# **Geostatistics and Reservoir Simulation**

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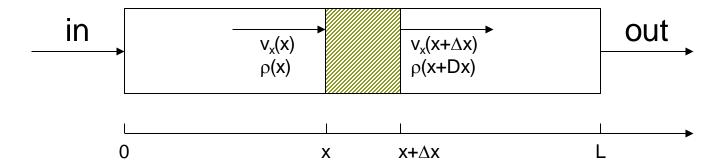


# Reservoir Simulation Equations: Single-phase, compressible flow

#### Mass Conservation

Considering a single phase flow in a numerical cell (Element) in x direction at any time we can write

Mass accumulation = Mass rate in – mass rate out + mass injection rate





$$Av_{x}(x)\rho(x) - Av_{x}(x + \Delta x)\rho(x + \Delta x) + q^{*}\Delta xA = \frac{\partial}{\partial t}(A\Delta x\bar{\varphi}\bar{\rho})$$

$$Av_{x}(x)\rho(x) - Av_{x}(x + \Delta x)\rho(x + \Delta x) + q^{*}\Delta xA = A\Delta x\frac{\partial}{\partial t}(\bar{\varphi}\bar{\rho})$$

q\* is a mass rate of inject. per unit vol. of reservoir

dividing by  $\Delta xA$  and taking the limit  $\Delta x \rightarrow 0$ , we have  $\bar{\rho} \rightarrow \rho$ ;  $\bar{\varphi} \rightarrow \varphi$ 

Continuity equation

$$-\frac{\partial(\rho v_{x})}{\partial x} + q^{*} = \frac{\partial}{\partial t}(\varphi \rho)$$

Similarly for y and z:

$$-\frac{\partial(\rho v_y)}{\partial y} + q^* = \frac{\partial}{\partial t}(\varphi \rho)$$
$$-\frac{\partial(\rho v_z)}{\partial z} + q^* = \frac{\partial}{\partial t}(\varphi \rho)$$



Then for three dimensional flow

$$-\frac{\partial(\rho v_x)}{\partial x} - \frac{\partial(\rho v_y)}{\partial y} - \frac{\partial(\rho v_z)}{\partial z} + q^* = \frac{\partial}{\partial t}(\varphi \rho)$$

In terms of differential operators:

Let  $u_x$ ,  $u_y$  and  $u_z$  be the x, y, and z component of vector  $\vec{u}$ 

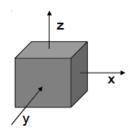
$$\vec{u} = u_x \vec{i} + u_y \vec{j} + u_z \vec{k}$$

 $\vec{l}$ ,  $\vec{j}$ ,  $\vec{k}$  are unit vectors for directions x, y, and z

$$\nabla = \frac{\partial}{\partial x}\vec{i} + \frac{\partial}{\partial y}\vec{j} + \frac{\partial}{\partial z}\vec{k}$$

The divergence of  $\vec{u}$  is

$$\nabla \cdot \vec{u} = \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z}$$





Thus, the continuity equation can be rewritten as

$$-\nabla \cdot (\rho \vec{v}) + q^* = \frac{\partial}{\partial t} (\phi \rho)$$
 General form of Continuity Equation

#### **Darcy equation**

1D representation with a gravity

$$v_{x} = \frac{k}{\mu} \left( \frac{\partial p}{\partial x} - \gamma \frac{\partial D}{\partial x} \right)$$

D is relative depth of an x location

 $\gamma = \rho g$  is specific gravity = density x acceleration due to gravity



Similarly Darcy's law can be written in y and z direction

$$v_y = \frac{k_y}{\mu} \left( \frac{\partial p}{\partial y} - \gamma \frac{\partial D}{\partial y} \right); v_z = \frac{k_z}{\mu} \left( \frac{\partial p}{\partial z} - \gamma \frac{\partial D}{\partial z} \right)$$

In terms of differential operators, we can write:

$$\vec{v} = \frac{\mathbf{k}}{\mu} (\nabla p + \gamma \nabla D);$$

where k is a permeability tensor, defined by nine parameters:

$$\boldsymbol{k} = \begin{bmatrix} k_{xx} & k_{xy} & k_{xz} \\ k_{yx} & k_{yy} & k_{yz} \\ k_{zx} & k_{zy} & k_{zz} \end{bmatrix}$$

