Computational Methods for Oil Recovery

PASI: Scientific Computing in the Americas

The Challenge of Massive Parallelism

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Table of contents

Table of contents

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  - The processes to be modeled are the motion of one phase or of two phases at most, without mass exchange between the phases.
  - Primary recovery ends when the oil field and the atmosphere reach pressure equilibrium.
  - The total recovery obtained at this stage is usually around 12-15% of the hydrocarbons contained in the reservoir (OIIP: oil initially in place).

Secondary Recovery

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  - The standard computational model to mimic such a system is technically known as the **black-oil** model.
  - Secondary recovery yields an additional 15-20% of the OIIP.
  - After this stage of production, 50% or more of the hydrocarbons often remains in the reservoir.

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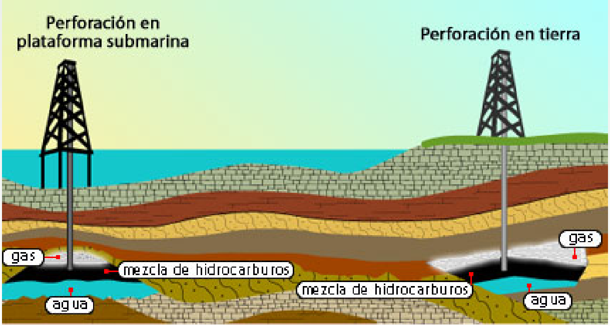
    3. Chemical injection: polymer/surfactant, caustic and micellar/polymer flooding.
    4. Thermal oil recovery: cyclic steam injection, steam-flooding, hot-water drive, in-situ combustion.

Table of contents

Petroleum reservoir

Is a subsurface pool of hydrocarbons contained in porous formations. The naturally occurring hydrocarbons, such as crude oil or natural gas, are trapped by overlying rock formations with lower permeability. It also can contains water, in such a way that in general we have three phases: oleic (o), aqueous (w) and gaseous (g).



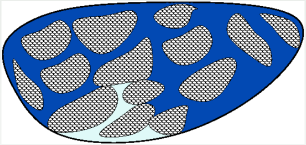
Rock: Pores, Porosity and Permeability (Chen [1]) I

- **Pores**: Pores are the tiny connected passages that exists in a permeable rock ($\approx$ 1–200μm).
- **Porosity**: is the fraction of a rock that is pore space. It measures the capacity of the reservoir to store productible fluids in its pores.

$$\phi = \frac{V_p}{V}$$

$$\phi_e = \frac{V_e}{V}$$

V_p interconnected and isolated pore spaces;
V_e interconnected pore spaces;
V total volume.



Porosity depends on pressure due to rock compressibility: $c_R = \frac{1}{\phi}\frac{d\phi}{dp}$

$$\phi = \phi^0 e^{c_R(p-p^0)} \Longrightarrow \phi = \phi^0 \left\{ 1 + c_R(p-p^0) + \frac{1}{2!}c_R^2(p-p^0) + \dots \right\}$$

Rock: Pores, Porosity and Permeability (Chen [1]) II

- **(Absolute) Permeability** : is the capacity of a rock to conduct fluids through its interconnected pores. In many practical situations, it is possible to assume:

$$\mathbf{k} = \begin{pmatrix} k_{11} & 0 & 0 \\ 0 & k_{22} & 0 \\ 0 & 0 & k_{33} \end{pmatrix}$$

$k_H = k_{11} = k_{22}$ in the horizontal plane;
$k_V = k_{33}$ in the vertical;
$k_H \neq k_V$.

Classification	Permeability range (md)
Poor fair	1 – 15
Moderate	15 – 20
Good	50 – 250
Very good	250 – 1000
Excellent	over 1000

- In many systems there is an approximate correlation between the permeability $\mathbf{k}$ and the porosity ϕ.
- In general, the larger the porosity, the higher the permeability.

Fluid: Phase and component (Chen [1])

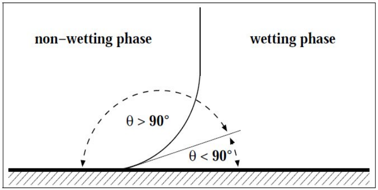
- **Phase** : refers to a chemically homogeneous region of fluid that is separated from another phase by an interface, e.g. oleic (o), aqueous (w), gaseous (g), or solid (rock).
- **Component** : is a single chemical species that may be present in a phase, e.g. oleic contains hundreds of components (C_1, C_2, ...)
- **Compressibility** : of a fluid can be defined in terms of the volume V or density ρ change with pressure:

$$c_f = -\frac{1}{V}\frac{\partial V}{\partial p}\Big|_T = \frac{1}{\rho}\frac{\partial \rho}{\partial p}\Big|_T \quad \text{at a fixed temperature } \; T$$

$$\rho = \rho^0 e^{c_f(p-p^0)} \Longrightarrow \rho = \rho^0 \left\{ 1 + c_f(p-p^0) + \frac{1}{2!}c_f^2(p-p^0) + \dots \right\}$$

Rock/Fluid, (Chen [1]) I

- **Wettability** : measures the preference of the rock surface to be wetted by a particular phase.



- *Water wet* formation is where water is the preferred wetting phase.
- *Oil wet* formation is where oil is the preferred wetting phase.

- **Fluid saturation** : is the fraction of the pore space that a phase occupies. For three-phase flow of oil, water and gas, if the three fluids jointly fill the pore space, then the saturations S_o, S_w and S_g satisfy: $S_o + S_w + S_g = 1$

Rock/Fluid, (Chen [1]) II

- **Residual saturation** : is the amount of a phase (fraction of pore space) that is trapped or irreducible ($S_{r\alpha}, \ \alpha = w, o, g$).
- **Capillary pressure** : In two phase flow, a discontinuity in fluid pressure occurs across an interface between any two immiscible fluids ($w - o$).
  - Suppose oil is the non-wetting phase and water is the wetting phase, then the capillary pressure is : $p_c = p_o - p_w$. In general, $p_c(S_\alpha)$.
  - For a three phase flow, two capillary pressures are needed: $p_{cow} = p_o - p_w$ and $p_{cgo} = p_g - p_o$.
  - A third capillary pressure can be obtained as follows : $p_{cgw} = p_g - p_w = p_{cow} + p_{cgo}$.
  - Usually is assumed that $p_{cow} = p_{cow}(S_w)$ and $p_{cgo} = p_{cgo}(S_g)$.

Rock/Fluid, (Chen [1]) III

- **Relative permeability**: is a quantity (fraction) that describes the amount of impairment to flow of one phase on another. The relative permeabilities to the water, oil, and gas phases are, respectively, denoted by k_{rw}, k_{ro}, and k_{rg}.
- **Mobility** : of a phase is defined as the ratio of the relative permeability and viscosity of that phase.
  - The relative permeabilities to the water, oil and gas phases are denoted $\lambda_w = k_{rw}/\mu_w$, $\lambda_o = k_{ro}/\mu_o$ and $\lambda_g = k_{rg}/\mu_g$ respectively.
  - The total mobility is the sum of all involved mobilities, for example in a three-phase flow: $\lambda = \lambda_w + \lambda_o + \lambda_g$.
- **Fractional flow** : is a quantity (fraction) that determines the fractional volumetric flow rate of a phase under a given pressure gradient in the presence of another phase. Notation for water, oil, and gas is: $f_w = \lambda_w/\lambda$, $f_o = \lambda_o/\lambda$, $f_g = \lambda_g/\lambda$.

