

# 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  $\mathbf{x}_{\text{drill}} := (0, 0)$ , we know the pressure  $p_{\text{drill}}(t)$ . Opposite of that, at  $\mathbf{x}_{\text{well}} := (1, 1)$  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

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

for water and

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

for oil. Here,  $p(\mathbf{x}, t)$  is the pressure,  $\mu_{\text{o}}, \mu_{\text{w}}$  are dynamic viscosities for oil and water,  $k(\mathbf{x}, t)$  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  $S_{\text{o}} \in [0, 1]$ :

$$k_{\text{rel, o}} = S_{\text{o}}^2 \quad (3)$$

$$k_{\text{rel, w}} = S_{\text{w}}^2. \quad (4)$$

The saturations are linked by the constitutive relation

$$S_{\text{o}} + S_{\text{w}} = 1. \quad (5)$$

$\mathbf{v}_{\text{o}}(\mathbf{x}, t), \mathbf{v}_{\text{w}}(\mathbf{x}, t)$  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

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

The term

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

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

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

$$q_{\text{tot}} := q_{\text{o}} + q_{\text{w}}. \quad (9)$$

$\phi$  is the porosity of the rock which is assumed to be constant over the domain.

Conservation of the total mass then reads

$$\text{div}(\mathbf{v}_{\text{tot}}) = q_{\text{tot}}, \quad (10)$$

where

$$\mathbf{v}_{\text{tot}} := \mathbf{v}_{\text{o}} + \mathbf{v}_{\text{w}} \quad (11)$$

is the total Darcy velocity.

We then introduce the mobilities

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

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

$$\lambda_{\text{tot}} := \lambda_{\text{o}} + \lambda_{\text{w}}. \quad (14)$$

Substituting in the  $\lambda$  from (12) into Darcy’s law (2), (1) and adding both sides of the results we get the total Darcy’s law

$$\mathbf{v}_{\text{tot}} = -\lambda_{\text{tot}} \text{grad}(p). \quad (15)$$

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

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

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

$$\mathbf{v}_{\text{w}} = \frac{\lambda_{\text{w}}}{\lambda_{\text{tot}}} \mathbf{v}_{\text{tot}}. \quad (17)$$

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

$$\frac{\partial}{\partial t} S_w + \text{div}(f(S_w) \mathbf{v}_{\text{tot}}) = \frac{q_w}{\phi}, \quad (18)$$

where  $f$  is the flux function

$$f(S_w) := \frac{S_w^2 / \phi}{S_w^2 + (1 - S_w)^2 \mu_w / \mu_o}. \quad (19)$$

#### A. Boundary and initial conditions

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

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

where we choose  $p_0$  such that the compatibility condition

$$\int_{\Omega} q_{\text{tot}} dA \stackrel{!}{=} \int_{\partial\Omega} \lambda_{\text{tot}} \text{grad}(p)^T \mathbf{n} dl \quad (21)$$

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

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

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  $\Omega$  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

$$\frac{1}{h^2} \int_{\partial K} \lambda_{\text{tot}} \text{grad}(p)^T \mathbf{n} dl = -\frac{1}{h^2} \int_K q_{\text{tot}} dA. \quad (23)$$

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

$$\begin{aligned} & \frac{1}{h} \left( (\lambda_{\text{tot}} \frac{\delta}{\delta x} p)|_E - (\lambda_{\text{tot}} \frac{\delta}{\delta x} p)|_W \right. \\ & \quad \left. + (\lambda_{\text{tot}} \frac{\delta}{\delta y} p)|_N - (\lambda_{\text{tot}} \frac{\delta}{\delta y} p)|_S \right) \\ &= -\frac{Q_{\text{tot}}}{h^2} \cdot \begin{cases} 1, & \text{if } K \text{ is the finite volume nearest to the well} \\ 0, & \text{otherwise} \end{cases} \end{aligned} \quad (24)$$