If the coordinate system is oriented accordingly with the directions of major and minor permeability values, the permeability tensor can be represented by

$$k_{xx}$$
,  $k_{yy}$ ,  $k_{zz}$ 



Replacing the Darcy's law in the continuity equation we have

$$\nabla \left( \frac{\rho \mathbf{k}}{\mu} (\nabla p - \gamma \nabla D) \right) + q^* = \frac{\partial}{\partial t} (\phi \rho)$$

In the case of isothermal condition we can assume:

$$\rho = \rho(p), \phi = \phi(p), \mu = \mu(p)$$

We can transfer the equation in different coordinates for single well studies in cylindrical coordinate system we have:

$$\frac{1}{r} \frac{\partial}{\partial r} \left[ r \frac{\rho k_h}{\mu} \left( \frac{\partial p}{\partial r} - \gamma \frac{\partial D}{\partial r} \right) \right] + \frac{\partial}{\partial z} \left[ \frac{\rho k_v}{\mu} \left( \frac{\partial p}{\partial z} - \gamma \frac{\partial D}{\partial z} \right) \right] \boldsymbol{k}$$

$$+ \frac{1}{r} \frac{\partial}{\partial \theta} \left[ \frac{\rho k_h}{\mu} \left( \frac{\partial p}{\partial \theta} - \gamma \frac{\partial D}{\partial \theta} \right) \right] = \frac{\partial (\phi \rho)}{\partial t}$$



#### Initial conditions: initial pressure distribution

At time zero without injection we have:

$$\vec{v} = 0 \to \frac{k}{\mu} (\nabla p - \gamma \nabla D) = 0 \to \nabla p - \gamma \nabla D = 0$$

In x and y direction  $\nabla D = 0$ ; in z direction  $\nabla D \neq 0$ , i.e.

$$\vec{v} = 0 \to \frac{k}{\mu} (\nabla p - \gamma \nabla D) = 0 \to \nabla p - \gamma \nabla D = 0$$

$$v_{x} = 0 = \frac{\partial p}{\partial x}$$

$$v_y = 0 = \frac{\partial p}{\partial y}$$

$$v_z = 0 = \frac{\partial p}{\partial z} - \gamma$$

$$v_y = 0 = \frac{\partial p}{\partial v} - p(x, y, z) = f(z); \frac{\partial p}{\partial z} = \gamma \rightarrow \int_{pref}^p \frac{dp'}{\gamma} = \int_{zref}^z dz'$$



#### Initial pressure distribution Cont.

$$\rightarrow$$
 1/  $\gamma$ (p - p<sub>ref</sub>) = z - z<sub>ref</sub>

$$\bar{\gamma} = \gamma(\bar{p}); \bar{p} \approx \frac{p + p_{ref}}{2}$$

$$\rightarrow p(z) = p_{ref} + \dot{\gamma}(z - z_{ref})$$

Observe that  $\gamma$  is a function of p, then the above equation is non-linear and must be solved iteratively.

Also, the following relationship can be used in the above equation:

$$\gamma = \rho(p).g$$



#### **Boundary conditions**

✓ Constant Pressure or (DIRICHLET type boundary condition)

$$p(x, y, z)_{x,y,z \text{ boundary}} = p_{boundary}$$

pressure at any time at the reservoir boundary

✓ Constant rate (NEUMMAN type boundary condition)

Assuming Darcy's law is valid:

$$\boldsymbol{v}_{\text{boundary}} = \frac{\boldsymbol{q}_{\text{boundary}}}{\boldsymbol{A}} = -\frac{\boldsymbol{k}}{\mu} \left( \frac{\partial \boldsymbol{p}}{\partial \boldsymbol{\eta}} - \gamma \frac{\partial \boldsymbol{D}}{\partial \boldsymbol{\eta}} \right)_{\boldsymbol{\eta} \perp \text{boundary}}$$

(η is any point perpendicular to the boundary interface)

$$\left(\frac{\partial \boldsymbol{p}}{\partial \boldsymbol{\eta}} - \gamma \frac{\partial \boldsymbol{D}}{\partial \boldsymbol{\eta}}\right) = -\frac{\mu}{\boldsymbol{k}\boldsymbol{A}} \boldsymbol{q} \bigg|_{\text{boundary}}$$



#### **Special Cases**

**Neglecting Gravitational Effects** 

For this case the flow equation can be simplified as follows:

$$\nabla \left( \frac{\rho \mathbf{k}}{\mu} \nabla \mathbf{p} \right) = \frac{\partial}{\partial \mathbf{t}} (\rho \phi) \tag{1}$$

