coefficient for dissolution of CO_2 in water



Towards Numerical Solution of Mass and Energy Balances
(space and time discretization)

- For a flow system of interest, we want to know P(x, t), C(x, t), S(x, t), T(x, t).
- Mass and energy balance equations can be solved in "closed form" only for very simple conditions.
- In general, will need to resort to numerical approaches that approximate the true solutions.
- Key to numerical solution approaches is discretizing the continuous space and time variables.
- Discretization inevitably introduces inaccuracies.



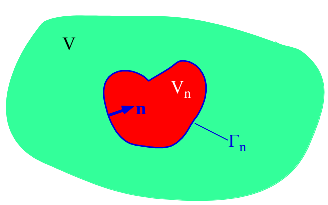
"finite differences" (FD)

$$\frac{\partial f}{\partial t} \longrightarrow \frac{\Delta f}{\Delta t} = \frac{f(x,t^{k+1}) - f(x,t^k)}{t^{k+1} - t^k}$$

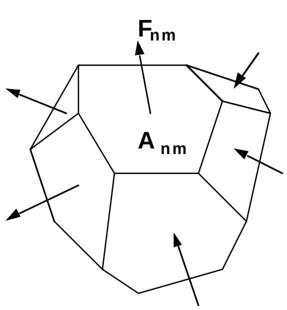
$$\frac{\partial f}{\partial x} \longrightarrow \frac{\Delta f}{\Delta x} = \frac{f(x_{n+1},t) - f(x_n,t)}{x_{n+1} - x_n}$$

Integral Finite Differences (IFD):

subdomain V_n, closed surface Γ_n, surface segments A_{nm}



$$\int_{V_n} M \, dV = V_n M_n$$

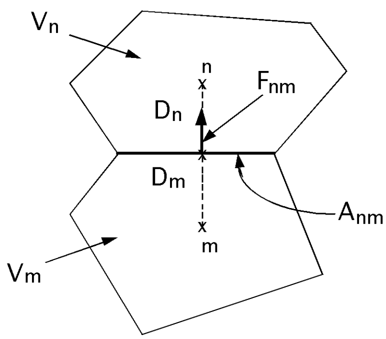


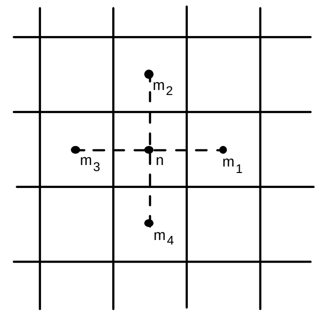
$$\int_{\Gamma_n} \mathbf{F} \bullet \mathbf{n} \, d\Gamma = \sum_m A_{nm} F_{nm}$$

$$\frac{dM_n^\kappa}{dt} = \frac{1}{V_n} \sum_m A_{nm} F_{nm}^\kappa + q_n^\kappa$$

Discretized Flow Term

$$F_{nm} = k_{nm}\left[\frac{\rho}{\mu}\right]_{nm}\left[\frac{P_m - P_n}{D_{nm}} + \rho_{nm}\, g_{nm}\right]$$





$$\frac{d M_n^{\kappa}}{d t} = \frac{1}{V_n}\sum_m A_{nm}\, F_{nm}^{\kappa} + q_n^{\kappa}$$

Time Discretization

$$\frac{dM_n^{\kappa}}{dt} = \frac{1}{V_n}\sum_m A_{nm}\, F_{nm}^{\kappa} + q_n^{\kappa}$$

$$\frac{M_n^{\kappa,k+1} - M_n^{\kappa,k}}{t^{k+1} - t^{k}} = \frac{1}{V_n}\sum_m A_{nm}\, F_{nm}^{\kappa,k+\theta} + q_n^{\kappa,k+\theta}$$

"fully implicit"

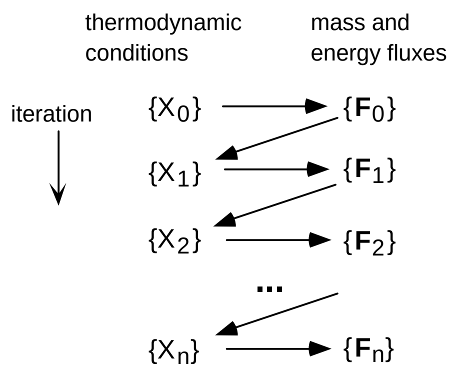
$$R_n^{\kappa,k+1} = M_n^{\kappa,k+1} - M_n^{\kappa,k} - \frac{\Delta t}{V_n}\left\{\sum_m A_{nm}\, F_{nm}^{\kappa,k+1} + V_n\, q_n^{\kappa,k+1}\right\} = 0$$

