Appendix A

Flow Simulation in SUQIB Code and Used Physical Properties

In SUQIB, simulation of two phase flow of oil and water in 2D black oil models has been implemented. It is desired to solve simultaneously the following system of two equations for pressure and water saturation:

$$\begin{cases} \dfrac{\partial S_w}{\partial t} + \nabla.\mathbf{V}_w = Q_w \\ \nabla.\left(\mathbf{V}_w + \mathbf{V}_o\right) = Q_w + Q_o \end{cases} \quad \text{(A.1)},$$

in which S_w and Q_w stand respectively for the water saturation and water production/injection volumetric rate over the unit volume. Darcy's law relates the water and oil fluxes ($\mathbf{V}_w$ and $\mathbf{V}_o$) to the corresponding phase flow potentials through following relations:

$$\begin{cases} \mathbf{V}_w = -\mathbf{K}\left(K_{rw}/\mu_w\right)\nabla\left(P_w + \rho_w g h\right) \\ \mathbf{V}_o = -\mathbf{K}\left(K_{ro}/\mu_o\right)\nabla\left(P_o + \rho_o g h\right) \end{cases} \quad \text{(A.2)},$$

where K_{ri}, μ_i, ρ_i, P_i stand respectively for the relative permeability, viscosity , density and the pressure of phase *i* when *i* points to both flowing phases. The following simplifying assumptions are applied:

1. Both phases are considered incompressible with constant density.
2. The viscosities of both phases are constant.
3. Capillarity is negligible, so there is no pressure drop across the common surface of two phases. We represent the common surface with *P* which $P = P_w = P_o$.
4. Relative permeability is a function of water saturation only.

We name the term $-\mathbf{K}\nabla\left(P+\rho_i gh\right)$ as the velocity of phase *i* at one-phase flow conditions and represent it with $\mathbf{V}_i^{1-phase}$. Therefore oil and water fluxes are expressed as $\mathbf{V}_i = \left(K_{ri} \diagup \mu_i\right)\mathbf{V}_i^{1-phase}$.

A.1 Temporal and Spatial Discretisation

Inserting Eq. A.2 into Eq. A.1 and integrating over the volume of each cell (Ω_C) followed by applying the Gauss divergence theorem results in the following set of equations:

$$\begin{cases} \dfrac{\partial S_w}{\partial t} + \dfrac{1}{V_{\Omega_C}} \displaystyle\int_{\Gamma_C} \left(K_{rw} \diagup \mu_w\right)\mathbf{n}_{\Gamma_C}{}^T \bullet \mathbf{V}_w^{1-phase} dA = Q_w \\ \displaystyle\int_{\Gamma_C} \left(\left(K_{rw} \diagup \mu_w\right)\mathbf{n}_{\Gamma_C}{}^T \bullet \mathbf{V}_w^{1-phase} + \left(K_{ro} \diagup \mu_o\right)\mathbf{n}_{\Gamma_C}{}^T \bullet \mathbf{V}_o^{1-phase} \right) dA = \left(Q_w + Q_o\right) V_{\Omega_C} \end{cases} \quad \text{(A.3)},$$

in which Γ_C is the external surface of the cell and it is defined as the collection of all interfaces of cell C (shown with I_C) with its immediate adjacent cells (cells sharing a common face with *C*) counted in the set $\widehat{C}(C) = \left\{\widehat{C}_k(C),\ k = 1,2,3,...,N\right\}$.

$$\Gamma_C = \left\{ I_C \mid I_C \in C \cap \widehat{C}_k(C), k = 1,2,...,N \right\} \quad \text{(A.4)}$$

Besides $\mathbf{n}_{\Gamma_C}$ is the normal outward vector drawn on Γ_C. Eq. A.3 is rearranged by decomposing the each integral over Γ_C into integrals over the segments I_C^k.

$$\begin{cases} \dfrac{\partial S_w}{\partial t} + \dfrac{1}{V_{\Omega_C}} \sum_{k=1}^{N} \int_{I_C^k} \left(K_{rw} / \mu_w \right) \mathbf{n}_{I_C^k}{}^T \bullet \mathbf{V}_w^{1-phase} dA = Q_w \\ \sum_{k=1}^{N} \int_{I_C^k} \left(\left(K_{rw} / \mu_w \right) \mathbf{n}_{I_C^k}{}^T \bullet \mathbf{V}_w^{1-phase} + \left(K_{ro} / \mu_o \right) \mathbf{n}_{I_C^k}{}^T \bullet \mathbf{V}_o^{1-phase} \right) dA = \left(Q_w + Q_o \right) V_{\Omega_C} \end{cases} \quad \text{(A.5)}$$

