Report for the semester thesis "Development of a Monte Carlo algorithm for optimal control problems"

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***Abstract*—TODO *CRITICAL: Do Not Use Symbols, Special Characters, Footnotes, or Math in Paper Title or Abstract.**

***Index Terms*—a, b, c**

I. Problem description

The problem we want to solve is a variant of the *quarter five spot problem* in literature. We model a cross section of an oil field as a two dimensional square $\Omega := [0,1]^2$. In the oilfield, there are two phases: water and oil. At the lower left corner $\boldsymbol{x}_{\text{drill}} := (0,0)$, we know the pressure $p_{\text{drill}}(t)$. Opposite of that, at $\boldsymbol{x}_{\text{well}} := (1,1)$ a well is located. There we can measure the pressure $p_{\text{well}}(t)$ as well as the total volumetric outflow

$$Q_{\text{tot}}(t) := Q_{\text{o}}(t) + Q_{\text{w}}(t)$$

per unit depth.

The flow rates for both phases are described by Darcy's law

$$\boldsymbol{v}_{\text{w}} = -\frac{k k_{\text{rel, w}}}{\mu_{\text{w}}} \operatorname{grad}(p), \tag{1}$$

for water and

$$\boldsymbol{v}_{\text{o}} = -\frac{k k_{\text{rel, o}}}{\mu_{\text{o}}} \operatorname{grad}(p) \tag{2}$$

for oil. Here, $p(\boldsymbol{x},t)$ is the pressure, μ_{o}, μ_{w} are dynamic viscosities for oil and water, $k(\boldsymbol{x},t)$ is the permeability. $k_{\text{rel, o}}(S)$, $k_{\text{rel, w}}(S)$ are relative permeabilities and are assumed to depend quadratically on the saturation of water $S_{\text{w}} \in [0,1]$ and the saturation of oil $S_{\text{o}} \in [0,1]$:

$$k_{\text{rel, o}} = S_{\text{o}}^2 \tag{3}$$

$$k_{\text{rel, w}} = S_{\text{w}}^2. \tag{4}$$

The saturations are linked by the constitutive relation

$$S_{\text{o}} + S_{\text{w}} = 1. \tag{5}$$

$\boldsymbol{v}_{\text{o}}(\boldsymbol{x},t)$, $\boldsymbol{v}_{\text{w}}(\boldsymbol{x},t)$ finally are the volumetric flow rates per unit area (Darcy velocities).

The saturation S is not assumed constant but instead is transported according to the equation

$$\phi \frac{\partial}{\partial t} S_{\text{w}} + \operatorname{div}(\boldsymbol{v}_{\text{w}}) = q_{\text{w}}. \tag{6}$$

The term

$$q_{\text{w}} := Q_{\text{w}} \delta(\boldsymbol{x} - \begin{pmatrix}1\\1\end{pmatrix}) \tag{7}$$

describes a line sink of water located at the well. Similarly, we use

$$q_{\text{o}} := Q_{\text{o}} \delta(\boldsymbol{x} - \begin{pmatrix}1\\1\end{pmatrix}) \tag{8}$$

$$q_{\text{tot}} := q_{\text{o}} + q_{\text{w}}. \tag{9}$$

ϕ is the porosity of the rock which is assumed to be constant over the domain.

Conservation of the total mass then reads

$$\operatorname{div}(\boldsymbol{v}_{\text{tot}}) = q_{\text{tot}}, \tag{10}$$

where

$$\boldsymbol{v}_{\text{tot}} := \boldsymbol{v}_{\text{o}} + \boldsymbol{v}_{\text{w}} \tag{11}$$

is the total Darcy velocity.

We then introduce the mobilities

$$\lambda_{\text{o}} := \frac{k k_{\text{rel, o}}}{\mu_{\text{o}}} \tag{12}$$

$$\lambda_{\text{w}} := \frac{k k_{\text{rel, w}}}{\mu_{\text{w}}} \tag{13}$$

$$\lambda_{\text{tot}} := \lambda_{\text{o}} + \lambda_{\text{w}}. \tag{14}$$

Substituting in the λ from (12) into Darcy's law (2), (1) and adding both sides of the results we get the total Darcy's law

$$\boldsymbol{v}_{\text{tot}} = -\lambda_{\text{tot}} \operatorname{grad}(p). \tag{15}$$