Table of contents

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- Fluid motion in a petroleum reservoir is governed by the
  - Balance of mass.
  - Balance of momentum.
  - Balance of energy.
- In the simulation of flow in the reservoir, the momentum equation is given in the form of Darcy's law [2].
  - Derived empirically, this law indicates a linear relationship between the fluid velocity relative to the solid and the pressure head gradient.
  - Its theoretical basis can be revised in, e.g. [3].

- The following assumptions are usually adopted:
  - The porous medium is saturated by the fluid.
  - The mass of the fluid is conserved.
- The model is based on only one extensive property:

$$M(t) \equiv \int_{B(t)} \phi(\vec{x},t)\rho(\vec{x},t)d\vec{x}.$$

- Then, the basic mathematical model for flow of a fluid through a porous media is

$$\frac{\partial(\phi\rho)}{\partial t} + \nabla \cdot \vec{f} = q \quad \text{where} \quad \vec{f} = \phi\rho\vec{v} - \vec{\tau}$$

- The velocity $\vec{v}$ is given by the Darcy's law:

$$\vec{u} = -\frac{1}{\mu}\underline{\underline{k}}(\nabla p - \rho \mathcal{G} \nabla D) \quad \text{where} \quad \vec{u} = \phi \vec{v}$$

- If we suppose no diffusion, i.e. $\vec{\tau} = 0$ then the general equation for single phase flow is:

$$\left(\phi \frac{\partial \rho}{\partial p} + \rho \frac{d\phi}{dp}\right) \frac{\partial p}{\partial t} = \nabla \cdot \left(\frac{\rho}{\mu}\underline{\underline{k}}(\nabla p - \rho \mathcal{G} \nabla D)\right) + q$$

- Equations of state: $c_R = \dfrac{1}{\phi}\dfrac{d\phi}{dp}$ and $c_f = \dfrac{1}{\rho}\dfrac{\partial \rho}{\partial p}\Big|_T$
- For slightly compressible rock we have:

$$\phi \approx \phi^0(1 + c_R(p - p^0)) \implies \frac{d\phi}{dp} = \phi^0 c_R$$

- Finally:

$$\boxed{\phi\rho c_t \frac{\partial p}{\partial t} = \nabla \cdot \left(\frac{\rho}{\mu} \underline{\underline{k}} (\nabla p - \rho \mathcal{G} \nabla D) \right) + q}$$

where $c_t = c_f + \frac{\phi^0}{\phi} c_R$ is the total compressibility.

- This equation is parabolic in p with ρ given by a state equation (e.g. slightly compressible fluid or ideal gas law).
- Boundary conditions:
  - **Dirichlet**: the pressure is specified as a known function of position and time on ∂B the condition is : $p = g_1$ on ∂B.
  - **Neumann**: the total mass flux is known on ∂B, the boundary condition is $\rho\vec{u} \cdot \vec{n} = g_2$ on ∂B. For impervious boundary $g_2 = 0$
  - **Robin**: this is a mixed boundary condition and takes the form: $g_p p + g_u \rho\vec{u} \cdot \vec{n} = g_3$ on ∂B.
- The initial condition can be defined in terms of p: $p(\vec{x}, 0) = p_0(\vec{x}), \quad \vec{x} \in B$.

Simple test

- Consider a horizontal domain of length $L = 100$.
- Assume: $\underline{\underline{k}} = cte$, $\mu = cte$, $c_T = cte$, no gravity and no sources.

$$\frac{\phi \mu c_T}{k} \frac{\partial p}{\partial t} = \frac{\partial^2 p}{\partial x^2}$$

- Boundary conditions: $p = 2$ on the left, and $p = 1$ on the right.
- Initial condition: $p_0 = 1$.
- Input data: $\phi = 0.2; \mu = 1.0; k = 1.0; c_T = 10^{-4}$

Applying TUNA

```
StructuredMesh<Uniform<double, 1> > mesh(length, num_nodes);
ScalarField1D p ( mesh.getExtentVolumes() );

DiagonalMatrix< double, 1> A(num_nodes);
ScalarField1D              b(num_nodes);

ScalarEquation< CDS<double, 1> > single_phase(p, A, b, mesh.getDeltas());
single_phase.setDeltaTime(dt);
single_phase.setGamma(Gamma);
single_phase.setDirichlet(LEFT_WALL);
single_phase.setDirichlet(RIGHT_WALL);

while (t <= Tmax) {
      single_phase.calcCoefficients();
      Solver::TDMA1D(single_phase);
      error = single_phase.calcErrorL1();
      single_phase.update();
      t += dt;
}
```

Result

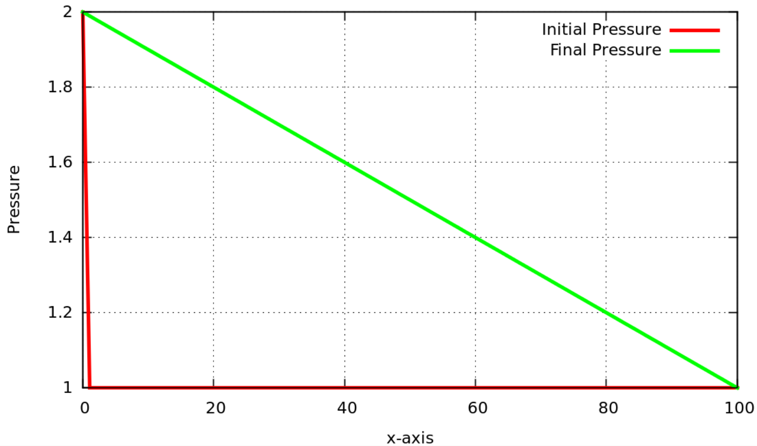

Initial Pressure
Final Pressure
Pressure
x-axis
2
1.8
1.6
1.4
1.2
1
0
20
40
60
80
100

Table of contents

- The following assumptions are usually adopted:
  - We consider two–phase flow where the fluids are immiscible (o, w).
  - There is no mass transfer between the phases.
  - One phase (w) wets porous medium more than the other (o).
  - The two fluids jointly fill the voids: $S_w + S_o = 1$.
  - The pressure in the wetting fluid is less than that in the non-wetting fluid. The pressure difference is given by the capillary pressure: $p_c = p_o - p_w$. And $p_c = p_c(S_w)$.
  - There is no diffusion $\vec{\tau} = 0$.
- Extensive properties: $M_\alpha(t) = \int\limits_{B(t)} \phi \rho_\alpha S_\alpha d\vec{x}$, $\alpha = w, o$.
- Intensive properties: $\psi = \phi \rho_\alpha S_\alpha$, $\alpha = w, o$.