Right hand side of the equation can be expanded as follows using chain rule:

$$\frac{d(\rho\phi)}{dt} = \rho \frac{d\phi}{dt} + \phi \frac{d\rho}{dt} = \rho \frac{d\phi}{dP} \frac{dP}{dt} + \phi \frac{d\rho}{dP} \frac{dP}{dt}$$

$$= \rho \phi \left[ \left( \frac{1}{\phi} \frac{d\phi}{dP} \right) + \left( \frac{1}{\rho} \frac{d\rho}{dP} \right) \right] \frac{dP}{dt}$$

$$= \rho \phi (c_{\phi} + c_{f}) \frac{dP}{dt},$$
(2)

 $C_f$  is the fluid and  $C_{\phi}$  is the rock compressibility values.  $C_T$  is defined as total compressibility that is  $C_T = C_{\phi} + C_f$ 



#### **Special Cases Cont.**

Now look at the left-hand side of equation 1

$$\nabla \left( \frac{\rho \mathbf{k}}{\mu} \nabla \mathbf{p} \right) = -\frac{d}{dx} \left[ \frac{-\rho k}{\mu} \frac{dP}{dx} \right] = \frac{k}{\mu} \left[ \rho \frac{d^2 P}{dx^2} + \frac{d\rho}{dx} \frac{dP}{dx} \right]$$

$$= \frac{k}{\mu} \left[ \rho \frac{d^2 P}{dx^2} + \frac{d\rho}{dP} \frac{dP}{dx} \frac{dP}{dx} \right]$$

$$= \frac{\rho k}{\mu} \left[ \frac{d^2 P}{dx^2} + \left( \frac{1}{\rho} \frac{d\rho}{dP} \right) \left( \frac{dP}{dx} \right)^2 \right]$$

$$= \frac{\rho k}{\mu} \left| \frac{d^2 P}{dx^2} + c_f \left( \frac{dP}{dx} \right)^2 \right|. \tag{3}$$



# **Special Cases Cont.**

#### Now substituting equations 2 and 3 in 1 we have:

$$\rightarrow \nabla (\nabla \mathbf{p}) + \mathbf{C}_{\mathsf{f}} (\nabla \mathbf{p})^2 = \frac{\phi \mu \mathbf{C}_{\mathsf{T}}}{\mathsf{k}} \frac{\partial \mathbf{p}}{\partial \mathsf{t}}$$

In the case of incompressible and slightly compressible flow fluid C<sub>f</sub>=0 or C is very small therefore:

$$C_f(\nabla p)^2 \cong 0$$

Rock (or Fluid) Type	c (1/Pa)
Clay	10 <sup>-6</sup> - 10 <sup>-8</sup>
Sand	10 <sup>-7</sup> - 10 <sup>-9</sup>
Gravel	10 <sup>-8</sup> - 10 <sup>-10</sup>
Intact rock	10 <sup>-9</sup> - 10 <sup>-11</sup>
Jointed rock	10 <sup>-10</sup> - 10 <sup>-12</sup>
Water	5 x 10 <sup>-10</sup>
Oil	10 <sup>-9</sup>

And simplified diffusivity equation can be obtained as:

$$\nabla(\nabla \mathbf{p}) = \frac{\phi \mu \mathbf{C}_{\mathrm{T}}}{\mathbf{k}} \frac{\partial \mathbf{p}}{\partial \mathbf{t}}$$

Diffusivity Equation



# Compressible flow (Gas Flow diffusivity Equation)

Compressibility Equation of State: pV = ZnRT = Z(m/Mol)RT

Gas density then can be obtained as:  $\rho_g = \frac{m}{V} = \frac{pMol}{ZRT}$ 

Substituting the gas density in diffusivity equation (1) we hav

$$\nabla \left( \frac{\rho_{g}}{\mu} \nabla \mathbf{p} \right) = \frac{1}{k} \frac{\partial}{\partial t} (\rho_{g} \phi)$$

$$\nabla \left(\frac{p}{\mu Z}\right) \frac{\text{Mol}}{\text{RT}} = \frac{1}{k} \frac{\partial}{\partial t} \left(\frac{\phi p}{Z}\right) \frac{\text{Mol}}{\text{RT}}$$

accumulation term



#### **Gas Flow Cont.**

Lets focus on accumulation term:

$$\begin{split} \frac{\partial}{\partial t}(\frac{\phi p}{Z}) &= \phi \frac{\partial}{\partial t} \left(\frac{p}{Z}\right) + \frac{p}{Z} \frac{\partial \phi}{\partial t} = \frac{\phi p}{Z} \left[\frac{Z}{p} \frac{d}{dp} \left(\frac{p}{Z}\right) + \frac{1}{\phi} \frac{d\phi}{dp}\right] \frac{\partial p}{\partial t} \\ \\ \frac{Z}{p} \frac{d}{dp} \left(\frac{p}{Z}\right) &= \frac{1}{p} - \frac{1}{Z} \frac{dZ}{dp} = \frac{1}{\rho_g} \frac{d\rho_g}{dp} = C_g \end{split}$$