$$R_n^{\kappa,k+1}\left(x_{i,p+1}\right) = R_n^{\kappa,k+1}\left(x_{i,p}\right) + \sum_i \left.\frac{\partial R_n^{\kappa,k+1}}{\partial x_i}\right|_p \left(x_{i,p+1} - x_{i,p}\right) + \ldots = 0$$

$$-\sum_i \left.\frac{\partial R_n^{\kappa,k+1}}{\partial x_i}\right|_p \left(x_{i,p+1} - x_{i,p}\right) = R_n^{\kappa,k+1}\left(x_{i,p}\right)$$

(Newton's method)

Iterative Procedure for a Time Step



Approach to Reservoir Simulation

- identify and understand the basic physical and chemical processes operating in a reservoir
- develop mathematical expressions for describing these processes (mass and energy balance equations)
- discretize continuous space variables (volume and areal averaging; approximate thermodynamic equilibrium locally)
- discretize time (time steps Δt)
- set up iteration for resulting non-linear algebraic equations
- perform linear equation solution at each iteration step
- “outer iteration”: march in time; “inner (Newtonian) iteration”: solve non-linear equations

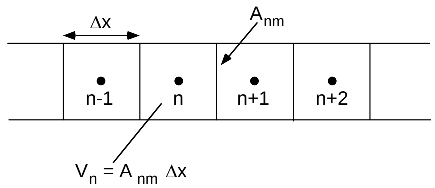
Data Needs

- hydrogeologic parameters of the formations (such as absolute and relative permeability, porosity, capillary pressure, etc.), including their spatial variation
- fluid properties (such as density, viscosity, enthalpy, vapor pressure, etc.), and their dependence on the thermodynamic conditions
- initial conditions throughout the system, and conditions at the outer boundary of the system for all times
- nature, location, and rates of sinks and sources
- discretized description of reservoir geometry (grid, mesh)
- simulation parameters (choice of approximations, time stepping controls, iteration and convergence parameters, linear equation solvers, output controls)

Words to the Wise

- When running simulations for field problems, where site-specific features should be modeled, much of the work ends up dealing with geometry (gridding).
- Large grids make simulations run more slowly, generate larger data files, and make it harder to understand what is going on.
- Start with a simple, coarse grid, and “debug” the problem.
  - facilitates data preparation
  - runs more easily and faster
  - smaller input and output files
  - makes it easier to understand what's happening
  - facilitates checking and debugging
- Can put most other problem features in place.
- After model is running satisfactorily, proceed to desired gridding and grid resolution.
- Check on grid sensitivity.

Heat Conduction in 1-D



$$\frac{d}{dt}\int_{V_n} M\,dV = \int_{\Gamma_n} \mathbf{G}\bullet\mathbf{n}\,d\Gamma \quad ===> \quad V_n \frac{d}{dt} M_n = \sum_m A_{nm} G_{nm}$$

$$G_{nm} \approx K\frac{T_m - T_n}{\Delta x} \qquad \frac{A_{nm}}{V_n} = \frac{1}{\Delta x} \qquad \frac{dM_n}{dt} \approx \rho c\frac{T_n^{k+1} - T_n^k}{\Delta t}$$

$$\frac{T_n^{k+1} - T_n^k}{\Delta t} = \frac{K}{\rho c}\frac{1}{\Delta x}\left(\frac{T_{n+1}^{k+1} - T_n^{k+1}}{\Delta x} + \frac{T_{n-1}^{k+1} - T_n^{k+1}}{\Delta x}\right) = \frac{K}{\rho c}\frac{1}{\Delta x^2}\left(T_{n+1}^{k+1} - 2T_n^{k+1} + T_{n-1}^{k+1}\right)$$

Compare PDE: $\frac{\partial T}{\partial t} = \frac{K}{\rho c}\frac{\partial^2 T}{\partial x^2}$

Space and Time Truncation Errors

Taylor series

$$T(x+h) = T(x) + h\frac{\partial T}{\partial x} + \frac{h^2}{2!}\frac{\partial^2 T}{\partial x^2} + \frac{h^3}{3!}\frac{\partial^3 T}{\partial x^3} + \ldots$$

$$==> \quad \frac{T(x+h) - T(x)}{h} = \frac{\partial T}{\partial x} + \frac{1}{h}\left\{\frac{h^2}{2!}\frac{\partial^2 T}{\partial x^2} + \frac{h^3}{3!}\frac{\partial^3 T}{\partial x^3} + \ldots\right\}$$

error terms

Discretization error for 1-D diffusion equation (Peaceman, 1977)

