# Simulation of oil recovery with miscible gas injection using a black oil model 

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## Motivations of compositional two phase oil gas models

■ Saturated or under saturated oil reservoirs: volatile Hydrocarbon Components (HC) evaporate with pressure drop
■ Oil recovery by miscible gas injection
■ Gas condensate reservoirs: liquid phase appears with pressure drop

## Oil-Gas Phase envelope



## Black Oil Model: definition

- Two phases: oil and gas
- Two components: heavy HC (h), and light HC: (I)
- The light component can dissolve into the oil phase
- The heavy component cannot evaporate into the gas phase


## Oil phase

## Gas phase



## Black Oil Model: conservation equations

$$
\left\{\begin{aligned}
\partial_{t}\left(\phi \rho^{\circ}(1-c) S^{o}\right)+ & \operatorname{div}\left((1-c) \rho^{o} \frac{k_{r, o}\left(S^{\circ}\right)}{\mu^{\circ}} \mathbf{V}^{o}\right)=0 \\
\partial_{t}\left(\phi\left[\rho^{o} c S^{o}+\rho^{g} S^{g}\right]\right) & +\operatorname{div}\left(c \rho^{o} \frac{k_{r, o}\left(S^{o}\right)}{\mu^{o}} \mathbf{V}^{o}\right) \\
& +\operatorname{div}\left(\rho^{g} \frac{k_{r, g}\left(S^{g}\right)}{\mu^{g}} \mathbf{V}^{g}\right)=0
\end{aligned} \quad \begin{array}{rl}
\mathbf{V}^{o}=-K\left(\nabla P-\rho^{\circ} \mathbf{g}\right), & \mathbf{V}^{g}=-K\left(\nabla P-\rho^{g} \mathbf{g}\right) \\
S^{o}+S^{g}=1 .
\end{array}\right.
$$

- Oil phase properties: $\rho^{o}(P, c), \mu^{o}(P, c)$
- Gas phase properties: $\rho^{g}(P), \mu^{g}(P)$


## Black Oil Model: thermodynamical equilibrium

If the oil and gas phases are both present, the thermodynamical equilibrium imposes that $c=\bar{c}(P)$.

$$
\left\{\begin{aligned}
S^{g}(\bar{c}(P)-c) & =0 \\
S^{g} & \geq 0 \\
(\bar{c}(P)-c) & \geq 0
\end{aligned}\right.
$$



## Black Oil Model

$$
\left\{\begin{array}{l}
\partial_{t}\left(\phi \rho^{o}(P, c)(1-c) S^{o}\right)+\operatorname{div}\left((1-c) \rho^{o}(P, c) \frac{k_{r, o}\left(S^{o}\right)}{\mu^{o}(P, c)} \mathbf{V}^{o}\right)=0, \\
\partial_{t}\left(\phi\left[\rho^{o}(P, c) c S^{o}+\rho^{g}(P) S^{g}\right]\right)+\operatorname{div}\left(c \rho^{o}(P, c) \frac{k_{r, o}\left(S^{o}\right)}{\mu^{\circ}(P, c)} \mathbf{V}^{o}\right) \\
\\
\\
\quad+\operatorname{div}\left(\rho^{g}(P) \frac{k_{r, g}\left(S^{g}\right)}{\mu^{g}(P)} \mathbf{V}^{g}\right)=0 \\
\mathbf{V}^{o}=-K\left(\nabla P-\rho^{o}(P, c) \mathbf{g}\right), \mathbf{V}^{g}=-K\left(\nabla P-\rho^{g}(P) \mathbf{g}\right), \\
S^{o}+S^{g}=1, \\
S^{g}(\bar{c}(P)-c)=0, \\
S^{g} \geq 0, \\
(\bar{c}(P)-c) \geq 0 .
\end{array}\right.
$$

Remarks:
■ Only one set of unknowns $P, S^{\circ}, S^{g}, c$ and equations because the oil phase is always present.

- No flash needed.


## Black Oil Model: $B_{o}, B_{g}$ and $R_{s}$

$$
\begin{gathered}
\mathrm{T}_{\mathrm{o}} \\
B_{o}=\frac{V_{o}}{V_{o, h, s}}=\frac{\rho_{h, s}}{\rho^{o}(P, c)(1-c)}, \quad B_{g}=\frac{V_{g}}{V_{g, l, s}}=\frac{\rho_{l, s}}{\rho^{g}(P)} \\
R_{s}=\frac{V_{o, l, s}}{V_{o, h, s}}=\frac{1-c}{c} \frac{\rho_{l, s}}{\rho_{h, s}}
\end{gathered}
$$

$\rho_{h, s}$ and $\rho_{l, s}$ are the "oil" and "gas" densities at surface conditions. $T$ is fixed.

