# RANDOM WALK PARTICLE MODELLING OF POLYMER INJECTION USING MATLAB RESERVOIR SIMULATION TOOLBOX

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BY

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# Approval of the Thesis:

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#### ABSTRACT

### RANDOM WALK PARTICLE MODELLING OF POLYMER INJECTION USING MATLAB RESERVOIR SIMULATION TOOLBOX

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Enhanced oil recovery (EOR) is essential to increase the maximum recoverable oil by natural means of production. Having chosen an EOR method, the effectiveness of the method should be analyzed before applying to a reservoir since the methods are generally costly. Polymer injection is a chemical EOR process, where the injected polymer with water increases the water viscosity, and help increasing the sweep efficiency in the reservoir. In order to model the effects of polymer injection, the random-walk particle tracking method is implemented on MATLAB Reservoir Simulation Toolbox (MRST), an open source code for MATLAB for reservoir modelling. Our approach is to utilize the random walk form of transport equation for the advection/diffusion of the injected chemical in the porous medium whereas the continuity equations are solved by the black-oil simulator MRST. Verification of MRST models integrity is done by comparing its simple transport model with a known analytical solution, and its polymer model with ECLIPSE 100 Black Oil Simulator's results. Then the particle tracking method is applied on one-dimensional and two-dimensional injection scenarios.

The method overcomes the numerical diffusion problem, which is a problem of finite difference/finite volume discretization techniques. We can also use the method to model the effect of dispersion coefficient, which is hard to obtain by normal methods. However,

the random nature of the solution sometimes causes convergence problems in some twodimensional simulations.

Keywords: Enhanced oil recovery, polymer injection, particle tracking method, reservoir modelling, dispersion

# MATLAB REZERVUAR SİMÜLASYON EKLENTİSİ KULLANARAK RASTLANTISAL PARÇACIK HAREKET METODU İLE POLİMER ENJEKSİYONU MODELLEMESİ

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Geliştirilmiş petrol üretimi (EOR) doğal yollardan kurtarılabilecek maksimum petrol miktarını arttırmak için gereklidir. EOR metodu seçildikten sonra, genellikle metotlar yüksek yatırım gerektirdiğinden dolayı uygulamadan önce metodun etkenliği analiz edilmelidir. Polimer enjeksiyonu, su ile birlikte enjekte edilen polimerin suyun viskozitesini arttırdığı ve rezervuardaki süpürme veriminin arttırıldığı bir kimyasal EOR metodudur. Polimer enjeksiyonunun etkilerini modellemek için düzensiz hareket metodunu kullanarak parçacık izleme metodu, rezervuar modellemede kullanılan açık kod MATLAB Reservoir Simulation Toolbox (MRST) üzerinde uygulanmıştır. Bu yaklaşımımızda enjekte edilen kimyasalın gözenekli ortamda taşınma denklemi düzensiz dağılım formunda çözülürken süreklilik denklemleri üç fazlı akışkan simülatörü MRST tarafından çözülmektedir. MRST modellerinin tutarlılığı, içerdiği basit taşıma modelinin bilinen bir analitik yöntemle ve polimer modelinin ECLIPSE 100 Black Oil Simulator'ün sonuçlarıyla kıyaslanarak doğrulanmıştır. Sonrasında parçacık izleme metodu tek boyutlu ve iki boyutlu enjeksiyon senaryoları üzerinde uygulanmıştır.

Metodun uygulaması sonlu kalan/sonlu hacim ayrıştırma tekniklerinin bir problemi olan sayısal dağılım probleminin üstesinden gelmektedir. Metot ayrıca normal metotlarla elde

edilmesi zor olan dağılım katsayısının etkilerinin gözlemlemek için de kullanılabilir. Ancak çözümün rastlantısal doğası nedeniyle bazı iki boyutlu simülasyon senaryolarında problemin bazen çözülememesine sebep olmaktadır.

Anahtar Kelimeler: Geliştirilmiş petrol üretimi, polimer enjeksiyonu, parçacık izleme metodu, rezervuar modelleme, dağılım

Don't Panic

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#### NOMENCLATURE

- A Flow area,  $cm^2$
- $b_{\alpha}$  Formation volume factor of phase  $\alpha$
- C Concentration, mol/cm<sup>3</sup> or kg/m<sup>3</sup>
- $C_p$  Injected polymer concentration, kg/m<sup>3</sup>
- $\hat{C}_p$  Adsorbed polymer concentration, kg/m<sup>3</sup>
- $D_0$  Diffusion coefficient, cm<sup>2</sup>/s
- $D_{\tau}$  Effective diffusion coefficient, cm<sup>2</sup>/s
- $D_L$  Longitudinal dispersion coefficient, cm<sup>2</sup>/s
- $D_T$  Transverse dispersion coefficient, cm<sup>2</sup>/s
- $D_C$  Dispersion coefficient used in the model, m<sup>2</sup>/s
- $d_p$  Average grain particle diameter, m<sup>2</sup>
- *E* Overall displacement efficiency (oil recovered by process / oil in place at start of process)
- $E_D$  Microscopic displacement efficiency
- $E_V$  Macroscopic displacement efficiency
- F Flux, mol/s/cm<sup>2</sup>
- $F_l$  Inhomogeneity factor of the porous medium
- $F_R$  Formation electrical resistivity factor
- $f_w$  Fractional flow of water
- *g* Gravitational acceleration factor  $m/s^2$

- *k* Absolute permeability, Darcy
- $k_{r\alpha}$  Relative permeability of phase  $\alpha$
- $k_{e\alpha}$  Effective permeability of phase  $\alpha$ , Darcy
- *L* Length of the porous medium, m
- *M* Mobility ratio
- $\mathcal{M}$  Polymer mass that can be adsorbed by unit mass of rock, kg/kg
- $m_{ads}$  Mass of polymer that can be adsorbed by grid cell, kg
- $m_{red}$  Particle mass to be reduced due to adsorption, kg
- $m_p$  Mobile polymer mass in a grid cell, kg
- $m_{\mu}$  Viscosity multiplier function for polymer
- *N* Moles of chemical injected, mol
- $\mathcal{N}$  Number of particles in a cell
- $P_{\alpha}$  Relative pressure of the phase  $\alpha$ , Pa
- Q Volumetric flow rate, cm<sup>3</sup>/sec
- RRF Residual resistance factor
- $r_s$  Solution gas oil ratio, scf/bbl
- $r_v$  Vaporized oil in gas phase, bbl/MMscf
- $S_{\alpha}$  Saturation of phase  $\alpha$
- Sor Residual oil saturation
- $S_{wc}$  Connate water saturation

 $S_{dpv}$  Dead pore volume

- t Time, s
- V Volume of a grid cell, m<sup>3</sup>
- v Interstitial velocity, m/s
- *x* Length, cm
- $\Delta x_{spread}$  Spreading distance of particle due to diffusion and dispersion
- $\alpha_L$  Longitudinal dispersivity, m
- $\mu_{\alpha}$  Viscosity of phase  $\alpha$ , cp
- $\mu_{w,eff}$  Effective water viscosity, cp
- $\mu_{p,eff}$  Effective polymer viscosity, cp
- $\mu_{fm}$  Fully mixed polymer and water solution viscosity
- $\mu_{pm}$  Partially mixed polymer and water solution viscosity
- $\lambda_{\alpha}$  Mobility of phase  $\alpha$
- au Tortuosity
- **Φ** Porosity
- $\sigma^2$  Variance of Gaussian distribution
- $\rho_{\alpha}$  Density of phase  $\alpha$ , kg/m<sup>3</sup>
- $\rho_{rock}$  Density of rock, kg/m<sup>3</sup>

#### CHAPTER 1

#### INTRODUCTION

Hydrocarbon reservoir performance under different conditions can be predicted through reservoir simulation, which combines physics, mathematics, reservoir engineering, and computer programming. Reservoir simulation is needed to forecast reservoir performance accurately because of the fact that the investments done on recovery projects may require high costs, and the risks of the development program should be evaluated and minimized. A set of partial differential equations (PDE) are developed and solved under reservoir's initial and boundary conditions. The main advantage of this approach is to have minimum amount of simplifying assumptions in the reservoir. The PDE's are discretized with finite-difference method in general (Ertekin, Abou-Kassem, & King, 2001). However, the transport equations solved introduces a numerical dispersion as Kinzelbach (1990) stated.

Polymer injection is an enhanced oil recovery (EOR) method used primarily to increase the injected solutions viscosity and improve sweep efficiency (Sheng, 2011). Accurate modelling of polymer injection programs are required as other recovery methods in the industry.

Zheng & Wang (1999) states in the user guide of MT3DMS, a modular multispecies transport model used in groundwater systems, that the numerical dispersion is an effect similar to physical dispersion in a system. However, numerical dispersion is introduced by truncation errors when solving the continuity equations in simulators. As stated in

CMG (2010) user guide, a commercial advanced process and thermal reservoir simulator CMG STARS, even in uniform reservoir models, numerical dispersion introduces errors in simulation results.

A random-walk particle tracking method can be used in order to model the effects of an injection process. The method does not require numerical solutions of PDE's (Liu, Bodvarsson, & Pan, 2000). The transport process of particles is solved as a linear equation. The solution therefore is virtually free of numerical dispersion effects (Zheng & Wang, 1999). In summary, the method calculates randomly injected/distributed equal mass particles' position representing a chemical in a system. Particle masses along with their position information can be used to calculate concentration and add the effects of the chemical to the system.