- Balance equations:

$$\frac{\partial(\phi\rho_\alpha S_\alpha)}{\partial t} + \nabla\cdot(\phi\rho_\alpha S_\alpha \vec{v}_\alpha) = q_\alpha \quad \text{for} \quad \alpha = w, o.$$

- Darcy's Law:

$$\vec{u}_\alpha = -\frac{k_{r\alpha}}{\mu_\alpha}\underline{\underline{k}}(\nabla p_\alpha - \rho_\alpha \mathcal{G}\nabla D) \quad \text{where} \quad \vec{u}_\alpha = \phi S_\alpha \vec{v}_\alpha$$

- Recall that:

$$S_w + S_o = 1 \quad \text{and} \quad p_c = p_o - p_w.$$

- We have six equations for six unknowns: $\rho_\alpha, \vec{u}_\alpha$ and S_α, for $\alpha = w, o$.

- Alternative differential equations:
  - **Formulation in phase pressures**

$$\text{Assume:} \quad S_w = p_c^{-1}(p_o - p_w).$$

We use p_w and p_o as the main unknowns:

$$\nabla \cdot \left(\frac{\rho_w}{\mu_w} k_{rw} \underline{\underline{k}} (\nabla p_w - \rho_w \mathcal{G} \nabla D) \right) = \frac{\partial(\phi \rho_w p_c^{-1})}{\partial t} - q_w$$

$$\nabla \cdot \left(\frac{\rho_o}{\mu_o} k_{ro} \underline{\underline{k}} (\nabla p_o - \rho_o \mathcal{G} \nabla D) \right) = \frac{\partial(\phi \rho_o (1 - p_c^{-1}))}{\partial t} - q_o$$

This system is commonly employed in the *simultaneos solution* (SS) scheme.

- **Formulation in phase pressure and saturation**
  We use p_o and S_w as the main variables:

$$\nabla \cdot \left(\frac{\rho_w}{\mu_w} k_{rw} \underline{\underline{k}} \left(\nabla p_o - \frac{dp_c}{dS_w} \nabla S_w - \rho_w \mathcal{G} \nabla D \right) \right) = \frac{\partial (\phi \rho_w S_w)}{\partial t} - q_w$$

$$\frac{1}{\rho_w} \nabla \cdot \left(\frac{\rho_w}{\mu_w} k_{rw} \underline{\underline{k}} \left(\nabla p_o - \frac{dp_c}{dS_w} \nabla S_w - \rho_w \mathcal{G} \nabla D \right) \right) +$$

$$\frac{1}{\rho_o} \nabla \cdot \left(\frac{\rho_o}{\mu_o} k_{ro} \underline{\underline{k}} \left(\nabla p_o - \rho_o \mathcal{G} \nabla D \right) \right) =$$

$$\frac{S_w}{\rho_w} \frac{\partial (\phi \rho_w)}{\partial t} + \frac{1 - S_w}{\rho_o} \frac{\partial (\phi \rho_o)}{\partial t} - \frac{q_w}{\rho_w} - \frac{q_w}{\rho_w}$$

  Saturation S_w is explicitly evaluated using the first equation. The second equation can be solved for p_o implicitly. This is the Implicit Pressure Explicit Saturation (IMPES) scheme.

Example: Pressure-Saturation Formulation I

- Phases: $\alpha =$ water(w) and oil(o).
- Phase mobility functions: $\lambda_\alpha = k_{r\alpha}/\mu_\alpha$
- Total mobility: $\lambda = \sum \lambda_\alpha$
- Fractional flow functions: $f_\alpha = \lambda_\alpha/\lambda$, $\sum f_\alpha = 1$
- Total velocity: $\vec{u} = \sum \vec{u}_\alpha$
- $p_o \equiv p$, $S_w \equiv S$, $p_{cow} \equiv p_c(S)$
- The capillary pressure gradient and permeability are expressed as:

$$\nabla p_c = \frac{dp_c}{dS}\nabla S \qquad \text{and} \qquad \underline{\underline{k}} \equiv \begin{pmatrix} k_{11} & 0 & 0 \\ 0 & k_{22} & 0 \\ 0 & 0 & k_{33} \end{pmatrix} = \begin{pmatrix} k & 0 & 0 \\ 0 & k & 0 \\ 0 & 0 & k \end{pmatrix}$$

- No gravity: $\mathcal{G} = 0$.

Example: Pressure-Saturation Formulation II

- Incompressible rock and fluids: $\rho_\alpha = cte$ and $\phi = cte$.
- Pressure equation (elliptic)

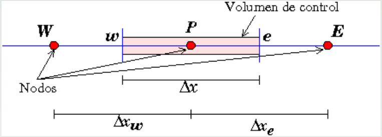
$$\nabla \cdot \underbrace{\left(-\underline{\underline{k}}\lambda \nabla p + \underline{\underline{k}}\lambda_w \frac{dp_c}{dS}\nabla S\right)}_{\text{flux function}} = q_w + q_o$$

- Saturation equation (parabolic, hiperbolic for $p_c = 0$)

$$\phi \frac{\partial S}{\partial t} + \nabla \cdot \underbrace{\left(\underline{\underline{k}}\lambda_w \frac{dp_c}{dS}\nabla S - \underline{\underline{k}}\lambda_w \nabla p\right)}_{\text{flux function}} = q_w$$

FVM: Pressure eq. 1D I

$$\int_{i-\frac{1}{2}}^{i+\frac{1}{2}} \nabla \cdot (-k\lambda \nabla p + kF_w \nabla S)\, dx = 0$$



$$F_w = \lambda_w \frac{dp_c}{dS}$$

$$-\left(\left(k\lambda\frac{dp}{dx}\right)_{i+\frac{1}{2}} - \left(k\lambda\frac{dp}{dx}\right)_{i-\frac{1}{2}}\right) + \left(kF_w\frac{dS}{dx}\right)_{i+\frac{1}{2}} - \left(kF_w\frac{dS}{dx}\right)_{i-\frac{1}{2}} = 0,$$

$$\boldsymbol{a}_i p_i - \boldsymbol{a}_{i+1} p_{i+1} - \boldsymbol{a}_{i-1} p_{i-1} - \boldsymbol{a}^*_i S_i + \boldsymbol{a}^*_{i+1} S_{i+1} + \boldsymbol{a}^*_{i-1} S_{i-1} = 0.$$