## Black Oil Model: phase properties in terms of $B_{o}, B_{g}$ and

 $R_{s}$$\bar{B}_{o}(P), \bar{R}_{s}(P), \bar{\mu}^{o}(P)$ are given at equilibrium (saturated oil). $B_{g}(P)$ and $\mu^{g}(P)$ are given.

For saturated oil $\left(c=\bar{c}(P)\right.$ or $\left.P=P_{b}(c)\right)$ and undersaturated oil $\left(c<\bar{c}(P)\right.$ or $\left.P>P_{b}(c)\right)$

$$
B_{o}\left(P, P_{b}\right)=\bar{B}_{o}\left(P_{b}\right)+c_{B_{o}}\left(P-P_{b}\right), \quad \mu^{o}\left(P, P_{b}\right)=\bar{\mu}^{o}\left(P_{b}\right)+c_{\mu_{o}}\left(P-P_{b}\right)
$$

$$
\left\{\begin{aligned}
\rho^{o}(P, c) & =\frac{\rho_{h, s}}{(1-c)\left(\bar{B}_{o}\left(P_{b}(c)\right)+c_{B_{o}}\left(P-P_{b}(c)\right)\right)}, \\
\mu^{o}(P, c) & =\bar{\mu}^{o}\left(P_{b}(c)\right)+c_{\mu_{o}}\left(P-P_{b}(c)\right), \\
\bar{c}(P) & =\frac{\rho_{l, s}}{\rho_{h, s} \bar{R}_{s}(P)+\rho_{l, s}}, \\
P_{b}(c) & =\bar{c}^{-1}(c), \\
\rho^{g}(P) & =\frac{\rho_{l, s}}{B_{g}(P)} .
\end{aligned}\right.
$$

## Discretization of Black Oil model: 2D fivespots test case



- 2D horizontal reservoir with 4 gas injectors at the corners and 1 producer at the center.
- Prescribed pressures $P^{\text {inj }}$ for the injection wells and $P^{\text {prod }}$ for the production well
- Initial state: under saturated oil at $P^{\text {prod }}<P_{\text {init }}<P^{\text {inj }}$ and $P_{b} \in\left(P^{\text {prod }}, P_{\text {init }}\right)$
- Gas will appear around the producer due to pressure drop
- Gas front will propagate from injectors to producer and saturate the oil phase behind the front


# Discretization of Black Oil model: diffusion fluxes and upwinding (without gravity) 

Diffusion fluxes (without gravity for simplicity)

$$
\left\{\begin{aligned}
F_{\kappa_{1}(\sigma), \sigma}^{\mathrm{int}} & =-F_{\kappa_{2}(\sigma), \sigma}^{\mathrm{int}}=T_{\sigma}^{\mathrm{int}}\left(p_{\kappa_{1}(\sigma)}-p_{\kappa_{2}(\sigma)}\right), \sigma \in \Sigma_{\mathrm{int}} \\
F_{\sigma_{w}}^{\mathrm{prod}} & =W I_{\sigma_{w}}^{\mathrm{prod}}\left(p_{\kappa_{\mathrm{prod}}\left(\sigma_{w}\right)}-p_{\sigma_{w}}^{\mathrm{prod}}\right), \sigma_{w} \in \Sigma^{\mathrm{prod}} \\
F_{\sigma_{w}}^{\mathrm{inj}} & =W I_{\sigma_{w}}^{\mathrm{inj}}\left(p_{\kappa_{\mathrm{inj}}\left(\sigma_{w}\right)}-p_{\sigma_{w}}^{\mathrm{inj}}\right), \sigma_{w} \in \Sigma^{\mathrm{inj}}
\end{aligned}\right.
$$

Upwinding (without gravity): for all $\sigma \in \Sigma_{\text {int }}$

$$
\kappa_{\mathrm{up}}(\sigma)=\left\{\begin{array}{l}
\kappa_{1}(\sigma)=\text { si } F_{\kappa_{1}(\sigma), \sigma}^{\text {int }}>0, \\
\kappa_{2}(\sigma)=\text { si } F_{\kappa_{1}(\sigma), \sigma}^{\text {int }} \leq 0 .
\end{array}\right.
$$

Five Spots example: $\Sigma^{\text {prod }}=$ one producer, $\Sigma^{\mathrm{inj}}=$ the four injectors.