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

$$\frac{\delta}{\delta x} p|_E = \frac{1}{h} (p_R - p_K) \quad (25)$$

$$\frac{\delta}{\delta x} p|_W = \frac{1}{h} (p_K - p_D) \quad (26)$$

$$\frac{\delta}{\delta y} p|_N = \frac{1}{h} (p_U - p_K) \quad (27)$$

$$\frac{\delta}{\delta y} p|_S = \frac{1}{h} (p_K - p_D). \quad (28)$$

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  $\lambda_{\text{tot}}$  at the boundaries are approximated by the harmonic mean of the total mobilities inside the adjacent finite volumes as

$$\lambda_{\text{tot}}|_E \approx \text{hm}(\lambda_{\text{tot}}|_K, \lambda_{\text{tot}}|_R) \quad (29)$$

$$\lambda_{\text{tot}}|_W \approx \text{hm}(\lambda_{\text{tot}}|_K, \lambda_{\text{tot}}|_L) \quad (30)$$

$$\lambda_{\text{tot}}|_N \approx \text{hm}(\lambda_{\text{tot}}|_K, \lambda_{\text{tot}}|_U) \quad (31)$$

$$\lambda_{\text{tot}}|_S \approx \text{hm}(\lambda_{\text{tot}}|_K, \lambda_{\text{tot}}|_D), \quad (32)$$

where

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

Explain why the harmonic mean

The discretized pressure Poisson equation reads

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

where

$$T_N = \text{hm}(\lambda_{\text{tot}}|_K, \lambda_{\text{tot}}|_U), \quad (35)$$

and so on.

### B. Discretizing the saturation equation

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

$$\begin{aligned} & \frac{\partial}{\partial t} \frac{1}{h^2} \int_K S_w dA \\ & + \frac{1}{h} \left( (f(S_w) v_{\text{tot},x})|_E - (f(S_w) v_{\text{tot},x})|_W \right. \\ & \quad \left. + (f(S_w) v_{\text{tot},y})|_N - (f(S_w) v_{\text{tot},y})|_S \right) \\ & = \frac{Q_w}{h^2 \phi} \begin{cases} 1, & \text{if } K \text{ is the finite volume nearest to the well} \\ 0, & \text{otherwise} \end{cases} \end{aligned} \quad (36)$$

We identify the volume average

$$\frac{1}{h^2} \int_K S_w dA =: S_K, \quad (37)$$

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  $v_{\text{tot}}$  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

$$\frac{d}{dS_w} f > 0 \quad (38)$$

and so instead of the advection velocity

$$\frac{\partial}{\partial S_w} (f \cdot v_{\text{tot}}) \quad (39)$$

we can use the Darcy velocity  $v_{\text{tot}}$ . We remember that this requires fixing the total Darcy velocity  $v_{\text{tot}}$  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.

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

where

$$\Delta p(t) := p_{\text{well}}(t) - p_{\text{drill}}(t) \quad (41)$$

$$\tilde{\Delta p}^{(i)} := p_{\text{well cell}}^{(i)} - p_{\text{drill cell}}^{(i)} \quad (42)$$

and  $\Delta t$  is the timestep.

## III. COMPUTING THE QUANTITIES FOR THE MONTE-CARLO ADJOINT SOLVER

First, we define the pressure residuals

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

where

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

The saturation residuals are given by

$$\begin{aligned} \Sigma_K^{(i)} &:= S_w^{(i)}|_K - S_w^{(i-1)}|_K \\ &+ \frac{\Delta t}{h} \left( (f(S_w^{(i-1)}) v_{\text{tot},x}^{(i-1)})|_E - (f(S_w^{(i-1)}) v_{\text{tot},x}^{(i-1)})|_W \right. \\ &\quad \left. + (f(S_w^{(i-1)}) v_{\text{tot},y}^{(i-1)})|_N - (f(S_w^{(i-1)}) v_{\text{tot},y}^{(i-1)})|_S \right) - \Delta t Q_{\text{tot},K}^{(i-1)}. \end{aligned} \quad (45)$$