Therefore we have:

$$\frac{\partial}{\partial t} \left( \frac{\phi p}{Z} \right) = \frac{\phi p}{Z} (C_g + C_r) \frac{\partial p}{\partial t} = \frac{\phi p}{Z} C_T \frac{\partial p}{\partial t}$$

The continuity equation then can be written as:

$$\nabla \left( \frac{p}{\mu_g \mathbf{Z}} \nabla p \right) = \frac{\phi \mathbf{C}_T \mu_g}{k} \frac{1}{\mu_g} \frac{p}{\mathbf{Z}} \frac{\partial p}{\partial t}$$



### Non-Darcy flow (High velocity flow)

At very high or very low velocities the relationship between velocity and pressure gradient is not linear anymore( Darcy's Law is not valid).

At very low velocities pre-Darcy flow exist that shows deviation from Darcy equation. At high velocities deviations from Darcy's law is determined by Forcheimmer (1901) for one-dimensional steady state flow without gravitational effects as follows:

$$-\frac{d\mathbf{p}}{d\mathbf{x}} = \frac{\mu}{\mathbf{k}} \mathbf{v}_{\mathbf{x}} + \beta \rho |\mathbf{v}_{\mathbf{x}}| \mathbf{v}_{\mathbf{x}}$$

where  $\beta$  is defined as turbulence factor (katz/1959)

Forcheimmer equation can be rearranged as follows:

$$-\frac{dp}{dx} = \frac{\mu}{k_x} v_x (1 + \beta \rho \frac{k_x}{\mu} | v_x |)$$



# Non-Darcy flow Cont.

Writing the equation for velocity and grouping the corrections to Darcy's law in a parameter called  $\delta$ , we have:

$$\delta = \frac{1}{1 + \beta \rho \frac{\mathbf{k}_{x}}{\mu} |\mathbf{v}_{x}|}$$

$$\rightarrow \mathbf{v}_{x} = -\delta_{x} \frac{\mathbf{k}_{x}}{\mu} \frac{\mathbf{dp}}{\mathbf{dx}}$$

δ is denominated turbulence correction factor



#### Non-Darcy flow Cont.

For numerical simulation purposes we are interested in the relationship between δ and pressure gradient.

Therefore we rearrange the turbulence correction as follows and solve for  $\delta$ 

$$\delta = \frac{1}{1 + \beta \rho \left(\frac{k}{\mu}\right)^2 \left|\frac{dp}{dx}\right| \delta} \qquad \qquad -\beta \rho \left(\frac{k}{\mu}\right)^2 \left|\frac{dp}{dx}\right| \delta^2 - \delta + 1 = 0$$

defining 
$$-\beta \rho \left(\frac{\mathbf{k}}{\mu}\right)^2 \left| \frac{\mathbf{dp}}{\mathbf{dx}} \right| = \mathbf{A}$$
, we have:

$$A\delta^2 - \delta - 1 = 0 \rightarrow \delta = \frac{-1 \pm \sqrt{1 + 4A}}{2A}$$

Since, at the limit  $\delta$  must be equal to 1 (Darcy's flow), we will adopt the following value:

$$\delta = \frac{2}{1 + \sqrt{1 + 4A}}$$

$$\delta = \frac{2}{1 + \sqrt{1 + 4A}} \qquad \text{or} \qquad \delta = \frac{2}{1 + \sqrt{1 + 4\beta \rho \left(\frac{k}{\mu}\right)^2 \left|\frac{dp}{dx}\right|}}$$



#### Non-Darcy flow Cont.

For fluids with constant compressibility and homogeneous and isotropic porous media (without sinks and sources and no gravitational effects), we have:

$$\nabla (\delta \nabla \mathbf{p}) = \frac{\phi \mu \mathbf{C}_{\mathsf{T}}}{\mathbf{k}} \frac{\partial \mathbf{p}}{\partial \mathbf{t}}$$