# Discretization of Black Oil Model: discrete system (without gravity) 

Heavy HC residual

$$
\left\{\begin{aligned}
R_{h, \kappa} & =\left(\rho^{o}\left(P_{\kappa}, c_{\kappa}\right) S_{\kappa}^{o}\left(1-c_{\kappa}\right)-m_{h, \kappa}^{n-1}\right) \frac{|\kappa|}{\Delta t} \\
& +\sum_{\sigma \in \Sigma_{\mathrm{int}} \cap \partial \kappa}\left(1-c_{\kappa_{\mathrm{up}}(\sigma)}\right) \rho^{o}\left(P_{\kappa_{\mathrm{up}}(\sigma)}, c_{\kappa_{\mathrm{up}}(\sigma)}\right) \frac{k_{r_{o}}\left(S_{\kappa_{\mathrm{up}}(\sigma)}^{o}\right)}{\mu^{o}\left(P_{\kappa_{\mathrm{up}}(\sigma)}, c_{\kappa_{\mathrm{up}}(\sigma)}\right)} F_{\kappa, \sigma}^{\mathrm{int}} \\
& +\sum_{\sigma_{w} \in \Sigma^{\text {prod }} \mid \kappa_{\text {prod }}\left(\sigma_{w}\right)=\kappa} \rho^{o}\left(P_{\kappa}, c_{\kappa}\right)\left(1-c_{\kappa}\right) \frac{k_{r_{o}}\left(S_{\kappa}^{o}\right)}{\mu^{o}\left(P_{\kappa}, c_{\kappa}\right)}\left(F_{\sigma_{w}}^{\text {prod }}\right)^{+}=0,
\end{aligned}\right.
$$

## Discretization of Black Oil Model: discrete system (without gravity)

## Light HC residual

$$
\begin{aligned}
R_{l, \kappa} & =\left(\rho^{o}\left(P_{\kappa}, c_{\kappa}\right) S_{\kappa}^{o} c_{\kappa}+\rho^{g}\left(P_{\kappa}\right) S_{\kappa}^{g}-m_{l, \kappa}^{n-1}\right) \frac{|\kappa|}{\Delta t} \\
& +\sum_{\sigma \in \Sigma_{\text {int }} \cap \partial \kappa} c_{\kappa_{\text {up }}(\sigma)} \rho^{o}\left(P_{\kappa_{\mathrm{up}}(\sigma)}, c_{\kappa_{\mathrm{up}}(\sigma)}\right) \frac{k_{r_{o}}\left(S_{\kappa_{\mathrm{up}}(\sigma)}^{o}\right)}{\mu^{o}\left(P_{\kappa_{\mathrm{up}}(\sigma)}, c_{\kappa_{\mathrm{up}}(\sigma)}\right)} F_{\kappa, \sigma}^{\mathrm{int}} \\
& +\sum_{\sigma \in \Sigma_{\text {int }} \cap \partial \kappa} \rho^{g}\left(P_{\kappa_{\mathrm{up}}(\sigma)}\right) \frac{k_{r_{g}}\left(S_{\kappa_{\mathrm{up}}(\sigma)}^{g}\right)}{\mu^{g}\left(P_{\kappa_{\mathrm{up}}(\sigma)}\right)} F_{\kappa, \sigma}^{\mathrm{int}} \\
& +\sum_{\sigma_{w} \in \sum_{\operatorname{prod}} \mid \kappa_{\text {prod }}\left(\sigma_{w}\right)=\kappa}\left[c_{\kappa} \rho^{o}\left(P_{\kappa}, c_{\kappa}\right) \frac{k_{r_{0}}\left(S_{\kappa}^{o}\right)}{\mu^{o}\left(P_{\kappa}, c_{\kappa}\right)}+\rho^{g}\left(P_{\kappa}\right) \frac{k_{r_{g}}\left(S_{\kappa}^{g}\right)}{\mu^{g}\left(P_{\kappa}\right)}\right]\left(F_{\sigma_{w}}^{\text {prod }}\right)^{+}=0, \\
& +\sum_{\sigma_{w} \in \Sigma^{\text {inj }} \mid \kappa_{\text {inj }}\left(\sigma_{w}\right)=\kappa} \rho_{g}\left(P_{\sigma_{w}}^{\text {inj }}\right) \frac{k_{r_{g}}(1)}{\mu_{g}\left(P_{\sigma_{w}}^{\text {inj }}\right)}\left(F_{\sigma_{w}}^{\text {inj }}\right)^{-}=0,
\end{aligned}
$$

