

# DTU



TECHNICAL UNIVERSITY  
OF DENMARK

SPECIAL COURSE - DHRTC

–

---

## **Fitting of Mass Transfer Coefficients for Simulation of DME flooding**

---

*Students:*

FREDERIK LEHN, s134594

*Supervisors:*

ALI AKBAR EFTEKHARI

HAMID NICK

March 19, 2018

# CONTENTS

<b>1 Abstract</b>	<b>1</b>
<b>2 Introduction</b>	<b>1</b>
<b>3 Governing Equations</b>	<b>1</b>
3.1 Model: No gravity, no capillary pressure, incompressible . . . . .	3
3.2 Model: Gravity, capillary pressure, compressible . . . . .	4
<b>4 Discretization</b>	<b>4</b>
4.1 Model: No gravity, no capillary pressure, incompressible . . . . .	4
4.2 Model: Gravity, capillary pressure, compressible . . . . .	5
<b>5 Optimization</b>	<b>5</b>
<b>6 Results</b>	<b>6</b>
6.1 Model: No gravity, no capillary pressure, incompressible . . . . .	6
6.2 Simulations using Optimal Mass Transfer Coefficients . . . . .	9
6.2.1 1D . . . . .	9
6.2.2 2D . . . . .	9
<b>7 Discussion</b>	<b>14</b>
<b>8 Conclusion</b>	<b>14</b>
<b>9 Appendix A</b>	<b>16</b>
9.1 Model: No gravity, no capillary pressure, incompressible . . . . .	16
9.2 Model: Gravity, capillary pressure, compressible . . . . .	17
<b>10 Appendix B</b>	<b>21</b>
10.1 Model: No gravity, no capillary pressure, incompressible . . . . .	21
10.1.1 Sub Division of Terms . . . . .	22
10.1.2 Coefficients of Terms . . . . .	22
10.2 Model: Gravity, capillary pressure, compressible . . . . .	23
10.2.1 Sub Division of Terms . . . . .	24
10.2.2 Coefficients of Terms . . . . .	25
<b>11 Appendix C</b>	<b>29</b>
11.1 Model: No gravity, no capillary pressure, incompressible . . . . .	30
11.2 Model: Gravity, capillary pressure, compressible . . . . .	30

# LIST OF FIGURES

1	Multiple simulations of various $k_w$ and $k_o$ values. . . . .	8
2	Heat-map of the error of the simulations . . . . .	8
3	Propagation fronts after 2 PVI water injection follows by 0.3 PVI DME injection (left). Progra- tion of fronts after 0.5 PVI of DME injection (right). . . . .	9
4	Relative permeabilities during water flooding (left). The relative permeabilities once the core is flooded to full DME concentration (right). . . . .	10

5	Concentration of DME in water after injecting 0.5 PVI, 1 PVI, 3 PVI and 6 PVI of DME respectively. . . . .	11
6	Concentration of DME in oil after injecting 0.5 PVI, 1 PVI, 3 PVI and 6 PVI of DME respectively. . . . .	11
7	Residual oil saturation after injecting 0.5 PVI, 1 PVI, 3 PVI and 6 PVI of DME respectively. . . . .	12
8	Pressure after injecting 0.5 PVI, 1 PVI, 3 PVI and 6 PVI of DME respectively. . . . .	12
9	Water saturation after injecting 0.5 PVI, 1 PVI, 3 PVI and 6 PVI of DME respectively. . . . .	13
10	Recovery factor after injecting 0.5 PVI, 1 PVI, 3 PVI and 6 PVI of DME respectively. . . . .	13

## LIST OF TABLES

1	History matched relative permeability parameters . . . . .	6
2	Simulation Parameters . . . . .	7

# 1. ABSTRACT

This paper investigates the effect of the mass transfer coefficients on the simulation of DME flooding. The results show that the coefficients have a significant impact on the simulated effects. Further, empirical formulations for estimating the coefficients yield order of magnitude errors compared to the optimal solutions, and thus fitting is required for obtaining realistic simulation results. It is also found, that trying to solve the problem as a least-squares problem with gradient-based algorithms are an ill-defined approach, and further investigation into this aspect is required to avoid manual, trial and error, fitting.

# 2. INTRODUCTION

It is well known that Enhanced Oil Recovery (EOR) methods increase the recovery factor, usually after primary and secondary recovery declines. The investments in EOR equipment (facilities, chemicals, etc.) are substantial, and hence the incremental recovery has to generate a higher cashflow than the investment. This requires the incremental recovery to be forecasted in order to substantiate an investment decision. There exists different types of EOR, and work is ongoing regarding understanding of the physical mechanisms that drive the increased recovery as well as building methods for forecasting the recovery of these methods. This paper is concerned with the EOR method Dimethyl Ether (DME) flooding, where DME is added to the injection water, which is then transferred to the oil-phase, affecting various physical parameters which increases the mobility of the fluid as well as lowering the residual oil saturation, allowing more oil to be recovered.

# 3. GOVERNING EQUATIONS

This section is heavily based on papers provided by Ali Akbar Eftekhari.

The concentration of Dimethyl Ether (DME) in the oleic and aqueous phase is assumed to be at equilibrium condition at the oil-water interface. DME is transferred between the two phases, by first diffusing from the bulk of the water phase, to the interface, then reaching equilibrium and then diffusing into the bulk of the oil phase. The flux of DME between the two phases may be written as

$$J_{DME} = K_w(c_w - c_w^*) = K_o(c_o^* - c_o) \quad (1)$$

where  $J_{DME}$  is the flux of DME [mol/(m<sup>2</sup>s)],  $c_w$  [mol/m<sup>3</sup>] is the concentration of DME in the bulk of water,  $c_o$  [mol/m<sup>3</sup>] is the concentration of DME in the bulk of oil,  $K_o$  [m/s] and  $K_w$  [m/s] are the overall mass transfer coefficients of oil and water respectively. The concentrations  $c_w^*$  [mol/m<sup>3</sup>] and  $c_o^*$  [mol/m<sup>3</sup>] are defined as follows, when the two phases are at equilibrium

$$\begin{aligned} c_w^* &= \frac{c_o}{K} \\ c_o^* &= Kc_w \end{aligned} \quad (2)$$

where  $K$  [-] is the partition coefficient (or equilibrium constant). The flux of DME may also be written differently, namely in terms of the flux within each phase, which is equal to the flux between the phases

$$J_{DME} = k_w(c_w - c_{w,i}) = k_o(c_{o,i} - c_o) \quad (3)$$

where  $k_{w,i}$  [m/s] and  $k_{o,i}$  [m/s] are the mass transfer coefficient of the respective phases and  $c_{o,i}$  and  $c_{w,i}$  are the concentrations of DME at equilibrium at the interface of the two phases. The following relationship exists between the the equilibrium concentrations at the interface, the equilibrium constant, overall mass

transfer coefficients and mass transfer coefficients

$$K = \frac{c_{o,i}}{c_{w,i}}$$

$$\frac{1}{K_w} = \frac{1}{Kk_o} + \frac{1}{k_w} \quad (4)$$

$$\frac{1}{K_o} = \frac{1}{k_o} + \frac{K}{k_w}$$

where it is relevant to isolate  $K_w$  and  $K_o$  respectively

$$K_w = \frac{1}{\frac{1}{Kk_o} + \frac{1}{k_w}} = \frac{Kk_o k_w}{Kk_o + k_w} \quad (5)$$

$$K_o = \frac{1}{\frac{1}{k_o} + \frac{K}{k_w}} = \frac{k_o k_w}{Kk_o + k_w} \quad (6)$$

The mass transport of DME boils down to a set of partial differential equations which are all variations of the transport equation. The two variations are coupled reactive transport and two phase flow respectively, which results in the following set of equations to be solved

$$\frac{\partial(\phi c_w S_w)}{\partial t} + \nabla \cdot (\mathbf{u}_w c_w - \mathcal{D}_w \phi \nabla c_w) + K_w a \phi (c_w - c_w^*) = 0 \quad (7)$$

$$\frac{\partial(\phi c_o S_o)}{\partial t} + \nabla \cdot (\mathbf{u}_o c_o - \mathcal{D}_o \phi \nabla c_o) + K_o a \phi (c_o - c_o^*) = 0 \quad (8)$$

$$\frac{\partial(\phi \rho_w S_w)}{\partial t} + \nabla \cdot (\rho_w \mathbf{u}_w) = 0 \quad (9)$$

$$\frac{\partial(\phi \rho_o S_o)}{\partial t} + \nabla \cdot (\rho_o \mathbf{u}_o) = 0 \quad (10)$$

$$S_w + S_o = 1 \quad (11)$$

where  $\phi$  [-] is the porosity,  $a$  [ $\text{m}^2/\text{m}^3$ ] is the specific surface area between the two fluid phases per unit volume,  $\rho_\alpha$  [ $\text{kg}/\text{m}^3$ ] is the density and  $S_\alpha$  is the saturation. Further, the velocities  $\mathbf{u}_o$  and  $\mathbf{u}_w$  are called Darcy velocities and are defined by

$$\mathbf{u}_w = -\frac{k k_{rw}}{\mu_w} (\nabla p_w - \rho_w \mathbf{g}) \quad (12)$$

$$\mathbf{u}_o = -\frac{k k_{ro}}{\mu_o} (\nabla p_o - \rho_o \mathbf{g}) \quad (13)$$

where  $k$  is the permeability,  $\mu_\alpha$  is the viscosity and the relative permeabilities,  $k_{ro}$  and  $k_{rw}$  are modelled using the Corey relations

$$k_{rw} = k_{rw}^0 \left( \frac{S_w - S_{wc}}{1 - S_{wc} - S_{or}} \right)^{n_w}$$

$$k_{ro} = k_{ro}^0 \left( \frac{1 - S_w - S_{or}}{1 - S_{wc} - S_{or}} \right)^{n_o} \quad (14)$$

where  $k_{rw}^0$  is the relative permeability of water at residual oil saturation,  $k_{ro}^0$  is the relative permeability of oil at irreducible saturation,  $S_{wc}$  is the irreducible water saturation,  $S_{or}$  is the residual oil saturation and  $n_\alpha$  are relative permeability exponents.

Due to capillary forces, there may occur a pressure difference between the water phase and oil phase, defined by

$$p_c = p_o - p_w \Leftrightarrow p_o = p_w + p_c \quad (15)$$

meaning the phase pressures reduce to one variable,  $p_w = p$  and  $p_o = p + p_c$  where  $p_c$  is the capillary pressure which may be modelled using any arbitrary model.

Similar to the reduction in the number of pressure variables, the number of saturation variables are reduced as well using (11), which allows for removing the variable  $S_o$  as follows

$$S_w + S_o = 1 \Leftrightarrow S_o = 1 - S_w \quad (16)$$

which may be substituted into all equations, and hence  $S_w = S$  and  $S_o = (1 - S)$ .

Two cases of (7)-(11) will be described and analytically derived. A simplified model where gravity is ignored, the formation and fluids are considered incompressible and capillary pressure is ignored. The second model includes gravity, fluid compressibility and capillary pressure.

### 3.1. Model: No gravity, no capillary pressure, incompressible

The simple model assumes the following: Gravity is ignored, the fluids are incompressible, the formation is incompressible, there is no capillary pressure, hence

$$p_c = p_o - p_w = 0 \Leftrightarrow p_o = p_w = p \quad (17)$$

the density & viscosity of oil as well as the viscosity of water are polynomial functions of  $c_o$ , the same goes for the residual oil saturation and relative permeability of oil at connate water saturation, which are both linear functions. The  $S_{or}$  is a function of the concentration of DME dissolved in the oleic phase

$$S_{or} = m_s c_o + S_{or,max} \quad (18)$$

where  $m_s < 0$  is the slope at which residual oil saturation changes with solvent concentration and  $S_{or,max}$  is the maximum residual oil saturation. The parameter,  $k_{ro}^0$ , is a linear function of the  $S_{or}$

$$k_{ro}^0 = m_k S_{or} + k_{ro,max}^0 \quad (19)$$

where  $m_k < 0$  is the slope at which relative permeability of oil at connate water saturation increases with decreasing  $S_{or}$ . It is also assumed that the residual oil saturation's dependency on  $c_o$  can be decoupled as well as  $k_{ro}^0$  dependency on  $S_{or}$ , and thus both are considered independent in the linearization.

The polynomial relationships of the densities and viscosities are found by fitting polynomials to experimental data from SPE-papers.

Density of oil (SPE-177919)

$$\rho_o(c_o) = 748 - 1.64 \cdot 10^{-3} c_o + 2.936 \cdot 10^{-7} c_o^2 - 4.107 \cdot 10^{-11} c_o^3 \quad (20)$$

Viscosity of oil (SPE-177919)

$$\mu_o(c_o) = 1.013 \cdot 10^{-3} - 2.529 \cdot 10^{-7} c_o + 2.387 \cdot 10^{-11} c_o^2 \quad (21)$$

Viscosity of water (SPE-177919)

$$\mu_w(c_w) = 4.071 \cdot 10^{-4} + 1.473 \cdot 10^{-7} c_w \quad (22)$$

The choice of order of polynomial is done based on a visual evaluation of the fit. The equilibrium constant could also be considered a function of the oil concentration, but appears to be approximately constant for a sufficient interval, and thus this mechanism is ignored.

### 3.2. Model: Gravity, capillary pressure, compressible

The complex model assumes the following: Gravity is included, the fluids are compressible (density only), the formation is incompressible, there is capillary pressure. The density & viscosity of oil as well as the viscosity of water and the equilibrium constant are polynomial functions of  $c_o$ , similarly the residual oil saturation is given by (18). This time the residual oil saturation's dependency on  $c_o$  is not considered decoupled and thus  $k_{rw}$  and  $k_{ro}$  are functions of  $c_o$ .  $k_{ro}^0$  dependency on  $S_{or}$  was a late addition to the simulations and has thus not yet been included in the complex model, as it is substantially more time consuming when it can not be considered decoupled from the remainder of the system.

The dependency of the viscosities will again be given by (21) and (22). The density of water will be given by

$$\rho_w(p) = \rho_w \cdot e^{\kappa_w(p-p_{ref})} \quad (23)$$

the density of oil

$$\rho_o(c_o, p) = \rho_o(c_o) \cdot e^{\kappa_o(p-p_{ref})} = (748 - 1.64 \cdot 10^{-3}c_o + 2.936 \cdot 10^{-7}c_o^2 - 4.107 \cdot 10^{-11}c_o^3) \cdot e^{\kappa_o(p-p_{ref})} \quad (24)$$

where  $\kappa_w$  [Pa<sup>-1</sup>] &  $\kappa_o$  [Pa<sup>-1</sup>] are compressibility factors and  $p_{ref}$  is the pressure at which the initial density is measured at. The equilibrium constant is given by

$$K(c_o) = 1,838 - 5,531 \cdot 10^{-5}c_o - 3.121 \cdot 10^{-8}c_o^2 + 2.308 \cdot 10^{-11}c_o^3 \quad (25)$$

## 4. DISCRETIZATION

In order to be able to discretize the system it first has to be linearized. The linearization of both the simple and complex model can be seen in appendix A.