Plugging this (15) into the conservation of mass (10) leads to the pressure equation

$$\boxed{\operatorname{div}(\lambda_{\text{tot}} \operatorname{grad}(p)) = -q_{\text{tot}}.} \tag{16}$$

Comparing the total Darcy's law (15) and the Darcy's law for water (1), we see that

$$\boldsymbol{v}_{\text{w}} = \frac{\lambda_{\text{w}}}{\lambda_{\text{tot}}} \boldsymbol{v}_{\text{tot}}. \tag{17}$$

We then plug in the model for the relative permeabilities in terms of the saturations (3), to get the final for of saturation transport equation

$$\boxed{\frac{\partial}{\partial t} S_{\mathrm{w}} + \operatorname{div}\left(f(S_{\mathrm{w}}) \boldsymbol{v}_{\mathrm{tot}}\right) = \frac{q_{\mathrm{w}}}{\phi},} \tag{18}$$

where f is the flux function

$$\boxed{f(S_{\mathrm{w}}) := \frac{S_{\mathrm{w}}^2/\phi}{S_{\mathrm{w}}^2 + (1 - S_{\mathrm{w}})^2 \mu_{\mathrm{w}}/\mu_{\mathrm{o}}}.} \tag{19}$$

A. Boundary and initial conditions

We assume the initial saturation of water to be given, which is $S_{\mathrm{w}}(\boldsymbol{x}, 0)$. For the pressure equation we use homogeneous Neumann boundary conditions (no flow), i.e.

$$\operatorname{grad}(p) = p_0 \begin{pmatrix} \delta(x - x_w) \\ \delta(y - y_w), \end{pmatrix}, \tag{20}$$

where we choose p_0 such that the compatibility condition

$$\int_{\Omega} q_{\mathrm{tot}} \mathrm{d}A \stackrel{!}{=} \int_{\partial\Omega} \lambda_{\mathrm{tot}} \operatorname{grad}(p)^{\mathsf{T}} \boldsymbol{n} \mathrm{d}l \tag{21}$$

is satisfied.

B. What to optimize?

To test the Monte-Carlo adjoint method, we want to match the pressure difference between drill and well, which is

$$c(T) := \int_0^T \left(\left(p_{\mathrm{drill}}(t) - p_{\mathrm{well}}(t)\right) - \left(\tilde{p}_{\mathrm{drill}}(t) - \tilde{p}_{\mathrm{well}}(t)\right) \right)^2 \mathrm{d}t, \tag{22}$$

where the variables with a tilde denote computed quantities and T is a final time.

C. What do we control?

We control the log-permeabilities $\ln(k)$, as these are hard to measure.

II. Discretization

We discretize the square domain Ω with $n \times n$ square finite volumes, thus getting a mesh width of $h := 1/n$.

An overview of the discretization technique is given in the following procedure:

1) Solve the pressure equation (16) as detailed in subsection II-A
2) Compute the total Darcy velocity as in (15), using the same approximation of the gradient as in the first step
3) Consider the total Darcy velocity to be independent of the saturation S_{w}.
4) With this assumption, solve the saturation equation (18) as in subsection II-B
5) Update the relative permeabilities according to (3) and repeat.

A. Discretizing the pressure Poisson equation

Averaging the pressure Poisson equation (16) over such a finite volume K, and using the divergence theorem leads to

$$\frac{1}{h^2} \int_{\partial K} \lambda_{\mathrm{tot}} \operatorname{grad}(p)^{\mathsf{T}} \boldsymbol{n} \mathrm{d}l = -\frac{1}{h^2} \int_K q_{\mathrm{tot}} \mathrm{d}A. \tag{23}$$

Using the four boundaries North, East, South and West of the finite volume K, we approximate (23) as

$$\begin{aligned} &\frac{1}{h}\Bigg((\lambda_{\mathrm{tot}} \frac{\delta}{\delta x} p)|_{\mathrm{E}} - (\lambda_{\mathrm{tot}} \frac{\delta}{\delta x} p)|_{\mathrm{W}} \\ &\qquad + (\lambda_{\mathrm{tot}} \frac{\delta}{\delta y} p)|_{\mathrm{N}} - \frac{\delta}{\delta y} p)|_{\mathrm{S}} \Bigg) \\ &= -\frac{Q_{\mathrm{tot}}}{h^2} \cdot \begin{cases} 1, & \text{if } K \text{ is the finite volume nearest to the well} \\ 0, & \text{otherwise} \end{cases} \end{aligned} \tag{24}$$