# Discretization of Black Oil Model: discrete system (without gravity) 

Local closure laws (volume conservation an thermodynamical equilibrium)

$$
\left\{\begin{aligned}
S_{\kappa}^{o}+S_{\kappa}^{g} & =1, \\
S_{\kappa}^{g}\left(\bar{c}\left(P_{\kappa}\right)-c_{\kappa}\right) & =0, \\
S_{\kappa}^{g} & \geq 0, \\
\left(\bar{c}\left(P_{\kappa}\right)-c_{\kappa}\right) & \geq 0 .
\end{aligned}\right.
$$

## Discretization of Black Oil Model: Newton type algorithm

- The oil phase is always present in all cells $\left(S_{\text {or }}>0\right)$
- Gas phase indicator for all cell $\kappa \in \mathcal{K}$

$$
\mathcal{I}_{\kappa}=\left\{\begin{array}{lll}
1 & \text { if } & \text { gas phase is present } \\
0 & \text { if } & \text { gas phase is absent }
\end{array}\right.
$$

- Given $\mathcal{I}_{\kappa}$ for all cells, the closure laws are eliminated at the non linear level:

$$
\begin{cases}\text { if } \mathcal{I}_{\kappa}=1: & S_{\kappa}^{\circ}=1-S_{\kappa}^{g}, \quad c_{\kappa}=\bar{c}\left(P_{\kappa}\right), \\ \text { if } \mathcal{I}_{\kappa}=0: & S_{\kappa}^{g}=0, S_{\kappa}^{\circ}=1,\end{cases}
$$

■ the unknowns $X_{\kappa}$ for the Newton linearization depend on $\mathcal{I}_{\kappa}$ for all cells:

$$
\begin{cases}\text { if } \mathcal{I}_{\kappa}=1: & X_{\kappa}=\left(P_{\kappa}, S_{\kappa}^{g}\right), \\ \text { if } \mathcal{I}_{\kappa}=0: & X_{\kappa}=\left(P_{\kappa}, c_{\kappa}\right) .\end{cases}
$$

## Solution of the discrete system of equations: Newton type algorithm

- The conservation equations are linearized with respect to the set of unknowns $X=\left(X_{\kappa}\right)_{\kappa \in \mathcal{K}}$ taking into account the previous elimination of the closure laws for a given $\mathcal{I}$ :

$$
R_{\kappa}(X)=\binom{R_{h, \kappa}(X)}{R_{l, \kappa}(X)}
$$

$R=\left(R_{\kappa}\right)_{\kappa \in \mathcal{K}}, d X=-\left(\frac{\partial R}{\partial X}\right)^{-1} R$

- On each cell $\kappa$ update of the unknowns $P_{\kappa}, S_{\kappa}, c_{\kappa}$ and of the Gas phase indicator $\mathcal{I}_{\kappa}$ to satisfy the inequality constraints $S_{\kappa}^{g} \geq 0$ and $c \leq \bar{c}\left(P_{\kappa}\right)$, $\kappa \in \mathcal{K}$.


## Solution of the discrete system of equations: algorithm

$$
\begin{aligned}
& P=\left(P_{\kappa}\right)_{\mathcal{K}}, \mathcal{I}=\left(\mathcal{I}_{\kappa}\right)_{\mathcal{K}}, S=\left(S_{\kappa}=S_{\kappa}^{g}\right)_{\mathcal{K}}, c=\left(c_{\kappa}\right)_{\mathcal{K}} . \\
& R=\left(R_{h, \kappa}, R_{l, \kappa}\right)_{\kappa \in \mathcal{K}} .
\end{aligned}
$$

- Initialization of $P=P^{0}, \mathcal{I}=\mathcal{I}^{0}, S=S^{0}, c=c^{0}$ and $\Delta t$ at $t=0$.
- Time loop: while $t<t_{f}: t=t+\Delta t$
- Compute the initial residual $R\left(P, S, c, P^{0}, S^{0}, c^{0}, \Delta t\right)$ and its norm $\|R\|_{0}=\|R\|$
- Newton Loop: while $\frac{\|R\|}{\|R\|_{0}}<\epsilon$ or Nit $_{\text {newton }}<$ Nit $_{\text {max }}$
- Linearization of the residuals $R(X)+\left(\frac{\partial R}{\partial X}\right) d X=0$
- $d X=-\left(\frac{\partial R}{\partial X}\right)^{-1} R$
- Update of $P, S, c$ and $I$