For flow of real gas we can write the equation as follows:

$$\nabla \left( \frac{\mathbf{p}}{\mu_{g} \mathbf{Z}} \delta \nabla \mathbf{p} \right) = \frac{\partial}{\partial t} \left( \frac{\phi \mathbf{p}}{\mathbf{Z}} \right)$$



#### Multiphase Flow in Porous Media

- → Black Oil Reservoir: the PVT behavior is represented by a simple form through oil formation volume factors and gas-oil solubility relationship.
- → In this case the global hydrocarbon composition inside the reservoir remains constant during the entire reservoir life.
- → General Concepts:
- → Three Phases Oil, Water and Gas
- → Gas -> (free gas, in solution in oil, in solution in water)
- → Oil -> dead oil, insoluble in water
- → Water -> insoluble in oil, ignore any water vapor in gas phase



#### Fluid Properties

→ Assuming isothermal process (Tres = Constant) and thermo dynamical equilibrium between all phases all over the reservoir, the PVT behavior can be described by the following equations

$$B_o(p_o) = \frac{(V_o + V_{gd})_{RES}}{(V_o)_{SUR}}$$
 Oil Formation Volume Factor

$$B_{g}(p_{g}) = \frac{(V_{g})_{RES}}{(V_{g})_{SUR}}$$
 Gas Formation Volume Factor

$$R_s(p_o) = \frac{(V_{gd})_{SUR}}{(V_o)_{SUR}}$$
 Solution Gas Oil Ratio



#### Fluid Properties (Cont.)

Relationship between parameters and density:

$$\rho_o = \frac{1}{B_o} (\rho_o + R_s \rho_g)_{SUR} \qquad \rho_g = \frac{(\rho_g)_{SUR}}{B_g} \qquad \rho_w = \frac{(\rho_w)_{SUR}}{B_w}$$

Value of Bw is practically constant and can be expressed

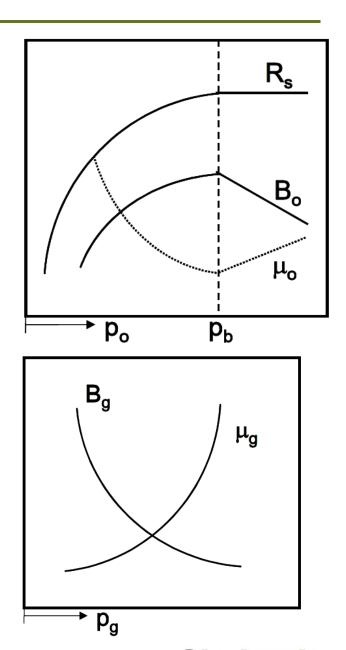
$$B_{w} = \frac{B_{wb}}{1 + C_{w} (p_{w} - p_{wb})}$$

where the subscript b indicates reference conditions.



#### Fluid Properties (Cont.)

- → Rso, Rsw -> gas solubility or solution GOR in oil, water
- → Bo = oil formation volume factor rm3/ m3
- → Bw = water formation volume factor
- → Bg = gas formation volume factor
- $\rightarrow \mu_0$ ,  $\mu_w$ ,  $\mu_g$ = viscosity of oil, aqueous and gas phase, respectively
- → Note: Usually the PVT information is given to the reservoir simulators in a table format. The simulators evaluate the PVT properties by means of linear interpolation.

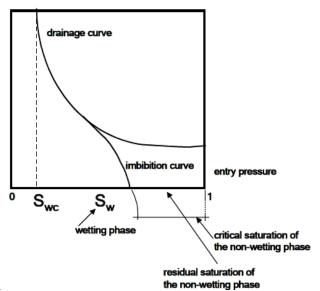




# **Capillary Pressure**

The capillary pressure is a function of:

- → Type of fluids;
- → Rock type;
- → Relative quantity of fluids (saturation);
- → History of the saturation process (drainage or imbibition).



$$P_{Cow}(Sw) = p_o - p_w$$

 $P_{Cog}(Sg) = p_g - p_o$ 

(oil: non wetting; water: wetting)

(gas: non wetting; oil: wetting)



Definition kro ,krw ,krg

$$\mathbf{k_r} = \frac{\mathbf{K_{effective}}}{\mathbf{K_{absolute}}}$$

 $k_f$  = phase f effective permeability = function of  $S_f$ 

Standard procedure is to use relative permeabilities:

$$k_{rf} = k_f / k$$
 and  $0 < k_{rf} < 1$ 

Three-phase Systems:

•water is the wetting phase

•gas is the non wetting phase

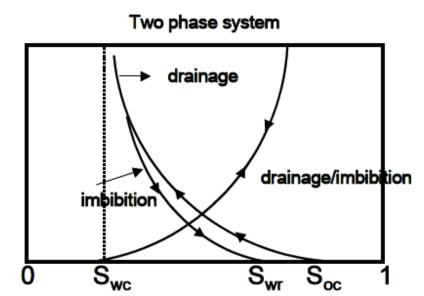
•oil is intermediary

In this respect we have that

$$k_{rw} = f(S_w)$$

$$k_{rg} = f(S_g)$$

$$k_{ro} = f(S_w, S_g)$$

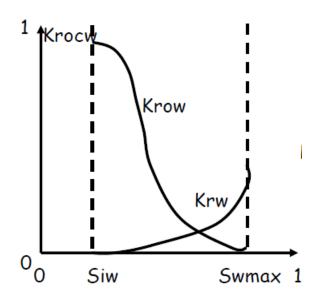




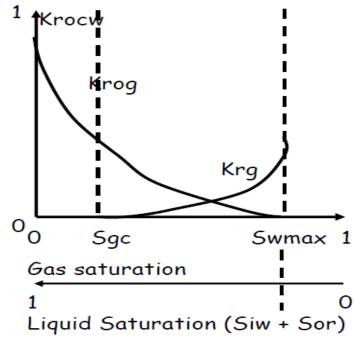
Since the experimental test to measure three-phase relative permeabilities is extremely difficult to execute,

Usually the three-phase relative permeabilities are generated from two phase experiments (oil-water and gas-liquid).

Oil-Water

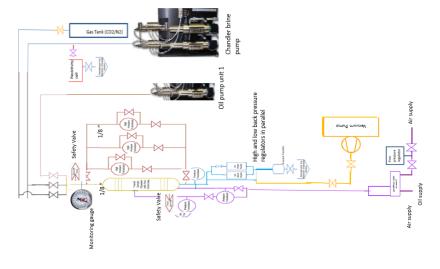


#### Gas-Liquid



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- → Steady State Method: output streams are identical to input. Calculate So, Sw ,Sg by Material Balance
- → Unsteady State Method (using pressure pulse decay)



Naar-Wygal-Henderson Equations:

$$k_{ro} = \frac{S_o^3 (1 - S_g + 2S_w - 3S_{iw})}{(1 - S_{iw})^4}$$

$$\mathbf{k}_{\mathrm{rw}} = \left(\frac{\mathbf{S}_{\mathrm{w}} - \mathbf{S}_{\mathrm{iw}}}{1 - \mathbf{S}_{\mathrm{iw}}}\right)^{4}$$

$$k_{rg} = \frac{S_g^3 (2 - S_g - 2S_{iw})}{(1 - S_{iw})^4}$$

$$k_{\rm ro} = 0 \quad S_{\rm o} \leq S_{\rm or}$$

$$k_{rg} = 0$$
  $S_g \le S_{gc}$ 

Stone's Model - Method I (1970):

Start with two-phase oil-water and oil-gas curves for 3 phases flow

$$k_{ro}(S_w, S_g) = \frac{S_o^* k_{row} k_{rog}}{k_{rocw} (1 - S_w^*) (1 - S_g^*)}$$

where,

$$\mathbf{S}_{o}^{\star} = \frac{\mathbf{S}_{o} - \mathbf{S}_{or}}{1 - \mathbf{S}_{iw} - \mathbf{S}_{or}}$$

$$S_{g}^{*} = \frac{S_{g}}{1 - S_{iw} - S_{or}}$$
 $S_{w}^{*} = \frac{S_{w} - S_{iw}}{1 - S_{iw} - S_{or}}$ 

$$\mathbf{S}_{\mathbf{w}}^{\star} = \frac{\mathbf{S}_{\mathbf{w}} - \mathbf{S}_{\mathbf{iw}}}{1 - \mathbf{S}_{\mathbf{iw}} - \mathbf{S}_{\mathbf{or}}}$$

 $S_{or}$  = oil residual saturation

Stone's Method II (1973): (does not take into account S<sub>or</sub> value)

$$\frac{k_{ro}}{k_{rocw}} = (k_{row} / k_{rocw} + k_{rw})(k_{rog} / k_{rocw} + k_{rg}) - (k_{rw} + k_{rg})$$

#### Multiphase Flow with Mass Transfer between Phases

#### Considerations:

- three phases (oil, gas and water);
- n<sub>c</sub> components;
- each component can be present in each one or all phases.

