Short solutions for exam in PET 565 spring 2016.

(a) A direct computation of derivatives u_t and u_x gives

$$u_t = u_0'(\cdot)\frac{\partial}{\partial t}[x - f'(u(x,t))t] = -u_0'(\cdot)[tf''(u(x,t))u_t + f'(u(x,t))]$$

and

$$u_x = u_0'(\cdot)\frac{\partial}{\partial x}[x - f'(u(x,t))t] = u_0'(\cdot)[1 - tf''(u(x,t))u_x],$$

that is,

$$f'(u)u_x = u_0'(\cdot)[f'(u) - tf''(u)f(u)_x].$$

Then it follows by adding

$$[u_t + f(u)_x] = -u_0'(\cdot)tf''(u)[u_t + f(u)_x].$$

Hence,

$$[u_t + f(u)_x] \cdot [1 + u_0'(\cdot)tf''(u)] = 0.$$

(b) By differentiating (***) with respect to x we get

$$u_x = u_0'(x_0)[1 - f''(u(x,t))u_x t], \qquad u(x,t) = u_0(x_0),$$

from which we find

$$u_x = \frac{u_0'(x_0)}{1 + u_0'(x_0)f''(u_0(x_0))t},$$

where $x_0 = x - f'(u_0(x_0))t$ and $u(x,t) = u_0(x_0)$.

Breaking time: The time when u_x blows up.
Characteristics will meet at that time possibly carrying different constant states, i.e., formation of jumps in the solution.

(c) The rectangle $[x_1, x_1 + \Delta x] \times [t_1, t_1 + \Delta t]$ is split by the shock into two triangles and the value of u is roughly constant in each. The integral form of the conservation law is obtained by integrating $u_t + f(u)_x = 0$ over $[x_1, x_1 + \Delta x] \times [t_1, t_1 + \Delta t]$:

$$\int_{x_1}^{x_1+\Delta x} u(x, t_1+\Delta t)\,dx - \int_{x_1}^{x_1+\Delta x} u(x, t_1)\,dx = \int_{t_1}^{t_1+\Delta t} f(u(x_1, t))\,dt - \int_{t_1}^{t_1+\Delta t} f(u(x_1+\Delta x, t))\,dt.$$

Using that u is essentially constant along each edge of the rectangle (either u_l or u_r) we get

$$\Delta x u_r - \Delta x u_l = \Delta t f(u_l) - \Delta t f(u_r) + O(\Delta t^2),$$

where $O(\Delta t^2)$ accounts for the variation in u. That is (for the case indicated in the figure where velocity of the jump is negative),

$$s = -\frac{\Delta x}{\Delta t} = \frac{f(u_l) - f(u_r)}{u_l - u_r} + O(\Delta t).$$

Letting $\Delta t \to 0$.

(d) At $x = 0$ we have a rarefaction wave, and at $x = 2$ we have a shock wave. The combined solution then reads

$$u(x,t) = \begin{cases} 0, & x \leq 0; \\ \frac{3}{2}\frac{x}{t}, & 0 < x < \frac{4}{3}t; \\ 2, & \frac{4}{3}t \leq x \leq \frac{2}{3}t + 2; \\ 0, & x > \frac{2}{3}t + 2; \end{cases}$$

After a time T_C, the rarefaction waves catches up to the shock. This must correspond to $\frac{4}{3}T_C = \frac{2}{3}T_C + 2$, giving $T_C = 3$.

(e) We want to compute the new shock $(u_l(t), 0)$ and its position $x_s(t)$ for times $t > T_C$. The Rankine-Hugoniot condition gives that $s = \frac{1}{3}u_l(t)$.
Furthermore, we expoit that $s(t) = \frac{d}{dt}x_s(t)$ and $x_s(t) = f'(u_l(t))t = \frac{2}{3}u_l(t)t$. This then leads to an equation of the form $u_l'(t) = -\frac{1}{2t}u_l(t)$.