### 4.1. Model: No gravity, no capillary pressure, incompressible

In general the system will be solved fully coupled, except for (18) and (19) which will not be coupled, to eliminate the dependency of the relative permeabilities on  $c_o$  and relative permeability of oil on  $S_{or}$ . Discretizing the linearized system of equations allows for defining a linear system of equations on algebraic form

$$\begin{bmatrix} \mathbf{M}_{c_w,1} + \mathbf{J}_{c_w,1} & \mathbf{M}_{c_o,1} & \mathbf{J}_{p,1} & \mathbf{J}_{S,1} \\ \mathbf{M}_{c_w,2} & \mathbf{M}_{c_o,2} + \mathbf{J}_{c_o,2} & \mathbf{J}_{p,2} & \mathbf{J}_{S,2} \\ \mathbf{J}_{c_w,3} & \mathbf{0} & \mathbf{M}_{p,3} + \mathbf{J}_{p,3} & \mathbf{J}_{S,3} \\ \mathbf{0} & \mathbf{J}_{c_o,4} & \mathbf{J}_{p,4} & \mathbf{M}_{S,4} + \mathbf{J}_{S,4} \end{bmatrix} \begin{bmatrix} \mathbf{c}_w \\ \mathbf{c}_o \\ \mathbf{p} \\ \mathbf{S} \end{bmatrix} = \begin{bmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \\ \mathbf{b}_3 \\ \mathbf{b}_4 \end{bmatrix} \quad (26)$$

where the variables are defined as

$$\mathbf{c}_w = \begin{bmatrix} c_{w,1} \\ \vdots \\ c_{w,n+2} \end{bmatrix}, \quad \mathbf{c}_o = \begin{bmatrix} c_{o,1} \\ \vdots \\ c_{o,n+2} \end{bmatrix}, \quad \mathbf{p} = \begin{bmatrix} p_1 \\ \vdots \\ p_{n+2} \end{bmatrix}, \quad \mathbf{S} = \begin{bmatrix} S_1 \\ \vdots \\ S_{n+2} \end{bmatrix} \quad (27)$$

Appendix B & C show how to construct the system matrix and RHS.

## 4.2. Model: Gravity, capillary pressure, compressible

For the complex model, everything is assumed to be fully coupled, including (18). The system may be written as a linear system of equations on algebraic form as follows

$$\begin{bmatrix} \mathbf{M}_{c_w,1} + \mathbf{J}_{c_w,1} & \mathbf{J}_{c_o,1} & \mathbf{J}_{p,1} & \mathbf{J}_{S,1} \\ \mathbf{J}_{c_w,2} & \mathbf{M}_{c_o,2} + \mathbf{J}_{c_o,2} & \mathbf{J}_{p,2} & \mathbf{J}_{S,2} \\ \mathbf{J}_{c_w,3} & \mathbf{J}_{c_o,3} & \mathbf{M}_{p,3} + \mathbf{J}_{p,3} & \mathbf{J}_{S,3} \\ \mathbf{0} & \mathbf{J}_{c_o,4} & \mathbf{J}_{p,4} & \mathbf{M}_{S,4} + \mathbf{J}_{S,4} \end{bmatrix} \begin{bmatrix} \mathbf{c}_w \\ \mathbf{c}_o \\ \mathbf{p} \\ \mathbf{S} \end{bmatrix} = \begin{bmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \\ \mathbf{b}_3 \\ \mathbf{b}_4 \end{bmatrix} \quad (28)$$

where the variables are defined as

$$\mathbf{c}_w = \begin{bmatrix} c_{w,1} \\ \vdots \\ c_{w,n+2} \end{bmatrix}, \quad \mathbf{c}_o = \begin{bmatrix} c_{o,1} \\ \vdots \\ c_{o,n+2} \end{bmatrix}, \quad \mathbf{p} = \begin{bmatrix} p_1 \\ \vdots \\ p_{n+2} \end{bmatrix}, \quad \mathbf{S} = \begin{bmatrix} S_1 \\ \vdots \\ S_{n+2} \end{bmatrix} \quad (29)$$

Appendix B & C show how to construct the system matrix and RHS.

## 5. OPTIMIZATION

The objective of the optimization is to find the optimal values of the mass transfer coefficients,  $k_o$  and  $k_w$ , for a specific sample tested in a lab. The objective function is a least-squares formulation of the difference between the observed and estimated recovery factors

$$\min_{k_o, k_w} r = ||R_{Lab} - R||_2 \quad (30)$$

where

$$R = \frac{\int_V \phi \rho_o (1 - S_{w,0}) dV - \int_V \phi \rho_o (1 - S_w) dV}{\int_V \phi \rho_o (1 - S_{w,0}) dV} \quad (31)$$

Both  $R_{lab}$  and  $R$  are vectors sampled at discrete times  $t$ .  $S_{w,0}$  is the initial water saturation of the core.

As for all optimization problems, an initial guess has to be provided for the optimal solution. A key issue with the specific problem at hand is computational efficiency, and the better the initial guess, the faster the solution converges (and also the more likely it is that it will converge). For this reason a heuristic is used to calculate the initial guess. Several empirical methods exist for estimating the mass transfer coefficients. The lab results considered here will be based on core samples, and is thus cylindrical. For this reason the relationship for a cylindrical shape is used

$$\text{Sh} = 0.023 \text{Re}^{0.83} \text{Sc}^{1/3} \quad (32)$$

where Sh (Sherwood), Re (Reynolds) and Sc (Schmidt) are dimensionless numbers given by

$$\begin{aligned} \text{Sh} &= \frac{k_\alpha d}{\mathcal{D}_\alpha} \\ \text{Re} &= \frac{\rho_\alpha v_\alpha d}{\mu_\alpha} \\ \text{Sc} &= \frac{\mu_\alpha}{\rho_\alpha \mathcal{D}_\alpha} \end{aligned} \quad (33)$$

hence the initial guess is estimated as

$$k_w = 0.023 \frac{\mathcal{D}_w}{d} \left( \frac{\rho_w v_w d}{\mu_w} \right)^{0.83} \left( \frac{\mu_w}{\rho_w \mathcal{D}_w} \right)^{1/3} \quad (34)$$

$$k_o = 0.023 \frac{\mathcal{D}_o}{d} \left( \frac{\rho_o v_o d}{\mu_o} \right)^{0.83} \left( \frac{\mu_o}{\rho_o \mathcal{D}_o} \right)^{1/3} \quad (35)$$

where  $d$  is the characteristic length of the domain (capillary diameter,  $\sqrt{k}$ ).



## 6. RESULTS

The effect of the mass transfer coefficients on the simulation of DME enhanced waterflooding will be tested on experiment 1 from [1]. History matched relative permeability coefficients have been provided by Ali Akbar Eftekhari.

**Table 1:** History matched relative permeability parameters

Variable	Symbol	Value	Unit
Connate water saturation	$S_{wc}$	0.206	-
Maximum residual oil saturation	$S_{or,max}$	0.1988	-
Minimum residual oil saturation	$S_{or,min}$	0.01	-
Maximum relative oil permeability (endpoint)	$k_{ro,max}^0$	0.95	-
Minimum relative oil permeability (endpoint)	$k_{ro,min}^0$	0.2498	-
Water Corey exponent	$n_w$	3.222	-
Oil Corey exponent	$n_o$	3.037	-

Notice however that the minimum residual oil saturation and maximum relative oil permeability endpoint are not history matched, but based on visual inspection of the recovery curve. As mentioned the variability of the residual oil saturation and relative oil permeability end point is a linear function. The slopes for the functions are calculated as follows

$$m_s = -\frac{S_{or,max} - S_{or,min}}{c_{o,max} - c_{o,min}} \quad (36)$$

where  $c_{o,max}$  is given as the two times the concentration of DME dissolved in the injection water and  $c_{o,min} = 0$ .

$$m_k = -\frac{k_{ro,max}^0 - k_{ro,min}^0}{S_{or,max} - S_{or,min}} \quad (37)$$

There are a wide array of variables which can be optimized in a simulation of flow through a porous medium, such as relative permeabilities, the geophysical parameters, etc. The parameters of interest in this project are the mass transfer coefficients of DME from the water phase, to the oil phase. What is especially of interest is the delayed response from when the DME slug is injected and until it can be seen by a bump in the recovery curve.

Having investigated the effect of  $k_w$  and  $k_o$  on the simulation results, as well as making multiple optimization runs with various start guesses, it is evident that the optimization problem is ill-defined for a gradient based optimization algorithm. For this reason a crude method has been adopted for optimizing the parameters, namely plotting them using a heat-map and visually assessing the region of interest. The various mass transfer values used for the runs will be permutations around the heuristics seen in (34) and (35).

Optimization results will only be provided using the simple model, because the complex model converges too slowly to be feasible for optimization.

### 6.1. Model: No gravity, no capillary pressure, incompressible

The parameters used in the simulation of the DME flooding are outlined in Tab. 2.

**Table 2:** *Simulation Parameters*

Variable	Symbol	General		Unit
Core length	$L_x$	0.104		m
Core diameter	$D$	0.025		m
Porosity	$\phi$	0.256		-
Permeability	$k$	$10^{-15}$		$\text{m}^2$
Density of matrix	$\rho_m$	2700		$\text{kg}/\text{m}^3$
Injection rate	$u_{inj}$	$9.21 \cdot 10^{-7}$		m/s
Equilibrium Constant	$K_{eq}$	2		-
Specific surface	$a$	4017600		$\text{m}^2/\text{m}^3$
Initial reservoir pressure	$p_{init}$	13.6		MPa
Saturation tolerance	-	$10^{-7}$		-
Concentration tolerance	-	$10^{-7}$		-
Variable	Symbol	Water	Oil	Unit
Diffusion constant	$\mathcal{D}$	$2 \cdot 10^{-9}$	$0.5 \cdot 10^{-9}$	$\text{m}^2/\text{s}$
Initial saturation	$S_{init}$	0.33	0.67	-
Initial DME condition	$c_{init}$	0	0	$\text{mol}/\text{m}^3$

In order to create a heat-map of the error,  $5 \times 5$  simulations are run with various combinations of  $k_w$  and  $k_o$ . The values are selected by applying the heuristic outlined in (34) and (35) and order of magnitude changes to these. The order of magnitude multipliers used are

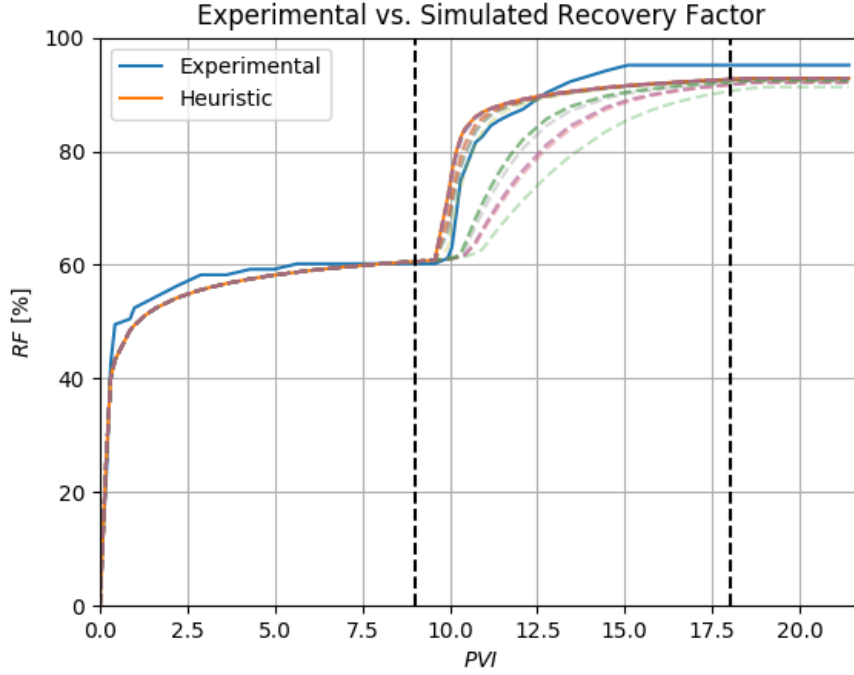
$$\left[10^{-4} \quad 10^{-3} \quad 10^{-2} \quad 10^{-1} \quad 10^1\right] \quad (38)$$

for both  $k_w$  and  $k_o$ , and the heuristic value is given by

$$k_{w,heu} = 3.08 \cdot 10^{-8} \quad (39)$$

and

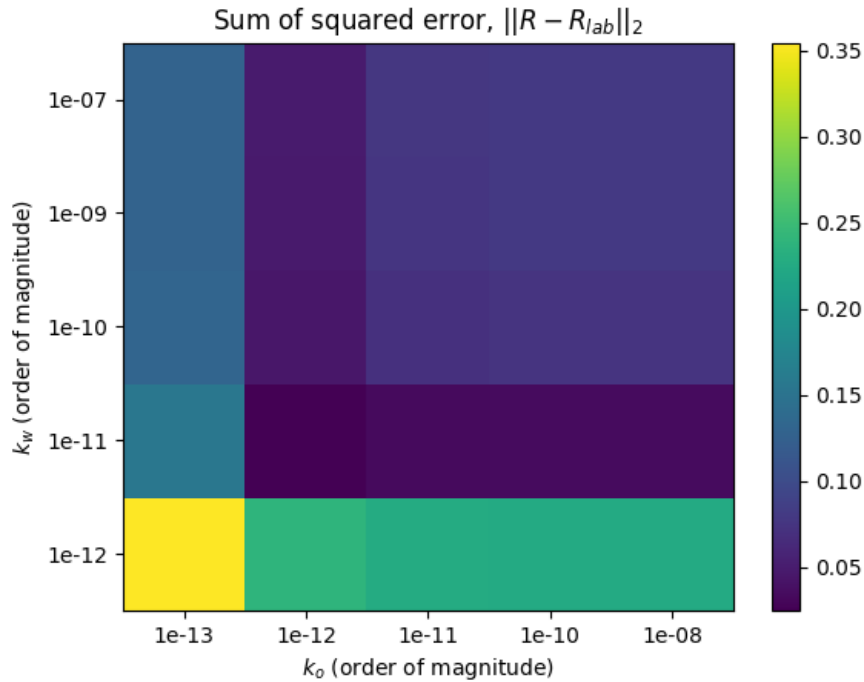
$$k_{o,heu} = 9.58 \cdot 10^{-9}. \quad (40)$$



**Figure 1:** Multiple simulations of various  $k_w$  and  $k_o$  values.

As can be seen from Fig. 1 the mass transfer coefficients have quite a significant impact on the delay of increased recovery, especially at low values. After reaching a certain level, an increase in the coefficients has no effect at all. This is because, once the coefficients reach a certain value, the mass transfer occurs faster than the advection of the DME, and thus it will have no further effect.

Heatmap of the error of the simulation with respect to the experimental data for the different simulations



**Figure 2:** Heat-map of the error of the simulations

Fig. 2 shows that the optimal mass transfer coefficients, i.e. the ones that minimize the sum of squared errors are at an order of magnitude of

$$k_w = 10^{-11}, \quad k_o = 10^{-12} \quad (41)$$

which corresponds to

$$k_{w,opt} = 3.08 \cdot 10^{-8} \cdot 10^{-3} = 3.08 \cdot 10^{-11}, \quad k_{o,opt} = 9.58 \cdot 10^{-9} \cdot 10^{-3} = 9.58 \cdot 10^{-12} \quad (42)$$

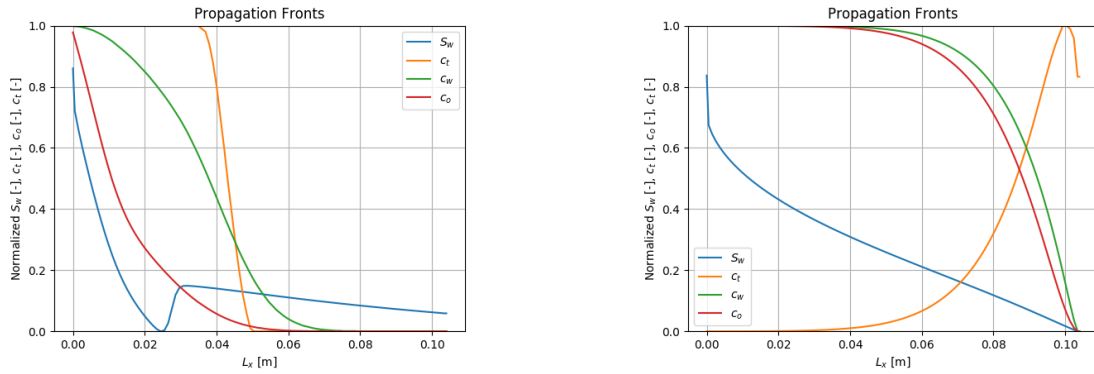
At this stage, it would be possible to narrow the area of interest to small perturbations around the optimized coefficients, and rerun the optimization to further refine the estimates. However, as will be shown in the following simulations, the result seems to be in good agreement with the experimental solution.