Random-walk particle tracking method can be used in different flow problems, as it is easy to apply and modify. The method is used to model the advection and diffusion/dispersion of chemicals in different studies. Kinzelbach (1990) used the method to simulate pollutant transport in groundwater for instance. Inoue, Takao, & Tanaka (2009) applies the method to delineate the capture zones in groundwater supply wells. Liu et al. (2000) used the method to model solute transport, while Stalgorova & Babadagli (2012) applies the method for tracer injection in fractured porous media. Method is used to investigate mixing in miscible displacements of tracer floods by John, Lake, Bryant, & Jennings (2010). Özdemir (2015) used the method to model marine sediment pollution by comparing the method with analytical and finite-difference models.

In this study, a particle method is implemented in MATLAB Reservoir Simulation Toolbox (MRST), an open source code for reservoir simulation, in order to simulate the effects of polymer injection. The thesis develops as:

- Definition of enhanced oil recovery
- Definition of some flow parameters & processes
- Information on polymers
- Information on general modelling equations
- Introduction of MATLAB Reservoir Simulation Toolbox and its verification
- Information on the developed particle model
- Statement of the problem
- Results and discussion
- Conclusion

#### **CHAPTER 2**

#### **ENHANCED OIL RECOVERY**

In this chapter, definitions of petroleum recovery processes and Enhanced Oil Recovery (EOR) methods are explained briefly.

#### 2.1 Reservoir Recovery

A petroleum reservoir can be described as a porous and permeable medium that contains oil, gas and brine, which can be produced by numerous recovery techniques. Oil recovery processes from a reservoir is divided into three groups: primary, secondary, and tertiary or enhanced oil recovery.

- 1. Primary recovery is the oil displacement process generally based on reservoir's natural energy. This energy is the pressure difference generated between reservoir and production well from numerous forces such as, natural gas expansion, gravitational force, water encroachment, and rock expansion. These forces can occur at the same time, or consecutively depending on the reservoir properties.
- 2. Secondary recovery processes start after the pressure difference between reservoir and production well is lowered due to primary recovery processes and is not enough. Reservoir pressure is partially increased by means of injecting water or gas into the reservoir with injection wells. Injected water or gas forces the oil in the reservoir to flow towards production wells and sweeps the reservoir.

 Enhanced oil recovery (EOR) starts after waterflooding and gas injection processes depleted the reservoir. The EOR processes are divided into three categories: thermal, miscible and chemical (Donaldson, Chilingarian, & Yen, 1989).

#### 2.2 Enhanced Oil Recovery

The term Enhanced Oil Recovery includes processes of injection of gases or liquid chemicals and use of thermal energy. Since some reservoirs may need EOR processes to start production, the term tertiary recovery is replaced by EOR. Aim of EOR is to provide extra energy to reservoir's natural energy and displace the oil remained. Additionally, reservoir conditions are changed favorably for oil flow with the interactions of injected fluids and rock/oil system. The displacement efficiency of the process is the product of macroscopic and microscopic efficiencies.

$$E = E_D E_V \tag{2.1}$$

where:

E = overall displacement efficiency (oil recovered by process / oil in place at start of process)

 $E_D$  = microscopic displacement efficiency

 $E_V$  = macroscopic displacement efficiency

Microscopic displacement efficiency is the process's ability to mobilize the oil at the pore scale. It is considered in the rock surface reached by the displacing fluid and is the measurement of displacement capacity in that area. Macroscopic displacement efficiency is the capacity of the injected fluid to sweep the oil in the reservoir volume towards production wells, both areally and vertically (Green & Willhite, 1998).

There is also the concept of Microbial Enhanced Oil Recovery (MEOR) present in the literature. In MEOR methods, microbes are injected in a reservoir in order to improve the oil recovery. Through microbial action in the reservoir, chemicals that can enhance the

recovery are produced in reservoir. Different mechanisms can occur in a reservoir such as viscosity reduction by produced gas, water viscosity increase by biopolymers etc. (Lacerda, Priimenko, & Pires, 2012).

Before selecting an EOR method, careful analysis of the reservoir is needed. Reservoir rock type, oil saturations, drive mechanisms should be studied to select the most efficient EOR method and should be continuously monitored during operations. The three main types of methods are explained below:

#### 2.2.1 Thermal Methods

For reservoirs with low gravity, high viscosity oil and high porosity, thermal methods are used. The idea is to create or apply heat energy in the reservoir to increase oil mobility. In other words, increasing reservoir temperature decreases oil viscosity, in turn, increases its mobility. In-situ combustion, wet combustion, and steam injection methods are used and they are counted as thermal EOR methods. In-situ combustion involves burning the crude oil near injection well and moving the burning zone through production wells with air injected with air behind the burning zone to use the heat left behind the zone to create superheated steam and evaporation front and decrease the amount of residual oil. Steam injection is done either continuously or in cycles to achieve lower viscosities in the reservoir. While both injection and production wells are used in continuous steam injection, one well is used to inject steam and produce oil in cyclic injection (Donaldson et al., 1989).

#### 2.2.2 Miscible Methods

In miscible EOR methods, a solvent that can dissolve the reservoir fluids and create a mixture that needs lower capillary forces to flow in the reservoir. Alcohols, refined hydrocarbons, condensed hydrocarbon gases, liquefied petroleum gases, or carbon dioxide are used in miscible floods. Injected fluid is followed by water or gas to push the solvent-oil mixture towards production wells. In some processes, a fluid that is miscible

with both oil and water is used to create a single phase flowing in the reservoir (Donaldson et al., 1989).

#### 2.2.3 Chemical Methods

Chemical EOR methods focus on mobility control in the reservoir. Chemical EOR processes include alkaline, surfactant, polymer and combinations of these chemicals injection to the reservoir. In surfactant injection, chemicals reduce the interfacial tension (IFT) between oil and displacing fluid. The effect of IFT is evaluated through the dimensionless capillary number, which relates viscous forces and capillary forces. The number is proportional with fluid viscosity and flow velocity, whereas inversely proportional to IFT and reservoir porosity (Dandekar, 2013). Capillary number is increased with reduced IFT and residual oil saturation decreases with the improved sweep efficiency. Alkaline injection method is based on applying surfactant to reduce IFT in reservoir conditions with chemical reactions between alkali and acids present in the reservoir. Polymer injection's main intention is to increase displacing phase viscosity and increase oil mobility (Sheng, 2011). Injected polymer's effects on reservoir and flow will be discussed in Chapter 4.

#### **CHAPTER 3**

#### FLOW PARAMETERS & PROCESSES

In this chapter, some flow parameters and processes will be presented in order to develop a better understanding on polymer injection and model used.

#### 3.1 Permeability

Permeability is the porous medium's capacity to transmit fluids. It can be measured by flow experiments in a reservoir rock. When the reservoir rock is 100% saturated with a fluid, the measured permeability is called the absolute permeability of the rock. It is a rock property and does not vary with fluid present in the reservoir. A French civil engineer, Henry Darcy's experiments on water flow through sand filters helped him to create the mathematical expressions that is used to calculate the absolute permeability. The general Darcy equation for fluid flow to calculate absolute permeability is given as:

$$Q = -\frac{k}{\mu}A\frac{dP}{dL}$$
(3.1)

where:

- Q = Volumetric flow rate, cm<sup>3</sup>/sec
- k = Absolute permeability, Darcy

 $\mu$  = Viscosity of fluid, cp

 $A = Flow area, cm^2$ 

dP = Pressure difference between upstream and downstream, atm

$$dL$$
 = Length of fluid flow, cm

The experiment and the formula used is based on some assumptions. The fluid is incompressible, horizontal, steady state, under laminar regime, and there is no reaction between the rock and fluid. However, reservoirs with a single-phase fluid rarely exists. Therefore, concept of effective permeability is needed to calculate flow. When there are more than one fluid flowing in the reservoir, flow of one phase affects the others. In such reservoirs, permeability is generally specified as relative permeability,  $k_r$ , which is defined usually by the ratio between effective permeability,  $k_e$ , of one phase to the absolute permeability of the rock.

$$k_r = \frac{k_e}{k} \tag{3.2}$$

Relative permeability also depends on fluid saturations in the rock, wetting characteristics of the fluids, and pore geometry. Relative permeability values of phases are given as a table or plotted at different saturation rates, which generally ranges between irreducible wetting-phase saturation and corresponding wetting-phase saturation of residual oil saturation, in general (Dandekar, 2013).