#### **Definitions:**

a) Mass fraction of component i in gas phase (C<sub>ig</sub>)

$$C_{ig} = \frac{mass \quad of \quad component \quad i}{mass \quad of \quad gas \quad phase}$$

b) Mass fraction of component i in oil phase (C<sub>io</sub>)

$$C_{io} = \frac{mass of component i}{mass of oil phase}$$

c) Mass fraction of component i in water phase (C<sub>iw</sub>)

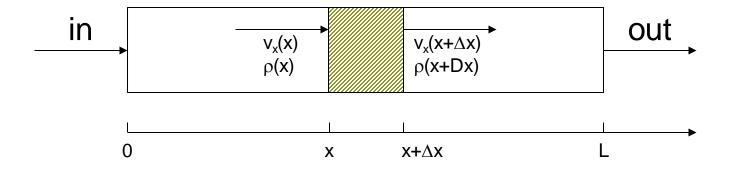
$$C_{iw} = \frac{mass \quad of \quad component \quad i}{mass \quad of \quad water \quad phase}$$

#### Multiphase Flow with Mass Transfer between Phases

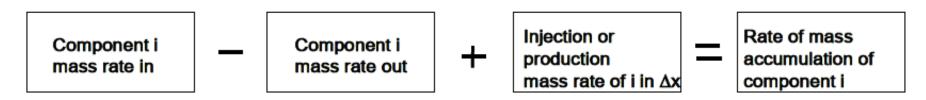
Each component mass much be conserved

Note: lets assume an isothermal process.

Assuming initially one dimensional flow, we have:



Applying mass conservation law to component i:





# Compositional Equations for Numerical Simulation – Flow Term

#### Rate of Mass of Component i IN:

```
In the oil phase = A(C_{io}\rho_o v_o)_x + 
In the gas phase = A(C_{ig}\rho_g v_g)_x + 
In the water phase = A(C_{iw}\rho_w v_w)_x
```

#### Rate of Mass of Component i OUT:

```
In the oil phase = A(C_{io}\rho_o v_o)_{x+\Delta x} + In the gas phase = A(C_{ig}\rho_g v_g)_{x+\Delta x} + In the water phase = A(C_{iw}\rho_w v_w)_{x+\Delta x}
```



# Compositional Equations for Numerical Simulation – Source/Sink Term

If  $q_0^*$  = injection/production rate of oil phase by unit of rock volume and similarly, we have  $q_g^*$  and  $q_w^*$ 

Mass injection/production rate of i in the elementary volume =

$$(C_{io} q_o^* + C_{ig} q_g^* + C_{iw} q_w^*) A x$$

Compositional Equations for Numerical Simulation – Accumulation Term

Rate of mass accumulation of component i in the elementary volume =

$$\mathbf{A} \Delta \mathbf{x} \frac{\partial}{\partial t} [\phi \mathbf{C}_{io} \mathbf{S}_{o} \rho_{o} + \phi \mathbf{C}_{ig} \mathbf{S}_{g} \rho_{g} + \phi \mathbf{C}_{iw} \mathbf{S}_{w} \rho_{w})$$



### **Compositional Equations**

Substituting all terms in the equation of mass conservation, rearranging, and dividing by A  $\Delta x$  and taking the limit when  $\Delta x \rightarrow 0$ 

we have:

$$\begin{split} -\frac{\partial}{\partial x} (\textbf{C}_{io} \rho_o \textbf{v}_{ox} + \textbf{C}_{ig} \rho_g \textbf{v}_{gx} + \textbf{C}_{iw} \rho_w \textbf{v}_{wx}) + \textbf{C}_{io} \textbf{q}_o^* + \textbf{C}_{ig} \textbf{q}_g^* + \textbf{C}_{iw} \textbf{q}_w^* = \\ = \frac{\partial}{\partial t} \Big[ \phi (\textbf{C}_{io} \textbf{S}_o \rho_o + \textbf{C}_{ig} \textbf{S}_g \rho_g + \textbf{C}_{iw} \textbf{S}_w \rho_w) \Big] \end{split}$$



# **Compositional Equations**

#### Considerations:

- -three phases (oil, gas and water);
- -nc components;
- -each component can be present in each one or all phases.