$\frac{\delta}{\delta \cdot}$ denote the standard finite difference quotients, i.e.

$$\frac{\delta}{\delta x} p|_{\mathrm{E}} = \frac{1}{h}(p_R - p_K) \tag{25}$$

$$\frac{\delta}{\delta x} p|_{\mathrm{W}} = \frac{1}{h}(p_K - p_D) \tag{26}$$

$$\frac{\delta}{\delta y} p|_{\mathrm{N}} = \frac{1}{h}(p_U - p_K) \tag{27}$$

$$\frac{\delta}{\delta y} p|_{\mathrm{S}} = \frac{1}{h}(p_K - p_D). \tag{28}$$

Here, U stands for the upper neighbor of K, D for the lower (down), R for the right and L for the left. p_K is the pressure at the center of the volume, which is taken to be the same as the volume averaged $\bar{p}$, as our scheme is just first order.

The total mobilities λ_{tot} at the boundaries are approximated by the harmonic mean of the total mobilities inside the adjacent finite volumes as

$$\lambda_{\mathrm{tot}}|_{\mathrm{E}} \approx \operatorname{hm}(\lambda_{\mathrm{tot}}|_K, \lambda_{\mathrm{tot}}|_R) \tag{29}$$

$$\lambda_{\mathrm{tot}}|_{\mathrm{W}} \approx \operatorname{hm}(\lambda_{\mathrm{tot}}|_K, \lambda_{\mathrm{tot}}|_L) \tag{30}$$

$$\lambda_{\mathrm{tot}}|_{\mathrm{N}} \approx \operatorname{hm}(\lambda_{\mathrm{tot}}|_K, \lambda_{\mathrm{tot}}|_U) \tag{31}$$

$$\lambda_{\mathrm{tot}}|_{\mathrm{S}} \approx \operatorname{hm}(\lambda_{\mathrm{tot}}|_K, \lambda_{\mathrm{tot}}|_D), \tag{32}$$

where

$$\operatorname{hm}(a, b) = 2ab/(a + b). \tag{33}$$

Explain why the harmonic mean

The discretized pressure Poisson equation reads

$$\begin{aligned} &T_E(p_K - p_R) + T_W(p_K - p_L) \\ &\qquad + T_N(p_K - p_U) + T_S(p_K - p_D) \\ &= Q_{\mathrm{tot}} \cdot \begin{cases} 1, & \text{if } K \text{ is the finite volume nearest to the well} \\ 0, & \text{otherwise} \end{cases}, \end{aligned} \tag{34}$$

where

$$T_N = \operatorname{hm}(\lambda_{\mathrm{tot}}|_K, \lambda_{\mathrm{tot}}|_U), \tag{35}$$

and so on.

B. Discretizing the saturation equation

The finite volume reformulation of the saturation equation (18) leads to the following:

$$\begin{aligned}&\frac{\partial}{\partial t}\frac{1}{h^2}\int_K S_\mathrm{w}\mathrm{d}A\\&\qquad+\frac{1}{h}\Big((f(S_\mathrm{w})v_{\mathrm{tot}\ ,x})|_E-(f(S_\mathrm{w})v_{\mathrm{tot}\ ,x})|_W\\&\qquad+(f(S_\mathrm{w})v_{\mathrm{tot}\ ,y})|_N-(f(S_\mathrm{w})v_{\mathrm{tot}\ ,y})|_S\Big)\\&=\frac{Q_\mathrm{w}}{h^2\phi}\cdot\begin{cases}1, & \text{if } K \text{ is the finite volume nearest to the well}\\0, & \text{otherwise}\end{cases}\end{aligned}\tag{36}$$

We identify the volume average

$$\frac{1}{h^2}\int_K S_\mathrm{w}\mathrm{d}A =: S_K,\tag{37}$$

with the saturation at the center of the volume S_K. This is legit, as our scheme is just first order.

For the total Darcy velocity $\boldsymbol{v}_\mathrm{tot}$ we use the same discretization of the pressure gradients as in the pressure equation, (25). This makes it available at the boundaries (N, S, E, W), as required by (36).