A series of relevant figures are shown for the DME flooding scenario with the optimized mass transfer coefficients. Initially the propagation fronts of the various variables are shown in 1D, and then a wider array of variables are shown in 2D. For these simulations, the same parameters as seen in Tab. 1 & 2 are used. For the 2D case there is the difference that a heterogeneous permeability field is used, as this provides a more interesting case, which better highlights effects such as flow paths.

## 6.2. Simulations using Optimal Mass Transfer Coefficients

### 6.2.1. 1D

The propagation of the fronts of the water saturation,  $S_w$ , a tracer injected at the same time as the DME,  $c_t$ , the concentration of DME in water,  $c_w$  and the concentration of DME in oil,  $c_o$  is shown on Fig. 3

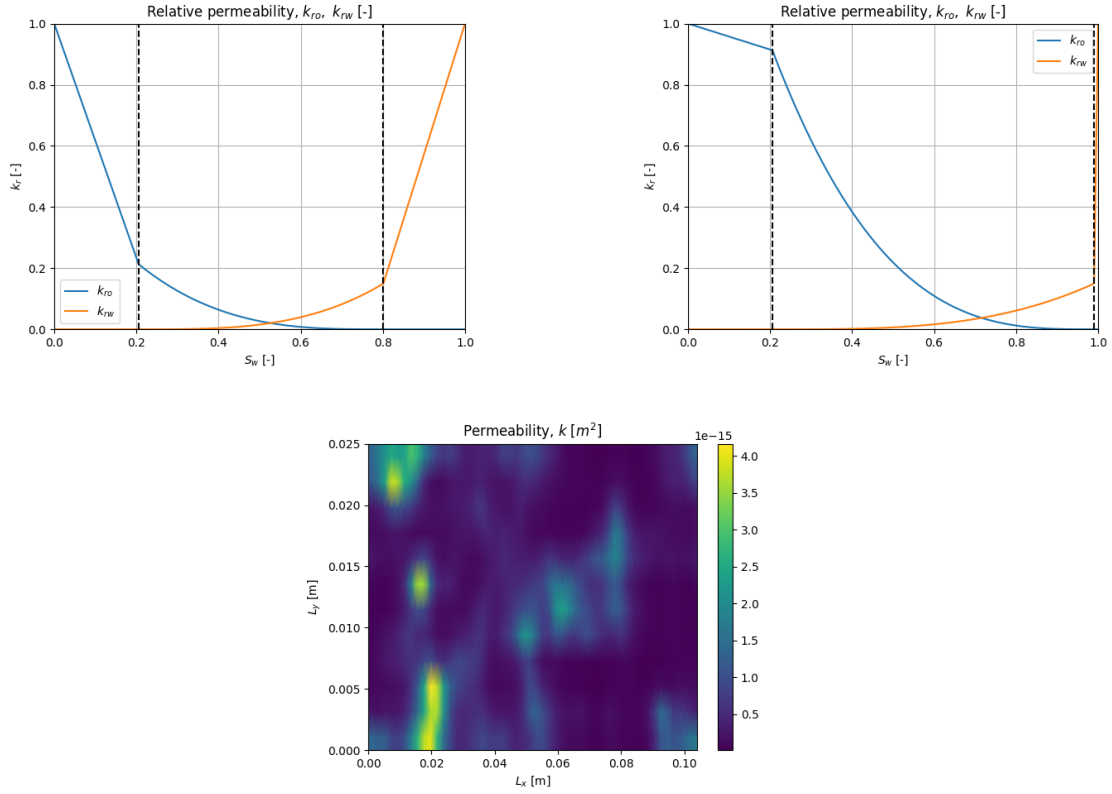


**Figure 3:** Propagation fronts after 2 PVI water injection followed by 0.3 PVI DME injection (left). Propagation of fronts after 0.5 PVI of DME injection (right).

As can be seen the tracer is the fastest, then the concentration of DME in water, then DME in oil and lastly the mobilized oil front. Fig. 3 also show a difference in how sharp the fronts are. The sharpness is related to the diffusivity of the property. The tracer is solved using a non-upwind advection scheme and thus has the sharpest front. Both the concentration of DME in water and in oil have a diffusive term with different diffusivity constants as wells as using an upwind advection scheme. The water saturation has no diffusive term, but an upwind convection scheme

### 6.2.2. 2D

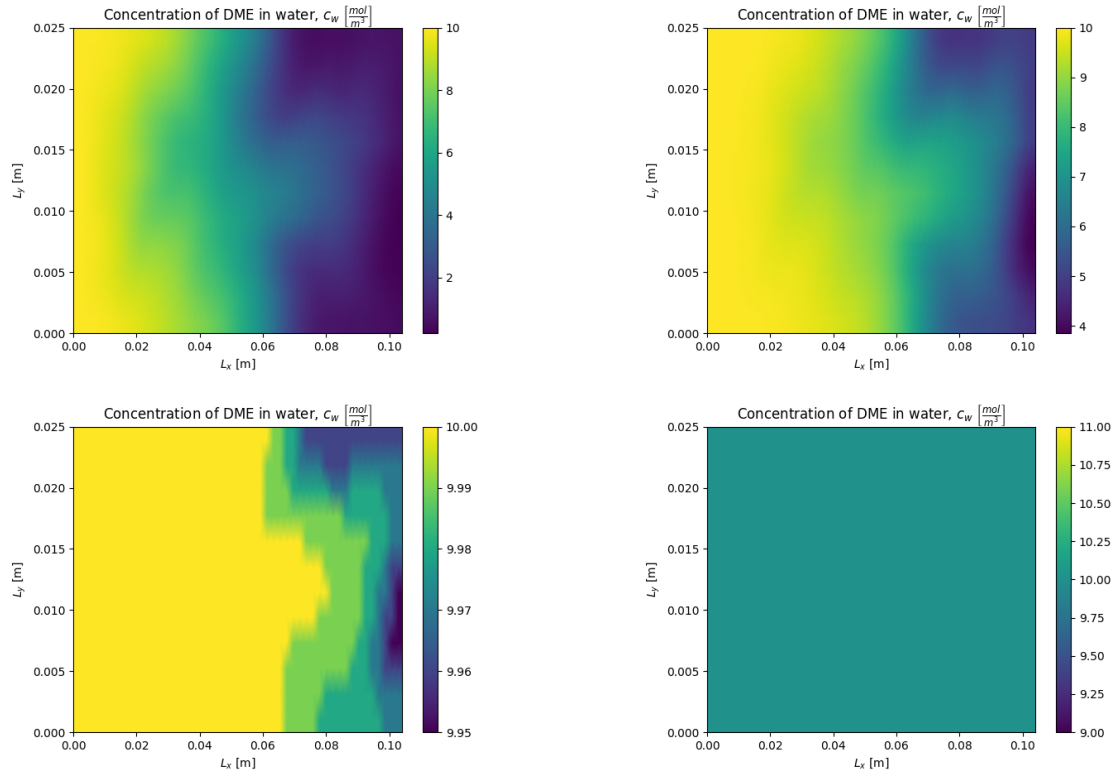
Fig. 4 shows the relative permeabilities at  $c_o = 0$  and  $c_o = c_{o,max}$  respectively, as well as the lognormally generated permeability field used for the simulations.



**Figure 4:** Relative permeabilities during water flooding (left). The relative permeabilities once the core is flooded to full DME concentration (right).

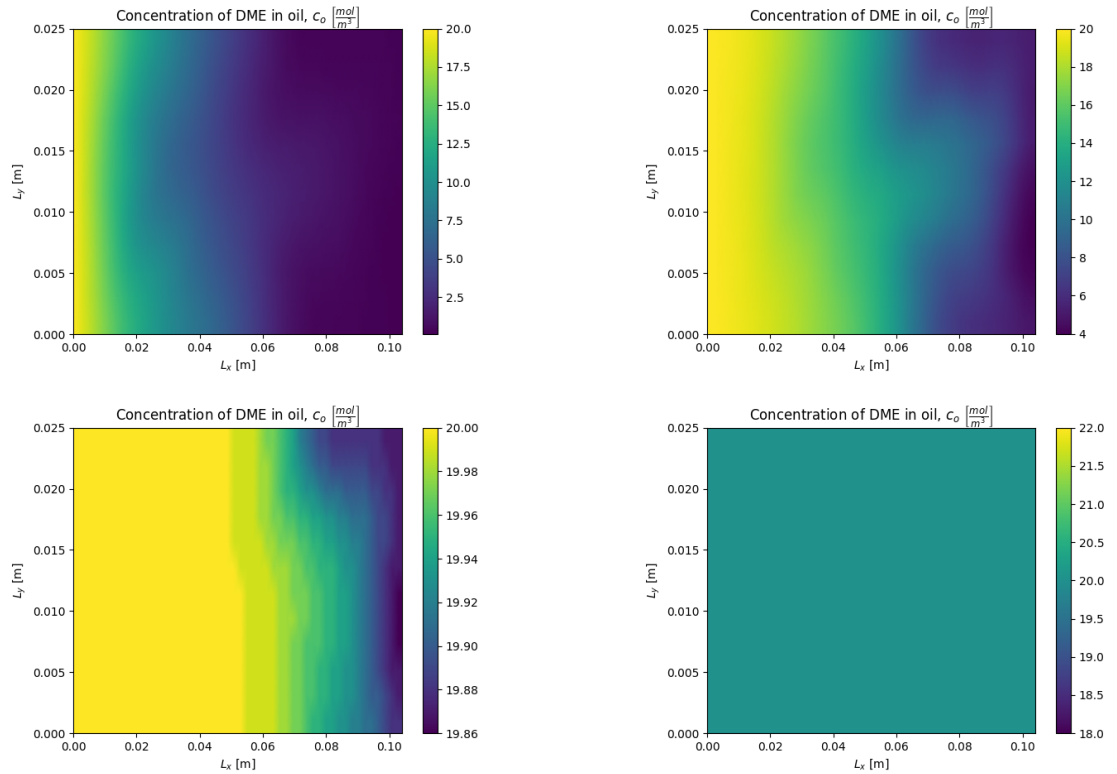
Four simulations are run. The first terminated after injecting 0.5 PVI of DME, the second after 1 PVI, the third after 3 PVI and the last after 6 PVI. All four simulations are preceded by a 9 PVI water flooding without DME.

## Concentration of DME in Water



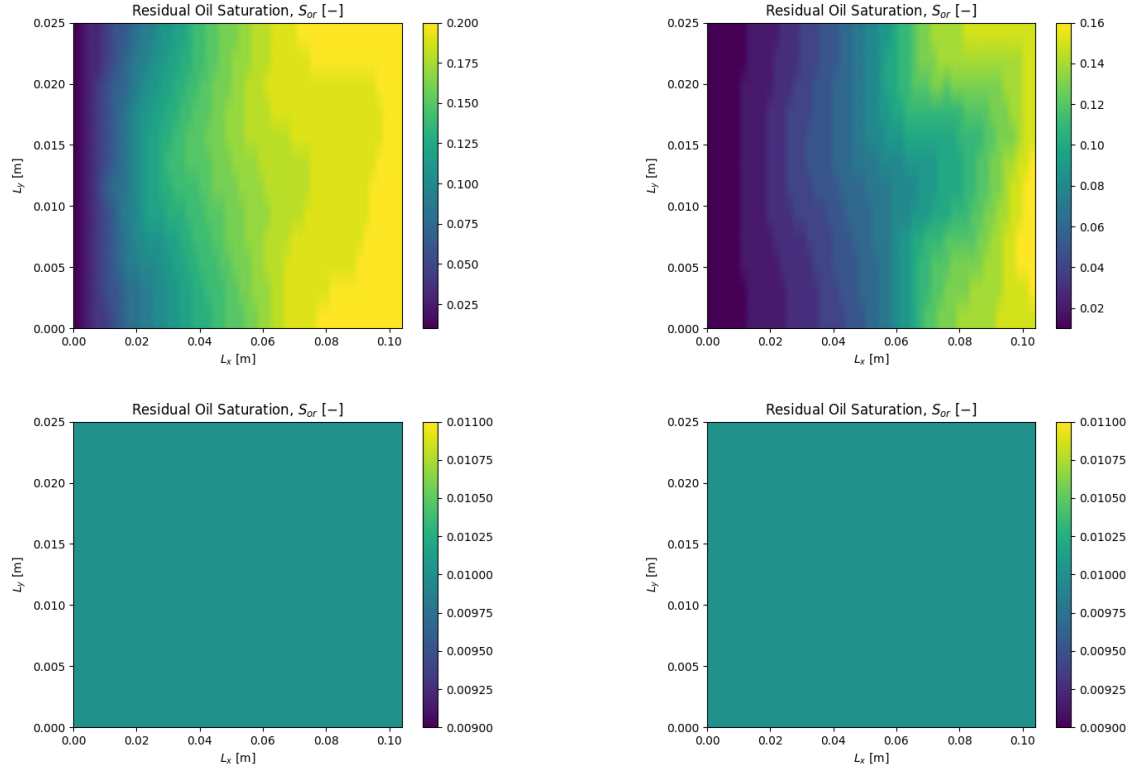
**Figure 5:** Concentration of DME in water after injecting 0.5 PVI, 1 PVI, 3 PVI and 6 PVI of DME respectively.

## Concentration of DME in Oil



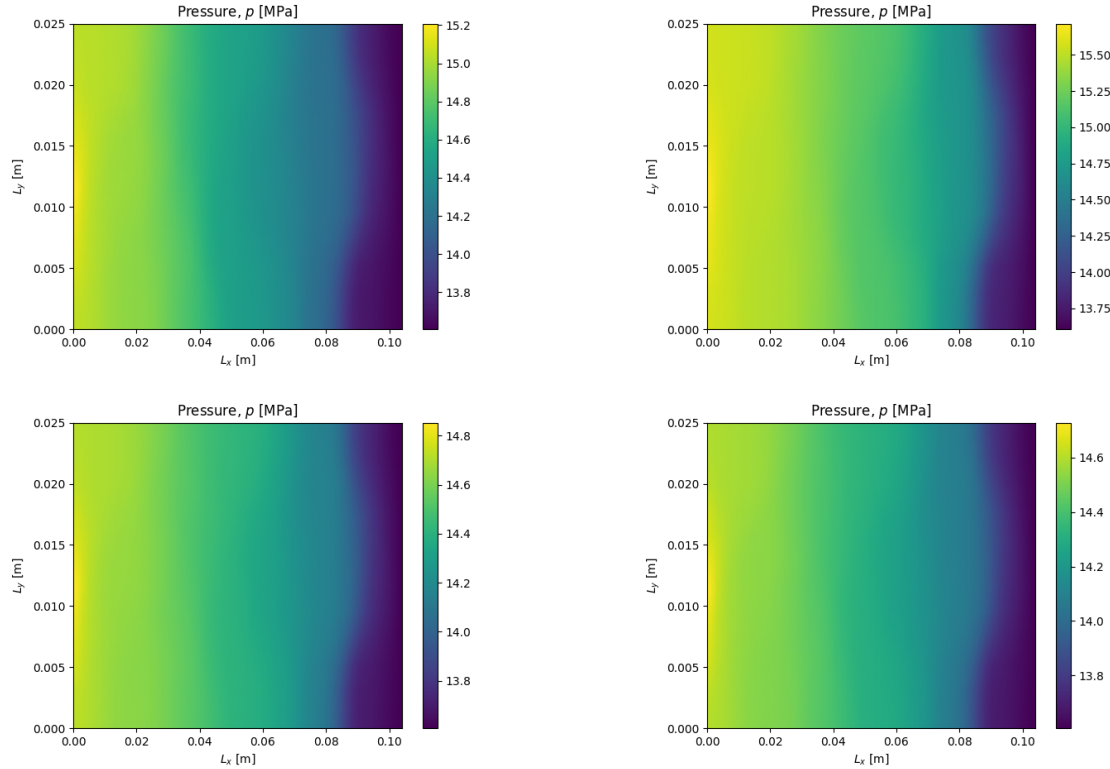
**Figure 6:** Concentration of DME in oil after injecting 0.5 PVI, 1 PVI, 3 PVI and 6 PVI of DME respectively.