We take out the phase mobilities $\left(K_{ri} / \mu_i \right)$ from the integral by assuming an average value over the interface for them. Then each integral $\int_{I_C^k} \mathbf{n}_{I_C^k}{}^T \bullet \mathbf{V}_i^{1-phase} dA$ is considered as the volumetric flux of phase *i* at single phase flow condition through the interface I_C^k and is shown with $f_{I_C^k}^i$. One can define two sets of cells:

1. $\hat{C}\left(I_C^k\right)$ is defined as the set of N_1 cells sharing at least one common point with I_C^k.
2. $\hat{\mathbb{C}}\left(I_C^k\right)$ is defined as the set of two adjacent cells sharing the whole interface I_C^k : $\hat{\mathbb{C}}\left(I_C^k\right) = \left\{C, \mathbb{C}^k\right\}$. Thus $\hat{\mathbb{C}}\left(I_C^k\right)$ is a subset of $\hat{C}\left(I_C^k\right)$.

Single phase fluxes ($f_{I_C^k}^i$) can be computed using the EEMPFA approach over all interfaces suffering from non-**K**-orthogonality problems and for the rest TPFA scheme would give the 2nd order accurate approximations of flux. In either of cases $f_{I_C^k}^i$ is expressed as a linear combination of potentials at centres of cells within one of above defined sets:

$$f_{I_C^k}^i = \begin{cases} \sum_{j=1}^{N_1} T_{\hat{C}_j(I_C)} \Phi^i_{\hat{C}_j\left(I_C^k\right)} & \text{EEMPFA} \\ \sum_{j=1}^{2} T_{\hat{\mathbb{C}}_j(I_C)} \Phi^i_{\hat{C}_j\left(I_C^k\right)} & \text{TPFA} \end{cases} \quad \text{(A.6).}$$

Remembering the fact that EEMPFA would vanish to TPFA for along the interfaces away from the non-**K**-orthogonality effects, one can come up with the final discretized form of Eq. A.5 as following:

$$\begin{cases} \Delta S_w = -\dfrac{\Delta t}{V_{\Omega_C}} \sum_{k=1}^{N} \left(K_{rw} \big/ \mu_w \right)_{I_C^k} \sum_{j=1}^{N_1} T_{\hat{C}_j\left(I_C^k\right)} \Phi^w_{\hat{C}_j\left(I_C^k\right)} + \Delta t Q_w \\ \sum_{k=1}^{N} \left(\left(K_{rw} \big/ \mu_w \right)_{I_C^k} \sum_{j=1}^{N_1} T_{\hat{C}_j\left(I_C^k\right)} \Phi^w_{\hat{C}_j\left(I_C^k\right)} + \left(K_{ro} \big/ \mu_o \right)_{I_C^k} \sum_{j=1}^{N_1} T_{\hat{C}_j\left(I_C^k\right)} \Phi^o_{\hat{C}_j\left(I_C^k\right)} \right) = \left(Q_w + Q_o \right) V_{\Omega_C} \end{cases} \quad \text{(A.7).}$$

Expressing flow potential as the summation of hydraulic and gravity heads, one would end up with:

$$\begin{cases} \Delta S_w = -\dfrac{\Delta t}{V_{\Omega_C}} \sum_{k=1}^{N} \left(K_{rw} \big/ \mu_w \right)_{I_C^k} \sum_{j=1}^{N_1} T_{\hat{C}_j\left(I_C^k\right)} \left(P_{\hat{C}_j\left(I_C^k\right)} + \rho_w g h_{\hat{C}_j\left(I_C^k\right)} \right) + \Delta t Q_w \\ \sum_{k=1}^{N} \left(\left(K_{rw} \big/ \mu_w \right)_{I_C^k} \sum_{j=1}^{N_1} T_{\hat{C}_j\left(I_C^k\right)} \left(P_{\hat{C}_j\left(I_C^k\right)} + \rho_w g h_{\hat{C}_j\left(I_C^k\right)} \right) + \left(K_{ro} \big/ \mu_o \right)_{I_C^k} \sum_{j=1}^{N_1} T_{\hat{C}_j\left(I_C^k\right)} \left(P_{\hat{C}_j\left(I_C^k\right)} + \rho_o g h_{\hat{C}_j\left(I_C^k\right)} \right) \right) = \left(Q_w + Q_o \right) V_{\Omega_C} \end{cases} \quad \text{(A.8).}$$