Mass Conservation Law and substituting Darcy's Equation and rewriting the previous equation in terms of differential operators we have:

$$\nabla\!\!\left[\frac{\boldsymbol{C_{io}\rho_{o}kk_{ro}(\!\nabla\boldsymbol{p_{o}}-\boldsymbol{\gamma_{o}}\!\nabla\boldsymbol{D})}{\mu_{o}} + \frac{\boldsymbol{C_{ig}\rho_{g}kk_{rg}(\!\nabla\boldsymbol{p_{g}}-\boldsymbol{\gamma_{g}}\!\nabla\boldsymbol{D})}{\mu_{g}} + \frac{\boldsymbol{C_{iw}\rho_{w}kk_{rw}(\!\nabla\boldsymbol{p_{w}}-\boldsymbol{\gamma_{w}}\!\nabla\boldsymbol{D})}{\mu_{w}}\right] + \frac{\boldsymbol{C_{iw}\rho_{w}kk_{rw}(\!\nabla\boldsymbol{p_{w}}-\boldsymbol{\gamma_{w}}\!\nabla\boldsymbol{D})}{\mu_{w}}$$

$$+ \mathbf{C}_{\mathsf{io}} \mathbf{q}_{\mathsf{o}}^{^{\star}} + \mathbf{C}_{\mathsf{ig}} \mathbf{q}_{\mathsf{g}}^{^{\star}} + \mathbf{C}_{\mathsf{iw}} \mathbf{q}_{\mathsf{w}}^{^{\star}} = \frac{\partial}{\partial t} [\phi (\mathbf{C}_{\mathsf{io}} \mathbf{S}_{\mathsf{o}} \boldsymbol{\rho}_{\mathsf{o}} + \mathbf{C}_{\mathsf{ig}} \mathbf{S}_{\mathsf{g}} \boldsymbol{\rho}_{\mathsf{g}} + \mathbf{C}_{\mathsf{iw}} \mathbf{S}_{\mathsf{w}} \boldsymbol{\rho}_{\mathsf{w}})]$$



#### Isothermal cases

→ for isothermal processes we have:

$$\begin{split} \rho_o &= \rho_o (\textbf{p}_o, \textbf{C}_{1o}, \textbf{C}_{2o}, ..., \textbf{C}_{nco}) & \rho_g &= \rho_g (\textbf{p}_g, \textbf{C}_{1g}, \textbf{C}_{2g}, ..., \textbf{C}_{ncg}) \\ & \rho_w &= \rho_w (\textbf{p}_w, \textbf{C}_{1w}, \textbf{C}_{2w}, ..., \textbf{C}_{ncw}) \\ & \mu_o &= \mu_o (\textbf{p}_o, \textbf{C}_{1o}, \textbf{C}_{2o}, ..., \textbf{C}_{nco}) & \mu_g &= \mu_g (\textbf{p}_g, \textbf{C}_{1g}, \textbf{C}_{2g}, ..., \textbf{C}_{ncg}) \\ & \mu_w &= \mu_w (\textbf{p}_w, \textbf{C}_{1w}, \textbf{C}_{2w}, ..., \textbf{C}_{ncw}) \end{split}$$

$$\mathbf{k}_{ro} = \mathbf{k}_{ro}(\mathbf{S}_{g}, \mathbf{S}_{w}) \qquad \mathbf{k}_{rg} = \mathbf{k}_{rg}(\mathbf{S}_{g}) \qquad \mathbf{k}_{rw} = \mathbf{k}_{rw}(\mathbf{S}_{w})$$



#### **Conclusion:**

Primary variables:

$$\mathsf{p}_{\mathrm{o}},\!\mathsf{p}_{\mathrm{g}},\!\mathsf{p}_{\mathrm{w}},\!\mathsf{S}_{\mathrm{o}},\!\mathsf{S}_{\mathrm{g}},\!\mathsf{S}_{\mathrm{w}}$$

$$\mathbf{C}_{\mathsf{io}}\,,\mathbf{C}_{\mathsf{ig}}\,,\mathbf{C}_{\mathsf{iw}}\,(\mathbf{i}=\mathbf{1,}\mathbf{2,}...,\mathbf{nc})$$

 $S_o + S_g + S_w = 1$ 

 $P_{cgo}(S_g) = p_g - p_o$ 

 $P_{cwo}(S_w) = p_o - p_w$ 

number of unknowns: 3nc + 6

Additional Equations

$$\begin{split} \sum_{i=1}^{nc} C_{io} &= 1, \\ \sum_{i=1}^{nc} C_{ig} &= 1, \\ \sum_{i=1}^{nc} C_{iw} &= 1 \\ f_{ig} &= f_{io} \\ f_{ig} &= f_{iw} \end{split}$$

i=1,2,...,nc (Phase Equilibrium Eq. / f = fugacity in pressure units)