For the flux function f at the boundaries, we use an upwind discretization. The standard formulation can be simplified by noting that

$$\frac{\mathrm{d}}{\mathrm{d}S_\mathrm{w}}f > 0\tag{38}$$

and so instead of the advection velocity

$$\frac{\partial}{\partial S_\mathrm{w}}(f\cdot\boldsymbol{v}_\mathrm{tot})\tag{39}$$

we can use the Darcy velocity $\boldsymbol{v}_\mathrm{tot}$. We remember that this requires fixing the total Darcy velocity $\boldsymbol{v}_\mathrm{tot}$ to be independent of the saturation S_w

For timestepping of the saturation equation (36) , we use explicit Euler, as this simplifies the Jacobian used in the Monte-Carlo adjoint.

C. Discretizing the cost function

The cost function (22) is discretized as a sum of squares over the timesteps, where the computed quantities with a tilde are taken to be the quantities in the volumes nearest to the well and the drill.

$$\sum_{i=1}^{n}(\Delta p(i\Delta t)-\tilde{\Delta p}^{(i)})^2,\tag{40}$$

where

$$\Delta_p(t) := p_\mathrm{well}(t)-p_\mathrm{drill}(t)\tag{41}$$

$$\tilde{\Delta p}^{(i)} := p^{(i)}_\mathrm{well\ cell}-p^{(i)}_\mathrm{drill\ cell}\tag{42}$$

and Δt is the timestep.

III. Computing the quantities for the Monte-Carlo adjoint solver

First, we define the pressure residuals

$$\Pi_K^{(i)} := \begin{cases}p_K^{(i)}-p_\mathrm{well}(i\Delta t), & \text{if } K \text{ is the cell nearest to the well}\\ T_E^{(i-1)}(p_K^{(i)}-p_R^{(i)})\\ +T_W^{(i-1)}(p_K^{(i)}-p_L^{(i)})\\ +T_N(p_K^{(i)}-p_U^{(i)})\\ +T_S^{(i-1)}(p_K^{(i)}-p_D^{(i)})-Q^{(i-1)}_\mathrm{tot,\ K}, & \text{else}\end{cases},\tag{43}$$

where

$$Q^{(i)}_\mathrm{tot,\ K} := Q_\mathrm{tot}(i\Delta t)\cdot\begin{cases}1, & \text{if } K \text{ is the cell nearest to the drill}\\0, & \text{otherwise}\end{cases}\tag{44}$$

The saturation residuals are given by

$$\begin{aligned}\Sigma_K^{(i)} :=\ & S_\mathrm{w}^{(i)}|_K-S_\mathrm{w}^{(i-1)}|_K\\&+\frac{\Delta t}{h}\Big((f(S_\mathrm{w}^{(i-1)})v^{(i-1)}_{\mathrm{tot}\ ,x})|_E-(f(S_\mathrm{w}^{(i-1)})v^{(i-1)}_{\mathrm{tot}\ ,x})|_W\\&+(f(S_\mathrm{w}^{(i-1)})v^{(i-1)}_{\mathrm{tot}\ ,y})|_N-(f(S_\mathrm{w}^{(i-1)})v^{(i-1)}_{\mathrm{tot}\ ,y})|_S\Big)-\Delta t Q^{(i-1)}_\mathrm{tot,\ K}.\end{aligned}\tag{45}$$

The nonzero derivatives for the diagonal blocks are given by

$$\frac{\partial}{\partial p_K^{(i)}}\Pi_K^{(i)} = T_E^{(i-1)}+T_W^{(i-1)}+T_N^{(i-1)}+T_S^{(i-1)}\tag{46}$$