#### 3.2 Mobility

Mobility,  $\lambda$ , of a phase in a reservoir is defined as the ratio between the effective permeability,  $k_e$ , and viscosity,  $\mu$ , of the phase. It can also be defined as relative mobility, using relative permeability of the phase.

$$\lambda = \frac{k}{\mu} \tag{3.3}$$

Mobility ratio, M, is the ratio between the displacing phase and displaced phase mobilities,  $\lambda_u$  and  $\lambda_d$ , respectively. A mobility ratio lower than one is desirable for a displacement process. Mobility control is an essential part of an EOR process. In processes such as polymer flooding, mobility ratio of the displacing fluid is lowered to increase oil production. In such cases, summation of the mobilities of displacing fluids, and displaced fluids are used to calculate total mobilities. Mobility ratio is also defined as the total mobility ratio and is desired to be lower than one. (Sheng, 2011).

$$M = \frac{\sum \lambda_u}{\sum \lambda_d} \tag{3.4}$$

#### 3.3 Diffusion & Dispersion

#### 3.3.1 Diffusion

Diffusion is an important transport mechanism in reservoirs. Diffusion is defined as the mixing of a material in a single phase in the absence of mechanical or convective mixing (Sheng, 2011). Pressure gradients, temperature gradients, and concentration gradients in a mixture can cause diffusion. Diffusion caused by concentration differences is called the molecular diffusion. Fick's law describes the concentration gradient flux of a material as:

$$F = -D_0 \frac{\partial C}{\partial x} \tag{3.5}$$

where:

 $F = Flux (mol/s/cm^2)$ 

 $D_0$  = Diffusion coefficient (cm<sup>2</sup>/s)

 $C = \text{Concentration (mol/cm}^3)$ 

x = Length(cm)

In the porous medium, flow takes place in a tortuous path. Tortuosity of the medium is the ratio,  $\tau$ , between the actual path length traveled by a fluid parcel and a single-line distance of the same path. To add the effect of tortuosity, the diffusion coefficient,  $D_0$ , is changed with effective diffusion coefficient,  $D_{\tau}$ . The relationship between  $D_{\tau}$  and  $D_0$  is:

$$D_{\tau} = \frac{D_0}{\tau^2} \tag{3.6}$$

Tortuosity can also be defined in terms of electrical formation resistivity factor of the medium,  $F_R$ , which is the ratio between electrical resistivity of the medium with a fluid that conducts electricity and the fluid in the medium, and porosity,  $\Phi$ .

$$\tau^2 = F_R \Phi \tag{3.7}$$

Empirical relationship between  $F_R$  and  $\Phi$  by Archie's law is:

$$F_R = \Phi^{-n} \tag{3.8}$$

The exponent n varies from 1.4 to 2.0. When n is taken to be 2, effective diffusion coefficient becomes:

$$D_{\tau} = D_0 \Phi \tag{3.9}$$

When mass balance in a small porous medium is written in one dimension, diffusion can be profiled as:

$$\frac{\partial C}{\partial t} = D_{\tau} \frac{\partial^2 C}{\partial x^2} \tag{3.10}$$

Equation 3.10 is known as the Fick's second law of diffusion.

Molecular diffusion results from the random motion of the molecules in a solution. Hence, it can be represented statistically. In a system with no chemical injected before t = 0, when N moles of chemical is injected at origin x = 0, concentration profile can be calculated with the stated function below (Sheng, 2011):

$$C(x,t) = \frac{N}{\sqrt{4\pi D_0 t}} \exp\left(-\frac{x^2}{4D_0 t}\right)$$
(3.11)

C(x, t) is in mol/cm. Concentration of the chemical is equal to 0 except at the origin at time t = 0. At the origin C $\rightarrow \infty$ . Equation 3.11 is similar to Gaussian distribution function (Sheng, 2011),

$$n(x) = \frac{N}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{x^2}{2\sigma^2}\right)$$
(3.12)

 $\sigma^2$  is the variance of the distribution. Using the similarity between equations 3.11 and 3.12, diffusion coefficient can be related with variance as:

$$\sigma^2 = 2D_0 t \tag{3.13}$$

Statistics states that the mean diffusion length can be estimated. The equation 3.14 represents distance traveled by the 68% of the original mass (Sheng, 2011).

$$\sigma = \sqrt{2D_0 t} \tag{3.14}$$

#### 3.3.2 Dispersion

In reservoir fluid flow, changes in velocity of the flow causes an uneven mixing of the chemicals. Added effect of gross fluid flow in chemical mixing or concentration gradients caused by the phenomena is called dispersion. Two types of dispersion is defined as the longitudinal dispersion,  $D_L$ , and the transverse dispersion,  $D_T$ . Longitudinal dispersion is the dispersion in gross fluid flow direction, whereas transverse dispersion is in transverse direction of it.

Dispersion is a highly scale dependent parameter, therefore quantifying is hard and done experimentally or empirically. Empirical correlation describes  $D_L$  as sum of molecular diffusion and convective dispersion components. Perkins & Johnston (1963) gives the correlation between  $D_L$  and  $D_0$ , based on the experiments held on different grain particle sized samples in the literature, as:

$$\frac{D_L}{D_0} = \frac{1}{F_R \Phi} + 0.5 \frac{\nu F_l d_p}{D_0}$$
(3.15)

For  $\nu F_l d_p / D_0 < 50$ , which is the effective ratio for diffusion to equalize the concentration in pore spaces, where:

v = Interstitial velocity, m/s

 $F_l$  = Inhomogeneity factor of the porous medium

 $d_p$  = Average grain particle diameter, m<sup>2</sup>

When the convective term is high, dispersion coefficient and velocity are proportional. When  $F_l$ ,  $d_p$ , and  $D_0$  are assumed constants in a reservoir, dispersivity parameter,  $\alpha_L$ , can be defined:

$$\alpha_L = \frac{D_L}{\nu} \tag{3.16}$$

Experimental and field data on the literature on longitudinal dispersivity is shown in Figure 3.1 and correlations are reported by Arya, Hewett, Larson, & Lake (1988) for field data and all data respectively as:

$$\alpha_L = 0.229 L^{0.755} \tag{3.17}$$

$$\alpha_L = 0.044L^{1.13} \tag{3.18}$$



Figure 3.1 Field & Lab Dispersivities (Arya et al., 1988)

Transverse dispersion and dispersivity are studied less in the literature and their effects are much less then longitudinal dispersion and dispersivity (Sheng, 2011).

## **CHAPTER 4**

#### POLYMERS

In this chapter, general information about polymers is given. Their structure, effect on flood conditions and adsorption is discussed.

#### 4.1 Structure

Rodriguez et al. (1993) states the polymer molecules dissolve in water via hydrogen bonding. Molecules dissolve in water but hold some of their structural identity in solution. Coils of polymer molecules holds large volumes of solvent. The connected coils deform and change shape under applied pressure, and drags other coils and solvent with them during flood. General polymer structures are given in Table 4.1. Sheng (2011) gives the good polymer properties as:

- Thermally stable (no hydroxyl group (-O-) in the carbon chain)
- Low adsorption rate on rock surface (negative ionic hydrophilic group)
- Good viscosifying powder
- Chemically stable (nonionic hydrophilic group)

The mostly used polymers are the synthetic type, hydrolyzed polyacrylamide (HPAM).

Structure	Characteristics	Sample Polymers
-O- in the backbone	Low thermal stability,	Polyoxyethylene, sodium
	thermal degradation at high	alginate, sodium
	T, only suitable at <80°C	carboxymethyl cellulose,
		HEC, xanthan gum
Carbon chain in the	Good thermal stability,	Polyvinyl, sodium
backbone	degradation not severe at	polyacrylate,
	<110°C	polyacrylamide, HPAM
-COO <sup>-</sup> chain in	Good viscosifier, less	Sodium alginate, sodium
hydrophilic group	adsorption on sandstones	carboxymethyl cellulose,
	due to the repulsion	HPAM, xanthan gum
	between chain links, but	
	precipitation with Ca <sup>2+</sup> and	
	Mg <sup>2+</sup> , less chemical	
	stability	
-OH or –CONH <sub>2</sub> in	No precipitation with Ca <sup>2+</sup>	Polyvinyl, HEC,
hydrophilic group	and Mg <sup>2+</sup> , good chemical	polyacrylamide, HPAM
	stability, but no repulsion	
	between chain links, thus	
	less viscosifying powder,	
	high adsorption due to	
	hydrogen bond formed on	
	sandstone rocks	
<b>Source:</b> (Sheng, 2011)	1	

# Table 4.1 General Polymer Characteristics

# 4.2 Adsorption

Adsorption is the phenomena that is caused by the interaction between polymer molecules and rock surface. Because of van der Waals forces and hydrogen bonding, molecules are bound to rock surface. Adsorption is the most important retention mechanism in the
reservoir because it is a major property of the solution-rock system. The process depends on the rock surface area exposed to the polymer solution. The other retention mechanisms are called mechanical entrapment and hydrodynamic retention. Since it is hard to distinguish the mechanisms, the term adsorption is generally used for retention and polymer loss. In general, mass of polymer adsorbed by the unit mass of rock is used as a unit for adsorption. To describe polymer adsorption, the Langmuir-type isotherm is used (Sheng, 2011):

$$\hat{C}_{p} = \min\left(C_{p}, \frac{a_{p}(C_{p} - \hat{C}_{p})}{1 + b_{p}(C_{p} - \hat{C}_{p})}\right)$$
(4.1)

where:

 $\hat{C}_p$  = Adsorbed polymer concentration

 $C_p$  = Injected polymer concentration

 $C_p - \hat{C}_p$  = Equilibrium concentration of the solution-rock system

 $a_p$ ,  $b_p$  = Empirical constants

However, this isotherm is used when adsorption process is reversible. It means that the concentration in the reservoir can increase by desorption of polymer molecules from the rock surface in time. In general, adsorption is accepted irreversible. Although small amounts can be recovered from rock surface with continuous water or brine injection, the recovery is not enough to calculate concentration properly. In other words, retention by adsorption is much higher than polymer removal. Therefore, if the process is taken to be irreversible as discussed, another parameter,  $\hat{C}_{p,max}$ , is added for observing the adsorption history.

$$\hat{C}_{p,max} = max \left\{ \left( \hat{C}_p \right)^1, \left( \hat{C}_p \right)^2, \dots, \left( \hat{C}_p \right)^n \right\}$$
(4.2)

Time steps are indicated with number 1, 2, ..., n where the current time step is n.  $\hat{C}_{p,max}$  cannot exceed the adsorption capacity. A typical adsorption curve can be seen on Figure 4.1 (Sheng, 2011).