■ Compute the residual $R\left(P, S, c, P^{0}, S^{0}, c^{0}, \Delta t\right)$ and its norm $\|R\|$

- If Nit $_{\text {newton }}=$ Nit $_{\text {max }}$ and $\frac{\|R\|}{\|R\|_{0}}>\epsilon$ then Restart the time step: $t=t-\Delta t$,

$$
\Delta t=\Delta t / 2, P=P^{0}, \mathcal{I}=\mathcal{I}^{0}, S=S^{0}, c=c^{0}
$$

■ Else new time step: update $\Delta t$ and set $P^{0}=P, \mathcal{I}^{0}=\mathcal{I}, S^{0}=S, c^{0}=c$

# Solution of the discrete system of equations: update of 

 $P, S, c$ and $\mathcal{I}$- $d X=-J^{-1} R$
- Newton update: for $\kappa=1, \cdots, N$ :
- $P_{\kappa} \leftarrow P_{\kappa}+d X(2 \kappa-1)$,
- if $\mathcal{I}_{\kappa}=1$ then $S_{\kappa} \leftarrow S_{\kappa}+d X(2 \kappa), c_{\kappa}=\bar{c}\left(P_{\kappa}\right)$
- else $c_{\kappa} \leftarrow c_{\kappa}+d X(2 \kappa), S_{\kappa}=0$.
- Gas phase indicator update: for $\kappa=1, \cdots, N$ :
- If $\mathcal{I}_{\kappa}=1$ then
- if $S_{\kappa}<0$ then

$$
\mathcal{I}_{\kappa} \leftarrow 0, S_{\kappa} \leftarrow 0, c_{\kappa} \leftarrow \bar{c}\left(P_{\kappa}\right)
$$

- else if $S_{\kappa}>1-S_{o r}$ then

$$
S_{\kappa} \leftarrow 1-S_{o r}
$$

- Else if $\mathcal{I}_{\kappa}=0$ then
- if $c_{\kappa}>\bar{c}\left(P_{\kappa}\right)$ then

$$
\mathcal{I}_{\kappa} \leftarrow 1, S_{\kappa} \leftarrow 0, c_{\kappa} \leftarrow \bar{c}\left(P_{\kappa}\right)
$$

## Solution of the discrete system of equations: computation of the residual $R\left(P, S, c, P^{0}, S^{0}, c^{0}, \Delta t\right)$

- numbering of the cells: $\kappa=1, \cdots, N$
- numbering of the equations:

$$
\left\{\begin{array}{l}
R_{\kappa}^{h} \rightarrow R(2 k-1), \kappa=1, \cdots, N \\
R_{\kappa}^{l} \rightarrow R(2 k), \kappa=1, \cdots, N
\end{array}\right.
$$

■ Loop on cells $\kappa=1, \cdots, N$

$$
\left\{\begin{aligned}
\rho_{\kappa}^{o} & =\rho^{o}\left(P_{\kappa}, c_{\kappa}\right), \\
\rho_{\kappa}^{g} & =\rho^{g}\left(P_{\kappa}\right), \\
R(2 \kappa-1) & \leftarrow R(2 \kappa-1)+\frac{\left(\rho_{\kappa}^{o}\left(1-S_{\kappa}\right)\left(1-c_{\kappa}\right)-\rho^{o}\left(P_{\kappa}^{0}, c_{\kappa}^{0}\right)\left(1-S_{\kappa}^{0}\right)\left(1-c_{\kappa}^{0}\right)\right)|\kappa|}{\Delta t} \\
R(2 \kappa) & \leftarrow R(2 \kappa)+\frac{\left(\rho_{\kappa}^{o}\left(1-S_{\kappa}\right) c_{\kappa}+\rho_{\kappa}^{g} S_{\kappa}-\rho^{o}\left(P_{\kappa}^{0}, c_{\kappa}^{0}\right)\left(1-S_{\kappa}^{0}\right) c_{\kappa}^{0}-\rho^{g}\left(P_{\kappa}^{0}\right) S_{\kappa}^{0}\right)|\kappa|}{\Delta t}
\end{aligned}\right.
$$

## Solution of the discrete system of equations: computation of the residual $R\left(P, S, c, P^{0}, S^{0}, c^{0}, \Delta t\right)$