$$\frac{\partial}{\partial p_R^{(i)}}\Pi_K^{(i)} = -T_E^{(i-1)}\tag{47}$$

$$\frac{\partial}{\partial p_L^{(i)}}\Pi_K^{(i)} = -T_W^{(i-1)}\tag{48}$$

$$\frac{\partial}{\partial p_N^{(i)}}\Pi_K^{(i)} = -T_U^{(i-1)}\tag{49}$$

$$\frac{\partial}{\partial p_S^{(i)}}\Pi_K^{(i)} = -T_D^{(i-1)}\tag{50}$$

for cells which are not nearest to the well and by

$$\frac{\partial}{\partial S_K^{(i)}}\Sigma_K^{(i)} = 1 \tag{51}$$

$$\begin{aligned}\frac{\partial}{\partial S_{\mathrm{w}}{}_K^{(i-1)}}\Sigma_K^{(i)} = &-1 + f'(S_{\mathrm{w}}{}_K^{(i-1)})\frac{\Delta t}{h}\cdot\Big(\mathbb{1}(v_{\text{tot, x}}|_E > 0)v_{\text{tot, x}}|_E \\ &- \mathbb{1}(v_{\text{tot, x}}|_W < 0)v_{\text{tot, x}}|_W + \mathbb{1}(v_{\text{tot, y}}|_N > 0)v_{\text{tot, y}}|_N \\ &- \mathbb{1}(v_{\text{tot, y}}|_S < 0)v_{\text{tot, y}}|_S\Big) \\ &+ \frac{\Delta t}{h}\cdot\Big(- f(S_{\mathrm{w}}{}_K^{(i-1)})|_E\frac{\partial}{\partial b}\mathrm{hm}(\\ &\lambda_{\text{tot, }R}, \lambda_{\text{tot, }K})\frac{\partial}{\partial S_{\mathrm{w}}}\lambda|_K\frac{\delta}{\delta x}p|_E \pm \dots\Big)\end{aligned} \tag{52}$$

$$\begin{aligned}\frac{\partial}{\partial S_{\mathrm{w}}{}_R^{(i-1)}}\Sigma_K^{(i)} = &f'(S_{\mathrm{w}}{}_R^{(i-1)})\frac{\Delta t}{h}\cdot\mathbb{1}(v_{\text{tot, x}}|_E < 0)v_{\text{tot, x}}|_E \\ &- \frac{\Delta t}{h}\frac{\partial}{\partial b}\mathrm{hm}(\lambda_{\text{tot, }K}, \lambda_{\text{tot, }R})\frac{\partial}{\partial S_{\mathrm{w}}}\lambda|_R\frac{\delta}{\delta x}p|_E\end{aligned} \tag{53}$$

where

$$f'(S_{\mathrm{w}}) = \frac{2\mu_{\mathrm{o}}\mu_{\mathrm{w}}(1-S_{\mathrm{w}})S_{\mathrm{w}}}{\phi\cdot(\mu_{\mathrm{w}}(1-S_{\mathrm{w}})^2 + \mu_{\mathrm{o}}S_{\mathrm{w}}^2)^2} \tag{54}$$

$$\mathbb{1}(b) = \begin{cases}1, & \text{if } b \text{ true}\\ 0, & \text{otherwise.}\end{cases} \tag{55}$$

For the off diagonal blocks, we have

$$\begin{aligned}\frac{\partial}{\partial p_K^{(i)}}\Sigma_K^{(i)} = -\frac{\Delta t}{h^2}\Big(&T_E^{(i-1)}f(S_{\mathrm{w}}^{(i-1)})|_E \\ &+ T_W^{(i-1)}f(S_{\mathrm{w}}^{(i-1)})|_W \\ &+ T_N^{(i-1)}f(S_{\mathrm{w}}^{(i-1)})|_N \\ &+ T_S^{(i-1)}f(S_{\mathrm{w}}^{(i-1)})|_S\Big)\end{aligned} \tag{56}$$

$$\frac{\partial}{\partial p_R^{(i)}}\Sigma_K^{(i)} = +\frac{\Delta t}{h^2}T_E^{(i-1)}f(S_{\mathrm{w}}^{(i-1)})|_E \tag{57}$$

$$\frac{\partial}{\partial p_L^{(i)}}\Sigma_K^{(i)} = +\frac{\Delta t}{h^2}T_W^{(i-1)}f(S_{\mathrm{w}}^{(i-1)})|_W \tag{58}$$

$$\tag{59}$$

$$\frac{\partial}{\partial p_U^{(i)}}\Sigma_K^{(i)} = +\frac{\Delta t}{h^2}T_N^{(i-1)}f(S_{\mathrm{w}}^{(i-1)})|_N \tag{60}$$

$$\frac{\partial}{\partial p_D^{(i)}}\Sigma_K^{(i)} = +\frac{\Delta t}{h^2}T_S^{(i-1)}f(S_{\mathrm{w}}^{(i-1)})|_S, \tag{61}$$

for cells not nearest to the well and

$$\frac{\partial}{\partial S_{\mathrm{w}}{}_K^{(i-1)}}\Pi_K^{(i)} = 2\frac{\partial}{\partial S_{\mathrm{w}}}\lambda_{\text{tot}}^{(i-1)}|_K \sum_{n\in\{U,D,L,R\}}\frac{(p_K^{(i-1)} - p_n^{(i-1)})\cdot(\lambda_{\text{tot, }n}^{(i-1)})^2}{(\lambda_{\text{tot, }K}^{(i-1)} + \lambda_{\text{tot, }n}^{(i-1)})^2} \tag{62}$$