Figure 4.1 Adsorption Curve (Sheng, 2011)

# 4.3 Effects on Mobility

Use of polymer solutions may increase the oil displacement efficiency in a reservoir. The increment in the efficiency rate is the result of lowered displacing phase mobility. Lowered mobility ratio causes the areal sweep efficiency and vertical coverage to improve. The mobility cut can be done by lowering permeability, increasing solution viscosity, or a combination of both (Rodriguez et al., 1993). The overall macroscopic displacement efficiency of polymer flooding over waterflooding can be seen on Figure 4.2.

Polymer solutions show higher resistance to flow than regular waterflooding. Hence, the mobility of the displacing phase is lowered and mobility ratio becomes more favorable. This resistance is caused by the swelled polymer molecules in a good solvent. The effect is greater with higher molecular weight of polymer. (Mungan, Smith, & Thompson, 1966). Polymer effect on solution viscosity increases with polymer concentration in solution. Effective water viscosity can be defined with Todd-Longstaff mixing model, which involves mixing rate of polymer and water, and viscosity multiplier function of solution with complete mixing (Bao et al., 2016).



Figure 4.2 Areal Sweep Efficiency of Water Flooding (*left*) & Polymer Flooding (*right*) (Sheng, 2011)

Gogarty (1967) states that the permeability reduction mechanism is more complicated. In the core-plug displacement experiments with 1200-ppm polymer solution, similar results with Figure 4.3 is realized. No polymer is produced until 1 pore volume (PV) of polymer solution is injected. Produced polymer concentration within the core is equal with the injection concentration after approximately 8 PV of injection is carried out. Late equalization means that polymer retention takes place in the porous medium during the flooding. Polymer retention is caused by the entrapment of polymer molecules in smaller pore openings and adsorption on the rock surfaces. Adsorption continues until the equalization in the concentration is completed. Since, effective viscosities decrease with the effect of polymer retention and permeability reduction, polymer flooding should be done with low adsorption rate.



Figure 4.3 Produced Concentration vs. Polymer Volume Injected (Gogarty, 1967)

The interfacial viscosity between polymer and oil also plays an important role in polymer flooding. Higher interfacial viscosity and shear stress between polymer and oil causes the polymer to have larger pull force on oil droplets. This effect helps pushing and pulling of oil droplets in dead-ends of porous medium. Higher push-pull force on oil droplets helps reducing the residual oil saturation,  $S_{or}$  (Sheng, 2011).

#### **CHAPTER 5**

#### **MODELLING EQUATIONS**

This chapter summarizes the equations solved in polymer flood modelling.

#### 5.1 Black-Oil Model Equations

Black-oil simulators are three phase simulators (i.e. oil, water and gas phases). This type of simulators defines the hydrocarbon fluids as oil and gas phases, being combined considered as combination of different weights of hydrocarbon components, which are not individually involved in the model. Depending on the reservoir pressure and hydrocarbon properties, the phases can be dissolved in each other either completely or partially at the reservoir conditions. There is also the aqueous phase of water present. Models used in this study defines boundaries of the reservoir as no-flow boundaries. The initial state of the reservoir, reservoir rock and fluid properties are input to the model manually. Bao et al. (2016) gives the continuity equations solved for the phases as:

$$\partial_t (\Phi b_w S_w) + \nabla (b_w v_w) - b_w q_w = 0 \tag{5.1}$$

$$\partial_t \left[ \Phi(b_o S_o + b_g r_v S_g) \right] + \nabla \left( b_o v_o + b_g r_v v_g \right) - \left( b_o q_o + b_g r_v q_g \right) = 0$$
(5.2)

$$\partial_t \left[ \Phi(b_g S_g + b_o r_s S_o) \right] + \nabla \left( b_g v_g + b_o r_s v_o \right) - \left( b_g q_g + b_o r_s q_o \right) = 0$$
(5.3)

$$S_o + S_g + S_w = 1 (5.4)$$

where  $b_{\alpha}$  denotes the formation volume factors.  $r_s$  is the solution gas oil ratio and  $r_v$  is the vaporized oil in gas phase in the reservoir. Darcy's law gives the phase fluxes as:

$$v_{\alpha} = -\lambda_{\alpha} k (\nabla P_{\alpha} - \rho_{\alpha} g \nabla z)$$
(5.5)

#### 5.2 **Polymer Equations**

MATLAB Reservoir Simulation Toolbox (MRST) is used in this study to model polymer flow in the reservoir. More information about MRST will be given in Chapter 7. The model assumes that the polymer is only present in the aqueous phase and do not interfere with hydrocarbon phases in the reservoir. Polymer properties such as the mixing parameter, adsorption values of polymer etc. are given to the model along with the initial reservoir conditions by the user. The continuity equation for the polymer is stated as (Bao et al., 2016):

$$\partial_t \left( \Phi \left( 1 - S_{dpv} \right) b_w S_w c \right) + \partial_t \left( \rho_r c^a (1 - \Phi) \right) + \nabla \left( b_w v_p c \right) - b_w q_w c = 0 \tag{5.6}$$
where:

 $c^a$  = Polymer adsorption concentration

 $\rho_r$  = Reservoir rock density, kg/m<sup>3</sup>

 $S_{dpv}$  = Dead pore volume (inaccessible pore space by polymer due to its larger molecular size than some pore diameters)

Equations solved adds the effect of the viscosity change and permeability reduction to the reservoir by means of polymer concentration in each grid block. Effective viscosity should be applied in the phase flux equations to add these effects. In polymer solution model, Darcy equations for water and polymer become:

$$v_w = -\frac{k_w S_w}{\mu_{w,eff}(c) R_k(c)} k(\nabla P_w - \rho_w g \nabla z)$$
(5.7)

$$v_p = -\frac{k_w S_w}{\mu_{p,eff}(c) R_k(c)} k(\nabla P_w - \rho_w g \nabla z)$$
(5.8)

The function  $R_k(c)$  defined in these equations represents the permeability reduction effect due to polymer adsorption and it is stated as:

$$R_k(c, c_{max}) = 1 + (RRF - 1) \frac{c^a(c, c_{max})}{c^a_{max}}$$
(5.9)

$$c_{max}(x,t) = \max_{s \le t} c(x,s)$$
 (5.10)

 $c_{max}^{a}$  is the maximum polymer concentration adsorbed and RRF (residual resistance factor) is the ratio between water relative permeability before and after polymer flood. Both of these qualities depend on the rock type.

The effect of viscosity change is calculated with the help of Todd-Longstaff mixing model. Displacement scenario and heterogeneity of the formation changes the Todd-Longstaff mixing parameter,  $\omega$ . Complete mixing is defined as  $\omega = 1$ , whereas complete segregation is  $\omega = 0$ . Fully mixed solution viscosity can be defined as (Bao et al., 2016):

$$\mu_{fm} = m_{\mu}(c)\mu_{w} \tag{5.11}$$

 $m_{\mu}$  is the viscosity multiplier function. Effective polymer viscosity is calculated by:

$$\mu_{p,eff} = \mu_{fm}^{\ w} \mu_p^{1-\omega} \tag{5.12}$$

Viscosity of a partially mixed solution,  $\mu_{pm}$ , and effective water viscosity are calculated as follows:

$$\mu_{pm} = \mu_{fm}^{\ w} \mu_w^{1-\omega} \tag{5.13}$$

Then the effective water viscosity is calculated by summing the polymer solution and pure water contributions as:

$$\frac{1}{\mu_{w,eff}} = \frac{1 - \bar{c}}{\mu_{pm}} + \frac{\bar{c}}{\mu_{p,eff}}$$
(5.14)

$$\mu_{w,eff} = \frac{m_{\mu}(c)^{\omega}\mu_{w}}{1 - \bar{c} + \bar{c}/m_{\mu}(c^{*})^{1-\omega}}$$
(5.15)

where  $\bar{c} = c/c^*$  and  $c^*$  is the maximum possible polymer concentration (Bao et al., 2016).

## **CHAPTER 6**

## MATLAB RESERVOIR SIMULATION TOOLBOX

MATLAB Reservoir Simulation Toolbox (MRST), solution method of its polymer model and is explained in this chapter. Theory on Buckley-Leverett waterflooding is also given for the simple verification of the toolbox.

## 6.1 MRST Description

MRST is an open-source code developed by SINTEF Applied Mathematics in Oslo. It is not a simulator, but a fast prototyping and demonstration tool for new methods and concepts for reservoir modelling, working with MATLAB. There are several modules for basic reservoir characterization and flow functions. For cases that are more specific many add-on modules can be activated for different physical models, solvers, etc. (Sintef, n.d.a)

In this thesis, the objective is to modify the source code of MRST to implement random movement particle tracking method to the system. Before implementing the method, integrity of MRST solutions is compared first by comparing MRST water flood solution with analytical Buckley-Leverett solution, then MRST 1D polymer flood solution with ECLIPSE solution of the same data.

## 6.2 Buckley-Leverett Analytical Solution

Before implementing the particle tracking method to MRST, integrity of MRST solutions is checked as stated before. One of the verification tools used was the analytical Buckley-Leverett solution of simple water flooding problem.