FVM: Pressure eq. 1D II

$$\boldsymbol{a}_{i+1} = \frac{k}{\Delta x}(\lambda)_{i+\frac{1}{2}}; \quad \boldsymbol{a}_{i-1} = \frac{k}{\Delta x}(\lambda)_{i-\frac{1}{2}}; \quad \boldsymbol{a}_{i} = \boldsymbol{a}_{i+1} + \boldsymbol{a}_{i-1}.$$

$$\boldsymbol{a}^*_{i+1} = \frac{k}{\Delta x}(F_w)_{i+\frac{1}{2}}; \quad \boldsymbol{a}^*_{i-1} = \frac{k}{\Delta x}(F_w)_{i-\frac{1}{2}}; \quad \boldsymbol{a}^*_{i} = \boldsymbol{a}^*_{i+1} + \boldsymbol{a}^*_{i-1}.$$

$$F_w = \lambda_w \frac{dp_c}{dS}$$

FVM: Saturation eq. 1D I

$$\int_{i-\frac{1}{2}}^{i+\frac{1}{2}} \int_{n}^{n+1} \phi \frac{\partial S}{\partial t} dt dx - \int_{n}^{n+1} \int_{i-\frac{1}{2}}^{i+\frac{1}{2}} \nabla \cdot \left(k\lambda_w \nabla p - k\lambda_w \frac{dp_c}{dS_w} \nabla S_w \right) dx dt = 0,$$

$$\phi \left(S_i^{n+1} - S_i^n \right) \Delta x - \left(\left(k\lambda_w \frac{\partial p}{\partial x} \right)_{i+\frac{1}{2}}^n - \left(k\lambda_w \frac{\partial p}{\partial x} \right)_{i-\frac{1}{2}}^n \right) \Delta t +$$

$$\left(\left(kF_w \frac{\partial S}{\partial x} \right)_{i+\frac{1}{2}}^n - \left(kF_w \frac{\partial S}{\partial x} \right)_{i-\frac{1}{2}}^n \right) \Delta t = 0$$

$$S_i^{n+1} = S_i^n + \boldsymbol{b}_i^* S_i^n - \boldsymbol{b}_{i+1}^* S_{i+1}^n - \boldsymbol{b}_{i-1}^* S_{i-1}^n - \boldsymbol{b}_i p_i^n + \boldsymbol{b}_{i+1} p_{i+1}^n + \boldsymbol{b}_{i-1} p_{i-1}^n.$$

FVM: Saturation eq. 1D II

$$\boldsymbol{b}_{i+1} = \frac{k\Delta t}{\phi \Delta x^2}(\lambda_w)^n_{i+\frac{1}{2}}; \quad \boldsymbol{b}_{i-1} = \frac{k\Delta t}{\phi \Delta x^2}(\lambda_w)^n_{i-\frac{1}{2}}; \quad \boldsymbol{b}_i = \boldsymbol{b}_{i+1} + \boldsymbol{b}_{i-1};.$$

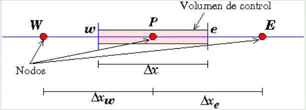
$$\boldsymbol{b}^*_{i+1} = \frac{k\Delta t}{\phi \Delta x^2}(F_w)^n_{i+\frac{1}{2}}; \quad \boldsymbol{b}^*_{i-1} = \frac{k\Delta t}{\phi \Delta x^2}(F_w)^n_{i-\frac{1}{2}}; \quad \boldsymbol{b}^*_i = \boldsymbol{b}^*_{i+1} + \boldsymbol{b}^*_{i-1}.$$

$$F_w = \lambda_w \frac{dp_c}{dS}$$

FVM: IMPES

- The coefficients are not constant and depend on λ, λ_w and F_w:

$$(\lambda)^n_{i\pm\frac{1}{2}}, \quad (\lambda_w)^n_{i\pm\frac{1}{2}}, \quad (F_w)^n_{i\pm\frac{1}{2}}$$



$$F_w = \lambda_w \frac{dp_c}{dS}$$

IMPES Algorithm

1: **while** $(t < T_{max})$ **do**
2: Calc. coeff. of pressure equation.
3: Solve the pressure equation implicitly.
4: Calc. coeff. of saturation equation.
5: Solve the saturation eq. explicitly.
6: $t \leftarrow t + \Delta t$
7: **end while**

```
while (t <= Tmax) {
  pressure.calcCoefficients();
  Solver::TDMA1D(pressure);
  pressure.update();

  saturation.calcCoefficients();
  Solver::solExplicit(saturation);
  saturation.update();

  t += dt;
}
```

Inheritance I

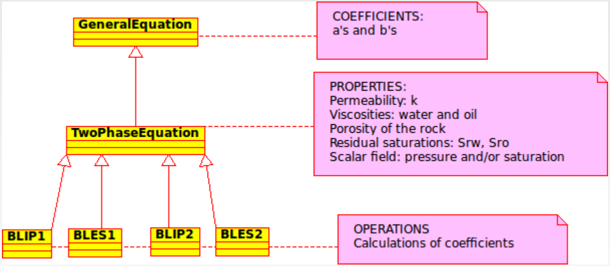
- General Equation:
  - Conservative form: $\frac{\partial}{\partial t}\int_{B(t)} \psi d\vec{x} + \int_{B(t)} \nabla \cdot \vec{f} d\vec{x} = \int_{B(t)} q d\vec{x}$
  - Discrete general equation:
    $\boldsymbol{a}_P^{n+1}\psi_P^{n+1} =$
    $\boldsymbol{a}_e^{n+1}\psi_e^{n+1} + \boldsymbol{a}_w^{n+1}\psi_w^{n+1} + \boldsymbol{a}_n^{n+1}\psi_n^{n+1} + \boldsymbol{a}_s^{n+1}\psi_s^{n+1} + \boldsymbol{a}_f^{n+1}\psi_f^{n+1} + \boldsymbol{a}_b^{n+1}\psi_b^{n+1} + q_P^n$
- Two phase immiscible and incompressible fluids:
  - Pressure and saturation equations are *derived* from general equation:

$$\nabla \cdot \left(-\underline{\underline{k}}\lambda \nabla p + \underline{\underline{k}}\lambda_w \frac{dp_c}{dS} \nabla S \right) = q_w + q_o$$

$$\phi \frac{\partial S}{\partial t} + \nabla \cdot \left(\underline{\underline{k}}\lambda_w \frac{dp_c}{dS} \nabla S - \underline{\underline{k}}\lambda_w \nabla p \right) = q_w$$

Inheritance II

- Inheritance is a way to share and reuse code by defining collections of attributes and behaviors, bundled into classes (*subclasses*), based on previously created classes (*superclasses*).



- Inheritance gives rise to hierarchies: complexity is reduced, but efficiency can be spoiled.

Object declaration

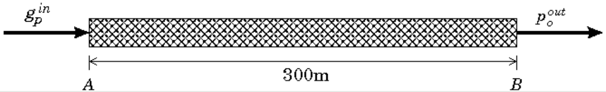
Pressure

```
TwoPhaseEquation< BLIP1<double, 1> > pressure(p, A, b, mesh.getDeltas());
pressure.setDeltaTime(dt);
pressure.setPermeability(permeability);
pressure.setPorosity(porosity);
pressure.setSrw(Srw);
pressure.setSro(Sro);
pressure.setViscosity_w(mu_w);
pressure.setViscosity_o(mu_o);
pressure.setNeumann(LEFT_WALL, injection);
pressure.setDirichlet(RIGHT_WALL);
pressure.setSaturation(Sw);
pressure.print();
```

Saturation

```
TwoPhaseEquation< BLES1<double, 1> > saturation(Sw, A, b, mesh.getDeltas());
saturation.setDeltaTime(dt);
saturation.setPermeability(permeability);
saturation.setPorosity(porosity);
saturation.setSrw(Srw);
saturation.setSro(Sro);
saturation.setViscosity_w(mu_w);
saturation.applyBounds(1, Sw.ubound(firstDim)-1);
saturation.setPressure(p);
saturation.print();
```