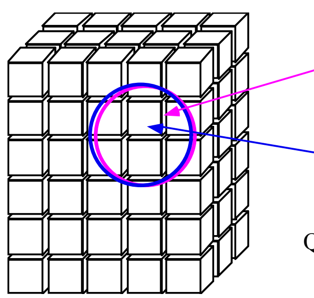
$$\varepsilon = \frac{\Delta x^2}{12}\frac{\partial^4 T}{\partial x^4} - \frac{\Delta t}{2}\frac{\rho c}{K}\frac{\partial^2 T}{\partial t^2}$$

- Due to the mathematical equivalence between FD and IFD methods, error estimates for FD are applicable to regular grid systems for IFD.
- For irregular grids, we are walking on less firm ground.

Flow in Fractured Media

- global flow vs. "interporosity" flow
- different approaches
  - explicit modeling of fractures
  - effective continuum model (ECM)
  - double porosity model (DPM)
  - dual permeability
  - multiple porosity, multiple interacting continua (MINC)

double porosity

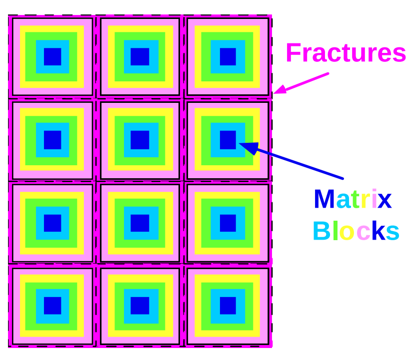


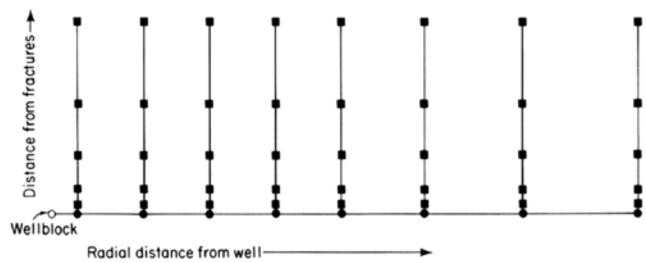
$$\hat{P}_f = \frac{1}{V_f} \int_{V_f} P\,dV$$

$$\hat{P}_m = \frac{1}{V_m} \int_{V_m} P\,dV$$

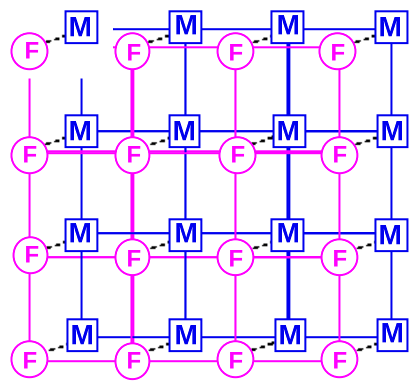
$$Q_{f \leftrightarrow m} \propto A_{fm} (\hat{P}_f - \hat{P}_m)$$

MINC





dual
permeability



Space Discretization by IFD

- In the Integral Finite Difference (IFD) method, space discretization is made directly from the integrals.
- The IFD does not make reference to a global coordinate system; the system geometry is described in terms of grid block (element) volumes, interface areas between grid blocks, nodal distances, and orientation of the nodal line with respect to the vertical.
- The IFD does not distinguish between 1-D, 2-D or 3-D systems, and allows great flexibility in dealing with irregular geometries.
- Even heterogeneous systems described by multiple overlapping continua can be treated without any coding changes in the simulator, simply by preprocessing of geometric data.
- This flexibility *does not come at a price* - for regular grids referred to global coordinates, IFD is equivalent to conventional finite differences.
- The geometric flexibility of the IFD must be used with caution, however, to avoid inaccurate results.

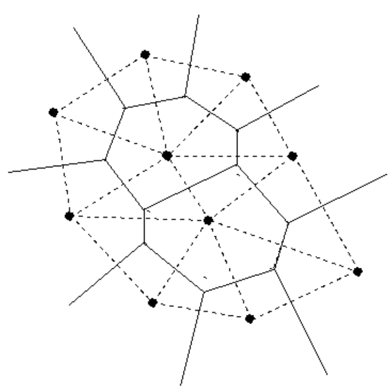
More on Space Discretization

- The basic space-discretized equations are valid regardless of how the discretization is made (including arbitrary irregular gridding).