As Dake (1998) mentioned, distance from injection well of any water saturation,  $S_w$ , at any time can be calculated in waterflooding applications. The equation is known as the Buckley-Leverett or frontal-advance equation. Darcy equation can be written for both water and oil phases respectively as:

$$q_w = -\frac{kk_w A}{\mu_w} \left(\frac{\partial P_w}{\partial x} + \frac{\rho_w g \sin \theta}{1.0133 x \, 10^6}\right) \tag{6.1}$$

$$q_o = -\frac{kk_o A}{\mu_o} \left(\frac{\partial P_o}{\partial x} + \frac{\rho_o g \sin \theta}{1.0133 x \, 10^6}\right) \tag{6.2}$$

$$q_t = q_w + q_o \tag{6.3}$$

where:

 $P_{\alpha}$  = Relative pressure of the phase, Pa

 $\rho_{\alpha}$  = Density of the phase, kg/m<sup>3</sup>

 $g = \text{Gravitational constant, m}^2/\text{s}$ 

$$\theta$$
 = Flow angle

When the relation in Equation 6.3 is applied,  $q_w$  can be written as:

$$q_w = -\left(\frac{\mu_w}{kk_w} + \frac{\mu_o}{kk_o}\right) = \frac{q_t\mu_o}{kk_o} + A\left(\frac{\partial P_c}{\partial x} - \frac{\Delta\rho g\sin\theta}{1.0133 x \, 10^6}\right) \tag{6.4}$$

where the capillary pressure gradient is:

$$\frac{\partial P_c}{\partial x} = \frac{\partial P_o}{\partial x} - \frac{\partial P_w}{\partial x}$$
(6.5)

Fractional flow of water in the reservoir is:

$$f_w = \frac{q_w}{q_t} \tag{6.6}$$

When the assumptions of horizontal flow, no gravity effect, and negligible capillary forces are made, the water fractional flow parameter can be defined by using the relations in the equations above, as:

$$f_w = \frac{1}{1 + \frac{k_o \mu_w}{k_w \mu_o}} \tag{6.7}$$

A typical fractional flow curve can be seen in Figure 6.1



Figure 6.1 Fractional Flow Curve (Dake, 1998)

If we write mass balance in a 1D system for water:

$$q_{w}\rho_{w}|_{x} - \left(q_{w}\rho_{w}|_{x} + \frac{\partial}{\partial x}(q_{w}\rho_{w})dx\right) = A\Phi dx \frac{\partial}{\partial t}(\rho_{w}S_{w})$$
(6.8)

When incompressible displacement is assumed, Equation 6.8 becomes:

$$\frac{\partial q_w}{\partial x}\Big|_t = -A\Phi \frac{\partial S_w}{\partial t}\Big|_x \tag{6.9}$$

Differential of water saturation is:

$$dS_w = \frac{\partial S_w}{\partial x}\Big|_t dx + \frac{\partial S_w}{\partial t}\Big|_x dt$$
(6.10)

Furthermore,

$$\left. \frac{\partial q_w}{\partial x} \right|_t = \left( \frac{\partial q_w}{\partial S_w} \frac{\partial S_w}{\partial x} \right)_t \tag{6.11}$$

Since we are trying to find the position of a constant water saturation, dSw can be taken 0 and when equations 6.6, 6.10 and 6.11 are substituted in 6.9, change of the position of a constant saturation can be found as:

$$\frac{dx_{Sw}}{dt} = \frac{q_t}{A\Phi} \left(\frac{\partial f_w}{\partial S_w}\right)_{S=S_w}$$
(6.12)

When integrated in time:

$$x_f = \frac{q_t}{A\Phi} \left(\frac{\partial f_w}{\partial S_w}\right)_f \tag{6.13}$$

However, discontinuity in the saturation function causes the result of equation 6.13 to give two saturation values for each position. A disconitnuity at the water front position is defined and areas below that position are balanced and the corrected water saturation profile can be obtained. Figure 6.2 shows an illusturation of the correction done on the analytical solution at different time steps by Craft & Hawkins (1991).

#### 6.3 Polymer Model of MRST

MRST solves the grid system and continuity equations given in Chapter 5 with respect to grid, reservoir, and polymer information defined in the input file by implicit discretization of the governing equations. Discrete continuous divergence and gradient operators are defined, and flow equations are discretized in very compact form. Implicit temporal discretization and standard two-point spatial discretization are used for conservation equations. The continuity equations, well rates, and well control equations are collected in a problem system. The nonlinear system of equations is solved using the Newton's method, and multidimensional Taylor expansions are used to derive the iterations.



Figure 6.2 Buckley-Leverett Analytical Solution of Water Saturation Profile (Craft & Hawkins, 1991)

The linearization (i.e. taking derivative of discretized nonlinear system equations with respect to unknown variables) is performed by the automatic differentiation (AD) method, one of the modules implemented in MRST, in the model. AD works with the created elementary arithmetic operations and functions of every function given, with respect to their known analytical derivatives. The method depends of evaluating the given functions and their derivatives simultaneously with predefined primary variables (Bao et al., 2016).

The black-oil models are in general computationally challenging. The mixed character of flow equations, parameter order-of-magnitude variations, discontinuities on fluid parameters etc. leads the solution not to converge efficiently unless preconditioners are used (Bao et al., 2016). The error introduced by the solving technique of the equations is called the numerical dispersion and it causes the system to act differently than theory.

The data structure containing reservoir rock, fluid and polymer properties, well specifications, injection rates and schedule are given as an ECLIPSE, an industry-standard simulation program, input file. Necessary unit conversions are done by MRST to use SI units in the models.

#### **CHAPTER 7**

## **PARTICLE MODEL**

Random-walk particle tracking model is explained in this chapter.

## 7.1 Random Walk Particle Model Description

Kinzelbach (1990) states in his work that the random walk method comes from statistical physics, which is used to solve diffusion and dispersion problems in porous medium. The main advantage of the method is that it does not show numerical dispersion in the solution. The transport equations in porous media are the second order initial value problem type partial differential equations. Their results are unreliable because of the combination of hyperbolic advection equation and parabolic diffusion/dispersion equation unless strict preconditioners are used. Random walk method is simple, can be added on any flow model, and matches with the analytical solution at comparable computational effort. However, due to its random nature, the method gives randomly fluctuated concentration profiles. Size of the fluctuations can be reduced by increasing the number of particles used in the simulations. Still, increased number of particles does not improve the result at the same rate because the statistical uncertainty is proportional to the inverse square root of the count of particles in a cell.

The method starts with the injection of the known-mass particles representing polymer mass/concentration in the water phase into the system at a uniform velocity. The positions of the particles are updated with the combinations of the effects of advection and diffusion.

Meaning that the particles moves with the water velocity of the cell for the time step and diffuses/disperses into the system. As discussed in Chapter 3, diffusion can be analyzed statistically and with normal distribution. Equation 3.14 is the distance travelled by 68% of the chemical injected. Cranmer, 2003 gives the probable distance travelled by a particle as:

$$\Delta x_{spread} = \mathcal{N}(\xi) \sqrt{2D_0 \Delta t} \tag{7.1}$$

where,  $\mathcal{N}(\xi)$  is a sample from a normal distribution with zero mean and unit variance.

$$\mathcal{N}(\xi) = \frac{1}{\sqrt{2\pi}} e^{-\xi^2/2}$$
(7.2)

Movement of the particle in the model can be shown schematically as in Figure 7.1.





Positions of the particles are updated as:

$$x_i^{n+1} = x_i^n + v_w^n \Delta t + \Delta x_{spread}$$
(7.3)

where  $x_i$  is the position of particle and superscript n denotes the time step. The terms after the old position of the particle are the advection and spreading terms respectively. Concentration profile can be obtained by counting the particles in each grid cell and dividing the mobile mass of particles to the water volume at the corresponding cell. The concentration distribution is fluctuated due to the randomness of the process as discussed before. There should be at least 20 particles in a cell to calculate the concentration properly. Duration of 5 to 10 time steps for a particle to leave a grid cell also helps the results to be smoother (Kinzelbach, 1990).

#### 7.2 Assumptions in the Model

In constructing the model during this study, some assumptions are made. In the model, it is assumed that the polymer only is present in water phase like MRST model does. Particles have the velocity of water in the porous medium. Advection of particles is carried out by the water velocity in each cell at the corresponding time step.

The spreading distance of the particles at each time step,  $\Delta t$ , due to diffusion and dispersion is calculated by taking the spreading length as  $\mathcal{N}(\xi)\sqrt{2D_c\Delta t}$ . The dispersion coefficient,  $D_c$ , used in the calculations involves effects of both diffusion and dispersion. Sheng (2011) states the typical diffusion coefficient as 4 x 10<sup>-10</sup> m<sup>2</sup>/s in the porous medium. This value is multiplied by the dispersivity of the reservoir using Equation 3.18 to find the dispersion coefficient,  $D_c$  in the model. Length term used in Equation 3.18 is the total length of reservoir in the problem. A normally distributed scalar, with mean of 0 and standard deviation of 1, at each time step for each particle is randomly generated to obtain  $\mathcal{N}(\xi)$ .

## 7.3 Movement of the Particles

Particles are injected with water at a constant rate and concentration in the problems. By using these information, mass of each particle is obtained and they are positioned in the center of the injection well at t = 0. Then a predetermined number of particles with calculated initial mass are released and then advected and dispersed at each time step along with the currently present particles in the system, and their mass is updated by adsorption process.

In the 1D problem, the movement occurs only in one direction, therefore advection and dispersion is modelled with ease. However, in the 2D scenarios, velocity vectors consists of x and y components at cell centers as averages. The releasing of particles should be in radial form. This condition is provided by assigning a uniformly distributed angle to each particle at the injection point. At the injection cell, instead of using the velocity field value for injection velocity, velocity calculated from the injection flow rate and wellbore cross sectional area is used. Newly released particles follow the same angle while in the injection cell. If a particle leaves the no-flow boundary, it is repositioned into the grid system by the distance it travelled outside of it in the same direction. By doing so, we prevent the system from giving errors because of misplaced particles.