Test 1: Buckley–Leverett (in collaboration with M. Diaz [7])



From Diaz *et al.* [7]

Property	Value
Length	300 m
k	1.0E-15 m^2
ϕ	0.2
μ_w	1.0E-03 Pa.s
μ_o	1.0E-03 Pa.s
S_{rw}	0
S_{ro}	0.2
g_p^{in}	3.4722E-07 m.s^{-1}
p^{out}	1E+07 Pa

- Zero capillary pressure
  - Pressure eq.

$$-\nabla \cdot \left(\underline{\underline{k}}\lambda \nabla p\right) = 0$$

  - Saturation eq.

$$\phi \frac{\partial S}{\partial t} - \nabla \cdot \left(\underline{\underline{k}}\lambda_w \nabla p\right) = 0.$$

Test 1: Buckley–Leverett I

- Constitutive Eqs.

$$k_{rw} = S_e^{\omega}; k_{ro} = (1 - S_e)^{\omega}, \quad \omega = 1, 2$$

$$S_e = \frac{S - S_{rw}}{1 - S_{rw} - S_{ro}}$$

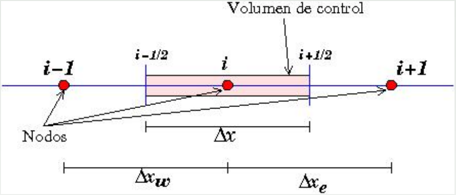
- Coefficients:

$$(\lambda)_{i\pm\frac{1}{2}} = \frac{1}{(1 - S_{rw} - S_{ro})^{\omega}} \left(\frac{(S_{i\pm\frac{1}{2}} - S_{rw})^{\omega}}{\mu_w} + \frac{(1 - S_{ro} - S_{i\pm\frac{1}{2}})^{\omega}}{\mu_o} \right)$$

$$(\lambda_w)^n_{i\pm\frac{1}{2}} = \frac{1}{\mu_w} \left(\frac{S^n_{i\pm\frac{1}{2}} - S_{rw}}{1 - S_{rw} - S_{ro}} \right)^{\omega}$$

Test 1: Buckley–Leverett II

- Upwind scheme for $S_{i\pm\frac{1}{2}}$.



if ($p^n_{i+1} >= p^n_i$) **then**
$S_{i+\frac{1}{2}} = S_{i+1}$
else
$S_{i+\frac{1}{2}} = S_i$
end if

Test 1: Buckley–Leverett III

- Adaptors: BLIP1 & BLES1

```
template<typename Tprec, int Dim>
class BLIP1 : public TwoPhaseEquation<BLIP1<Tprec, Dim> > {
public:
  inline void calcCoefficients1D();
  inline void calcCoefficients2D();
  inline void calcCoefficients3D();
};

template<typename Tprec, int Dim>
inline void BLIP1<Tprec, Dim>::calcCoefficients1D () {
    static prec_t Sw_e, Sw_w;
    static prec_t mult_o = k / ( (1 - Srw - Sro) * mu_o * dx ) ;
    static prec_t mult_w = k / ( (1 - Srw - Sro) * mu_w * dx ) ;
    aE = 0.0; aW = 0.0; aP = 0.0; sp = 0.0;
    for (int i =  bi; i <= ei; ++i) {
      if ( phi_0(i+1) >= phi_0(i) ) Sw_e = S(i+1);
      else                          Sw_e = S(i);
      if ( phi_0(i-1) >= phi_0(i) ) Sw_w = S(i-1);
      else                          Sw_w = S(i);
      aE (i) = (1 - Sro - Sw_e) * mult_o + (Sw_e - Srw) * mult_w ;
      aW (i) = (1 - Sro - Sw_w) * mult_o + (Sw_w - Srw) * mult_w ;
      aP (i) = aE (i) + aW (i);
    }
    applyBoundaryConditions1D();
}
```

Test 1: Buckley–Leverett IV

```
template<typename Tprec, int Dim>
class BLES1 : public TwoPhaseEquation<BLES1<Tprec, Dim> >
{
  public:
    inline void calcCoefficients1D();
    inline void calcCoefficients2D();
    inline void calcCoefficients3D();
};

template<typename Tprec, int Dim>
inline void BLES1<Tprec, Dim>::calcCoefficients1D ()
{
    static prec_t Sw_e, Sw_w;
    static prec_t mult = k * dt / ( porosity * dx * dx * (1 - Srw - Sro) * mu_w );
    aE = 0.0; aW = 0.0; aP = 0.0; sp = 0.0;

    for (int i =  bi; i <= ei; ++i) {
      if ( phi_0(i+1) >= phi_0(i) ) Sw_e = phi_0(i+1);
      else                          Sw_e = phi_0(i);
      if ( phi_0(i-1) >= phi_0(i) ) Sw_w = phi_0(i-1);
      else                          Sw_w = phi_0(i);

      aE (i) = (Sw_e - Srw) * mult;
      aW (i) = (Sw_w - Srw) * mult;
      aP (i) = aE (i) + aW (i);
    }
```

Test 1: Buckley–Leverett V

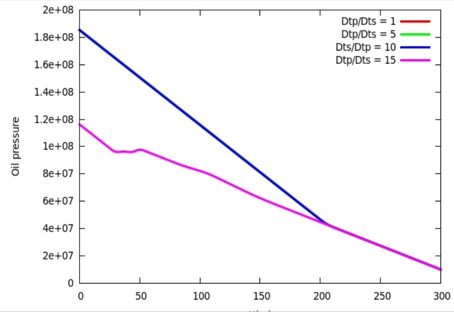
```
    // Dirichlet right side
    aP(ei) += aE(ei);
    sp(ei) = 2 * aE(ei) * p(ei+1);
    aE(ei) = 0;

    // Neumann left side
    aP(bi) -= aW(bi) ;
    sp(bi) = aW(bi) * dx * ( 3.47e-7 * mu_w / k) ;
    aW(bi) = 0;
}
```

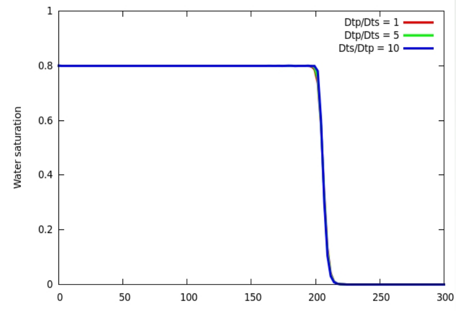
- 2D rectangular mesh: 300×10
- Time steps = 1100 days and $\Delta t = 60$ secs. (1,584,000 steps)
- Cases:
  1. $\omega = 1$ and $\mu_w/\mu_o = 1$ (lineal01)
  2. $\omega = 1$ and $\mu_w/\mu_o = 2$ (lineal02)
  3. $\omega = 1$ and $\mu_w/\mu_o = 2/3$ (lineal2_3)
  4. $\omega = 2$ and $\mu_w/\mu_o = 2/3$ (quadratic2_3)

Improved IMPES

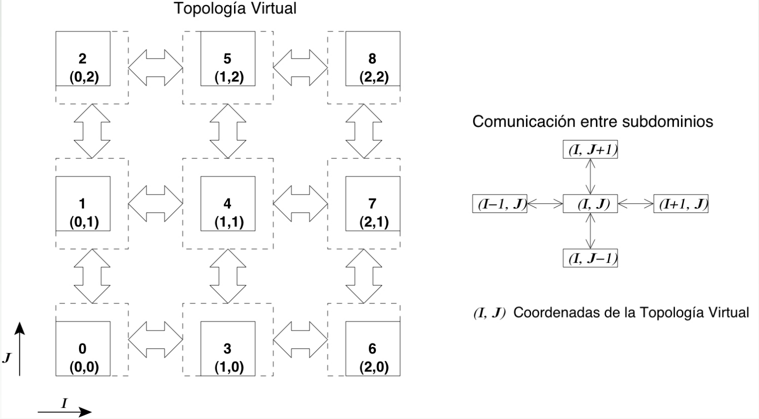
- As described in Chen *et al.* [8] the improved IMPES consists in to take a bigger time step for the calculation of pressure.