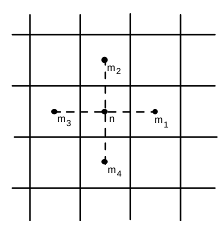
$$\frac{d}{dt}\int_{V_n} M\,dV = \int_{\Gamma_n} \mathbf{F} \bullet \mathbf{n}\, d\Gamma \quad ===> \quad V_n \frac{d}{dt} M_n = \sum_m A_{nm} F_{nm}$$

- Practical limitations for how discretization is made arise from two sources:
  - ➢We need to be able to obtain fluxes between grid blocks from averages of intensive quantities (pressure, temperature, etc.) within grid blocks: $F_{nm} \propto \left([M_m - M_n]/D_{nm}\right)$
  - ➢We need to be able to keep track of where the grid blocks are, so we can understand what is happening in the simulation, and can plot results.

More on Space Discretization (cont'd)



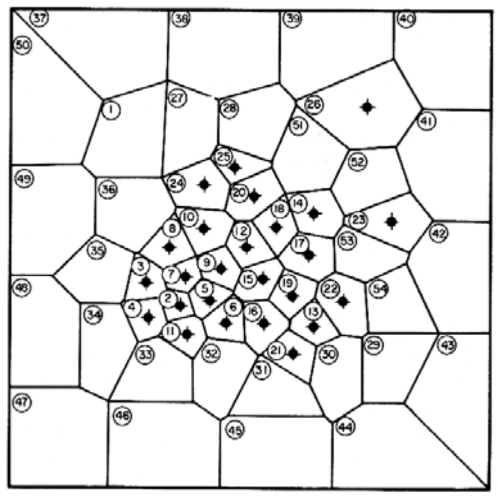
(J. Krämer, 1995)



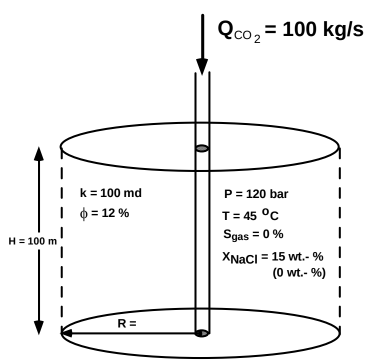
- ➢ start with arbitrary nodal points
- ➢ draw nodal lines (dashed)
- ➢ draw perpendicular bisectors
- ➢ partition plane into polygons (Voronoi tesselation)

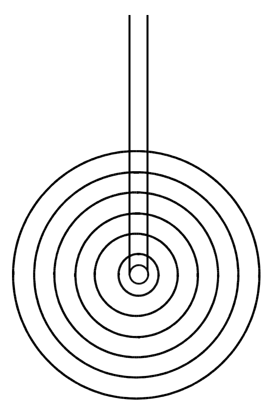
Areal View of Grid for Olkaria/Kenya

(from Bodvarsson et al., 1985)