MRST solution provides the x and y components of the velocity vector field at cell centers as averages. In order to provide more realistic velocity values for particles, the interpolated velocity at their exact location in the grid system is used for advection. This approach is better in 2D problems, because it provides a better distribution pattern.

Concentration in each cell is calculated as described in Chapter 8.1 at each time step as:

$$c = \frac{m_p}{V \Phi S_w} \tag{8.4}$$

where:

 $m_p$  = Mobile polymer mass in the cell, kg

$$V =$$
 Volume of the cell, m<sup>3</sup>

This concentration information is used to calculate the amount of polymer to be adsorbed to the rock surface. Concentration of polymer and corresponding polymer mass that can be adsorbed by unit mass of rock is given as a table by the user to the system.

$$m_{ads}^n = \mathcal{M}\rho_r V(1 - \Phi(1 - S_{dpv})) \tag{8.5}$$

where:

 $m_{ads}^n$  = Mass of polymer that can be adsorbed by the cell at the current time step, kg

 $\mathcal{M}$  = Mass of polymer that can be adsorbed by unit mass of rock, kg

If  $m_{ads}^n$  is greater than  $m_{ads}^{n-1}$ , which is the already adsorbed polymer mass at the previous time steps, the difference between  $m_{ads}^n$  and  $m_{ads}^{n-1}$  is taken to be the adsorbed at the current time step. Then, mass of each particle in the cell is reduced equally to add the adsorption effect.

$$m_{red} = \frac{m_{ads}^n - m_{ads}^{n-1}}{\mathcal{N}} \tag{8.6}$$

where  $m_{red}$  is the mass to be reduced from each particle, and N is the number of particles present in the cell.

The particles that reaches the production well during the simulation are reduced to zero mass and positioned at the production well location to ignore their effects on the process.

#### **CHAPTER 8**

#### STATEMENT OF PROBLEM

The aim of this study is to use random walk particle tracking method with MRST to model polymer injection. Discretization of the continuity equations solved in black-oil simulators by numerical methods involves an error, which is called numerical dispersion. Numerical dispersion causes the system to act differently than theory. The particle tracking method is used to overcome the effects of numerical dispersion on polymer distribution. The continuity equation for the polymer phase is solved by introducing particles representing a known mass of polymer. Effects of polymer injection in the system is included by calculating the concentration field, from particles' position and mass information. The method uses water phase velocity obtained from MRST to introduce advection on the particles. Dispersion of the particles is modelled by assigning a dispersivity coefficient and random walk method. Polymer adsorption on rock surface is added by updating particle masses with respect to concentration and adsorption capacity of rock. The polymer concentration field calculated by MRST is updated with the concentration field from the particle tracking method at each time step. MRST then utilizes the field in calculation of flow characteristics of the oil and water phases.

## **CHAPTER 9**

## **RESULTS & DISCUSSION**

## 9.1 Verification of MRST Models

Before implementing the random walk particle tracking method into MRST, a verification study on MRST solutions has been carried out as stated in Chapter 6.

#### 9.1.1 Buckley-Leverett Verification

For verification of MRST solvers, a basic 1D problem with 100 grids is created and solved with both MRST and Buckley-Leverett analytical solution. Reservoir and fluid properties of the problem are obtained from Willhite (1986) and stated below:

- The reservoir is 300 ft wide, 20 ft thick, and 1000 ft long
- $\Phi = 0.15$
- $S_{wc} = 0.363, S_{or} = 0.205$
- Sw = 0.363, So = 0.637
- Injection well is located in one end of the reservoir and  $q_t = 53.7 \text{ m}^3/\text{day}$
- $\mu_w = 1.0 \text{ cp}, \ \mu_o = 2.0 \text{ cp}$
- $k_o = (1 S_{wD})^{2.56}$
- $k_w = 0.78 S_{wD}^{3.72}$
- $S_{wD} = \frac{S_w S_{wc}}{1 S_{or} S_{wc}}$

Corresponding relative permeability and fractional water flow curves are obtained in MATLAB and given below in Figures 9.1 and 9.2.



Figure 9.1 Relative Permeability Curve



Figure 9.2 Fractional Flow & Derivative

The problem is solved with no flow boundary conditions and incompressible transport, using block system of linear equations of interface fluxes and cell pressures at the next time step. Water saturation profile of the MRST solution is compared with the flood front position gathered from Equation 6.13 throughout 400 days of injection. Gathered profiles can be seen on Figure 9.3.



**Figure 9.3** Comparison of Flood Front Position (*a*) t = 100 days (*b*) t = 200 days



**Figure 9.3 (cont'd)** Comparison of Flood Front Position (c) t = 400 days

The movement of flood front of both analytical and MRST solutions are coherent with each other.

## 9.1.2 ECLIPSE Verification

ECLIPSE is a simulator developed by the company Schlumberger having various modelling options and methods used in the industry. ECLIPSE 100, the black-oil simulator, is used in this study to compare the consistency of polymer model of MRST. A fully implicit model is used in the system to treat oil/water/gas/polymer/brine system (Schlumberger, 2015).

For the sake of verification, dataset downloaded from MRST polymer tutorial website (Sintef, n.d.-b) is modified to be a one dimensional continuous polymer injection problem. The dataset is run on ECLIPSE and concentration profile is obtained from each grid cell in the model. Concentration profile from both MRST and ECLIPSE solutions plotted together against distance to injection well to see their match in MATLAB at different times of the injection. Plotted results can be seen on Figure 9.4.

Figure 9.4 shows that the concentration profile obtained from MRST solution matches with ECLIPSE solution.



**Figure 9.4** Comparison of Polymer Concentration Profiles (*a*) t = 200 days (*b*) t = 600 days (*c*) t = 1000 days

# 9.2 Numerical Dispersion

### 9.2.1 Water Flooding Problem

In order to show the effect of numerical dispersion, Buckley-Leverett problem and a modified 1D problem is solved with different grid numbers of the same problems. Figure 9.5 shows flood front position of water flooding problem given in Chapter 9.1.1 at different time steps at different number of grids and analytical solution front position.



Figure 9.5 Flood Front Movement with Different Grid Numbers (a) t = 100 days (b) t = 200 days



Figure 9.5 (cont'd) Flood Front Movement with Different Grid Numbers (c) t = 400 days

All obtained saturation profiles from different number of grid systems of the same problem shows a curvature at the front position. The curvature observed is the result of numerical dispersion and the rate of divergence from the theoretical front position does not improve much after 300 grids. The effect of numerical dispersion is always present in the numerical solution.

#### 9.2.2 1D Polymer Injection Problem

In all of our problems, a modified MRST polymer tutorial dataset obtained from MRST website (Sintef, n.d.-b) is used to create and solve an oil/water/polymer problem. All polymer injection scenarios use complete mixing of polymer with water. The effect of polymer on water viscosity and adsorption capacity of the rock are given as tables in the input file, and are not modified. Corresponding plots of viscosity multiplier and adsorption curve can be seen on Figure 9.6 and 9.7 respectively. Polymer adsorption process in the reservoir is taken irreversible.



Figure 9.7 Polymer Adsorption Curve

In our 1D polymer injection scenario, injection well is positioned in the first grid cell and production well is at the last grid cell of the system. Rest of the important properties are given in the Table 9.1.

Property	Value
Total Dimensions (x-y-z)	200  m - 20  m - 4  m
Porosity	30 %
Permeability	100 mD
S <sub>dpv</sub>	5 %
RRF	1.1
$ ho_{rock}$	2000 kg/m <sup>3</sup>
Water Injection Flow Rate	$10 \text{ m}^3/\text{day}$
Injected Polymer Concentration	0.8 kg/m <sup>3</sup>
$\Delta t$	0.5 days
Total Simulation Time	500 days

Table 9.1 One Dimensional Problem Properties

In order to observe the effect of numerical dispersion, the problem given above is solved with different number of grids. Figure 9.8 shows polymer concentration profile movement plotted at two different time steps.



Figure 9.8 Polymer Concentration Profile with Different Grid Numbers (a) t = 100 days



Figure 9.8 (cont'd) Polymer Concentration Profile with Different Grid Numbers (b) t = 200 days

Figure 9.8 shows the effect of numerical dispersion decreases with increasing number of grids in the system. However, it is not completely removed and the computation time increase with increasing number of grids also. The numerical dispersion is not smoothed much after 400 grids representation of the 1D problem. Therefore, 400 grids are used for this problem in the rest of the study. The numerical dispersion effect can also be smoothed with shorter time steps, since it leads to better representation of flow process. However, the numerical solution would still cause numerical dispersion in the results.

## 9.3 Implementation of Model into MRST

Idea behind the implementation of the random walk particle tracking method into MRST is initializing and moving the particles, then updating the concentration profile that MRST calculates by our profile at each time step. MRST solves all the equations given in Chapter 5 at each time step, including polymer phase. Our model solves the particle system simultaneously with MRST at each time step by using water phase velocity calculated from MRST. Interpolated water phase velocity field is used for particles' exact positions in the problems. Effect of interpolation is better seen on 2D problems, therefore will be explained later. Working principle of particle model with MRST is summarized in the flow chart seen on Figure 9.9 at each time step.



Figure 9.9 Solution Flow Chart

By updating concentration field information of MRST solution at the end of each time step, we aim to eliminate the effects of polymer continuity equations.