## Residual Oil Saturation



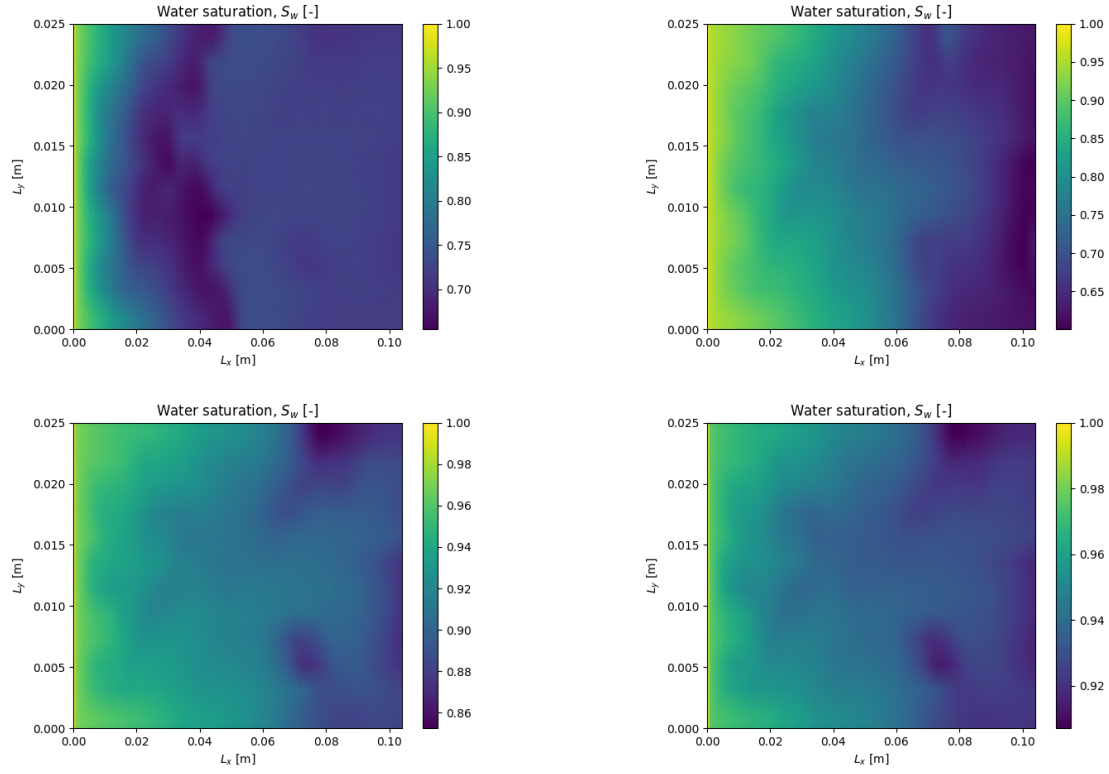
**Figure 7:** Residual oil saturation after injecting 0.5 PVI, 1 PVI, 3 PVI and 6 PVI of DME respectively.

## Pressure



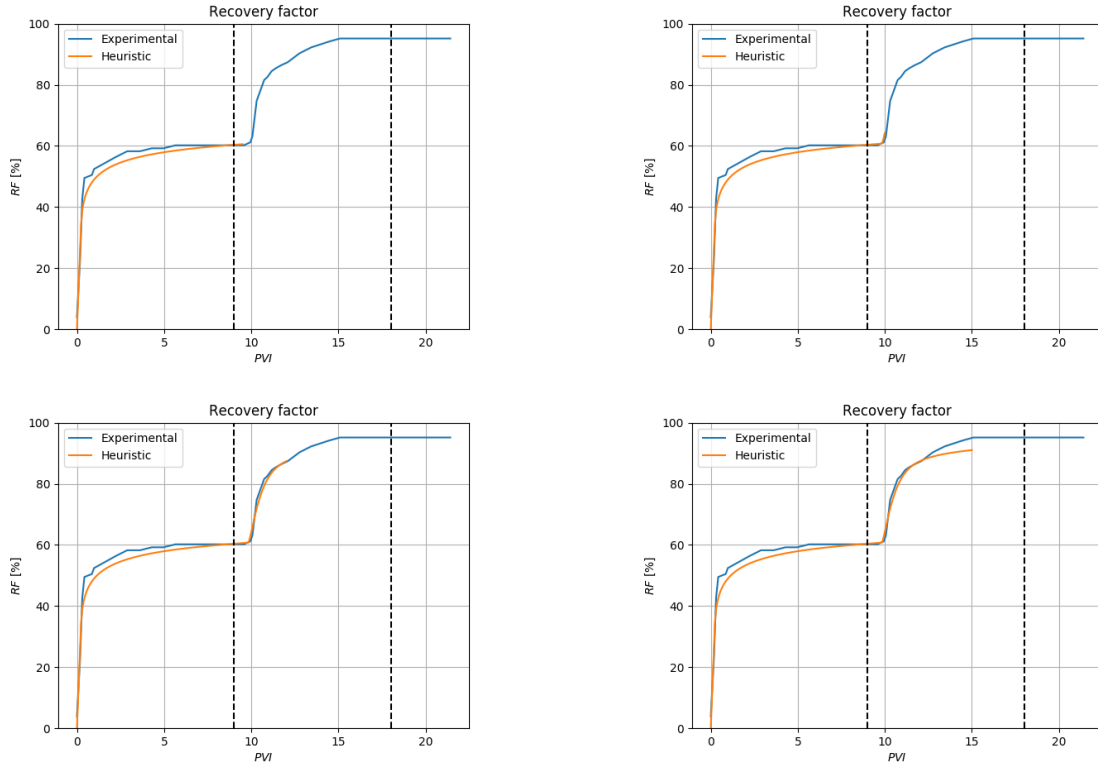
**Figure 8:** Pressure after injecting 0.5 PVI, 1 PVI, 3 PVI and 6 PVI of DME respectively.

## Water Saturation



**Figure 9:** Water saturation after injecting 0.5 PVI, 1 PVI, 3 PVI and 6 PVI of DME respectively.

## Recovery Factor



**Figure 10:** Recovery factor after injecting 0.5 PVI, 1 PVI, 3 PVI and 6 PVI of DME respectively.



In general the simulations behave as expected. It can be seen on Fig. 5 & 6 that the front of the DME in oil is behind the front of DME in water. Similarly Fig. 7 shows that the residual oil saturation is reduced in a pattern following the concentration of DME in oil. Fig. 9 (upper left) shows a front of low water saturation (higher oil saturation) moving through the core, due to previously residual oil being mobilized by the DME flooding.

A key issue is seen on Fig. 10, where the first three graphs, up until 12 PVI in total, shows that the simulated RF matches the experimental RF almost perfectly. However at 12 PVI and onward, the simulated RF tapers off, at the same time where it almost appears as though the experimental one experiences an additional bump in recovery. As seen on Fig. 1, the simulated RF never catches up, and ends at  $\approx 3 - 5\%$  lower than the experimental.

## 7. DISCUSSION

As outlined in the results section, the mass transfer coefficients,  $k_w$  &  $k_o$ , have a significant impact on the delay seen in incremental recovery seen after DME injection. However, this effect has a limit, which is reached once the transfer between the phases are as fast or faster than the advection of the DME. The results also showed that the heuristic formula is not a particularly good estimate of the coefficients, being three orders of magnitude too large, compared to the optimal solution.

Several attempts showed that various gradient based optimization algorithms had difficulties finding an optimal solution, both being very dependent on the initial guess as well as the resulting parameters being the same as the initial guess or only varied slightly. This means a manual approach had to be used, which most likely resulted in a more imprecise estimate. Though not investigated here, it is quite possible that either using a global optimization algorithm or redefining the optimization problem to something other than a least-squares problem, might allow for using an algorithm rather than a manual approach.

Also, as mentioned in the results sections, there is an issue with the recovery factor, where the simulation does not quite reach the same level as the experimental one. This is most likely due to one of two reasons. Either the DME creates additional physical effects, not taken into account in the reservoir simulator, or some of the parameters are not properly history matched. Most likely it is a combination of the two. Namely because a few of the relative permeabilities parameters, at the time of DME injection, is not history matched and the remaining relative permeability coefficients are assumed unaffected by the DME. This is not realistic, as there is a good chance the DME will change the wettability of the core and thus the relative permeability coefficients. There could also be a problem with the permeability field, which is heterogeneous for the RF seen in Fig. 10. However, since Fig. 1 shows the same behaviour for a homogeneous permeability field, this is doubtful.

Also, as can be seen from (34) and (35), the mass transfer coefficients are a function of viscosity, density and velocity. Since these properties are also functions of the concentration of DME in oil, it would mean that the mass transfer coefficients are not constant, but should vary as a function of the DME. This would result in different mass transfer coefficients through out the core.

## 8. CONCLUSION

There are several conclusions to be drawn. First and foremost, is that the mass transfer coefficients have a significant impact on the simulation of the DME effect. Secondly, the heuristic formulas do not provide a good estimate, and optimization of the parameters is required to get a realistic result. Further, the problem is ill-defined for using gradient based optimization algorithms to solve it, however

this part will require further investigation, by trying different algorithms or redefining the objective function.

Further, it appears that either some of the used parameters requires additional history matching, or perhaps that some physical effects of the DME has not been taken into account in the reservoir simulator, based on the mismatch between simulated and experimental recovery at high PVI's.

## 9. APPENDIX A

The system of equations (7)-(11) are non-linear, and thus have to be linearized in order to be able to solve the system. The linearization is done using 1<sup>st</sup>-order Taylor-expansion.

### 9.1. Model: No gravity, no capillary pressure, incompressible

#### Coupled Reactive Transport, water

The equation to be linearized is

$$\phi \frac{\partial c_w S}{\partial t} + \nabla \cdot \left( -\frac{k k_{rw}}{\mu_w} \nabla p - \mathcal{D}_w \phi \nabla c_w \right) + \frac{K k_o k_w}{K k_o + k_w} a \phi \left( c_w - \frac{c_o}{K} \right) = 0 \quad (43)$$

Transient

$$c_w S \approx c_o S_0 + S_0 \frac{\partial c_w}{\partial c_w} (c_w - c_o) + c_o \frac{\partial S}{\partial S} (S - S_0) = -S_0 c_o + S_0 c_w + c_o S \quad (44)$$

$$\frac{\partial S c_w}{\partial t} \approx \frac{\partial (-S_0 c_o + S_0 c_w + S c_o)}{\partial t} = S_0 \frac{\partial c_w}{\partial t} + c_o \frac{\partial S}{\partial t} \quad (45)$$

Advective

$$\frac{k_{rw}}{\mu_w} c_w \nabla p \approx \left( \frac{c_w}{\mu_w} \right)_{c_o} (k_{rw})_{S_0} \nabla p + \left( \frac{\partial \frac{c_w}{\mu_w}}{\partial c_w} \right)_{c_o} (k_{rw})_{S_0} \nabla p_0 (c_w - c_o) + \left( \frac{c_w}{\mu_w} \right)_{c_o} \left( \frac{\partial k_{rw}}{\partial S} \right)_{S_0} \nabla p_0 (S - S_0) \quad (46)$$

#### Coupled Reactive Transport, oil

The equation to be linearized is

$$\phi \frac{\partial c_o (1 - S)}{\partial t} + \nabla \cdot \left( -\frac{k k_{ro}}{\mu_o} \nabla p - \mathcal{D}_o \phi \nabla c_o \right) + \frac{k_o k_w}{K k_o + k_w} a \phi (c_o - K c_w) = 0 \quad (47)$$

Transient

$$c_o (1 - S) \approx c_o (1 - S_0) + (1 - S_0) \frac{\partial c_o}{\partial c_o} (c_o - c_o) + c_o \frac{\partial (1 - S)}{\partial S} (S - S_0) = S_0 c_o + (1 - S_0) c_o - c_o S \quad (48)$$

$$\frac{\partial c_o (1 - S)}{\partial t} \approx \frac{\partial (S_0 c_o + (1 - S_0) c_o - c_o S)}{\partial t} = (1 - S_0) \frac{\partial c_o}{\partial t} - c_o \frac{\partial S}{\partial t} \quad (49)$$

Advective

$$\frac{k_{ro}}{\mu_o} c_o \nabla p \approx \left( \frac{c_o}{\mu_o} \right)_{c_o} (k_{ro})_{S_0} \nabla p + \left( \frac{\partial \frac{c_o}{\mu_o}}{\partial c_o} \right)_{c_o} (k_{ro})_{S_0} \nabla p_0 (c_o - c_o) + \left( \frac{c_o}{\mu_o} \right)_{c_o} \left( \frac{\partial k_{ro}}{\partial S} \right)_{S_0} \nabla p_0 (S - S_0) \quad (50)$$

#### Two-Phase Flow, water

The equation to be linearized is

$$\phi \frac{\partial \rho_w S}{\partial t} + \nabla \cdot \left( -\rho_w \frac{k k_{rw}}{\mu_w} \nabla p \right) = 0 \quad (51)$$

Transient

$$\frac{\partial \rho_w S}{\partial t} = \rho_w \frac{\partial S}{\partial t} \quad (52)$$

Advective

$$\rho_w \frac{k_{rw}}{\mu_w} \nabla p \approx \rho_w \left( \frac{1}{\mu_w} \right)_{c_o} (k_{rw})_{S_0} \nabla p + \rho_w \left( \frac{\partial \frac{1}{\mu_w}}{\partial c_w} \right)_{c_o} (k_{rw})_{S_0} \nabla p_0 (c_w - c_o) + \rho_w \left( \frac{1}{\mu_w} \right)_{c_o} \left( \frac{\partial k_{rw}}{\partial S} \right)_{S_0} \nabla p_0 (S - S_0) \quad (53)$$

## Two-Phase Flow, oil

The equation to be linearized is

$$\phi \frac{\partial \rho_o(1-S)}{\partial t} + \nabla \cdot \left( -\rho_o \frac{k k_{ro}}{\mu_o} \nabla p \right) = 0 \quad (54)$$

Transient

$$\begin{aligned} \rho_o(1-S) &\approx (\rho_o)_{c_0}(1-S_0) + (1-S_0) \left( \frac{\partial \rho_o}{\partial c_o} \right)_{c_0} (c_o - c_0) + (\rho_o)_{c_0} \left( \frac{\partial(1-S)}{\partial S} \right)_{S_0} (S - S_0) \\ &= (\rho_o)_{c_0} + (1-S_0) \left( \frac{\partial \rho_o}{\partial c_o} \right)_{c_0} (c_o - c_0) - (\rho_o)_{c_0} S \end{aligned} \quad (55)$$

$$\frac{\partial \rho_o(1-S)}{\partial t} \approx -(\rho_o)_{c_0} \frac{\partial S}{\partial t} + (1-S_0) \left( \frac{\partial \rho_o}{\partial c_o} \right)_{c_0} \frac{\partial(c_o - c_0)}{\partial t} = (1-S_0) \left( \frac{\partial \rho_o}{\partial c_o} \right)_{c_0} \frac{\partial c_o}{\partial t} - (\rho_o)_{c_0} \frac{\partial S}{\partial t} \quad (56)$$

Advective

$$\rho_o \frac{k_{ro}}{\mu_o} \nabla p \approx \left( \frac{\rho_o}{\mu_o} \right)_{c_0} (k_{ro})_{S_0} \nabla p + \left( \frac{\partial \frac{\rho_o}{\mu_o}}{\partial c_o} \right)_{c_0} (k_{ro})_{S_0} \nabla p_0 (c_o - c_0) + \left( \frac{\rho_o}{\mu_o} \right)_{c_0} \left( \frac{\partial k_{ro}}{\partial S} \right)_{S_0} \nabla p_0 (S - S_0) \quad (57)$$

## 9.2. Model: Gravity, capillary pressure, compressible

### Coupled Reactive Transport, water

The equation to be linearized is

$$\phi \frac{\partial c_w S}{\partial t} + \nabla \cdot \left( -\frac{k k_{rw}}{\mu_w} (\nabla p - \rho_w \mathbf{g}) - \mathcal{D}_w \phi \nabla c_w \right) + \frac{K k_o k_w}{K k_o + k_w} a \phi \left( c_w - \frac{c_o}{K} \right) = 0 \quad (58)$$

The saturation is still not coupled with  $c_w$  or  $c_o$  in any way, so the transient terms are similar to (45) and (49).