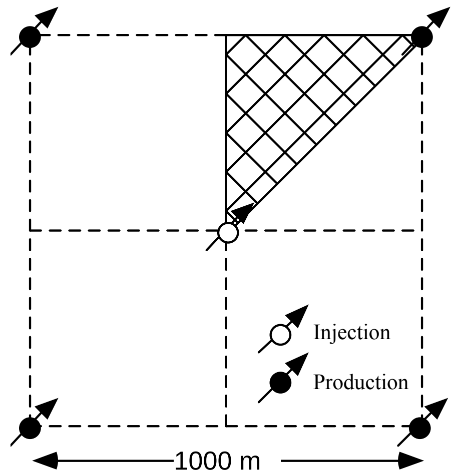


Radial Flow

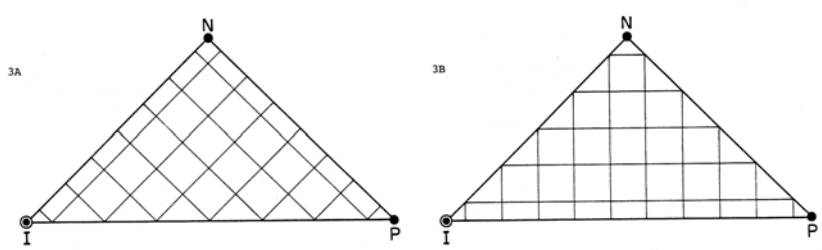




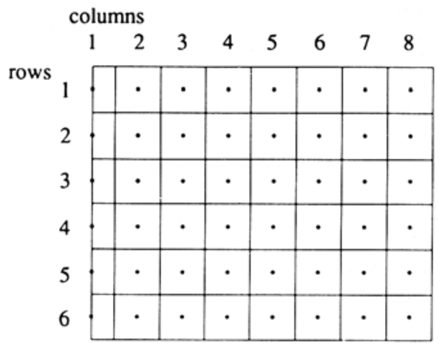
Five-Spot Production-Injection System



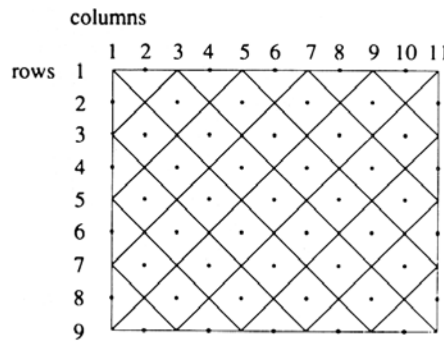
Diagonal and Parallel Grids



“Grid Orientation Effects”

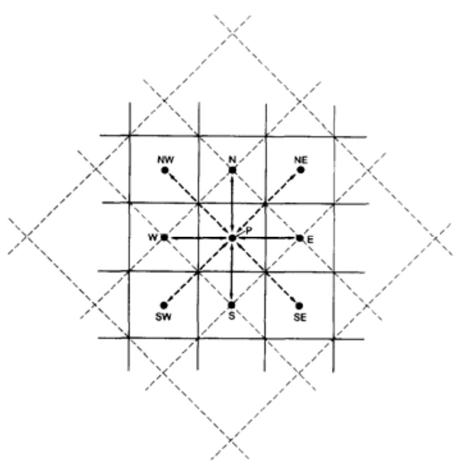


parallel grid

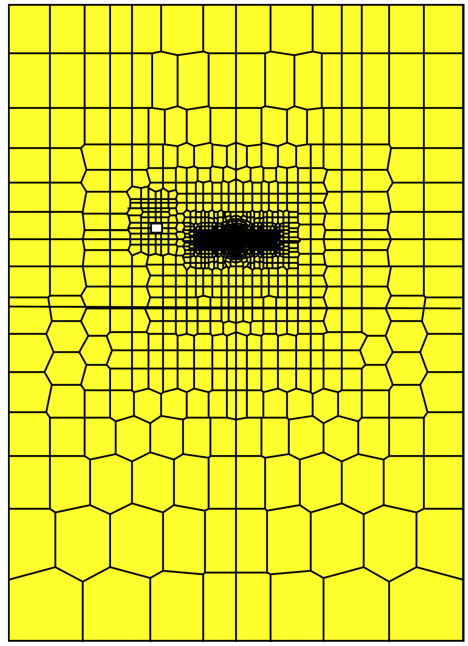


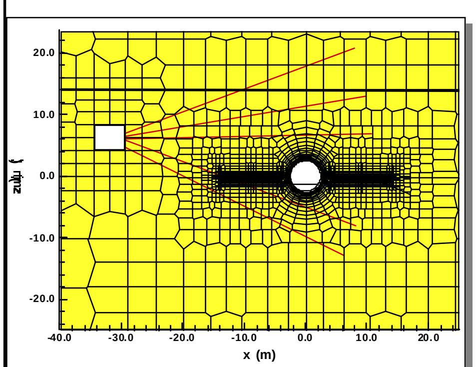
diagonal grid

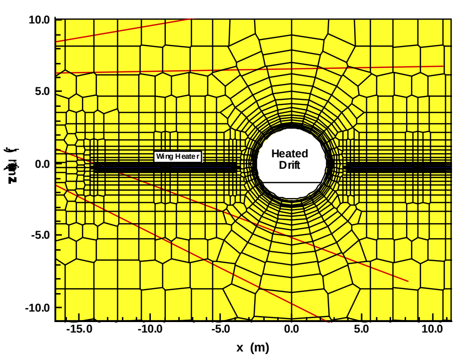
Five- and Nine-Point Finite Difference Approximations