- Loop on interior faces:

$$
\begin{aligned}
& F_{\sigma}^{h}=\left(1-c_{\kappa_{\text {up }}(\sigma)}\right) \rho_{\kappa_{\text {up }}(\sigma)}^{o} \frac{k_{\kappa_{0}}\left(1-S_{\kappa_{\text {up }}(\sigma)}\right)}{\mu^{\circ}} F_{\kappa_{1}(\sigma), \sigma}^{\text {int }} \\
& F_{\sigma}^{\prime}=\left[c_{\kappa_{\mathrm{up}}(\sigma)} \rho_{\kappa_{\mathrm{up}}(\sigma)}^{o} \frac{k_{\kappa_{\mathrm{o}}}\left(1-S_{\kappa_{\mathrm{up}}(\sigma)}\right)}{\mu^{o}}+\rho_{\kappa_{\mathrm{up}}(\sigma)}^{g} \frac{k_{\mathrm{rg}_{g}}\left(S_{\kappa_{\mathrm{up}}(\sigma)}\right.}{\mu^{g}}\right] F_{\kappa_{1}(\sigma), \sigma}^{\mathrm{int}} \\
& R\left(2 \kappa_{1}(\sigma)-1\right) \leftarrow R\left(2 \kappa_{1}(\sigma)-1\right)+F_{\sigma}^{h} \\
& R\left(2 \kappa_{2}(\sigma)-1\right) \leftarrow R\left(2 \kappa_{2}(\sigma)-1\right)-F_{\sigma}^{h} \\
& R\left(2 \kappa_{1}(\sigma)\right) \leftarrow R\left(2 \kappa_{1}(\sigma)\right)+F_{\sigma}^{\prime} \\
& R\left(2 \kappa_{2}(\sigma)\right) \leftarrow R\left(2 \kappa_{2}(\sigma)\right)-F_{\sigma}^{\prime}
\end{aligned}
$$

# Solution of the discrete system of equations: computation of the residual $R\left(P, S, c, P^{0}, S^{0}, c^{0}, \Delta t\right)$ 

- Loop on injector wells $\sigma_{w}$ :

$$
R\left(2 \kappa_{\mathrm{inj}}\left(\sigma_{w}\right)\right) \leftarrow R\left(2 \kappa_{\mathrm{inj}}\left(\sigma_{w}\right)\right)+\rho_{g}\left(P_{\sigma_{w}}^{\mathrm{inj}}\right) \frac{k_{r_{g}}(1)}{\mu_{g}}\left(F_{\sigma_{w}}^{\mathrm{inj}}\right)^{-}
$$

- Producer well $\sigma_{w}$

$$
\left\{\begin{array}{l}
R\left(2 \kappa_{\text {prod }}\left(\sigma_{w}\right)-1\right) \leftarrow R\left(2 \kappa_{\text {prod }}\left(\sigma_{w}\right)-1\right)+\rho_{\kappa}^{o}\left(1-c_{\kappa}\right) \frac{k_{r_{o}}\left(1-S_{\kappa}\right)}{\mu^{o}}\left(F_{\sigma_{w}}^{\text {prod }}\right)^{+} \\
R\left(2 \kappa_{\text {prod }}\left(\sigma_{w}\right)\right) \leftarrow R\left(2 \kappa_{\text {prod }}\left(\sigma_{w}\right)\right)+\left[c_{\kappa} \rho_{\kappa}^{o} \frac{k_{r_{0}}\left(1-S_{\kappa}\right)}{\mu^{\circ}}+\rho_{\kappa}^{g} \frac{k_{r_{g}}\left(S_{\kappa}\right)}{\mu^{g}}\right]\left(F_{\sigma_{w}}^{\text {prod }}\right)^{+}
\end{array}\right.
$$

Solution of the discrete system of equations: Newton linearization $R(X)+\left(\frac{\partial R}{\partial X}\right) d X=0$

- Unknowns numbering for the Newton linearization: $\kappa=1, \cdots, N$

$$
\left\{\begin{aligned}
d X(2 \kappa-1) & =d P_{\kappa}, \\
d X(2 \kappa) & =\left\{\begin{array}{lll}
d S_{\kappa} & \text { if } \mathcal{I}_{\kappa}=1, \\
d c_{\kappa} & \text { if } \mathcal{I}_{\kappa}=0 .
\end{array}\right.
\end{aligned}\right.
$$

- Notation

$$
\left(X^{1}, X^{2}\right)= \begin{cases}(P, S) & \text { if } \mathcal{I}=1 \rightarrow c=\bar{c}(P) \\ (P, c) & \text { if } \mathcal{I}=0 \rightarrow S=0\end{cases}
$$