In each scenario, 100 particles per time step is used. However, only 20 particles per each time step is plotted in order to visualize the particles with ease and reduce computation time. Time step length and total time required are arranged to see the effect of polymer after it reaches to production wells.

# 9.4 1D Problem

In our 1D polymer injection scenario, problem set described in Chapter 9.2.2 is used with 400 grids. First, we checked the polymer concentration obtained from the MRST solution, in order to see the model behavior. In Figure 9.10, polymer concentration and saturation movement throughout the reservoir can be seen at different time steps.

Two saturation front occurs as expected and stated in Pope, 1980 throughout the injection process. The first front is the result of increasing saturation velocity in the upstream as in a waterflooding application. The following saturation front occurs at the polymer concentration front, which is the connection point of polymer water and connate water of the system. This trend can be seen on Figure 9.10 also.



**Figure 9.10** MRST Polymer Concentration & Saturation Profiles (*a*) t = 100 days (*b*) t = 300 days



Figure 9.10 (cont'd) MRST Polymer Concentration & Saturation Profiles (c) t = 500 days

Then our profile is replaced with MRST at each time step and profiles are plotted. Figure 9.11 shows the concentration and saturation movement at different time steps. Saturation profiles of both of the solutions can be seen in the Figure 9.11 also.



**Figure 9.11** Particle Polymer Concentration & Saturation Profiles (*a*) t = 100 days (*b*) t = 300 days


**Figure 9.11 (cont'd)** Polymer Concentration & Saturation Profiles (c) t = 500 days

Most of the particles that falls ahead of the concentration front has lost their mass to reservoir rock due to adsorption. Those particles are not counted in particle concentration calculation and not plotted in Figure 9.11. The random nature of the particles can be seen as fluctuations in the profile but it seems to agree with injection concentration in the reservoir. Effect of the fluctuations can also be seen on both saturation profiles in Figure 9.11. Production curves are obtained at the end of injection and in Figure 9.12, comparison of MRST and Particle production curves of four different realizations, in other words, four different possibilities of the solution, is plotted. The effect of random movement can also be seen on Figure 9.12 after polymer reaches the production well in the reservoir.



Figure 9.12 1D Production Curve Comparisons

Particle method concentration front is more piston like and falls behind the MRST concentration profile in time in Figure 9.11. Numerical dispersion causes MRST profile to move faster and polymer to reach earlier to the production well. This effect and the piston like movement of the saturation profiles can also be seen in Figure 9.11 in particle method profiles as it follows the concentration front. The effect of numerical dispersion can be clearly seen on both figures 9.11 and 9.12. MRST profile reaches earlier and shows a curved nature instead of a steep change.

## 9.4.1 Effect of Dispersion Coefficient

If the flow is advection dominant in the reservoir, movement of flood fronts and shape of production curve should be more piston like. If reservoir has high heterogeneities, the flow can be dispersion dominant. The dispersion is not taken into account in continuity equations solved in the system normally. The dispersion effect only comes numerically. This effect can be modelled by changing the dispersion coefficient used in particle method. In order to see the effect of dispersion coefficient on polymer application, Equation 3.18 is changed in other realizations. Figure 9.13 shows the effect of dispersion coefficient changes on concentration profile movement at 200<sup>th</sup> day of injection.



**Figure 9.13** Effect of Dispersivity Coefficient on Polymer Concentration Movement The effect of dispersion coefficient on production curves is also plotted on Figure 9.14.



Figure 9.14 Effect of Dispersivity Coefficient (a) Dc x 0.1 (b) Dc x 1 (c) Dc x 10 (d) Dc x 50



Figure 9.14 (cont'd) Effect of Dispersivity Coefficient (e) Dc x 100 (f) Dc x 200 (g) Dc x 300 (h) Dc x 500

Figures 9.13 and 9.14 shows that when we increase the dispersion coefficient used in the model, it converges more to the MRST solution. However, the uncertainties also increase with the increased dispersion coefficient.

## 9.4.2 Effect of Particle Number Injected

Number of particles injected to the system defines the number of particles to be present in a grid during the simulation. With increased number of particles, particle masses that represent polymer mass injected are reduced. If low number of particles are used, we should see more uncertainties in terms of concentration calculation. The same 1D problem is solved with four different total particle number injected throughout the simulation to see its effect on calculations. In four different simulations of the same problem, 10, 50, 100, and 200 particles per time step are injected respectively. Figure 9.15 shows the concentration profile movement at 200<sup>th</sup> time step of simulation and the concentration profile obtained from MRST solution only, without visualizing the particle positions.



Figure 9.15 Polymer Concentration Profile with Different Number of Particles (*a*) 10000 particles



Figure 9.15 (cont'd) Polymer Concentration Profile with Different Number of Particles (*b*) 50000 particles (*c*) 100000 particles (*d*) 200000 particles

The uncertainties on concentration calculation causes the solution not to give good production results of simulation with low number of particles injected. After 100 particles per time step injected, the results does not change much.

## 9.5 2D Problem

### 9.5.1 Velocity Field Interpolation

MRST provides the components of the velocity vector field, as stated in Chapter 7.3. Direct use of the vectors for advection therefore causes the particles to move along the resultant velocity vector after they leave the injection cell. Instead of using the velocity vectors directly, they are interpolated in grid cells with respect to particle position for each particle to provide a proper advection path. Interpolated velocity field is used in both 1D and 2D problems but its effects are more obvious in 2D problems. In order to visualize the effect of interpolation on the velocity field, an example constant velocity field is obtained and used to inject particles in a grid system of 30 m x 30 m. Figure 9.16 shows the velocity vectors and movement of particles in a short time period, and the need for interpolation to provide a proper distribution.



**Figure 9.16** Effect of Velocity Field Interpolation on Particle Distribution, without Interpolation (*a*), with Interpolation (*b*)

# 9.5.2 1<sup>st</sup> Scenario

In our 2D problem, 1D problem dataset is updated to have equal dimension grid blocks and a square reservoir representation. Our 1<sup>st</sup> scenario includes one injection well on the lower left grid, and one production well on the upper right grid of the system. Rest of the properties of the scenario can be seen on Table 9.2. Particles are released into the system with as explained in Chapter 7.3.

Property	Value
Grids $(x - y - z)$	30 - 30 - 1
Total Dimensions $(x - y - z)$	180  m - 180  m - 2  m
Porosity	30 %
Permeability	100 mD
S <sub>dpv</sub>	5 %
RRF	1.1
ρ <sub>rock</sub>	2000 kg/m <sup>3</sup>
Water Injection Flow Rate	10 m <sup>3</sup> /day
Injected Polymer Concentration	0.8 kg/m <sup>3</sup>
$\Delta t$	1 days
Total Simulation Time	1400 days

Table 9.2 Two Dimensional Problem 1<sup>st</sup> Scenario Properties

Polymer concentration profiles can be plotted as a color map in this scenario. Figure 9.17 shows the MRST and particle concentration profiles at different time steps. In Figure 9.18, distribution of particles can be seen areally. Obtained production results of four different realizations is again plotted and shown in Figure 9.19.



Figure 9.17 2D Concentration Distribution Comparison ( $1^{st}$  Scenario), MRST (*above*), Particle (*below*) (*a*) t = 200 days (*b*) t = 600 days



**Figure 9.17 (cont'd)** 2D Concentration Distribution Comparison (1<sup>st</sup> Scenario), MRST (above), Particle (below) (c) t = 1000 days (d) t = 1400 days



**Figure 9.18** Particle Distribution Profiles ( $1^{st}$  Scenario) (a) t = 200 days (b) t = 600 days (c) t = 1000 days (d) t = 1400 days



Figure 9.19 2D Production Curve Comparison (1<sup>st</sup> Scenario)

4<sup>th</sup> realization of this scenario gave a different production curve than the rest of the runs. Randomly generated angles used for injection and random numbers used on dispersion of the particles can lead the particles to accumulate in some regions of the system. The effect of accumulation affects the system and different results can be seen in some simulations. However, the other results seems to agree with each other and the effect of numerical dispersion is not seen on the results.

## 9.5.3 2<sup>nd</sup> Scenario

In our 2<sup>nd</sup> scenario, the dataset is updated to have one production well on the lower left and one on the upper right grid of the system, and one injection well at the center grid. Particle releasing on the system is the same and the rest of the properties of the scenario can be seen on Table 9.3.

Property	Value
Grids $(x - y - z)$	30 - 30 - 1
Total Dimensions $(x - y - z)$	180 m – 180 m – 2 m
Porosity	30 %
Permeability	100 mD
S <sub>dpv</sub>	5 %
RRF	1.1
ρ <sub>rock</sub>	2000 kg/m <sup>3</sup>
Water Injection Flow Rate	10 m <sup>3</sup> /day
Injected Polymer Concentration	$0.8 \text{ kg/m}^3$
$\Delta t$	1 days
Total Simulation Time	1000 days

**Table 9.3** Two Dimensional Problem 2<sup>nd</sup> Scenario Properties

Figure 9.20 shows the concentration distribution at different time steps of the injection. Figure 9.21 shows the particle distributions. Comparison of MRST and Particle production curves are plotted on Figure 9.22.