$$\frac{\partial}{\partial S_{\mathrm{w}}{}_R^{(i-1)}}\Pi_K^{(i)} = 2\frac{\partial}{\partial S_{\mathrm{w}}}\lambda_{\text{tot}}^{(i-1)}|_R\cdot\frac{(p_K^{(i-1)} - p_R^{(i-1)})\cdot(\lambda_{\text{tot, }K}^{(i-1)})^2}{(\lambda_{\text{tot, }K}^{(i-1)} + \lambda_{\text{tot, }R}^{(i-1)})^2} \tag{63}$$

$$\frac{\partial}{\partial S_{\mathrm{w}}{}_L^{(i-1)}}\Pi_K^{(i)} = 2\frac{\partial}{\partial S_{\mathrm{w}}}\lambda_{\text{tot}}^{(i-1)}|_L\cdot\frac{(p_K^{(i-1)} - p_L^{(i-1)})\cdot(\lambda_{\text{tot, }K}^{(i-1)})^2}{(\lambda_{\text{tot, }K}^{(i-1)} + \lambda_{\text{tot, }L}^{(i-1)})^2} \tag{64}$$

$$\frac{\partial}{\partial S_{\mathrm{w}}{}_U^{(i-1)}}\Pi_K^{(i)} = 2\frac{\partial}{\partial S_{\mathrm{w}}}\lambda_{\text{tot}}^{(i-1)}|_U\cdot\frac{(p_K^{(i-1)} - p_U^{(i-1)})\cdot(\lambda_{\text{tot, }K}^{(i-1)})^2}{(\lambda_{\text{tot, }K}^{(i-1)} + \lambda_{\text{tot, }U}^{(i-1)})^2} \tag{65}$$

$$\frac{\partial}{\partial S_{\mathrm{w}}{}_D^{(i-1)}}\Pi_K^{(i)} = 2\frac{\partial}{\partial S_{\mathrm{w}}}\lambda_{\text{tot}}^{(i-1)}|_D\cdot\frac{(p_K^{(i-1)} - p_D^{(i-1)})\cdot(\lambda_{\text{tot, }K}^{(i-1)})^2}{(\lambda_{\text{tot, }K}^{(i-1)} + \lambda_{\text{tot, }D}^{(i-1)})^2} \tag{66}$$

where

$$\frac{\partial}{\partial S_{\mathrm{w}}}\lambda_{\text{tot}} = 2k\left(\frac{S_{\mathrm{w}}-1}{\mu_{\mathrm{o}}} + \frac{S_{\mathrm{w}}}{\mu_{\mathrm{w}}}\right). \tag{67}$$

For solving the adjoint equations, we also need the derivatives of the residuals with respect to the parameters, in our case $\ln(k)$.

For the pressure residuals and if K is not the cell at the well, those read

$$\frac{\partial}{\partial \ln(k)_K}\Pi_K^{(i)} = \lambda^{(i-1)}|_K\sum_{n\in\{L,R,U,D\}}(p_K^{(i)} - p_n^{(i)})\frac{\partial}{\partial b}\mathrm{hm}(\lambda^{(i-1)}|_n, \lambda_{\text{tot}}^{(i-1)}|_K) \tag{68}$$

$$\frac{\partial}{\partial \ln(k)_L}\Pi_K^{(i)} = (p_K^{(i)} - p_L^{(i)})\lambda_{\text{tot}}^{(i-1)}|_L\frac{\partial}{\partial b}\mathrm{hm}(\lambda_{\text{tot}}^{(i-1)}|_K, \lambda_{\text{tot}}^{(i-1)}|_L) \tag{69}$$

$$\frac{\partial}{\partial \ln(k)_R}\Pi_K^{(i)} = (p_K^{(i)} - p_R^{(i)})\lambda_{\text{tot}}^{(i-1)}|_R\frac{\partial}{\partial b}\mathrm{hm}(\lambda_{\text{tot}}^{(i-1)}|_K, \lambda_{\text{tot}}^{(i-1)}|_R) \tag{70}$$