- Derivatives: example of $\rho^{\circ}(P, c)$ :

$$
\begin{gathered}
\frac{\partial \rho^{o}}{\partial X^{1}}=\left[\frac{\partial \rho^{o}}{\partial P}(P, c)+\frac{\partial \rho^{o}}{\partial c}(P, c) \frac{\partial \bar{c}}{\partial P}(P)\right] \mathcal{I}+\left[\frac{\partial \rho^{o}}{\partial P}(P, c)\right](1-\mathcal{I}) \\
\frac{\partial \rho^{o}}{\partial X^{2}}=\left[\frac{\partial \rho^{o}}{\partial c}(P, c)\right](1-\mathcal{I})
\end{gathered}
$$

Solution of the discrete system of equations: Newton linearization $R(X)+\left(\frac{\partial R}{\partial X}\right) d X=0$

- Jacobian: example of the accumulation term for $R_{\kappa}^{h}$ :

$$
\frac{\left(\rho_{\kappa}^{o}\left(1-S_{\kappa}\right)\left(1-c_{\kappa}\right)-\rho^{o}\left(P_{\kappa}^{0}, c_{\kappa}^{0}\right)\left(1-S_{\kappa}^{0}\right)\left(1-c_{\kappa}^{0}\right)\right)|\kappa|}{\Delta t}
$$

- Loop on cells $\kappa$

$$
\begin{aligned}
& J(2 \kappa-1,2 \kappa-1) \leftarrow J(2 \kappa-1,2 \kappa-1)+\mathcal{I}_{\kappa}\left[-\rho_{\kappa}^{o}\left(1-S_{\kappa}\right) \frac{\partial \bar{c}}{\partial P}\left(P_{\kappa}\right)\right. \\
& \left.+\left(1-S_{\kappa}\right)\left(1-c_{\kappa}\right)\left(\frac{\partial \rho^{o}}{\partial P}\left(P_{\kappa}, c_{\kappa}\right)+\frac{\partial \rho^{o}}{\partial c}\left(P_{\kappa}, c_{\kappa}\right) \frac{\partial \bar{c}}{\partial P}\left(P_{\kappa}\right)\right)\right] \frac{|\kappa|}{\Delta t} \\
& +\left(1-\mathcal{I}_{\kappa}\right)\left[\frac{\partial \rho^{\circ}}{\partial P}\left(P_{\kappa}, c_{\kappa}\right)\left(1-S_{\kappa}\right)\left(1-c_{\kappa}\right)\right] \frac{|\kappa|}{\Delta t} \\
& \quad J(2 \kappa-1,2 \kappa) \leftarrow J(2 \kappa-1,2 \kappa)+\mathcal{I}_{\kappa}\left[-\rho_{\kappa}^{o}\left(1-c_{\kappa}\right)\right] \frac{|\kappa|}{\Delta t} \\
& \quad+\left(1-\mathcal{I}_{\kappa}\right)\left[\frac{\partial \rho^{\circ}}{\partial c}\left(P_{\kappa}, c_{\kappa}\right)\left(1-S_{\kappa}\right)\left(1-c_{\kappa}\right)-\rho_{\kappa}^{\circ}\left(1-S_{\kappa}\right)\right] \frac{|\kappa|}{\Delta t}
\end{aligned}
$$

## Solution of the discrete system of equations: Newton

 linearization $R(X)+\left(\frac{\partial R}{\partial X}\right) d X=0$- Jacobian: example of the interior face flux term:

$$
F_{\sigma}^{h}=\left(1-c_{\kappa_{\text {up }}(\sigma)}\right) \rho_{\kappa_{\text {up }}(\sigma)}^{o} \frac{k_{\mathrm{r}}\left(1-S_{\kappa_{\text {up }}(\sigma)}\right)}{\mu^{\circ}} F_{\kappa_{1}(\sigma), \sigma}^{\mathrm{int}}
$$