The nonzero derivatives for the diagonal blocks are given by

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

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

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

$$\frac{\partial}{\partial p_U^{(i)}} \Pi_K^{(i)} = -T_N^{(i-1)} \quad (49)$$

$$\frac{\partial}{\partial p_D^{(i)}} \Pi_K^{(i)} = -T_S^{(i-1)} \quad (50)$$

for cells which are not nearest to the well

and by

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

$$\begin{aligned} \frac{\partial}{\partial S_{wK}^{(i-1)}} \Sigma_K^{(i)} = & -1 + f'(S_{wK}^{(i-1)}) \frac{\Delta t}{h} \cdot \left( \mathbb{1}(v_{\text{tot}, x}|_E > 0) v_{\text{tot}, x}|_E \right. \\ & + \mathbb{1}(v_{\text{tot}, x}|_W < 0) v_{\text{tot}, x}|_W + \mathbb{1}(v_{\text{tot}, y}|_N > 0) v_{\text{tot}, y}|_N \\ & \left. + \mathbb{1}(v_{\text{tot}, y}|_S < 0) v_{\text{tot}, y}|_S \right) \end{aligned} \quad (52)$$

$$\frac{\partial}{\partial S_{wR}^{(i-1)}} \Sigma_K^{(i)} = f'(S_{wR}^{(i-1)}) \frac{\Delta t}{h} \cdot \mathbb{1}(v_{\text{tot}, x}|_E < 0) v_{\text{tot}, x}|_E \quad (53)$$

$$\frac{\partial}{\partial S_{wL}^{(i-1)}} \Sigma_K^{(i)} = f'(S_{wL}^{(i-1)}) \frac{\Delta t}{h} \cdot \mathbb{1}(v_{\text{tot}, x}|_W > 0) v_{\text{tot}, x}|_W \quad (54)$$

$$\frac{\partial}{\partial S_{wU}^{(i-1)}} \Sigma_K^{(i)} = f'(S_{wU}^{(i-1)}) \frac{\Delta t}{h} \cdot \mathbb{1}(v_{\text{tot}, y}|_N < 0) v_{\text{tot}, y}|_N \quad (55)$$

$$\frac{\partial}{\partial S_{wD}^{(i-1)}} \Sigma_K^{(i)} = f'(S_{wD}^{(i-1)}) \frac{\Delta t}{h} \cdot \mathbb{1}(v_{\text{tot}, y}|_S > 0) v_{\text{tot}, y}|_S, \quad (56)$$

where

$$f'(S_w) = \frac{2\mu_0\mu_w(1-S_w)S_w}{\phi \cdot (\mu_w(1-S_w)^2 + \mu_0 S_w^2)^2} \quad (57)$$

$$\mathbb{1}(b) = \begin{cases} 1, & \text{if } b \text{ true} \\ 0, & \text{otherwise.} \end{cases} \quad (58)$$

For the off diagonal blocks, we have

$$\begin{aligned} \frac{\partial}{\partial p_K^{(i)}} \Sigma_K^{(i)} = & \frac{\Delta t}{h^2} \left( T_E^{(i-1)} f(S_w^{(i-1)})|_E \right. \\ & + T_W^{(i-1)} f(S_w^{(i-1)})|_W \\ & + T_N^{(i-1)} f(S_w^{(i-1)})|_N \\ & \left. + T_S^{(i-1)} f(S_w^{(i-1)})|_S \right) \end{aligned} \quad (59)$$

$$\frac{\partial}{\partial p_R^{(i)}} \Sigma_K^{(i)} = -\frac{\Delta t}{h^2} T_E^{(i-1)} f(S_w^{(i-1)})|_E \quad (60)$$

$$\frac{\partial}{\partial p_L^{(i)}} \Sigma_K^{(i)} = -\frac{\Delta t}{h^2} T_W^{(i-1)} f(S_w^{(i-1)})|_W \quad (61)$$

$$\frac{\partial}{\partial p_U^{(i)}} \Sigma_K^{(i)} = -\frac{\Delta t}{h^2} T_N^{(i-1)} f(S_w^{(i-1)})|_N \quad (62)$$

$$\frac{\partial}{\partial p_D^{(i)}} \Sigma_K^{(i)} = -\frac{\Delta t}{h^2} T_S^{(i-1)} f(S_w^{(i-1)})|_S, \quad (63)$$

$$\frac{\partial}{\partial p_D^{(i)}} \Sigma_K^{(i)} = -\frac{\Delta t}{h^2} T_S^{(i-1)} f(S_w^{(i-1)})|_S, \quad (64)$$