Advective (pressure)

$$\begin{aligned} \frac{k_{rw}}{\mu_w} c_w \nabla p &\approx \left( \frac{c_w}{\mu_w} \right)_{c_{w,0}} (k_{rw})_{c_{o,0},S_0} \nabla p \\ &+ \left( \frac{\partial \frac{c_w}{\mu_w}}{\partial c_w} \right)_{c_{w,0}} (k_{rw})_{c_{o,0},S_0} \nabla p_0 (c_w - c_{w,0}) \\ &+ \left( \frac{c_w}{\mu_w} \right)_{c_{w,0}} \left( \frac{\partial k_{rw}}{\partial c_o} \right)_{c_{o,0},S_0} \nabla p_0 (c_o - c_{o,0}) \\ &+ \left( \frac{c_w}{\mu_w} \right)_{c_{w,0}} \left( \frac{\partial k_{rw}}{\partial S} \right)_{c_{o,0},S_0} \nabla p_0 (S - S_0) \end{aligned} \quad (59)$$

Advective (gravity)

$$\begin{aligned} \rho_w \frac{k_{rw}}{\mu_w} c_w \mathbf{g} &\approx (\rho_w)_{p_0} \left( \frac{c_w}{\mu_w} \right)_{c_{w,0}} (k_{rw})_{c_{o,0},S_0} \mathbf{g} \\ &+ (\rho_w)_{p_0} \left( \frac{\partial \frac{c_w}{\mu_w}}{\partial c_w} \right)_{c_{w,0}} (k_{rw})_{c_{o,0},S_0} \mathbf{g} (c_w - c_{w,0}) \\ &+ (\rho_w)_{p_0} \left( \frac{c_w}{\mu_w} \right)_{c_{w,0}} \left( \frac{\partial k_{rw}}{\partial c_o} \right)_{c_{o,0},S_0} \mathbf{g} (c_o - c_{o,0}) \\ &+ \left( \frac{\partial \rho_w}{\partial p} \right)_{p_0} \left( \frac{c_w}{\mu_w} \right)_{c_{w,0}} (k_{rw})_{c_{o,0},S_0} \mathbf{g} (p - p_0) \\ &+ (\rho_w)_{p_0} \left( \frac{c_w}{\mu_w} \right)_{c_{w,0}} \left( \frac{\partial k_{rw}}{\partial S} \right)_{c_{o,0},S_0} \mathbf{g} (S - S_0) \end{aligned} \quad (60)$$

because the equilibrium constant,  $K$  is now considered dependent on  $c_o$  the DME mass transfer terms also have to be linearized

$$K_w(c_w - c_w^*) = K_w c_w - K_o c_o = \frac{K k_o k_w}{K k_o + k_w} c_w - \frac{k_o k_w}{K k_o + k_w} c_o \quad (61)$$

one term at a time

$$\frac{K k_o k_w}{K k_o + k_w} c_w = \left( \frac{K k_o k_w}{K k_o + k_w} \right)_{c_{o,0}} c_{w,0} + \left( \frac{K k_o k_w}{K k_o + k_w} \right)_{c_{o,0}} \left( \frac{\partial c_w}{\partial c_o} \right) (c_w - c_{w,0}) + c_{w,0} \left( \frac{\partial \frac{K k_o k_w}{K k_o + k_w}}{\partial c_o} \right)_{c_{o,0}} (c_o - c_{o,0}) \quad (62)$$

$$\frac{k_o k_w}{K k_o + k_w} c_o = \left( \frac{k_o k_w}{K k_o + k_w} c_o \right)_{c_{o,0}} + \left( \frac{\partial \frac{k_o k_w}{K k_o + k_w} c_o}{\partial c_o} \right)_{c_{o,0}} (c_o - c_{o,0}) \quad (63)$$

### Coupled Reactive Transport, oil

The equation to be linearized is

$$\phi \frac{\partial c_o(1-S)}{\partial t} + \nabla \cdot \left( -\frac{k k_{ro}}{\mu_o} (\nabla p + \nabla p_c - \rho_o \mathbf{g}) - \mathcal{D}_o \phi \nabla c_o \right) + \frac{k_o k_w}{K k_o + k_w} a \phi (c_o - K c_w) = 0 \quad (64)$$

Advective (pressure)

$$\begin{aligned} \frac{k_{ro}}{\mu_o} c_o \nabla p &\approx \left( \frac{c_o}{\mu_o} \right)_{c_{o,0}} (k_{ro})_{c_{o,0}, S_0} \nabla p \\ &+ \left( \frac{\partial \frac{k_{ro}}{\mu_o} c_o}{\partial c_o} \right)_{c_{o,0}, S_0} \nabla p_0 (c_o - c_{o,0}) \\ &+ \left( \frac{c_o}{\mu_o} \right)_{c_{o,0}} \left( \frac{\partial k_{ro}}{\partial S} \right)_{c_{o,0}, S_0} \nabla p_0 (S - S_0) \end{aligned} \quad (65)$$

Advective (capillary pressure)

$$\begin{aligned} \frac{k_{ro}}{\mu_o} c_o \nabla p_c &= \frac{k_{ro}}{\mu_o} c_o \frac{dp_c}{dS} \nabla S \approx \left( \frac{c_o}{\mu_o} \right)_{c_{o,0}} (k_{ro})_{c_{o,0}, S_0} \left( \frac{dp_c}{dS} \right)_{c_{o,0}, S_0} \nabla S \\ &+ \left( \frac{\partial \frac{k_{ro}}{\mu_o} c_o \frac{dp_c}{dS}}{\partial c_o} \right)_{c_{o,0}, S_0} \nabla S_0 (c_o - c_{o,0}) \\ &+ \left( \frac{c_o}{\mu_o} \right)_{c_{o,0}} \left( \frac{\partial k_{ro} \frac{dp_c}{dS}}{\partial S} \right)_{c_{o,0}, S_0} \nabla S_0 (S - S_0) \end{aligned} \quad (66)$$

Advective (gravity)

$$\begin{aligned} \rho_o \frac{k_{ro}}{\mu_o} c_o \mathbf{g} &\approx (\rho_o)_{c_{o,0}, p_0} \left( \frac{c_o}{\mu_o} \right)_{c_{o,0}} (k_{ro})_{c_{o,0}, S_0} \mathbf{g} \\ &+ \left( \frac{\partial \rho_o \frac{k_{ro}}{\mu_o} c_o}{\partial c_o} \right)_{c_{o,0}, p_0, S_0} \mathbf{g} (c_o - c_{o,0}) \\ &+ \left( \frac{\partial \rho_o}{\partial p} \right)_{c_{o,0}, p_0} \left( \frac{c_o}{\mu_o} \right)_{c_{o,0}} (k_{ro})_{c_{o,0}, S_0} \mathbf{g} (p - p_0) \\ &+ (\rho_o)_{c_{o,0}, p_0} \left( \frac{c_o}{\mu_o} \right)_{c_{o,0}} \left( \frac{\partial k_{ro}}{\partial S} \right)_{c_{o,0}, S_0} \mathbf{g} (S - S_0) \end{aligned} \quad (67)$$

DME mass transfer

$$K_o(c_o - c_o^*) = K_o c_o - K_w c_w = \frac{k_o k_w}{K k_o + k_w} c_o - \frac{K k_o k_w}{K k_o + k_w} c_w \quad (68)$$

where the two linearized terms are given by (62) and (63).

## Two-Phase Flow, water

The equation to be linearized is

$$\phi \frac{\partial \rho_w S}{\partial t} + \nabla \cdot \left( -\rho_w \frac{k k_{rw}}{\mu_w} (\nabla p - \rho_w \mathbf{g}) \right) = 0 \quad (69)$$

Transient

$$\rho_w S = (\rho_w)_{p_0} S_0 + S_0 \left( \frac{\partial \rho_w}{\partial p} \right)_{p_0} (p - p_0) + (\rho_w)_{p_0} \left( \frac{\partial S}{\partial S} \right)_{S_0} (S - S_0) = S_0 \left( \frac{\partial \rho_w}{\partial p} \right)_{p_0} (p - p_0) + (\rho_w)_{p_0} S \quad (70)$$

$$\frac{\partial \rho_w S}{\partial t} = \frac{\partial \left( S_0 \left( \frac{\partial \rho_w}{\partial p} \right)_{p_0} (p - p_0) + (\rho_w)_{p_0} S \right)}{\partial t} = S_0 \left( \frac{\partial \rho_w}{\partial p} \right)_{p_0} \frac{\partial p}{\partial t} + (\rho_w)_{p_0} \frac{\partial S}{\partial t} \quad (71)$$

Advective (pressure)

$$\begin{aligned} \rho_w \frac{k_{rw}}{\mu_w} \nabla p \approx & (\rho_w)_{p_0} \left( \frac{1}{\mu_w} \right)_{c_{w,0}} (k_{rw})_{c_{o,0},S_0} \nabla p \\ & + (\rho_w)_{p_0} \left( \frac{\partial \frac{1}{\mu_w}}{\partial c_w} \right)_{c_{w,0}} (k_{rw})_{c_{o,0},S_0} \nabla p_0 (c_w - c_{w,0}) \\ & + (\rho_w)_{p_0} \left( \frac{1}{\mu_w} \right)_{c_{w,0}} \left( \frac{\partial k_{rw}}{\partial c_o} \right)_{c_{o,0},S_0} \nabla p_0 (c_o - c_{o,0}) \\ & + \left( \frac{\partial \rho_w}{\partial p} \right)_{p_0} \left( \frac{1}{\mu_w} \right)_{c_{w,0}} (k_{rw})_{c_{o,0},S_0} \nabla p_0 (p - p_0) \\ & + (\rho_w)_{p_0} \left( \frac{1}{\mu_w} \right)_{c_{w,0}} \left( \frac{\partial k_{rw}}{\partial S} \right)_{c_{o,0},S_0} \nabla p_0 (S - S_0) \end{aligned} \quad (72)$$

Advective (gravity)

$$\begin{aligned} \rho_w^2 \frac{k_{rw}}{\mu_w} \mathbf{g} \approx & (\rho_w^2)_{p_0} \left( \frac{1}{\mu_w} \right)_{c_{w,0}} (k_{rw})_{c_{o,0},S_0} \mathbf{g} \\ & + (\rho_w^2)_{p_0} \left( \frac{\partial \frac{1}{\mu_w}}{\partial c_w} \right)_{c_{w,0}} (k_{rw})_{c_{o,0},S_0} \mathbf{g} (c_w - c_{w,0}) \\ & + (\rho_w^2)_{p_0} \left( \frac{1}{\mu_w} \right)_{c_{w,0}} \left( \frac{\partial k_{rw}}{\partial c_o} \right)_{c_{o,0},S_0} \mathbf{g} (c_o - c_{o,0}) \\ & + \left( \frac{\partial \rho_w^2}{\partial p} \right)_{p_0} \left( \frac{1}{\mu_w} \right)_{c_{w,0}} (k_{rw})_{c_{o,0},S_0} \mathbf{g} (p - p_0) \\ & + (\rho_w^2)_{p_0} \left( \frac{1}{\mu_w} \right)_{c_{w,0}} \left( \frac{\partial k_{rw}}{\partial S} \right)_{c_{o,0},S_0} \mathbf{g} (S - S_0) \end{aligned} \quad (73)$$

## Two-Phase Flow, oil

The equation to be linearized is

$$\phi \frac{\partial \rho_o (1 - S)}{\partial t} + \nabla \cdot \left( -\rho_o \frac{k k_{ro}}{\mu_o} (\nabla p + \nabla p_c - \rho_o \mathbf{g}) \right) = 0 \quad (74)$$

Transient

$$\begin{aligned}
\rho_o(1-S) &= (\rho_o)_{c_o,0,p_0}(1-S_0) \\
&\quad + (1-S_0) \left( \frac{\partial \rho_o}{\partial c_o} \right)_{c_o,0,p_0} (c_o - c_{o,0}) \\
&\quad + (1-S_0) \left( \frac{\partial \rho_o}{\partial p} \right)_{c_o,0,p_0} (p - p_0) \\
&\quad + (\rho_o)_{c_o,0,p_0} \left( \frac{\partial(1-S)}{\partial S} \right)_{S_0} (S - S_0) \\
&= (\rho_o)_{c_o,0,p_0} \\
&\quad + (1-S_0) \left( \frac{\partial \rho_o}{\partial c_o} \right)_{c_o,0,p_0} (c_o - c_{o,0}) \\
&\quad + (1-S_0) \left( \frac{\partial \rho_o}{\partial p} \right)_{c_o,0,p_0} (p - p_0) \\
&\quad - (\rho_o)_{c_o,0,p_0} S
\end{aligned} \tag{75}$$

and the transient derivative

$$\begin{aligned}
\frac{\partial \rho_o(1-S)}{\partial t} &= \frac{\partial \left( (\rho_o)_{c_o,0,p_0} + (1-S_0) \left( \frac{\partial \rho_o}{\partial c_o} \right)_{c_o,0,p_0} (c_o - c_{o,0}) + (1-S_0) \left( \frac{\partial \rho_o}{\partial p} \right)_{c_o,0,p_0} (p - p_0) - (\rho_o)_{c_o,0,p_0} S \right)}{\partial t} \\
&= (1-S_0) \left( \frac{\partial \rho_o}{\partial c_o} \right)_{c_o,0,p_0} \frac{\partial c_o}{\partial t} + (1-S_0) \left( \frac{\partial \rho_o}{\partial p} \right)_{c_o,0,p_0} \frac{\partial p}{\partial t} - (\rho_o)_{c_o,0,p_0} \frac{\partial S}{\partial t}
\end{aligned} \tag{76}$$

Advective (pressure)

$$\begin{aligned}
\rho_o \frac{k_{ro}}{\mu_o} \nabla p &\approx (\rho_o)_{c_o,0,p_0} \left( \frac{1}{\mu_o} \right)_{c_o,0} (k_{ro})_{c_o,0,S_0} \nabla p \\
&\quad + \left( \frac{\partial \rho_o \frac{k_{ro}}{\mu_o}}{\partial c_o} \right)_{c_o,0,S_0,p_0} \nabla p_0 (c_o - c_{o,0}) \\
&\quad + \left( \frac{\partial \rho_o}{\partial p} \right)_{p_0} \left( \frac{1}{\mu_o} \right)_{c_o,0} (k_{ro})_{c_o,0,S_0} \nabla p_0 (p - p_0) \\
&\quad + (\rho_o)_{p_0} \left( \frac{1}{\mu_o} \right)_{c_o,0} \left( \frac{\partial k_{ro}}{\partial S} \right)_{c_o,0,S_0} \nabla p_0 (S - S_0)
\end{aligned} \tag{77}$$

Advective (capillary pressure)

$$\begin{aligned}
\rho_o \frac{k_{ro}}{\mu_o} \nabla p_c &= \rho_o \frac{k_{ro}}{\mu_o} \frac{dp_c}{dS} \nabla S \approx (\rho_o)_{c_o,0,p_0} \left( \frac{1}{\mu_o} \right)_{c_o,0} (k_{ro})_{c_o,0,S_0} \left( \frac{dp_c}{dS} \right)_{c_o,0,S_0} \nabla S \\
&\quad + \left( \frac{\partial \rho_o \frac{k_{ro}}{\mu_o} \frac{dp_c}{dS}}{\partial c_o} \right)_{c_o,0,p_0,S_0} \nabla S_0 (c_o - c_{o,0}) \\
&\quad + \left( \frac{\partial \rho_o}{\partial p} \right)_{c_o,0,p_0} \left( \frac{1}{\mu_o} \right)_{c_o,0} (k_{ro})_{c_o,0,S_0} \left( \frac{dp_c}{dS} \right)_{c_o,0,S_0} \nabla S_0 (p - p_0) \\
&\quad + (\rho_o)_{c_o,0,p_0} \left( \frac{1}{\mu_o} \right)_{c_o,0} \left( \frac{\partial k_{ro} \frac{dp_c}{dS}}{\partial S} \right)_{c_o,0,S_0} \nabla S_0 (S - S_0)
\end{aligned} \tag{78}$$