$\Delta t_p/\Delta t_S$	SP_p	SP_T
1	1.0	1.00
5	4.7	2.50
10	9.6	3.19





Overlapping method I



Overlapping method II

```
CartComm<2> cart(argc, argv, rank);   // MPI::COMM_WORLD.Create_cart()
Isub = cart.get_I();
Jsub = cart.get_J();
num_subdom_x = cart.getNumProc_I();
num_subdom_y = cart.getNumProc_J();

SubDomain<double, 2> subdom(cart);

double ovlp_l = subdom.createOverlap(LEFT,  nc_ovlp_l, dx);
double ovlp_r = subdom.createOverlap(RIGHT, nc_ovlp_r, dx);
double ovlp_d = subdom.createOverlap(DOWN,  nc_ovlp_d, dy);
double ovlp_u = subdom.createOverlap(UP,    nc_ovlp_u, dy);

while (t <= Tmax) {  // IMPES loop
//...
  subdom.infoExchange1(p);
  pressure.updatePhi(p);

  subdom.infoExchange1(Sw);
  saturation.updatePhi(Sw);
}
```

Overlapping method III

- Results on a Quadcore computer.

Procs.	Subdom	CPU time$_p$	CPU time$_S$	Speed up	Eff.
1	1	614.51	170.09	–	–
2	2×1	351.45	155.32	1.55	0.75
4 (1)	4×1	165.61	42.79	3.76	0.94
4 (2)	1×4	322.26	76.07	1.97	0.49
4 (3)	2×2	218.45	57.48	2.84	0.71

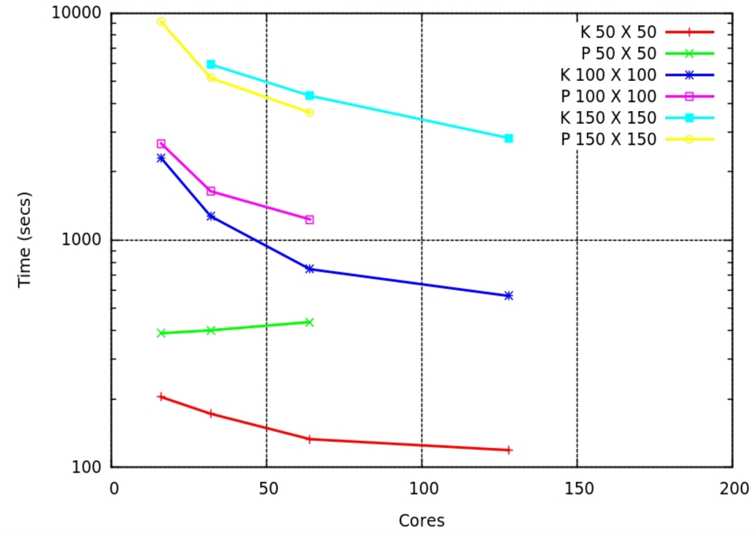
Multipliers–Free DDM

- Non–overlapping DDM : Unified theory of multipliers–free DDM methods, Herrera and Yates [9, 10]

Elliptic Operator – Subdomains = 32 × 32 = 1024[1]						
Nx × Ny	50 × 50 2,560,000		100 × 100 10,240,000		150 × 150 23,040,000	
Proc.	K[2]	P[3]	K	P	K	P
16 (64)	204	389	2303	2670	–	9158
32 (32)	172	401	1274	1641	5937	5178
64 (16)	133	436	745	1234	4326	3647
128 (8)	119	–	568	–	2818	–

[1] Recently results from A. Carrillo and R. Yates
[2] K ≡ KanBalam 1360 AMD Opteron 2.6 GHz, 8 GB per 4 cores, Net 10 Gbps
[3] P ≡ Pohualli 100 Intel Xeon 2.33 GHz, 32 GB per 8 cores, Net 1 Gbps

Multipliers–Free DDM



Test 2: Five–spots

- Classical five-spots pattern.
- Four water injection wells: a well in each corner of the domain.
- One oil production well: in the center of the domain.
- Only one quarter of the domain is simulated.
- No flux on the boundaries.

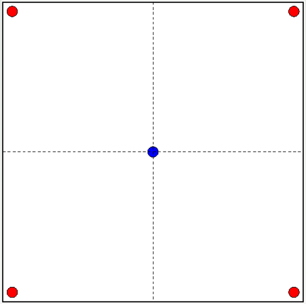


Table of contents

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  8. The system is in thermal equilibrium.
  9. There is no chemical reactions.
  10. Three components: W = water component, O = liquid hydrocarbon component, G = gaseous hydrocarbon component.
  11. Water phase: wetting phase, Oil phase: intermediate wetting phase, Gas phase: non-wetting phase.

	Phases		
Component	**Aqueos** (w)	**Oleic** (o)	**Gaseous** (g)
W	$\phi\rho_w S_w \ \ (\rho_{Ww} \equiv \rho_w)$		
O		$\phi\rho_{Oo} S_w$	
G		$\phi\rho_{Go} S_o$ (dg)	$\phi\rho_g S_g \ \ (\rho_{Gg} \equiv \rho_g)$ (fg)

dg : dissolved gas; fg : free gas.

- Balance equations:
  - Water component: $\dfrac{\partial(\phi\rho_w S_w)}{\partial t} = -\nabla \cdot (\rho_w \vec{u}_w) + q_W$
  - Oil component: $\dfrac{\partial(\phi\rho_{Oo} S_o)}{\partial t} = -\nabla \cdot (\rho_{Oo} \vec{u}_o) + q_O$
  - Gas component:

$$\frac{\partial(\overbrace{\phi\rho_{Go} S_o}^{\text{dg}} + \overbrace{\phi\rho_g S_g}^{\text{fg}}))}{\partial t} = -\nabla \cdot (\underbrace{\rho_{Go}\vec{u}_o}_{\text{flow dg}} + \overbrace{\rho_g \vec{u}_g}^{\text{flow fg}}) + q_G$$

- Darcy's Law:

$$\vec{u}_w = -\frac{k_{rw}}{\mu_w}\underline{\underline{k}}(\nabla p_w - \rho_w \mathcal{G} \nabla D)$$

$$\vec{u}_o = -\frac{k_{ro}}{\mu_o}\underline{\underline{k}}(\nabla p_o - \rho_o \mathcal{G} \nabla D) \qquad (\text{where } \rho_o = \rho_{Oo} + \rho_{Go})$$

$$\vec{u}_g = -\frac{k_{rg}}{\mu_g}\underline{\underline{k}}(\nabla p_g - \rho_g \mathcal{G} \nabla D)$$

- Saturation constrain: $S_w + S_o + S_g = 1$.
- Capillary pressures: $p_{cgw} = p_g - p_w$; $p_{cow} = p_o - p_w$; $p_{cgo} = p_g - p_o$.