for cells not nearest to the well and

$$\frac{\partial}{\partial S_{wK}^{(i-1)}} \Pi_K^{(i)} = 2 \frac{\partial}{\partial S_w} \lambda_{\text{tot}}^{(i-1)}|_K \quad (65)$$

$$\begin{aligned} \sum_{n \in \{U, D, L, R\}} \frac{(p_K^{(i-1)} - p_n^{(i-1)}) \cdot (\lambda_{\text{tot}, n}^{(i-1)})^2}{(\lambda_{\text{tot}, K}^{(i-1)} + \lambda_{\text{tot}, n}^{(i-1)})^2} \\ \frac{\partial}{\partial S_{wR}^{(i-1)}} \Pi_K^{(i)} = 2 \frac{\partial}{\partial S_w} \lambda_{\text{tot}}^{(i-1)}|_R \cdot \frac{(p_K^{(i-1)} - p_R^{(i-1)}) \cdot (\lambda_{\text{tot}, K}^{(i-1)})^2}{(\lambda_{\text{tot}, K}^{(i-1)} + \lambda_{\text{tot}, R}^{(i-1)})^2} \end{aligned} \quad (66)$$

$$\frac{\partial}{\partial S_{wL}^{(i-1)}} \Pi_K^{(i)} = 2 \frac{\partial}{\partial S_w} \lambda_{\text{tot}}^{(i-1)}|_L \cdot \frac{(p_K^{(i-1)} - p_L^{(i-1)}) \cdot (\lambda_{\text{tot}, K}^{(i-1)})^2}{(\lambda_{\text{tot}, K}^{(i-1)} + \lambda_{\text{tot}, L}^{(i-1)})^2} \quad (67)$$

$$\frac{\partial}{\partial S_{wU}^{(i-1)}} \Pi_K^{(i)} = 2 \frac{\partial}{\partial S_w} \lambda_{\text{tot}}^{(i-1)}|_U \cdot \frac{(p_K^{(i-1)} - p_U^{(i-1)}) \cdot (\lambda_{\text{tot}, K}^{(i-1)})^2}{(\lambda_{\text{tot}, K}^{(i-1)} + \lambda_{\text{tot}, U}^{(i-1)})^2} \quad (68)$$

$$\frac{\partial}{\partial S_{wD}^{(i-1)}} \Pi_K^{(i)} = 2 \frac{\partial}{\partial S_w} \lambda_{\text{tot}}^{(i-1)}|_D \cdot \frac{(p_K^{(i-1)} - p_D^{(i-1)}) \cdot (\lambda_{\text{tot}, K}^{(i-1)})^2}{(\lambda_{\text{tot}, K}^{(i-1)} + \lambda_{\text{tot}, D}^{(i-1)})^2} \quad (69)$$

where

$$\frac{\partial}{\partial S_w} \lambda_{\text{tot}} = 2k \left( \frac{S_w - 1}{\mu_0} + \frac{S_w}{\mu_w} \right). \quad (70)$$

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

$$\frac{\partial}{\partial \ln(k)_K} \Pi_K^{(i)} = \lambda_{\text{tot}}^{(i-1)}|_K \sum_{n \in \{L, R, U, D\}} (p_K^{(i)} - p_n^{(i)}) \frac{\partial}{\partial b} \text{hm}(\lambda_{\text{tot}}^{(i-1)}|_n, \lambda_{\text{tot}}^{(i-1)}|_K) \quad (71)$$

$$\begin{aligned} \lambda_{\text{tot}}^{(i-1)}|_K \\ \frac{\partial}{\partial \ln(k)_L} \Pi_K^{(i)} = (p_K^{(i)} - p_L^{(i)}) \lambda_{\text{tot}}^{(i-1)}|_L \frac{\partial}{\partial b} \text{hm}(\lambda_{\text{tot}}^{(i-1)}|_K, \lambda_{\text{tot}}^{(i-1)}|_L) \end{aligned} \quad (72)$$

$$\frac{\partial}{\partial \ln(k)_R} \Pi_K^{(i)} = (p_K^{(i)} - p_R^{(i)}) \lambda_{\text{tot}}^{(i-1)}|_R \frac{\partial}{\partial b} \text{hm}(\lambda_{\text{tot}}^{(i-1)}|_K, \lambda_{\text{tot}}^{(i-1)}|_R) \quad (73)$$