The relative permeability (and viscosity in general) at interfaces is calculated by means of single point upstream weighting which is a 1st order accurate scheme.

$$\left(K_{ri} \big/ \mu_i \right)_{I_C^k} = \begin{cases} \left(K_{ri} \big/ \mu_i \right)_C & \int_{I_C^k} \mathbf{n}_{I_C^k}{}^T \bullet \mathbf{V}_i^{1-phase} dA = \sum_{j=1}^{N_1} T_{\hat{C}_j\left(I_C\right)} \Phi^i_{\hat{C}_j\left(I_C^k\right)} > 0 \\ \left(K_{ri} \big/ \mu_i \right)_{\in^k} & \int_{I_C^k} \mathbf{n}_{I_C^k}{}^T \bullet \mathbf{V}_i^{1-phase} dA = \sum_{j=1}^{N_1} T_{\hat{C}_j\left(I_C\right)} \Phi^i_{\hat{C}_j\left(I_C^k\right)} < 0 \end{cases} \quad \text{(A.9)}$$

A.2 Coupling Scheme

System of mass conservation equations for water phase and both phases can be solved for the pressure and water saturation via one of conventionally used approaches in reservoir simulation. Both IMPES (IMplicit Pressure Explicit Saturation) and fully implicit approaches have been implemented in SUQIB code. In IMPES approach water saturations would be updated at each time-step from the water conservation equation using the pressure and saturation information of the current time step ($S_w{}^n$ and P^n). The resulting water saturations are used to compute fluid mobilities (relative permeability and viscosity) and source/sink terms (Q_w, Q_o) at new time-step. Inserting renewed fluid mobilities in total conservation equation eventuates in a system of $\mathbb{N}$ (number of cells) equations for pressures at cell centres.

$$\begin{cases} S_w^{n+1} = S_w^{n} - \dfrac{\Delta t}{V_{\Omega_C}} \sum_{k=1}^{N} \left(K_{rw} \big/ \mu_w \right)_{I_C^k}^{n} \sum_{j=1}^{N_1} T_{\hat{C}_j\left(I_C^k\right)} \left(P_{\hat{C}_j\left(I_C^k\right)}^{\ n} + \rho_w g h_{\hat{C}_j\left(I_C^k\right)} \right) + \Delta t Q_w^{\ n} \\ \sum_{i=w,o} \sum_{k=1}^{N} \left(\left(K_{ri} \big/ \mu_i \right)_{I_C^k}^{n+1} \sum_{j=1}^{N_1} T_{\hat{C}_j\left(I_C^k\right)} \left(P_{\hat{C}_j\left(I_C^k\right)}^{\ n+1} + \rho_i g h_{\hat{C}_j\left(I_C^k\right)} \right) \right) = V_{\Omega_C} \sum_{i=w,o} Q_i^{\ n+1} \end{cases} \quad \text{(A.10)}$$

Comprised system of equation obtained from discretized total conservation equation ($\mathbf{A}_{\mathbb{N}\times\mathbb{N}}\mathbf{P}_{\mathbb{N}\times 1} = \mathbf{B}_{\mathbb{N}\times 1}$) are solved with preconditioner routines and matrix solvers provided by PETSc (The Portable, Extensible Toolkit for Scientific Computation) developed at the Mathematics and Computer Science Division of Argonne National Laboratory. Considering the reduced sparsity of solution matrix due to using EEMPFA instead of TPFA near to reservoir boundaries, we have tried several pairs of Preconditioner/Matrix Solvers. The best results with least non-physical solutions are obtained when Block Jacobi Preconditioner and BiCGSTAB (BiConjugate Gradient Stabilized) matrix solver is utilised. However satisfactory results for smaller anisotropy and heterogeneity can be obtained when any pair of Preconditioner/Matrix Solver among those listed in table A.1 is chosen.