Advective (gravity)

$$\begin{aligned}
\rho_o^2 \frac{k_{ro}}{\mu_o} \mathbf{g} \approx & (\rho_o^2)_{c_o,0,p_0} \left( \frac{1}{\mu_o} \right)_{c_o,0} (k_{ro})_{c_o,0,S_0} \mathbf{g} \\
& + \left( \frac{\partial \rho_o^2 \frac{k_{ro}}{\mu_o}}{\partial c_o} \right)_{c_o,0,S_0} \mathbf{g} (c_o - c_{o,0}) \\
& + \left( \frac{\partial \rho_o^2}{\partial p} \right)_{c_o,0,p_0} \left( \frac{1}{\mu_o} \right)_{c_o,0} (k_{ro})_{c_o,0,S_0} \mathbf{g} (p - p_0) \\
& + (\rho_o^2)_{c_o,0,p_0} \left( \frac{1}{\mu_o} \right)_{c_o,0} \left( \frac{\partial k_{ro}}{\partial S} \right)_{c_o,0,S_0} \mathbf{g} (S - S_0)
\end{aligned} \tag{79}$$

## 10. APPENDIX B

The discretization given in (26) is a high level view of the system block matrix. This appendix subdivides these various matrices into individual terms, and whether these sub divided terms are transient, advective, diffusive, linear or constant. The subscripts that will be used are  $t$ ,  $adv$ ,  $diff$ :

Essentially subscript  $t$  means it is a matrix of coefficients, discretizing a term of the form

$$\mathbf{M}_{t,\psi} = \mathbf{M}_{t,\psi}(\beta) \equiv \beta \frac{\partial \psi}{\partial t} \tag{80}$$

subscript  $adv$  means it is a matrix of coefficients, discretizing a term of the form

$$\mathbf{M}_{adv,\psi} = \mathbf{M}_{adv,\psi}(\beta) \equiv \nabla \cdot (\mathbf{u}(\beta)\psi) \tag{81}$$

where  $\mathbf{u}$  is a vector and a function of  $\beta$ . Subscript  $diff$  means it is a matrix of coefficients, discretizing a term of the form

$$\mathbf{M}_{diff,\psi} = \mathbf{M}_{diff,\psi}(\beta) \equiv \nabla \cdot (\beta \nabla \psi) \tag{82}$$

i.e. a discretization of the divergence of the gradient of variable  $\psi$  with some constant  $\beta$ . Subscript  $lin$  means it is a matrix of coefficients, discretizing a term of the form

$$\mathbf{M}_{lin,\psi} = \mathbf{M}_{lin,\psi}(\beta) \equiv \beta \psi \tag{83}$$

I.e. a linear source term. Subscript  $div$ , means it is a vector of coefficients, discretizing a term of the form

$$\mathbf{b}_{div,\mathbf{g}} = \mathbf{b}_{div,\mathbf{g}}(\beta) \equiv \nabla \cdot (\beta \mathbf{g}) \tag{84}$$

I.e. the divergence of a given vector  $\mathbf{g}$ . Subscript  $const$ , means it is a vector of coefficients, discretizing a term of the form

$$\mathbf{b}_{const,\mathbf{g}} = \mathbf{b}_{const,\mathbf{g}}(\beta) \equiv \beta \mathbf{g} \tag{85}$$

For subscript  $bc$  it is constructed from the boundary conditions and will thus be a function of those. In order to make it very clear how the individual matrices are defined, they are written as a function of the constant they are a function of.

### 10.1. Model: No gravity, no capillary pressure, incompressible

The following extended subscript notation will be used:  $(term, variable, row)$ , so an advective term, for saturation in row 3 will be  $adv,S,3$



### 10.1.1. Sub Division of Terms

and the individual matrices in the block matrix and RHS can be subdivided as:

System-matrices

$$\begin{aligned}
\mathbf{M}_{c_w,1} &= -\mathbf{M}_{diff,c_w} + \frac{Kk_0k_w}{Kk_0 + k_w}a\phi + \mathbf{M}_{bc,c_w}, & \mathbf{M}_{c_o,1} &= -\frac{k_0k_w}{Kk_0 + k_w}a\phi \\
\mathbf{M}_{c_w,2} &= -\frac{k_0k_w}{k_0 + k_w}a\phi, & \mathbf{M}_{c_o,2} &= -\mathbf{M}_{diff,c_o} + \frac{Kk_0k_w}{Kk_0 + k_w}a\phi + \mathbf{M}_{bc,c_o} \\
\mathbf{M}_{p,3} &= \mathbf{M}_{bc,p} \\
\mathbf{M}_{S,4} &= \mathbf{M}_{bc,S}
\end{aligned} \tag{86}$$

Jacobians (from (49) and (50))

$$\begin{aligned}
\mathbf{J}_{c_w,1} &= \mathbf{J}_{t,c_w,1} + \mathbf{J}_{adv,c_w,1}, & \mathbf{J}_{p,1} &= \mathbf{J}_{diff,p,1}, & \mathbf{J}_{S,1} &= \mathbf{J}_{t,S,1} + \mathbf{J}_{adv,S,1} \\
\mathbf{J}_{c_o,2} &= \mathbf{J}_{t,c_o,2} + \mathbf{J}_{adv,c_o,2}, & \mathbf{J}_{p,2} &= \mathbf{J}_{diff,p,2}, & \mathbf{J}_{S,2} &= \mathbf{J}_{t,S,2} + \mathbf{J}_{adv,S,2} \\
\mathbf{J}_{c_w,3} &= \mathbf{J}_{adv,c_w,3}, & \mathbf{J}_{p,3} &= \mathbf{J}_{diff,p,3}, & \mathbf{J}_{S,3} &= \mathbf{J}_{t,S,3} + \mathbf{J}_{adv,S,3} \\
\mathbf{J}_{c_o,4} &= \mathbf{J}_{t,c_o,4} + \mathbf{J}_{adv,c_o,4}, & \mathbf{J}_{p,4} &= \mathbf{J}_{diff,p,4}, & \mathbf{J}_{S,4} &= \mathbf{J}_{t,S,4} + \mathbf{J}_{adv,S,4}
\end{aligned} \tag{87}$$

RHS's

$$\begin{aligned}
\mathbf{b}_1 &= \mathbf{b}_{bc,c_w} + \mathbf{b}_{t,c_w,1} + \mathbf{b}_{t,S,1} + \mathbf{b}_{adv,c_w,1} + \mathbf{b}_{adv,S,1} \\
\mathbf{b}_2 &= \mathbf{b}_{bc,c_o} + \mathbf{b}_{t,c_o,2} + \mathbf{b}_{t,S,2} + \mathbf{b}_{adv,c_o,2} + \mathbf{b}_{adv,S,2} \\
\mathbf{b}_3 &= \mathbf{b}_{bc,p} + \mathbf{b}_{t,S,3} + \mathbf{b}_{adv,c_w,3} + \mathbf{b}_{adv,S,3} \\
\mathbf{b}_4 &= \mathbf{b}_{bc,S} + \mathbf{b}_{t,c_o,4} + \mathbf{b}_{t,S,4} + \mathbf{b}_{adv,c_o,4} + \mathbf{b}_{adv,S,4}
\end{aligned} \tag{88}$$

### 10.1.2. Coefficients of Terms

#### Coupled Reactive Transport, water

System Matrices

$$\mathbf{M}_{diff,c_w} = \mathbf{M}_{diff,c_w}(\mathcal{D}_w\phi) \tag{89}$$

Jacobians

$$\begin{aligned}
\mathbf{J}_{t,c_w,1} &= \mathbf{J}_{t,c_w,1}(\phi S_0) \\
\mathbf{J}_{adv,c_w,1} &= \mathbf{J}_{adv,c_w,1} \left( -k \left( \frac{\partial \frac{c_w}{\mu_w}}{\partial c_w} \right)_{c_0} (k_{rw})_{S_0} \nabla p_0 \right) \\
\mathbf{J}_{diff,p,1} &= \mathbf{J}_{diff,p,1} \left( -k \left( \frac{1}{\mu_w} \right)_{c_w} (k_{rw})_{S_0} c_0 \right) \\
\mathbf{J}_{t,S,1} &= \mathbf{J}_{t,S,1}(\phi c_0) \\
\mathbf{J}_{adv,S,1} &= \mathbf{J}_{adv,S,1} \left( -k \left( \frac{c_w}{\mu_w} \right)_{c_0} \left( \frac{\partial k_{rw}}{\partial S} \right)_{S_0} \nabla p_0 \right)
\end{aligned} \tag{90}$$

#### Coupled Reactive Transport, oil

System Matrices

$$\mathbf{M}_{diff,c_o} = \mathbf{M}_{diff,c_o}(\mathcal{D}_o\phi) \tag{91}$$

Jacobians

$$\begin{aligned}
\mathbf{J}_{t,c_o,2} &= \mathbf{J}_{t,c_o,2}(\phi(1 - S_0)) \\
\mathbf{J}_{adv,c_o,2} &= \mathbf{J}_{adv,c_o,2} \left( -k \left( \frac{\partial \frac{c_o}{\mu_o}}{\partial c_o} \right)_{c_0} (k_{ro})_{S_0} \nabla p_0 \right) \\
\mathbf{J}_{diff,p,2} &= \mathbf{J}_{diff,p,2} \left( -k \left( \frac{1}{\mu_o} \right)_{c_0} (k_{ro})_{S_0} c_0 \right) \\
\mathbf{J}_{t,S,2} &= \mathbf{J}_{t,S,2}(-\phi c_0) \\
\mathbf{J}_{adv,S,2} &= \mathbf{J}_{adv,S,2} \left( -k \left( \frac{c_o}{\mu_o} \right)_{c_0} \left( \frac{\partial k_{ro}}{\partial S} \right)_{S_0} \nabla p_0 \right)
\end{aligned} \tag{92}$$

## Two-Phase Flow, water

Jacobians

$$\begin{aligned}
\mathbf{J}_{adv,c_w,3} &= \mathbf{J}_{adv,c_w,3} \left( -k \left( \frac{\partial \frac{1}{\mu_w}}{\partial c_w} \right)_{c_0} (k_{rw})_{S_0} \rho_w \nabla p_0 \right) \\
\mathbf{J}_{diff,p,3} &= \mathbf{J}_{diff,p,3} \left( -k \left( \frac{1}{\mu_w} \right)_{c_0} (k_{rw})_{S_0} \rho_w \right) \\
\mathbf{J}_{t,S,3} &= \mathbf{J}_{t,S,3}(\phi \rho_w) \\
\mathbf{J}_{adv,S,3} &= \mathbf{J}_{adv,S,3} \left( -k \left( \frac{1}{\mu_w} \right)_{c_0} \left( \frac{\partial k_{rw}}{\partial S} \right)_{S_0} \rho_w \nabla p_0 \right)
\end{aligned} \tag{93}$$

## Two-Phase Flow, oil

Jacobians

$$\begin{aligned}
\mathbf{J}_{t,c_o,4} &= \mathbf{J}_{t,c_o,4} \left( \phi(1 - S_0) \left( \frac{\partial \rho_o}{\partial c_o} \right)_{c_0} \right) \\
\mathbf{J}_{adv,c_o,4} &= \mathbf{J}_{adv,c_o,4} \left( -k \left( \frac{\partial \frac{\rho_o}{\mu_o}}{\partial c_o} \right)_{c_0} (k_{ro})_{S_0} \nabla p_0 \right) \\
\mathbf{J}_{diff,p,4} &= \mathbf{J}_{diff,p,4} \left( -k \left( \frac{\rho_o}{\mu_o} \right)_{c_0} (k_{ro})_{S_0} \right) \\
\mathbf{J}_{t,S,4} &= \mathbf{J}_{t,S,4}(-\phi(\rho_o)_{c_0}) \\
\mathbf{J}_{adv,S,4} &= \mathbf{J}_{adv,S,4} \left( -k \left( \frac{\rho_o}{\mu_o} \right)_{c_0} \left( \frac{\partial k_{ro}}{\partial S} \right)_{S_0} \nabla p_0 \right)
\end{aligned} \tag{94}$$

All RHS's will be a function of the same constants as the corresponding Jacobian, i.e.  $\mathbf{b}_{t,c_o,1}$  is a function of the same constant as  $\mathbf{J}_{t,c_o,1}$ , etc.

## 10.2. Model: Gravity, capillary pressure, compressible

The following extended subscript notation will be used: *(term of eq., variable(term of var.), row)*, so if the term being linearized is the advective term in one of the four equations, and the variable is the saturation related to the gravity part of the advective term, in row 3, then the subscript will be *(adv, S(g), 3)*. The individual matrices in the block matrix and RHS can be subdivided as:

### 10.2.1. Sub Division of Terms

#### System Matrices

$$\begin{aligned}
\mathbf{M}_{c_w,1} &= -\mathbf{M}_{diff,c_w} + \mathbf{M}_{bc,c_w} \\
\mathbf{M}_{c_o,2} &= -\mathbf{M}_{diff,c_o} + \mathbf{M}_{bc,c_o} \\
\mathbf{M}_{p,3} &= \mathbf{M}_{bc,p} \\
\mathbf{M}_{S,4} &= \mathbf{M}_{bc,S}
\end{aligned} \tag{95}$$

#### Jacobians

##### Coupled Reactive Transport, water

$$\begin{aligned}
\mathbf{J}_{c_w,1} &= \mathbf{J}_{t,c_w,1} + \mathbf{J}_{adv,c_w(p),1} - \mathbf{J}_{adv,c_w(g),1} + \mathbf{J}_{lin,c_w(c_w),1} \\
\mathbf{J}_{c_o,1} &= \mathbf{J}_{adv,c_o(p),1} - \mathbf{J}_{adv,c_o(g),1} + \mathbf{J}_{lin,c_o(c_w),1} - \mathbf{J}_{lin,c_o(c_o),1} \\
\mathbf{J}_{p,1} &= -\mathbf{J}_{adv,p(g),1} + \mathbf{J}_{diff,p,1} \\
\mathbf{J}_{S,1} &= \mathbf{J}_{t,S,1} + \mathbf{J}_{adv(p),S,1} - \mathbf{J}_{adv(g),S,1}
\end{aligned} \tag{96}$$

##### Coupled Reactive Transport, oil

$$\begin{aligned}
\mathbf{J}_{c_w,2} &= -\mathbf{J}_{lin,c_w(c_w),2} \\
\mathbf{J}_{c_o,2} &= \mathbf{J}_{t,c_o,2} + \mathbf{J}_{adv,c_o(p),2} + \mathbf{J}_{adv,c_o(p_c),2} - \mathbf{J}_{adv,c_o(g),2} - \mathbf{J}_{lin,c_o(c_w),2} + \mathbf{J}_{lin,c_o(c_o),2} \\
\mathbf{J}_{p,2} &= -\mathbf{J}_{adv,p(g),2} + \mathbf{J}_{diff,p,2} \\
\mathbf{J}_{S,2} &= \mathbf{J}_{t,S,2} + \mathbf{J}_{adv,S(p),2} + \mathbf{J}_{adv,S(p_c),2} - \mathbf{J}_{adv,S(g),2} + \mathbf{J}_{diff,S(p_c),2}
\end{aligned} \tag{97}$$