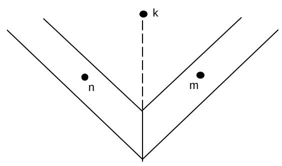
Heater Test at Yucca Mountain

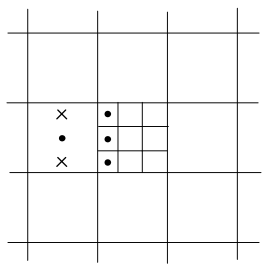


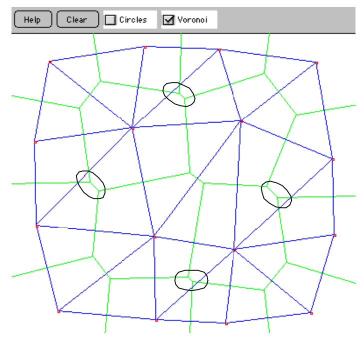




Problematic Gridding







http://cage.rug.ac.be/~dc/alhtml/Delaunay.html

Interface Weighting

- Space-discretized expressions for fluxes (advection, diffusion, heat conduction) generally involve the product of a driving force (gradient of pressure, species concentrations, temperature) with a conductance-type “strength parameter” (permeability, diffusivity, thermal conductivity, etc.).

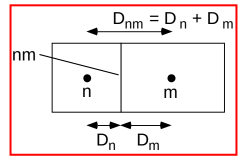
  Example: single-phase flow without gravity.

$$F_{nm} = k_{nm} \left[\frac{\rho}{\mu}\right]_{nm} \left[\frac{P_m - P_n}{D_{nm}}\right]$$

- The rock and fluid parameters in the conductance term (k, ρ, μ) will in general be different for the two grid blocks. This raises the question, how to obtain the appropriate strength parameter at the interface in terms of those of the two grid blocks?

Interface Weighting (cont'd)

Simplify notation by abbreviating $K_{nm} = k_{nm}\left[\frac{\rho}{\mu}\right]_{nm}$



Then have $F_{nm} = K_{nm}\left[\frac{P_m - P_n}{D_{nm}}\right]$

Introduce the (unknown) fluid pressure P_{nm} at the interface and write

$$F_{nm} = K_m\left[\frac{P_m - P_{nm}}{D_m}\right] = K_n\left[\frac{P_{nm} - P_n}{D_n}\right]$$

Setting this equal to the above flux expression gives two equations for the two unknowns P_{nm} and K_{nm}.

$$\boxed{\frac{D_m}{K_m(P_m - P_{nm})} = \frac{D_{nm}}{K_{nm}(P_m - P_n)}} \qquad \boxed{\frac{D_n}{K_n(P_{nm} - P_n)} = \frac{D_{nm}}{K_{nm}(P_m - P_n)}}$$

Multiply the first equation with $(P_m - P_{nm})$, the second with $(P_{nm} - P_n)$ and add:

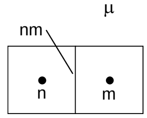
$$\frac{D_m}{K_m} + \frac{D_n}{K_n} = \frac{D_{nm}(P_m - P_{nm} + P_{nm} - P_n)}{K_{nm}(P_m - P_n)} = \frac{D_{nm}}{K_{nm}}$$

"harmonic weighting"

Interface Weighting (cont'd)

How do we proceed in more complicated circumstances? For example, consider solute transport (C = concentration).

$$\mathbf{F}^\kappa = -k\frac{\rho}{\mu}C\nabla P \qquad F^\kappa_{nm} = k_{nm}\left[\frac{\rho}{\mu}\right]_{nm} C_{nm}\left[\frac{P_m - P_n}{D_{nm}}\right]$$



One might think of interpolating, $C_{nm} = \frac{1}{2}(C_n + C_m)$

However...

Let us suppose flow is from m to n, and $C_m < C_n$. Then $C_{mn} > C_m$, and by flowing from m to n we would remove fluid from m that has a higher concentration than is present in m. Concentrations in m could even become negative, for example when $C_m = 0$. Similar considerations apply for heat flow: we could be transferring heat from the colder region to the hotter one, while cooling the colder region, in violation of the Second Law of Thermodynamics.

To avoid this kind of unphysical behavior, employ "total variation diminishing" (TVD) interpolation schemes. The simplest such scheme is "upstream weighting":

$$C_{nm} = \begin{cases} C_m & \text{if flow is from m to n} \\ C_n & \text{if flow is from n to m} \end{cases}$$

Interface Weighting (cont'd)

transient two-phase flow

uniform medium	composite medium
k (constant) **k_r** (upstream)	**k**, **k_r** } upstream

steady two-phase flow

k k_r harmonic

single-phase flow

k harmonic
k_r (none)