Figure 9.20 2D Concentration Distribution Comparison ( $2^{nd}$  Scenario), MRST (*above*), Particle (*below*) (a) t = 100 days (b) t = 400 days



Figure 9.20 (cont'd) 2D Concentration Distribution Comparison ( $2^{nd}$  Scenario), MRST (*above*), Particle (*below*) (c) t = 700 days (d) t = 1000 days



Figure 9.21 Particle Distribution Profiles  $(2^{nd} Scenario)(a) t = 100 \text{ days } (b) t = 400 \text{ days } (c) t = 700 \text{ days } (d) t = 1000 \text{ days}$ 



Figure 9.22 2D Production Curve Comparison (2<sup>nd</sup> Scenario)

Since there are two production wells at this scenario, the production curve is the summation of both of the wells. The physical effect of dispersion is seen less and the results vary more than the other scenarios, but still the overall profiles agree with MRST solution. In some runs, the problem did not converge because of high accumulation of particles at some cells. Generated random numbers, effect of polymer on velocity fields, and overall velocity field generated by the MRST might cause the high accumulation in this problem.

#### **CHAPTER 10**

#### CONCLUSION

Random-walk particle tracking method gives an alternative modelling option for polymer flooding. The technique is used to solve polymer advection and diffusion/dispersion equation to add the effects of injected polymer to a reservoir. MRST model solves the set of equations for the system. Simultaneously polymer concentration profile is calculated with the updated position and mass information of particles' at each time step. The effects of polymer on other properties in the reservoir and flow are dependent on polymer concentration in the reservoir. In order to eliminate the equations solved for polymer phase in the MRST model, concentration profile calculated by MRST model is updated with the profile calculated from the polymer concentration at each time step.

MRST model does not include the dispersion process. Effect of dispersion occurs numerically on MRST model solutions of simple water flooding and 1D problem even though finer grid systems are used to overcome the effect. Particle tracking method allows us to define a dispersion parameter that is used to calculate the transport of polymer probabilistically. Since the transportation of polymer is calculated with a linear equation, it does not involve numerical errors. Dispersion coefficient used can be changed easily in the model. A high dispersivity reservoir shows similar results with MRST solution. The model can be used to determine the dispersivity of a reservoir with field data in simple 1D problems.

Oscillations in the concentration calculations are the result of the random nature of the problem. They can be lowered with higher particle numbers released into the system. If small numbers of particles or long time steps are applied, the number of particles in a cell leads to more oscillations and uncertainties in the calculations. Increasing the number of particles injected does not improve much after some point, but it also increases the computation time of the model.

In 2D scenarios, particle solution shows a general consistency with some exceptions. Generated random numbers used in injection modelling can cause the particles to accumulate in an area with the combined effect of water velocity profiles obtained from MRST solution. This effect is seen on the production curve generated in our 1<sup>st</sup> scenario, whereas in the 2<sup>nd</sup> scenario, the problem might not converge to a solution at some simulations.

As a result, random-walk particle tracking method can be a tool to overcome the effect of numerical dispersion in simple 1D models, whereas it can still be an alternative in 2D scenarios in polymer injection modelling.

For future works, reservoir heterogeneities, different grid orientations, effect of salinity can be worked with the model. In addition to different reservoir and chemical systems, some smoothing methods can be introduced to the model in order to reduce the oscillations in the calculations.

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## **APPENDIX** A

## **CODE IMPLEMENTED**

Appendix A gives implemented code in MRST model for particle tracking method for 1D problem. Arrays model, schedule, and state are obtained from MRST solution.

Section below shows code for initialization of particle and input parameters:

dt = schedule.step.val; % time step information taken from model nSteps = numel(dt); % number of time steps

% Injection input (hard-coded) Ci = 0.8; % polymer injection concentration, kg/m3 qi = 10.0/86400; % water injection flow rate, m3/day Simu = '1D';

% Set up random walk parameters nPstep = 100; % particles to be injected per time step nPtotal = nSteps \* nPstep; % total particle number nPnow = 0; % active particle count in the system

```
part.x = zeros(nPtotal,1); % particle distance information
part.i = zeros(nPtotal,1); % particle grid information
part.k = randperm(nPtotal); % random permutation; to locate the particle on y-axis
part.m = ones(nPtotal,1)*qi*Ci*dt(1)/nPstep; % particle mass, kg
```

nc = model.G.cells.num; % total grid number of the system
partmassads = zeros(nc, 1); % adsorbed particle mass in each cell
partmassads1 = zeros(nc, 1); % adsorption capacity of the cell at the current time
step
mobmass = zeros(nc, 1); % mobile particle mass at the time step in each cell
massdiff = zeros(nc, 1); % mass to be adsorbed by rock in each cell
% Set dispersion parameters
diffC = 4.0e-10; % a typical diff. coeff., m^2/s
dispX = 0.044\*model.G.nodes.coords(end,1)^1.13; % dispersivity multiplier
dispC = dispX \* diffC \* 1; % dispersion coefficient used
dispL = sqrt(2\*dispC\*dt(1)); % dispersion length

Section below is used for updating the position information of particles to injection well location.

dx = model.inputdata.GRID.DX(1); inji = cell2mat(model.inputdata.SCHEDULE.control.WELSPECS(end,3)); % injection well position part.x = ones(nPtotal,1)\*((inji-1)\*dx+dx/2); % reposition particles to injection point

Rest of the code given below is repeated in each time step. First part computes interpolated velocity field and introduces advection and dispersion to active particles in the system.

% Compute interstial water phase velocities fW = state.flux(:,1); % water phase flux given by MRST solution sW = state.s(:,1); % water saturation given by MRST solution poro = model.rock.poro; % porosity information vW = bsxfun(@rdivide,faceFlux2cellVelocity(model.G, fW),poro.\*sW); % water phase velocity in each cell Fx = griddedInterpolant(dist,vW(:,1),'cubic','cubic'); % interpolated velocity handle Xq = part.x(1:nPnow); % positions of the active particles xVq = Fx(Xq); % advection velocity for active particles part.x(1:nPnow) = part.x(1:nPnow) + xVq.\*dT; % advection of active particles % Introduce dispersion part.x(1:nPnow) = part.x(1:nPnow) + randn([nPnow 1])\*dispL; % dispersion of active particles

Second part is used for releasing new particles to the system at the current time step

```
% Release new particles with average cell velocities of their position
vW(1,1) = vW(1,1)*2; % velocity is doubled in the first cell
dTpart = dT/nPstep; % mini time step for continious release of particle during time
step
for id = 1:nPstep
  currentcell = 1; % current position of newly released particles
  for t = 1:(nPstep + 1 - id) % loop to update position particle in case it leaves
injection cell
     part.x(nPnow + id) = part.x(nPnow + id) + vW(currentcell,1)*dTpart; %
advection of newly released particle
     part.x(nPnow + id) = part.x(nPnow + id) + randn()*sqrt(2*dispC*dTpart); %
dispersion of newly released particle
     pos = floor(part.x(nPnow + id)/dx) + 1; % position of particle at the end of mini
time step
     if pos > currentcell % position check
       currentcell = pos;
     end
  end
end
% increase active particle count
nPnow = nPnow + nPstep;
```

After moving the particles, positions are checked and polymer concentration is calculated with code below

```
% Check and correct the particle positions against the boundaries
partidx = part.x(1:nPnow)<0;
part.x(partidx) = 0;
% Correct produced particle location an masses
iprod = part.x(1:nPnow)>model.G.nodes.coords(end,1)-dx/2;
part.x(iprod) = model.G.nodes.coords(end,1)-dx/2;
part.m(iprod) = 0.0;
% Update particle grid information
part.i(1:nPnow) = floor(part.x(1:nPnow)/dx) + 1;
```

```
% Sum the mass of the particles in each cells and
% compute the cell contration using the accumulated particle masses
idx = part.i(1:nPnow); idxmax = max(idx);
mobmass(1:idxmax) = accumarray(idx,part.m(1:nPnow));
% Divide the accumulated mass by the water volume of each cell to calculate
% concentration
concpart = mobmass ./ (model.G.cells.volumes .* poro .* sW);
```

Adsorption is added as the last step and concentration field of MRST is updated at the end.

```
% Calculate adsorption capacity of each cell at their current polymer
% concentration
partmassads1(1:idx) = model.fluid.ads(concpart(1:idx)) .*...
  model.fluid.rhoR .* model.G.cells.volumes(1:idx) .*...
  (1 - poro(1:idx)*(1-model.fluid.dps));
% find the grids in which more adsorption can occur
k = find(partmassads1(1:idx) > partmassads(1:idx))';
massdiff(1:idx) = partmassads1(1:idx) - partmassads(1:idx); \% mass to be adsorbed
by rock
for idC = 1:size(k,2) %loop to update particle mass in cells that adsorption can occur
  control1 = k(idC);
  if mobmass(control1) > massdiff(control1) % if mobile mass is greater than mass
to be adsorbed, calculate mass fraction to be removed from each particle
     control2 = find(idx == control1); % particles that are in the grid
     control3 = find(part.m(control2) == 0); \% particles that has 0 mass
     control2(control3) = []; % remove 0 mass particles out of equation
     massfrac = massdiff(control1) / mobmass(control1); % fraction of mass to be
adsorbed
     part.m(control2) = part.m(control2).*(1 - massfrac); % update masses of the
particles in the grid
     partmassads(control1) = partmassads(control1) + massdiff(control1); % update
adsorbed mass information of the grid
```

else % if mobile mass is less than mass to be adsorbed, reduce mass of each particle in that grid to 0

```
control2 = find(idx == control1);
control3 = find(part.m(control2) == 0);
control2(control3) = [];
part.m(control2) = 0;
partmassads(control1) = partmassads(control1) + mobmass(control1); % update
adsorbed mass information of the grid
end
end
state.c = concpart; % update concentration array of MRST with particle method
concentration
```