##### Two-Phase Flow, water

$$\begin{aligned}
\mathbf{J}_{c_w,3} &= \mathbf{J}_{adv,c_w(p),3} - \mathbf{J}_{adv,p(g),3} \\
\mathbf{J}_{c_o,3} &= \mathbf{J}_{adv,c_o(p),3} - \mathbf{J}_{adv,p(g),3} \\
\mathbf{J}_{p,3} &= \mathbf{J}_{t,p,3} + \mathbf{J}_{adv,p(p),3} - \mathbf{J}_{adv,p(g),3} + \mathbf{J}_{diff,p,3} \\
\mathbf{J}_{S,3} &= \mathbf{J}_{t,S,3} + \mathbf{J}_{adv,S(p),3} - \mathbf{J}_{adv,S(g),3}
\end{aligned} \tag{98}$$

##### Two-Phase Flow, oil

$$\begin{aligned}
\mathbf{J}_{c_o,4} &= \mathbf{J}_{t,c_o,4} + \mathbf{J}_{adv,c_o(p),4} + \mathbf{J}_{adv,c_o(p_c),4} - \mathbf{J}_{adv,c_o(g),4} \\
\mathbf{J}_{p,4} &= \mathbf{J}_{t,p,4} + \mathbf{J}_{adv,S(p),4} + \mathbf{J}_{adv,S(p_c),4} - \mathbf{J}_{adv,S(g),4} + \mathbf{J}_{diff,p,4} \\
\mathbf{J}_{S,4} &= \mathbf{J}_{t,S,4} + \mathbf{J}_{adv,S(p),4} + \mathbf{J}_{adv,S(p_c),4} - \mathbf{J}_{adv,S(g),4} + \mathbf{J}_{diff,S(p_c),4}
\end{aligned} \tag{99}$$

#### RHS

##### Coupled Reactive Transport, water

$$\begin{aligned}
\mathbf{b}_1 &= \mathbf{b}_{bc,c_w} + \mathbf{b}_{t,c_w,1} + \mathbf{b}_{adv,c_w(p),1} - \mathbf{b}_{adv,c_w(g),1} + \mathbf{b}_{lin,c_w(c_w),1} - \mathbf{b}_{const,c_w(c_w),1} \\
&\quad + \mathbf{b}_{adv,c_o(p),1} - \mathbf{b}_{adv,c_o(g),1} + \mathbf{b}_{lin,c_o(c_w),1} - \mathbf{b}_{lin,c_o(c_o),1} + \mathbf{b}_{const,c_o(c_o),1} \\
&\quad - \mathbf{b}_{adv,p(g),1} \\
&\quad + \mathbf{b}_{t,S,1} + \mathbf{b}_{adv,S(p),1} - \mathbf{b}_{adv,S(g),1} \\
&\quad + \mathbf{b}_{div,g,1}
\end{aligned} \tag{100}$$

##### Coupled Reactive Transport, oil

$$\begin{aligned}
\mathbf{b}_2 &= -\mathbf{b}_{lin,c_w(c_w),2} + \mathbf{b}_{const,c_w(c_w),2} \\
&\quad + \mathbf{b}_{bc,c_o} + \mathbf{b}_{t,c_o,2} + \mathbf{b}_{adv,c_o(p),2} + \mathbf{b}_{adv,c_o(p_c),2} - \mathbf{b}_{adv,c_o(g),2} - \mathbf{b}_{lin,c_o(c_w),2} + \mathbf{b}_{lin,c_o(c_o),2} - \mathbf{b}_{const,c_o(c_o),2} \\
&\quad - \mathbf{b}_{adv,p(g),2} \\
&\quad + \mathbf{b}_{t,S,2} + \mathbf{b}_{adv,S(p),2} + \mathbf{b}_{adv,S(p_c),2} - \mathbf{b}_{adv,S(g),2} \\
&\quad + \mathbf{b}_{div,g,2}
\end{aligned} \tag{101}$$

Two-Phase Flow, water

$$\begin{aligned}
\mathbf{b}_3 = & \mathbf{b}_{adv,c_w(p),3} - \mathbf{b}_{adv,c_w(g),3} \\
& + \mathbf{b}_{adv,c_o(p),3} - \mathbf{b}_{adv,c_o(g),3} \\
& + \mathbf{b}_{bc,p} + \mathbf{b}_{t,p,3} + \mathbf{b}_{adv,p(p),3} - \mathbf{b}_{adv,p(g),3} \\
& + \mathbf{b}_{t,S,3} + \mathbf{b}_{adv,S(p),3} - \mathbf{b}_{adv,S(g),3} \\
& + \mathbf{b}_{div,\mathbf{g},3}
\end{aligned} \tag{102}$$

Coupled Reactive Transport, water

$$\begin{aligned}
\mathbf{b}_4 = & \mathbf{b}_{t,c_o,4} + \mathbf{b}_{adv,c_o(p),4} + \mathbf{b}_{adv,c_o(p_c),4} - \mathbf{b}_{adv,c_o(g),4} \\
& + \mathbf{b}_{t,p,4} + \mathbf{J}_{adv,p(p),4} + \mathbf{b}_{adv,p(p_c),4} - \mathbf{b}_{adv,p(g),4} \\
& + \mathbf{b}_{bc,S} + \mathbf{b}_{t,S,4} + \mathbf{b}_{adv,S(p),4} + \mathbf{b}_{adv,S(p_c),4} - \mathbf{b}_{adv,S(g),4} \\
& + \mathbf{b}_{div,\mathbf{g},4}
\end{aligned} \tag{103}$$

### 10.2.2. Coefficients of Terms

Coupled Reactive Transport, water

System Matrices

$$\mathbf{M}_{diff,c_w} = \mathbf{M}_{diff,c_w}(\mathcal{D}_w\phi) \tag{104}$$

Jacobians

$$\begin{aligned}
\mathbf{J}_{t,c_w,1} &= \mathbf{J}_{t,c_w,1}(\phi S_0) \\
\mathbf{J}_{adv,c_w(p),1} &= \mathbf{J}_{adv,c_w(p),1} \left( -k \left( \frac{\partial \frac{c_w}{\mu_w}}{\partial c_w} \right)_{c_w,0} (k_{rw})_{c_o,0,S_0} \nabla p_0 \right) \\
\mathbf{J}_{adv,c_w(g),1} &= \mathbf{J}_{adv,c_w(g),1} \left( -k(\rho_w) p_0 \left( \frac{\partial \frac{c_w}{\mu_w}}{\partial c_w} \right)_{c_w,0} (k_{rw})_{c_o,0,S_0} \mathbf{g} \right) \\
\mathbf{J}_{lin,c_w(c_w),1} &= \mathbf{J}_{lin,c_w(c_w),1} \left( \left( \frac{Kk_o k_w}{Kk_o + k_w} \right)_{c_o,0} a\phi \right) \\
\mathbf{J}_{adv,c_o(p),1} &= \mathbf{J}_{adv,c_o(p),1} \left( -k \left( \frac{c_w}{\mu_w} \right)_{c_w,0} \left( \frac{\partial k_{rw}}{\partial c_o} \right)_{c_o,0,S_0} \nabla p_0 \right) \\
\mathbf{J}_{adv,c_o(g),1} &= \mathbf{J}_{adv,c_o(g),1} \left( -k(\rho_w) p_0 \left( \frac{c_w}{\mu_w} \right)_{c_w,0} \left( \frac{\partial k_{rw}}{\partial c_o} \right)_{c_o,0,S_0} \mathbf{g} \right) \\
\mathbf{J}_{lin,c_o(c_w),1} &= \mathbf{J}_{lin,c_o(c_w),1} \left( \left( \frac{\partial \frac{Kk_o k_w}{Kk_o + k_w}}{\partial c_o} \right)_{c_o,0} a\phi c_{w,0} \right) \\
\mathbf{J}_{lin,c_o(c_o),1} &= \mathbf{J}_{lin,c_o(c_o),1} \left( \left( \frac{\partial \frac{k_o k_w}{Kk_o + k_w} c_o}{\partial c_o} \right)_{c_o,0} a\phi \right) \\
\mathbf{J}_{adv,p(g),1} &= \mathbf{J}_{adv,p(g),1} \left( -k \left( \frac{\partial \rho_w}{\partial p} \right)_{p_0} \left( \frac{c_w}{\mu_w} \right)_{c_w,0} (k_{rw})_{c_o,0,S_0} \mathbf{g} \right) \\
\mathbf{J}_{diff,p,1} &= \mathbf{J}_{diff,p,1} \left( -k \left( \frac{c_w}{\mu_w} \right)_{c_w,0} (k_{rw})_{c_o,0,S_0} \right) \\
\mathbf{J}_{t,S,1} &= \mathbf{J}_{t,S,1}(\phi c_0) \\
\mathbf{J}_{adv,S(p),1} &= \mathbf{J}_{adv,S(p),1} \left( -k \left( \frac{c_w}{\mu_w} \right)_{c_w,0} \left( \frac{\partial k_{rw}}{\partial S} \right)_{c_o,0,S_0} \nabla p_0 \right) \\
\mathbf{J}_{adv,S(g),1} &= \mathbf{J}_{adv,S(g),1} \left( -k(\rho_w) p_0 \left( \frac{c_w}{\mu_w} \right)_{c_w,0} \left( \frac{\partial k_{rw}}{\partial S} \right)_{c_o,0,S_0} \mathbf{g} \right)
\end{aligned} \tag{105}$$

Constant RHS terms

$$\begin{aligned}
\mathbf{b}_{const,c_w(c_w),1} &= \mathbf{b}_{const,c_w(c_w),1} \left( \left( \frac{Kk_o k_w}{Kk_o + k_w} \right)_{c_o,0} a\phi c_{w,0} \right) \\
\mathbf{b}_{const,c_o(c_o),1} &= \mathbf{b}_{const,c_o(c_o),1} \left( \left( \frac{k_o k_w}{Kk_o + k_w} c_o \right)_{c_o,0} a\phi \right) \\
\mathbf{b}_{div,g,1} &= \mathbf{b}_{div,g,1} \left( -k(\rho_w) p_0 \left( \frac{c_w}{\mu_w} \right)_{c_w,0} (k_{rw})_{c_o,0,S_0} \mathbf{g} \right)
\end{aligned} \tag{106}$$

All advective terms will have a corresponding RHS,  $\mathbf{b}_{adv}$ , with the same coefficients. Similarly all transient terms will also have a corresponding RHS,  $\mathbf{b}_t$ . The diffusive terms will not have a RHS, and the mass transfer terms (subscript  $K$ ) will also have corresponding RHS,  $\mathbf{b}_K$ .

### Coupled Reactive Transport, oil

System Matrices

$$\mathbf{M}_{diff,c_o} = \mathbf{M}_{diff,c_o} (\mathcal{D}_o \phi) \tag{107}$$

$$\begin{aligned}
\mathbf{J}_{lin,c_w(c_w),2} &= \mathbf{J}_{lin,c_w(c_w),2} \left( \left( \frac{Kk_0k_w}{Kk_0+k_w} \right)_{c_{o,0}} a\phi \right) \\
\mathbf{J}_{t,c_o,2} &= \mathbf{J}_{t,c_o,2}(\phi(1-S_0)) \\
\mathbf{J}_{adv,c_o(p),2} &= \mathbf{J}_{adv,c_o(p),2} \left( -k \left( \frac{\partial \frac{k_{ro}}{\mu_o} c_o}{\partial c_o} \right)_{c_{o,0},S_0} \nabla p_0 \right) \\
\mathbf{J}_{adv,c_o(p_c),2} &= \mathbf{J}_{adv,c_o(p_c),2} \left( -k \left( \frac{\partial \frac{k_{ro}}{\mu_o} c_o \frac{dp_c}{dS}}{\partial c_o} \right)_{c_{o,0},S_0} \nabla S_0 \right) \\
\mathbf{J}_{adv,c_o(g),2} &= \mathbf{J}_{adv,c_o(g),2} \left( -k \left( \frac{\partial \rho_o \frac{k_{ro}}{\mu_o} c_o}{\partial c_o} \right)_{c_{o,0},p_0,S_0} \mathbf{g} \right) \\
\mathbf{J}_{lin,c_o(c_w),2} &= \mathbf{J}_{lin,c_o(c_w),2} \left( \left( \frac{\partial \frac{Kk_0k_w}{Kk_0+k_w}}{\partial c_o} \right)_{c_{o,0}} a\phi c_{w,0} \right) \\
\mathbf{J}_{lin,c_o(c_o),2} &= \mathbf{J}_{lin,c_o(c_o),2} \left( \left( \frac{\partial \frac{k_0k_w}{Kk_0+k_w} c_o}{\partial c_o} \right)_{c_{o,0}} a\phi \right) \\
\mathbf{J}_{adv,p(g),2} &= \mathbf{J}_{adv,p(g),2} \left( -k \left( \frac{\partial \rho_o}{\partial p} \right)_{p_0} \left( \frac{c_o}{\mu_o} \right)_{c_{o,0}} (k_{ro})_{c_{o,0},S_0} \mathbf{g} \right) \\
\mathbf{J}_{diff,p,2} &= \mathbf{J}_{diff,p,2} \left( -k \left( \frac{c_o}{\mu_o} \right)_{c_{o,0}} (k_{ro})_{c_{o,0},S_0} \right) \\
\mathbf{J}_{t,S,2} &= \mathbf{J}_{t,S,2}(-\phi c_0) \\
\mathbf{J}_{adv,S(p),2} &= \mathbf{J}_{adv,S(p),2} \left( -k \left( \frac{c_o}{\mu_o} \right)_{c_{o,0}} \left( \frac{\partial k_{ro}}{\partial S} \right)_{c_{o,0},S_0} \nabla p_0 \right) \\
\mathbf{J}_{adv,S(p_c),2} &= \mathbf{J}_{adv,S(p_c),2} \left( -k \left( \frac{c_o}{\mu_o} \right)_{c_{o,0}} \left( \frac{\partial k_{ro} \frac{dp_c}{dS}}{\partial S} \right)_{c_{o,0},S_0} \nabla S_0 \right) \\
\mathbf{J}_{adv,S(g),2} &= \mathbf{J}_{adv,S(g),2} \left( -k(\rho_o)_{p_0} \left( \frac{c_o}{\mu_o} \right)_{c_{o,0}} \left( \frac{\partial k_{ro}}{\partial S} \right)_{c_{o,0},S_0} \mathbf{g} \right) \\
\mathbf{J}_{diff,S(p_c),2} &= \mathbf{J}_{diff,S(p_c),2} \left( -k \left( \frac{c_o}{\mu_o} \right)_{c_{o,0}} (k_{ro})_{c_{o,0},S_0} \left( \frac{dp_c}{dS} \right)_{c_{o,0},S_0} \right)
\end{aligned} \tag{108}$$

Constant RHS terms

$$\begin{aligned}
\mathbf{b}_{const,c_w(c_w),2} &= \mathbf{b}_{const,c_w(c_w),2} \left( \left( \frac{Kk_0k_w}{Kk_0+k_w} \right)_{c_{o,0}} a\phi c_{w,0} \right) \\
\mathbf{b}_{const,c_o(c_o),2} &= \mathbf{b}_{const,c_o(c_o),2} \left( \left( \frac{k_0k_w}{Kk_0+k_w} c_o \right)_{c_{o,0}} a\phi \right) \\
\mathbf{b}_{div,g,2} &= \mathbf{b}_{div,g,2} \left( -k(\rho_o)_{c_{o,0},p_0} \left( \frac{c_o}{\mu_o} \right)_{c_{o,0}} (k_{ro})_{c_{o,0},S_0} \mathbf{g} \right)
\end{aligned} \tag{109}$$