■ Loop on interior faces $\sigma: \kappa_{1}=\kappa_{1}(\sigma), \kappa_{2}=\kappa_{2}(\sigma), \kappa_{\text {up }}=\kappa_{\text {up }}(\sigma)$

$$
\begin{aligned}
& G_{\sigma}^{h}=\left(1-c_{\kappa_{\text {up }}}\right) \rho_{\kappa_{\text {up }}}^{o} \frac{k_{\text {ro }}\left(1-S_{\kappa_{\text {up }}}\right)}{\mu^{\circ}} \\
& J\left(2 \kappa_{1}-1,2 \kappa_{1}-1\right) \leftarrow J\left(2 \kappa_{1}-1,2 \kappa_{1}-1\right)+G_{\sigma}^{h} T_{\sigma}^{\text {int }} \\
& J\left(2 \kappa_{2}-1,2 \kappa_{2}-1\right) \leftarrow J\left(2 \kappa_{2}-1,2 \kappa_{2}-1\right)+G_{\sigma}^{h} T_{\sigma}^{\text {int }} \\
& J\left(2 \kappa_{1}-1,2 \kappa_{2}-1\right) \leftarrow J\left(2 \kappa_{1}-1,2 \kappa_{2}-1\right)-G_{\sigma}^{h} T_{\text {To }}^{\text {int }} \\
& J\left(2 \kappa_{2}-1,2 \kappa_{1}-1\right) \leftarrow J\left(2 \kappa_{2}-1,2 \kappa_{1}-1\right)-G_{\sigma}^{h} T_{\sigma}^{\text {int }}
\end{aligned}
$$

to be continued ...

Solution of the discrete system of equations: Newton linearization $R(X)+\left(\frac{\partial R}{\partial X}\right) d X=0$

- suite of the interior flux term $F_{\sigma}^{h}$

$$
\begin{aligned}
& \gamma=\left(\mathcal { I } _ { \kappa } \left[\left(1-c_{\kappa_{\text {up }}}\right) \frac{\partial \rho^{o}}{\partial P}\left(P_{\kappa_{\text {up }}}, c_{\kappa_{\text {up }}}\right)+\left(1-c_{\kappa_{\text {up }}}\right) \frac{\partial \rho^{o}}{\partial c}\left(P_{\kappa_{\text {up }}}, c_{\kappa_{\text {up }}}\right) \frac{\partial \bar{c}}{\partial P}\left(P_{\kappa_{\text {up }}}\right)\right.\right. \\
& \left.\left.-\frac{\partial \bar{c}}{\partial P}\left(P_{\kappa_{\text {up }}}\right) \rho_{\kappa_{\text {up }}}^{o}\right]+\left(1-\mathcal{I}_{\kappa}\right)\left[\left(1-c_{\kappa_{\text {up }}}\right) \frac{\partial \rho^{o}}{\partial P}\left(P_{\kappa_{\text {up }}}, c_{\kappa_{\text {up }}}\right)\right]\right) \frac{k_{\kappa_{0}}\left(1-S_{\kappa_{\text {up }}}\right)}{\mu^{\circ}} F_{\kappa_{1}, \sigma}^{\text {int }} \\
& \delta=\mathcal{I}_{\kappa}\left[-\frac{\left(1-c_{\kappa_{\text {up }}}\right) \rho_{\kappa_{\text {up }}}^{o}}{\mu^{o}} \frac{\partial k_{\text {ro }}}{\partial S}\left(\left(1-S_{\kappa_{\text {up }}}\right)\right] F_{\kappa_{1}, \sigma}^{\text {int }}\right. \\
& +\left(1-\mathcal{I}_{\kappa}\right)\left[-\rho_{\kappa_{\text {up }}}^{o}+\left(1-c_{\kappa_{\text {up }}}\right) \frac{\partial \rho^{o}}{\partial c}\left(P_{\kappa_{\text {up }}}, c_{\kappa_{\text {up }}}\right)\right] \frac{k_{\text {ro }}\left(1-S_{\text {upp }}\right)}{\mu^{\circ}} F_{\kappa_{1}, \sigma}^{\text {int }} \\
& J\left(2 \kappa_{1}-1,2 \kappa_{\text {up }}-1\right) \leftarrow J\left(2 \kappa_{1}-1,2 \kappa_{\text {up }}-1\right)+\gamma \\
& J\left(2 \kappa_{2}-1,2 \kappa_{\text {up }}-1\right) \leftarrow J\left(2 \kappa_{2}-1,2 \kappa_{\text {up }}-1\right)-\gamma \\
& J\left(2 \kappa_{1}-1,2 \kappa_{\text {up }}\right) \leftarrow J\left(2 \kappa_{1}-1,2 \kappa_{\text {up }}\right)+\delta \\
& J\left(2 \kappa_{2}-1,2 \kappa_{\text {up }}\right) \leftarrow J\left(2 \kappa_{2}-1,2 \kappa_{\text {up }}\right)-\delta
\end{aligned}
$$

- to be continued for all remaining terms of the Jacobian ...