$$\frac{\partial}{\partial \ln(k)_U} \Pi_K^{(i)} = (p_K^{(i)} - p_U^{(i)}) \lambda_{\text{tot}}^{(i-1)}|_U \frac{\partial}{\partial b} \text{hm}(\lambda_{\text{tot}}^{(i-1)}|_K, \lambda_{\text{tot}}^{(i-1)}|_U) \quad (74)$$

$$\frac{\partial}{\partial \ln(k)_D} \Pi_K^{(i)} = (p_K^{(i)} - p_D^{(i)}) \lambda_{\text{tot}}^{(i-1)}|_D \frac{\partial}{\partial b} \text{hm}(\lambda_{\text{tot}}^{(i-1)}|_K, \lambda_{\text{tot}}^{(i-1)}|_D) \quad (75)$$

where

$$\frac{\partial}{\partial b} \text{hm}(a, b) := \frac{2a^2}{(a+b)^2}. \quad (76)$$

On the other hand, the saturation residuals  $\Sigma_K$  lead to the following derivatives

$$\begin{aligned}
\frac{\partial}{\partial \ln(k)_K} \Sigma_K = & \lambda_{\text{tot}}^{(i-1)}|_K \frac{\Delta t}{h} \left( \right. \\
& (f(S_{\text{w}}^{(i-1)})v_{\text{tot},x}^{(i-1)})|_E \frac{\partial}{\partial b} \text{hm}(\lambda_{\text{tot}}^{(i-1)}|_E, \lambda_{\text{tot}}^{(i-1)}|_K) \\
& - (f(S_{\text{w}}^{(i-1)})v_{\text{tot},x}^{(i-1)})|_W \frac{\partial}{\partial b} \text{hm}(\lambda_{\text{tot}}^{(i-1)}|_W, \lambda_{\text{tot}}^{(i-1)}|_K) \\
& + (f(S_{\text{w}}^{(i-1)})v_{\text{tot},y}^{(i-1)})|_N \frac{\partial}{\partial b} \text{hm}(\lambda_{\text{tot}}^{(i-1)}|_N, \lambda_{\text{tot}}^{(i-1)}|_K) \\
& \left. - (f(S_{\text{w}}^{(i-1)})v_{\text{tot},y}^{(i-1)})|_S \frac{\partial}{\partial b} \text{hm}(\lambda_{\text{tot}}^{(i-1)}|_E, \lambda_{\text{tot}}^{(i-1)}|_S) \right)
\end{aligned} \tag{77}$$

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

$$\begin{aligned}
\frac{\partial}{\partial \ln(K)_L} \Sigma_K = & -\lambda_{\text{tot}}^{(i-1)}|_L \frac{\Delta t}{h} f(S_{\text{w}}^{(i-1)})v_{\text{tot},x}^{(i-1)}|_W \frac{\partial}{\partial b} \text{hm}(\lambda_{\text{tot}}^{(i-1)}|_K, \lambda_{\text{tot}}^{(i-1)}|_L)
\end{aligned} \tag{79}$$

$$\begin{aligned}
\frac{\partial}{\partial \ln(K)_U} \Sigma_K = & \lambda_{\text{tot}}^{(i-1)}|_U \frac{\Delta t}{h} f(S_{\text{w}}^{(i-1)})v_{\text{tot},x}^{(i-1)}|_N \frac{\partial}{\partial b} \text{hm}(\lambda_{\text{tot}}^{(i-1)}|_K, \lambda_{\text{tot}}^{(i-1)}|_U)
\end{aligned} \tag{80}$$

$$\begin{aligned}
\frac{\partial}{\partial \ln(K)_D} \Sigma_K = & -\lambda_{\text{tot}}^{(i-1)}|_D \frac{\Delta t}{h} f(S_{\text{w}}^{(i-1)})v_{\text{tot},x}^{(i-1)}|_S \frac{\partial}{\partial b} \text{hm}(\lambda_{\text{tot}}^{(i-1)}|_K, \lambda_{\text{tot}}^{(i-1)}|_D)
\end{aligned} \tag{81}$$