**Two-Phase Flow, water**  
Jacobians

$$\begin{aligned}
\mathbf{J}_{adv,c_w(p),3} &= \mathbf{J}_{adv,c_w(p),3} \begin{pmatrix} -k(\rho_w)_{p_0} \left( \frac{\partial \frac{1}{\mu_w}}{\partial c_w} \right)_{c_{w,0}} & (k_{rw})_{c_{o,0},S_0} \nabla p_0 \end{pmatrix} \\
\mathbf{J}_{adv,c_w(g),3} &= \mathbf{J}_{adv,c_w(g),3} \begin{pmatrix} -k(\rho_w^2)_{p_0} \left( \frac{\partial \frac{1}{\mu_w}}{\partial c_w} \right)_{c_{w,0}} & (k_{rw})_{c_{o,0},S_0} \mathbf{g} \end{pmatrix} \\
\mathbf{J}_{adv,c_o(p),3} &= \mathbf{J}_{adv,c_o(p),3} \begin{pmatrix} -k(\rho_w)_{p_0} \left( \frac{1}{\mu_w} \right)_{c_{w,0}} \left( \frac{\partial k_{rw}}{\partial c_o} \right)_{c_{o,0},S_0} \nabla p_0 \end{pmatrix} \\
\mathbf{J}_{adv,c_o(g),3} &= \mathbf{J}_{adv,c_o(g),3} \begin{pmatrix} -k(\rho_w^2)_{p_0} \left( \frac{1}{\mu_w} \right)_{c_0} \left( \frac{\partial k_{rw}}{\partial c_o} \right)_{c_{o,0},S_0} \mathbf{g} \end{pmatrix} \\
\mathbf{J}_{t,p,3} &= \mathbf{J}_{t,p,3} \left( \phi S_0 \left( \frac{\partial \rho_w}{\partial p} \right)_{p_0} \right) \\
\mathbf{J}_{adv,p(p),3} &= \mathbf{J}_{adv,p(p),3} \begin{pmatrix} -k \left( \frac{\partial \rho_w}{\partial p} \right)_{p_0} \left( \frac{1}{\mu_w} \right)_{c_{w,0}} & (k_{rw})_{c_{o,0},S_0} \nabla p_0 \end{pmatrix} \\
\mathbf{J}_{adv,p(g),3} &= \mathbf{J}_{adv,p(g),3} \begin{pmatrix} -k \left( \frac{\partial \rho_w^2}{\partial p} \right)_{p_0} \left( \frac{1}{\mu_w} \right)_{c_{w,0}} & (k_{rw})_{c_{o,0},S_0} \mathbf{g} \end{pmatrix} \\
\mathbf{J}_{diff,p,3} &= \mathbf{J}_{diff,p,3} \begin{pmatrix} -k(\rho_w)_{p_0} \left( \frac{1}{\mu_w} \right)_{c_0} & (k_{rw})_{c_{o,0},S_0} \end{pmatrix} \\
\mathbf{J}_{t,S,3} &= \mathbf{J}_{t,S,3} (\phi(\rho_w)_{p_0}) \\
\mathbf{J}_{adv,S(p),3} &= \mathbf{J}_{adv,S(p),3} \begin{pmatrix} -k(\rho_w)_{p_0} \left( \frac{1}{\mu_w} \right)_{c_0} \left( \frac{\partial k_{rw}}{\partial S} \right)_{c_{o,0},S_0} \nabla p_0 \end{pmatrix} \\
\mathbf{J}_{adv,S(g),3} &= \mathbf{J}_{adv,S(g),3} \begin{pmatrix} -k(\rho_w^2)_{p_0} \left( \frac{1}{\mu_w} \right)_{c_{w,0}} \left( \frac{\partial k_{rw}}{\partial S} \right)_{c_{o,0},S_0} \mathbf{g} \end{pmatrix}
\end{aligned} \tag{110}$$

Constant RHS terms

$$\mathbf{b}_{div,g,3} = \mathbf{b}_{div,g,3} \begin{pmatrix} -k(\rho_w^2)_{p_0} \left( \frac{1}{\mu_w} \right)_{c_{w,0}} & (k_{rw})_{c_{o,0},S_0} \mathbf{g} \end{pmatrix} \tag{111}$$

**Two-Phase Flow, oil**  
Jacobians

$$\begin{aligned}
\mathbf{J}_{t,c_o,A} &= \mathbf{J}_{t,c_o,A} \left( \phi(1-S_0) \left( \frac{\partial \rho_o}{\partial c_o} \right)_{c_{o,0},p_0} \right) \\
\mathbf{J}_{adv,c_o(p),A} &= \mathbf{J}_{adv,c_o(p),A} \left( -k \left( \frac{\partial \rho_o \frac{k_{ro}}{\mu_o}}{\partial c_o} \right)_{c_{o,0},S_0} \nabla p_0 \right) \\
\mathbf{J}_{adv,c_o(p_c),A} &= \mathbf{J}_{adv,c_o(p_c),A} \left( -k \left( \frac{\partial \rho_o \frac{k_{ro}}{\mu_o} \frac{dp_c}{dS}}{\partial c_o} \right)_{c_{o,0},p_{c,0},S_0} \nabla S_0 \right) \\
\mathbf{J}_{adv,c_o(g),A} &= \mathbf{J}_{adv,c_o(g),A} \left( -k \left( \frac{\partial \rho_o^2 \frac{k_{ro}}{\mu_o}}{\partial c_o} \right)_{c_{o,0},S_0} \mathbf{g} \right) \\
\mathbf{J}_{t,p,A} &= \mathbf{J}_{t,p,A} \left( \phi(1-S_0) \left( \frac{\partial \rho_o}{\partial p} \right)_{c_{o,0},p_0} \right) \\
\mathbf{J}_{adv,p(p),A} &= \mathbf{J}_{adv,p(p),A} \left( -k \left( \frac{\partial \rho_o}{\partial p} \right)_{c_{o,0},p_0} \left( \frac{1}{\mu_o} \right)_{c_{o,0}} (k_{ro})_{c_{o,0},S_0} \nabla p_0 \right) \\
\mathbf{J}_{adv,p(p_c),A} &= \mathbf{J}_{adv,p(p_c),A} \left( -k \left( \frac{\partial \rho_o}{\partial p_c} \right)_{c_{o,0},p_{c,0}} \left( \frac{1}{\mu_o} \right)_{c_{o,0}} (k_{ro})_{c_{o,0},S_0} \left( \frac{dp_c}{dS} \right)_{S_0} \nabla S_0 \right) \\
\mathbf{J}_{adv,p(g),A} &= \mathbf{J}_{adv,p(g),A} \left( -k \left( \frac{\partial \rho_o^2}{\partial p} \right)_{c_{o,0},p_0} \left( \frac{1}{\mu_o} \right)_{c_{o,0}} (k_{ro})_{c_{o,0},S_0} \mathbf{g} \right) \\
\mathbf{J}_{diff,p,A} &= \mathbf{J}_{diff,p,A} \left( -k(\rho_o)_{c_{o,0},p_0} \left( \frac{1}{\mu_o} \right)_{c_0} (k_{ro})_{c_{o,0},S_0} \right) \\
\mathbf{J}_{t,S,A} &= \mathbf{J}_{t,S,A} (-\phi(\rho_o)_{c_{o,0},p_0}) \\
\mathbf{J}_{adv,S(p),A} &= \mathbf{J}_{adv,S(p),A} \left( -k(\rho_o)_{c_{o,0},p_0} \left( \frac{1}{\mu_o} \right)_{c_0} \left( \frac{\partial k_{ro}}{\partial S} \right)_{c_{o,0},S_0} \nabla p_0 \right) \\
\mathbf{J}_{adv,S(p_c),A} &= \mathbf{J}_{adv,S(p_c),A} \left( -k(\rho_o)_{c_{o,0},p_{c,0}} \left( \frac{1}{\mu_o} \right)_{c_{o,0}} \left( \frac{\partial k_{ro} \frac{dp_c}{dS}}{\partial S} \right)_{c_{o,0},S_0} \nabla S_0 \right) \\
\mathbf{J}_{adv,S(g),A} &= \mathbf{J}_{adv,S(g),A} \left( -k(\rho_o^2)_{c_{o,0},p_0} \left( \frac{1}{\mu_o} \right)_{c_{o,0}} \left( \frac{\partial k_{ro}}{\partial S} \right)_{c_{o,0},S_0} \mathbf{g} \right) \\
\mathbf{J}_{diff,S(p_c),A} &= \mathbf{J}_{diff,S(p_c),A} \left( -k(\rho_o)_{c_{o,0},p_{c,0}} \left( \frac{1}{\mu_o} \right)_{c_{o,0}} (k_{ro})_{c_{o,0},S_0} \left( \frac{dp_c}{dS} \right)_{S_0} \right)
\end{aligned} \tag{112}$$

Constant RHS terms

$$\mathbf{b}_{div,g,A} = \mathbf{b}_{div,g,A} \left( -k(\rho_o^2)_{c_{o,0},p_0} \left( \frac{1}{\mu_o} \right)_{c_{o,0}} (k_{ro})_{c_{o,0},S_0} \mathbf{g} \right) \tag{113}$$

All RHS's will be a function of the same constants as the corresponding Jacobian, i.e.  $\mathbf{b}_{t,c_o,1}$  is a function of the same constant as  $\mathbf{J}_{t,c_o,1}$ , etc.

## 11. APPENDIX C

Some of the terms listed in Appendix A are derivatives. These derivatives will be listed explicitly here.



### 11.1. Model: No gravity, no capillary pressure, incompressible

Derivatives of  $c_w$

$$\begin{aligned}\frac{\partial \frac{c_w}{\mu_w}}{\partial c_w} &= \frac{\mu_w - c_w \mu'_w}{\mu_w^2} \\ \frac{\partial \frac{1}{\mu_w}}{\partial c_w} &= \frac{-\mu'_w}{\mu_w^2}\end{aligned}\tag{114}$$

Derivatives of  $c_o$

$$\begin{aligned}\frac{\partial \frac{c_o}{\mu_o}}{\partial c_o} &= \frac{\mu_o - c_o \mu'_o}{\mu_o^2} \\ \frac{\partial \rho_o}{\partial c_o} &= \rho'_o \\ \frac{\partial \frac{\rho_o}{\mu_o}}{\partial c_o} &= \frac{\rho'_o \mu_o - \rho_o \mu'_o}{\mu_o^2}\end{aligned}\tag{115}$$

Derivatives of  $S$

$$\begin{aligned}\frac{\partial k_{ro}}{\partial S} &= -\frac{n_o k_{ro}^0}{1 - S_{wc} - S_{or}} \left( \frac{1 - S - S_{or}}{1 - S_{wc} - S_{or}} \right)^{n_o - 1} \\ \frac{\partial k_{rw}}{\partial S} &= \frac{n_w k_{rw}^0}{S - S_{wc}} \left( \frac{S - S_{wc}}{1 - S_{wc} - S_{or}} \right)^{n_w - 1}\end{aligned}\tag{116}$$

### 11.2. Model: Gravity, capillary pressure, compressible

Derivatives of  $c_w$

$$\begin{aligned}\frac{\partial \frac{c_w}{\mu_w}}{\partial c_w} &= \frac{\mu_w - c_w \mu'_w}{\mu_w^2} \\ \frac{\partial \frac{1}{\mu_w}}{\partial c_w} &= \frac{-\mu'_w}{\mu_w^2}\end{aligned}\tag{117}$$

Derivatives of  $c_o$

$$\begin{aligned}\frac{\partial \frac{K k_o k_w}{K k_o + k_w}}{\partial c_o} &= \frac{k_o k_w}{K k_o + k_w} K' - \frac{K k_o^2 k_w}{(K k_o + k_w)^2} K' \\ \frac{\partial \frac{k_o k_w}{K k_o + k_w} c_o}{\partial c_o} &= \frac{k_o k_w}{K k_o + k_w} - \frac{k_o^2 k_w c_o}{(K k_o + k_w)^2} K' \\ \frac{\partial \frac{k_{ro}}{\mu_o} c_o}{\partial c_o} &= \frac{c_o}{\mu_o} k'_{ro} + \frac{k_{ro}}{\mu_o} - \frac{c_o k_{ro}}{\mu_o^2} \mu'_o \\ \frac{\partial \rho_o}{\partial c_o} &= \rho'_o \\ \frac{\partial \rho_o \frac{k_{ro}}{\mu_o}}{\partial c_o} &= \frac{k_{ro}}{\mu_o} \rho'_o + \frac{\rho_o}{\mu_o} k'_{ro} - \frac{\rho_o k_{ro}}{\mu_o^2} \mu'_o \\ \frac{\partial \rho_o^2 \frac{k_{ro}}{\mu_o}}{\partial c_o} &= \frac{2 \rho_o k_{ro}}{\mu_o} \rho'_o + \frac{\rho_o^2}{\mu_o} k'_{ro} - \frac{\rho_o^2 k_{ro}}{\mu_o^2} \mu'_o \\ \frac{\partial \rho_o \frac{k_{ro}}{\mu_o} c_o}{\partial c_o} &= \frac{c_o k_{ro}}{\mu_o} \rho'_o + \frac{\rho_o c_o}{\mu_o} k'_{ro} + \frac{\rho_o k_{ro}}{\mu_o} - \frac{\rho_o c_o k_{ro}}{\mu_o^2} \mu'_o \\ \frac{\partial \frac{k_{ro}}{\mu_o} c_o \frac{dp_c}{dS}}{\partial c_o} &= \frac{c_o}{\mu_o} \frac{dp_c}{dS} k'_{ro} + \frac{k_{ro}}{\mu_o} \frac{dp_c}{dS} + \frac{k_{ro} c_o}{\mu_o} \frac{d^2 p_c}{dS dc_o} - \frac{k_{ro} c_o}{\mu_o^2} \frac{dp_c}{dS} \mu'_o \\ \frac{\partial \rho_o \frac{k_{ro}}{\mu_o} \frac{dp_c}{dS}}{\partial c_o} &= \frac{k_{ro}}{\mu_o} \frac{dp_c}{dS} \rho'_o + \frac{\rho_o}{\mu_o} \frac{dp_c}{dS} k'_{ro} + \frac{\rho_o k_{ro}}{\mu_o} \frac{d^2 p_c}{dS dc_o} - \frac{\rho_o k_{ro}}{\mu_o^2} \frac{dp_c}{dS} \mu'_o\end{aligned}\tag{118}$$

Derivatives of  $p$

$$\begin{aligned}
\frac{\partial \rho_w}{\partial p} &= \rho'_w \\
\frac{\partial \rho_o}{\partial p} &= \rho'_o \\
\frac{\partial \rho_w^2}{\partial p} &= 2\rho_w \rho'_w \\
\frac{\partial \rho_o^2}{\partial p} &= 2\rho_o \rho'_o
\end{aligned} \tag{119}$$

Derivatives of  $S$

$$\begin{aligned}
\frac{\partial k_{rw}}{\partial S} &= \frac{n_w k_{rw}^0}{1 - S_{wc} - S_{or}} \left( \frac{S - S_{wc}}{1 - S_{wc} - S_{or}} \right)^{n_w - 1} \\
\frac{\partial k_{ro}}{\partial S} &= -\frac{n_o k_{ro}^0}{1 - S_{wc} - S_{or}} \left( \frac{1 - S - S_{or}}{1 - S_{wc} - S_{or}} \right)^{n_o - 1} \\
\frac{\partial k_{ro} \frac{dp_c}{dS}}{\partial S} &= k'_{ro} \frac{dp_c}{dS} + k_{ro} \frac{d^2 p_c}{dS^2}
\end{aligned} \tag{120}$$

Derivatives related to specific models chosen in this paper (relative permeability and capillary pressure)

$$\begin{aligned}
\frac{\partial k_{rw}}{\partial c_o} &= \frac{n_w k_{rw}^0}{1 - S_{wc} - S_{or}} \left( \frac{S - S_{wc}}{1 - S_{wc} - S_{or}} \right)^{n_w} S'_{or} \\
\frac{\partial k_{ro}}{\partial c_o} &= \frac{k_{ro}^0 n_o (1 - S_{wc} - S_{or})}{1 - S - S_{or}} \left( \frac{1 - S - S_{or}}{1 - S_{wc} - S_{or}} \right)^{n_o} \left( \frac{(1 - S - S_{or}) S'_{or}}{(1 - S_{wc} - S_{or})^2} - \frac{S'_{or}}{1 - S_{wc} - S_{or}} \right)
\end{aligned} \tag{121}$$

## REFERENCES

- [1] A. Chernetsky, et al. (2015). *A Novel Enhanced Oil Recovery Technique: Experimental Results and Modelling Workflow of the DME Enhanced Waterflood Technology*. Society of Petroleum Engineers, SPE-177919.