$$\frac{\partial}{\partial \ln(k)_U}\Pi_K^{(i)} = (p_K^{(i)} - p_U^{(i)})\lambda_{\text{tot}}^{(i-1)}|_U\frac{\partial}{\partial b}\mathrm{hm}(\lambda_{\text{tot}}^{(i-1)}|_K, \lambda_{\text{tot}}^{(i-1)}|_U) \tag{71}$$

$$\frac{\partial}{\partial \ln(k)_D}\Pi_K^{(i)} = (p_K^{(i)} - p_D^{(i)})\lambda_{\text{tot}}^{(i-1)}|_D\frac{\partial}{\partial b}\mathrm{hm}(\lambda_{\text{tot}}^{(i-1)}|_K, \lambda_{\text{tot}}^{(i-1)}|_D) \tag{72}$$

where

$$\frac{\partial}{\partial b}\mathrm{hm}(a,b) := \frac{2a^2}{(a+b)^2}. \tag{73}$$

On the other hand, the saturation residuals Σ_K lead to the following derivatives

$$
\begin{aligned}
\frac{\partial}{\partial \ln(k)_K}\Sigma_K = \lambda_{\text{tot}}^{(i-1)}|_K \frac{\Delta t}{h}\Big(\\
&(f(S_{\text{w}}^{(i-1)})v_{\text{tot},x}^{(i-1)})|_E \frac{\partial}{\partial b}\text{hm}(\lambda_{\text{tot}}^{(i-1)}|_E, \lambda_{\text{tot}}^{(i-1)}|_K) \\
&-(f(S_{\text{w}}^{(i-1)})v_{\text{tot},x}^{(i-1)})|_W \frac{\partial}{\partial b}\text{hm}(\lambda_{\text{tot}}^{(i-1)}|_W, \lambda_{\text{tot}}^{(i-1)}|_K) \\
&+(f(S_{\text{w}}^{(i-1)})v_{\text{tot},y}^{(i-1)})|_N \frac{\partial}{\partial b}\text{hm}(\lambda_{\text{tot}}^{(i-1)}|_N, \lambda_{\text{tot}}^{(i-1)}|_K) \\
&-(f(S_{\text{w}}^{(i-1)})v_{\text{tot},y}^{(i-1)})|_S \frac{\partial}{\partial b}\text{hm}(\lambda_{\text{tot}}^{(i-1)}|_E, \lambda_{\text{tot}}^{(i-1)}|_S) \\
&\Big)
\end{aligned}
\tag{74}
$$

$$
\frac{\partial}{\partial \ln(K)_R}\Sigma_K = \lambda_{\text{tot}}^{(i-1)}|_R \frac{\Delta t}{h} f(S_{\text{w}}^{(i-1)})v_{\text{tot},x}^{(i-1)})|_E \frac{\partial}{\partial b}\text{hm}(\lambda_{\text{tot}}^{(i-1)}|_K, \lambda_{\text{tot}}^{(i-1)}|_E) \tag{75}
$$

$$
\frac{\partial}{\partial \ln(K)_L}\Sigma_K = -\lambda_{\text{tot}}^{(i-1)}|_L \frac{\Delta t}{h} f(S_{\text{w}}^{(i-1)})v_{\text{tot},x}^{(i-1)})|_W \frac{\partial}{\partial b}\text{hm}(\lambda_{\text{tot}}^{(i-1)}|_K, \lambda_{\text{tot}}^{(i-1)}|_L) \tag{76}
$$

$$
\frac{\partial}{\partial \ln(K)_U}\Sigma_K = \lambda_{\text{tot}}^{(i-1)}|_U \frac{\Delta t}{h} f(S_{\text{w}}^{(i-1)})v_{\text{tot},x}^{(i-1)})|_N \frac{\partial}{\partial b}\text{hm}(\lambda_{\text{tot}}^{(i-1)}|_K, \lambda_{\text{tot}}^{(i-1)}|_U) \tag{77}
$$

$$
\frac{\partial}{\partial \ln(K)_D}\Sigma_K = -\lambda_{\text{tot}}^{(i-1)}|_D \frac{\Delta t}{h} f(S_{\text{w}}^{(i-1)})v_{\text{tot},x}^{(i-1)})|_S \frac{\partial}{\partial b}\text{hm}(\lambda_{\text{tot}}^{(i-1)}|_K, \lambda_{\text{tot}}^{(i-1)}|_D) \tag{78}
$$