- We have: 3 mass conservation eqs, 3 Darcy's Law eqs, 1 sat. constrain, 2 capillary pressure. Total: 9 eqs.
- We have 9 unknowns: $p_w, p_o, p_g, \vec{u}_w, \vec{u}_o, \vec{u}_g, S_w, S_o$, and S_g.

Pressure–Saturation Formulation for Black–Oil Model

Pressure equation (oil)

$$c_T \frac{\partial p}{\partial t} + \nabla \cdot \underline{u} = \sum_\alpha \frac{1}{\rho_\alpha} \left\{ q_\alpha - \rho_\alpha^0 c_\alpha \underline{u}_\alpha \cdot \nabla p \right\}, \quad \alpha = w, o, g,$$

Saturation equation (water and gas)

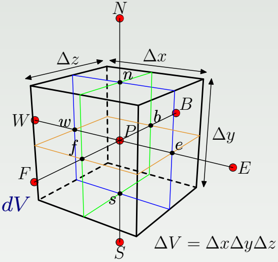
$$\begin{aligned} \rho_\alpha \phi \frac{\partial s_\alpha}{\partial t} + \rho_\alpha \nabla \cdot \underline{u}_\alpha \quad &= \quad -(s_\alpha \rho_\alpha \phi^0 c_p + \phi s_\alpha \rho_\alpha^0 c_\alpha) \frac{\partial p}{\partial t} \\ &\quad\; -\rho_\alpha^0 c_\alpha \underline{u}_\alpha \cdot \nabla p + q_\alpha, \qquad \alpha = w, g. \end{aligned}$$

Discrete pressure equation

- Integrating on ΔV and Δt:

$$\int_{\Delta V}\int_{\Delta t}\left[\left(\phi^0 c_p + \sum_{\alpha}\frac{\phi s_\alpha}{\rho_\alpha}\rho_\alpha^0 c_\alpha\right)\frac{\partial p}{\partial t} + \nabla\cdot\underline{u}\right] dt\, dV$$

$$= \int_{\Delta V}\int_{\Delta t}\left[\sum_{\alpha}\frac{1}{\rho_\alpha}\left(q_\alpha - \rho_\alpha^0 c_\alpha \underline{u}_\alpha\cdot\nabla p\right)\right] dt\, dV$$



- Using convenient approximations and $\theta = 1$ we get :

$$\left(a_P^0 + a_P\right)p_P^{n+1} - a_E p_E^{n+1} - a_W p_W^{n+1}$$
$$- a_N p_N^{n+1} - a_S p_S^{n+1} - a_F p_F^{n+1} - a_B p_B^{n+1} = S$$

Coefficients

$$a_E = -\sum_\alpha \left\{ \frac{\rho^0_{\alpha,P}}{\rho^n_{\alpha,P}} c_{\alpha,P} \left(u^n_{\alpha,e} + u^n_{\alpha,w} \right) \right\} \frac{\Delta V \Delta t}{8\delta x_e} \qquad a_W = \sum_\alpha \left\{ \frac{\rho^0_{\alpha,P}}{\rho^n_{\alpha,P}} c_{\alpha,P} \left(u^n_{\alpha,e} + u^n_{\alpha,w} \right) \right\} \frac{\Delta V \Delta t}{8\delta x_w}$$

$$a_N = -\sum_\alpha \left\{ \frac{\rho^0_{\alpha,P}}{\rho^n_{\alpha,P}} c_{\alpha,P} \left(v^n_{\alpha,n} + v^n_{\alpha,s} \right) \right\} \frac{\Delta V \Delta t}{8\delta y_n} \qquad a_S = \sum_\alpha \left\{ \frac{\rho^0_{\alpha,P}}{\rho^n_{\alpha,P}} c_{\alpha,P} \left(v^n_{\alpha,n} + v^n_{\alpha,s} \right) \right\} \frac{\Delta V \Delta t}{8\delta y_s}$$

$$a_F = -\sum_\alpha \left\{ \frac{\rho^0_{\alpha,P}}{\rho^n_{\alpha,P}} c_{\alpha,P} \left(w^n_{\alpha,f} + w^n_{\alpha,b} \right) \right\} \frac{\Delta V \Delta t}{8\delta z_f} \qquad a_B = \sum_\alpha \left\{ \frac{\rho^0_{\alpha,P}}{\rho^n_{\alpha,P}} c_{\alpha,P} \left(w^n_{\alpha,f} + w^n_{\alpha,b} \right) \right\} \frac{\Delta V \Delta t}{8\delta z_b}$$

$$a^0_P = \phi^0_P c_{p,P} \Delta V + \left[\sum_\alpha \frac{\rho^0_{\alpha,P}}{\rho^n_{\alpha,P}} c_{\alpha,P} s^n_{\alpha,P} \right] \phi^n_P \Delta V \qquad a_P = a_E + a_W + a_N + a_S + a_F + a_B$$

$$S = \left(a^0_P - a_P \right) p^n_P + a_E p^n_E + a_W p^n_W + a_N p^n_N + a_S p^n_S + a_F p^n_F + a_B p^n_B + S^0$$

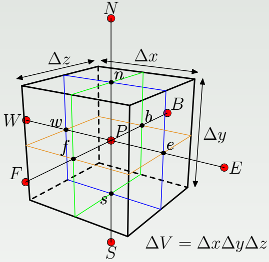
$$S^0 = \left(\sum_\alpha \frac{q^n_{\alpha,P}}{\rho^n_{\alpha,P}} \right) \Delta V \Delta t - \left(\frac{u^n_e - u^n_w}{\Delta x} + \frac{v^n_n - v^n_s}{\Delta y} + \frac{w^n_f - w^n_b}{\Delta z} \right) \Delta V \Delta t$$

Discrete saturation equation ($\alpha = w, g$)

- Integrating on ΔV and Δt:

$$\int_{\Delta V}\int_{\Delta t}\left[\phi\frac{\partial s_\alpha}{\partial t} + \nabla\cdot\underline{u}_\alpha + c_\alpha\frac{\rho_\alpha^0}{\rho_\alpha}\underline{u}_\alpha\cdot\nabla p\right] dt\, dV$$

$$= \int_{\Delta V}\int_{\Delta t}\left[\frac{q_\alpha}{\rho_\alpha} - \left(s_\alpha\phi^0 c_p + s_\alpha\phi c_\alpha\frac{\rho_\alpha^0}{\rho_\alpha}\right)\frac{\partial p}{\partial t}\right] dt\, dV$$