Preconditioner	Matrix Solver
Jacobi	Transpose-Free Quasi-Minimal Residual
Incomplete Lower Upper (ILU)	BiConjugate Gradient
Successive Over-Relaxation (SOR)	Chebychev

Table A.1: Used Preconditioners and Matrix Solvers resulting in less-oscillatory solutions

In fully implicit approach, all pressure or water saturation dependent terms are calculated in the next time-step. In effect all unknown pressure and saturation terms are non-linearly coupled. This would constitute a non-linear system of $2\mathbb{N}$ equations in the form $\mathbf{F}(\mathbf{X}) = \mathbf{0}$, in which:

$$\mathbf{X}_{\mathbb{N}\times 1} = \left[\left[P_1, S_{w1}\right]^T, \left[P_2, S_{w2}\right]^T, ..., \left[P_{\mathbb{N}}, S_{w\mathbb{N}}\right]^T \right]^T \quad \text{(A.11)},$$

$$\mathbf{F}=\left[\mathbf{F}_1,\mathbf{F}_2,...,\mathbf{F}_{\mathbb{N}}\right]^T,$$

$$\mathbf{F}_C=\begin{bmatrix} {S_w}^{n+1}-{S_w}^{n}+\dfrac{\Delta t}{V_{\Omega_C}}\sum_{k=1}^{N}\left(K_{rw}/\mu_w\right)_{I_C^k}{}^{n+1}\sum_{j=1}^{N_1}T_{\hat{C}_j\left(I_C^k\right)}\left(P_{\hat{C}_j\left(I_C^k\right)}{}^{n+1}+\rho_w g h_{\hat{C}_j\left(I_C^k\right)}\right)-\Delta t{Q_w}^{n+1} \\ \sum_{i=w,o}\sum_{k=1}^{N}\left(\left(K_{ri}/\mu_i\right)_{I_C^k}{}^{n+1}\sum_{j=1}^{N_1}T_{\hat{C}_j\left(I_C^k\right)}\left(P_{\hat{C}_j\left(I_C^k\right)}{}^{n+1}+\rho_i g h_{\hat{C}_j\left(I_C^k\right)}\right)\right)-V_{\Omega_C}\sum_{i=w,o}{Q_i}^{n+1}\end{bmatrix}$$

(A.12).

We have employed the SNES routine of PETSc which solves the non-linear equation through an iterative Newton-Raphson method which improves the initial guess of solution ($\mathbf{X}_0^{n+1}$) via following relation:

$$\begin{aligned}&\mathbf{X}_{k+1}^{n+1}=\mathbf{X}_k^n-\mathbf{Y}_k^n,\\&\mathbf{F}'\left(\mathbf{X}_k^n\right)\mathbf{Y}_k^n=\mathbf{F}\left(\mathbf{X}_k^n\right)\end{aligned}\qquad\text{(A.13).}$$

$\mathbf{F}'\left(\mathbf{X}_k^n\right)_{\mathbb{N}\times\mathbb{N}}$ is the Jacobian matrix of vector $\mathbf{F}\left(\mathbf{X}_k^n\right)_{\mathbb{N}\times 1}$ and can be evaluated using either the analytic relation of Jacobian matrix or by letting the PETSc to calculate it by finite difference approximation. For our examined problems, more stable (less spuriously oscillatory) solutions with faster convergence are obtained when the analytic Jacobian is applied. SNES convergence is monitored with Line-Search method. Besides in our implementation, solution of internal system of equations occurring at each iteration ($\mathbf{F}'\left(\mathbf{X}_k^n\right)\mathbf{Y}_k^n=\mathbf{F}\left(\mathbf{X}_k^n\right)$) is carried out through Preconditioner/Solver pair of Jacobi/BICGSTAB. When the flux and matrix splitting idea (discussed in Chapter 4) is utilised, the modified vector $\mathbf{F}_C$ by means of flux/matrix splitting method would be written as:

$$\mathbf{F}_C=\begin{bmatrix} {S_w}^{n+1}-{S_w}^{n}+\dfrac{\Delta t}{V_{\Omega_C}}\sum_{k=1}^{N}\left(K_{rw}/\mu_w\right)_{I_C^k}{}^{n+1}\left(\begin{array}{l}\displaystyle\sum_{j=1}^{2}T_{\hat{\mathbb{C}}_j\left(I_C^k\right)}\left(P_{\hat{\mathbb{C}}_j\left(I_C^k\right)}{}^{n+1}+\rho_w g h_{\hat{\mathbb{C}}_j\left(I_C^k\right)}\right)+\\ \displaystyle\sum_{\hat{C}_j\left(I_C^k\right)\notin\hat{\mathbb{C}}\left(I_C^k\right)}T_{\hat{C}_j\left(I_C^k\right)}\left(P_{\hat{C}_j\left(I_C^k\right)}{}^{n}+\rho_w g h_{\hat{C}_j\left(I_C^k\right)}\right)\end{array}\right)-\Delta t{Q_w}^{n+1} \\ \displaystyle\sum_{i=w,o}\sum_{k=1}^{N}\left(\left(K_{ri}/\mu_i\right)_{I_C^k}{}^{n+1}\left(\begin{array}{l}\displaystyle\sum_{j=1}^{2}T_{\hat{\mathbb{C}}_j\left(I_C^k\right)}\left(P_{\hat{\mathbb{C}}_j\left(I_C^k\right)}{}^{n+1}+\rho_i g h_{\hat{\mathbb{C}}_j\left(I_C^k\right)}\right)+\\ \displaystyle\sum_{\hat{C}_j\left(I_C^k\right)\notin\hat{\mathbb{C}}\left(I_C^k\right)}T_{\hat{C}_j\left(I_C^k\right)}\left(P_{\hat{C}_j\left(I_C^k\right)}{}^{n}+\rho_i g h_{\hat{C}_j\left(I_C^k\right)}\right)\end{array}\right)\right)-V_{\Omega_C}\sum_{i=w,o}{Q_i}^{n+1}\end{bmatrix}$$

(A.14).

In this method, at each cell unknown pressures all immediate adjacent cells (those with a common interface) are written at next time-step, but all pressures belonging to non-immediate adjacent cells are written in current time-step and are known. This method were used to increase the sparsity of Jacobian matrix, this would allow for faster convergence of solving the denser Jacobian matrices and would reduce the possibility of non-physical results at large anisotropy and large cross terms.

A.3 Physical properties used in simulator

A.3.1: Relative Permeability

Stone's two-phase model-1 (Aziz and Settari [1979]) is used to compute relative permeabilities, on which one set of data for 2-phase relative permeabilities (for water/oil flow) associated with the knowledge of residual oil saturation (S_{orw}), connate water saturation (S_{wc}), oil relative permeability at connate water saturation (k_{rowc}) and water relative permeability at maximum water saturation (k_{rwi}) are used to approximate relative permeabilities in terms of a function of water saturation.

$$k_{ro} = \begin{cases} k_{rowc} & S_w \le S_{wc} \\ k_{rowc}\left[\dfrac{1-S_w-S_{orw}}{1-S_{wc}-S_{orw}}\right]^{\alpha_o} & S_{wc} < S_w < 1-S_{orw} \\ 0 & S_w > 1-S_{orw} \end{cases} \tag{A.15}$$

$$k_{rw} = \begin{cases} 0 & S_w \le S_{wc} \\ k_{rwi}\left[\dfrac{S_w-S_{wc}}{1-S_{wc}-S_{orw}}\right]^{\alpha_w} & S_{wc} < S_w < 1-S_{orw} \\ k_{rwi} & S_w > 1-S_{orw} \end{cases} \tag{A.16}$$

Values we have used for the constants in Stone's model are as followings:

$$\begin{cases} S_{wc} = 0.1, S_{orw} = 0.1 \\ k_{rwi} = 0.5, k_{rowc} = 0.3 \\ \alpha_w = 1.5, \alpha_{ow} = 2 \end{cases} \tag{A.17}.$$

A.3.2: Viscosity:

Water and oil viscosities are assumed to be constants independent of pressure and saturation. The values measured in Cent-Poise are given as:

$$\mu_w = 0.4\ cp, \mu_o = 0.05\ \ cp \tag{A.18}$$

A.3.3: PVT Data:

All flowing phases are proposed to be incompressible; their constant densities are:

$$\rho_w = 55\ \text{lbm/ft}^3, \rho_o = 55\ \text{lbm/ft}^3 \tag{A.19}$$