- Using convenient approximations we get and $\theta = 0$:

$$s_{\alpha,P}^{n+1} = b_P s_{\alpha,P}^n + d_P$$

$$b_P = b_P(\phi_P^n, \rho_{\alpha,P}^n, p_P^n, p_P^{n+1})$$

$$d_P = d_P(\phi_P^n, \rho_{\alpha,P}^n, q_P^n, p^n, \underline{u}_\alpha^n)$$

Explicit equation for saturation ($\alpha = w, g$)

$$
\begin{aligned}
s_{\alpha,P}^{n+1} = & s_{\alpha,P}^{n} - s_{\alpha,P}^{n}\left[c_{p,P}\frac{\phi_P^0}{\phi_P^n} + c_{\alpha,P}\frac{\rho_{\alpha,P}^0}{\rho_{\alpha,P}^n}\right]\left(p_P^{n+1} - p_P^n\right) + \frac{q_{\alpha,P}^n}{\rho_{\alpha,P}^n\phi_P^n}\Delta t \\
& - \frac{\Delta t}{\phi_P^n}\left[\frac{u_{\alpha,e}^n - u_{\alpha,w}^n}{\Delta x} + \frac{v_{\alpha,n}^n - v_{\alpha,s}^n}{\Delta y} + \frac{w_{\alpha,f}^n - w_{\alpha,b}^n}{\Delta z}\right] \\
& - \frac{\rho_{\alpha,P}^0 c_{\alpha,P}}{\rho_{\alpha,P}^n\phi_P^n}\Delta t\left[\frac{u_{\alpha,e}^n + u_{\alpha,w}^n}{4}\left(\frac{p_E^n - p_P^n}{\delta x_e} - \frac{p_W^n - p_P^n}{\delta x_w}\right) + \right. \\
& \qquad \frac{v_{\alpha,n}^n + v_{\alpha,s}^n}{4}\left(\frac{p_N^n - p_P^n}{\delta y_n} - \frac{p_S^n - p_P^n}{\delta y_s}\right) + \\
& \qquad \left. \frac{w_{\alpha,f}^n + w_{\alpha,b}^n}{4}\left(\frac{p_F^n - p_P^n}{\delta z_f} - \frac{p_B^n - p_P^n}{\delta z_b}\right)\right]
\end{aligned}
$$

Solution Algorithm

Algorithm 1 IMPES

$s_\alpha^0, p^0, \underline{u}^0, \phi^0, \rho_\alpha^0, q_\alpha^0, p_{c\alpha o}, c_\alpha, c_p$

while $t < T_{max}$ **do**

    $p^{n+1} \leftarrow solve(s_\alpha^n, p^n, \underline{u}^n, \phi^n, \rho_\alpha^n, q_\alpha^n, c_\alpha, c_p)$

    $s_\alpha^{n+1} \leftarrow solve(s_\alpha^n, \phi^n, \rho_\alpha^n, p^n, p^{n+1}, \underline{u}_\alpha^n, q_\alpha^n)$

    $\phi^{n+1}, \rho_\alpha^{n+1}, \lambda^{n+1} \leftarrow update(p^{n+1})$

    $\underline{u}_\alpha^{n+1} \leftarrow update(p^{n+1}, \lambda^{n+1}, \rho_\alpha^{n+1})$

    $\underline{u}^{n+1} \leftarrow update(p^{n+1}, \lambda^{n+1}, \rho_\alpha^{n+1})$

    $t \leftarrow t + \Delta t$

end while

Table of contents

- Assumptions:
  - Compositional flow involves many components and mass transfer between phases in a general fashion.
  - The flow process is isothermal.
  - The components form at most three phases.
  - There is no mass transfer between the water phase and the hydrocarbon phases.
- Total mass is conserved for each component:
  - Water component:

$$\frac{(\phi \xi_w S_w)}{\partial t} + \nabla \cdot (\xi_w \vec{u}_w) = q_w$$

where ξ_w is the molar density of the water.

- Hydrocarbon components:

$$\frac{\phi(x_{io}\xi_o S_o + x_{ig}\xi_g S_g)}{\partial t} + \nabla \cdot (x_{io}\xi_o \vec{u}_o + x_{ig}\xi_g \vec{u}_g) +$$

$$\nabla \cdot (\underline{\underline{d}}_{io} + \underline{\underline{d}}_{ig}) = q_i, \quad i = 1, \ldots, N_c$$

  where ξ_{io}, $x_{i\alpha}$ and $\underline{\underline{d}}_{i\alpha}$ represents the molar densities, the mole fraction, and the difussive fluxes of componet i in the phase α, respectively. $\alpha = o, g$. N_c is the number of hydrocarbon components,

- Darcy's Law:

$$\vec{u}_\alpha = -\frac{k_{r\alpha}}{\mu_\alpha}\underline{\underline{k}}(\nabla p_\alpha - \rho_\alpha \mathcal{G} \nabla D) \quad \text{for} \quad \alpha = w, o, g.$$

- The mole fraction balance implies: $\sum_{i=1}^{N_c} x_{io} = 1$ and $\sum_{i=1}^{N_c} x_{ig} = 1$
- Saturation constrain: $S_w + S_o + S_g = 1$.
- Capillary pressures: $p_{cow} = p_o - p_w$; $p_{cgo} = p_g - p_o$.
- We have $N_c + 9$ equations and $2N_c + 9$ unknowns: $x_{io}, x_{ig}, \vec{u}_\alpha, \rho_\alpha$ and S_α, for $\alpha = w, o, g$ and $i = 1, \ldots, N_c$.
- The aditional N_c relations are provided by the *equilibrium relations* that relate the numbers of moles:

$$f_{io}(p_o, x_{1o}, \ldots x_{N_c o}) = f_{ig}(p_g, x_{1g}, \ldots x_{N_c g})$$

- Typical (moderate) simulation: grid nodes $\sim 10^5$ and $N_c = 10 \Longrightarrow \sim 3 \times 10^6$ unknowns by time step.

Table of contents

Solution Schemes I

- An important problem in the numerical simulation is to develop stable, efficient, robust, accurate, and self-adaptive time stepping techniques.
- IMPES method.
  - This scheme works well for problems of intermediate difficulty and nonlinearity (e.g., for two-phase incompressible flow) and is still widely used in the petroleum industry.
  - However, it is not efficient for problems with strong nonlinearities, particularly for problems involving more than two fluid phases.
- Simultaneous solution (SS) method.
  - Solves all of the coupled nonlinear equations simultaneously and implicitly.
  - This technique is stable and can take very large time steps while stability is maintained.

Solution Schemes II

- For the black oil and thermal models (with a few components) is a good choice.
- However, for complex problems that involve many chemical components (e.g., the compositional and chemical compositional flow problems), the size of system matrices to be solved is too large.

- Sequential methods, implicit fashion without a full coupling.
  - They are less stable but more computationally efficient than the SS scheme, and more stable but less efficient than the IMPES scheme.
  - The sequential schemes are very suitable for the compositional and chemical compositional flow problems that involve many chemical components.
- Adaptive implicit scheme can be employed in reservoir simulation.

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