Rewriting and then integrating over $[T_C, t]$ and $[2, u_l(t)]$ gives us the equation
$ln(\frac{T_C}{t})^{\frac{1}{2}} = ln(\frac{u_l}{2})$.
We then find that $u_l(t) = 2(\frac{3}{t})^{\frac{1}{2}}$.
We also note that $x_s(t) = \frac{2}{3}u_l(t)t = 4(3)^{-\frac{1}{2}}t^{\frac{1}{2}}$.
The solution for $t >= T_C$ then reads

$$u(x,t) = \begin{cases} 0, & x \leq 0; \\ \frac{3}{2}\frac{x}{t}, & 0 < x < x_s(t); \\ 0, & x \geq x_s(t); \end{cases}$$

Exercise 2

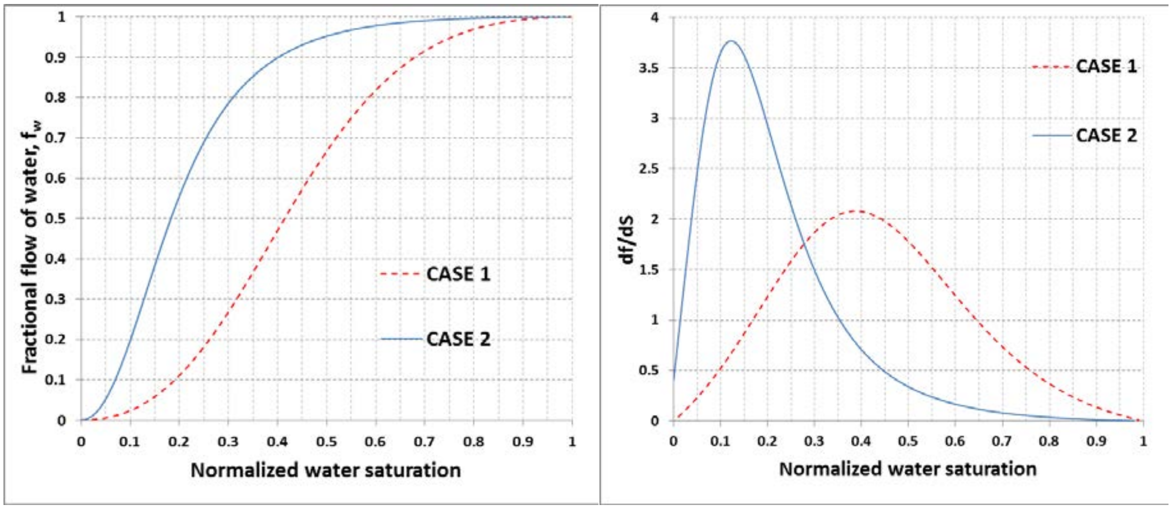


Fig. 1. Fractional flow curves vs. normalized water saturation for CASE 1 and CASE 2 to the left and corresponding df/dS curves to the right.

The Buckley-Leverett (B-L) equation for water-oil transport (horizontal flow) is given by:

$$\frac{\partial S}{\partial t} + \frac{\partial f(S)}{\partial x} = 0 \qquad x \in [0,1] \qquad (*)$$

where S is normalized water saturation, t is dimensionless time and x is normalized length.

The equation (*) can further be developed to (**) below.

$$\frac{\partial S}{\partial t} + f'(S)\frac{\partial S}{\partial x} = 0 \qquad (**)$$

a) Show how (**) can be derived from (*). What is the quantify f’(S) representing?
b) Sketch the general steps involved for determining the water saturation shock front height and the water saturation profile behind the front ($S > S_f$) for a system with a given fractional flow curve.
c) Determine the time when water breakthrough occurs for CASE 1 (called TB1) and CASE 2 (called TB2)?
d) Let water be injected into two different core samples having fractional flow curve characteristics corresponding to CASE 1 and CASE 2 above. What is the expected water-cut exactly at the time when water is breaking through at the outlet of the core sample for CASE 1 and CASE 2? We assume that water-cut is equal to water fractional flow value meaning that we assume $B_w = B_o$ which should be a reasonable assumption in a laboratory test using dead oil and low pressures during in the experiments.

e) Calculate oil recovery for both cases at the time when water breakthrough occurs for CASE 1 i.e., at TB1.

Solution

a) $\frac{\partial S}{\partial t} + \frac{\partial f(S)}{\partial x} = 0$

Using chain rule: $\frac{\partial S}{\partial t} + \frac{\partial f(S)}{\partial x} = \frac{\partial S}{\partial t} + \frac{df(S)}{dS}\frac{\partial S}{\partial x} = \frac{\partial S}{\partial t} + f'(S)\frac{\partial S}{\partial x} = 0$

f'(S) represents the dimensionless velocity for a certain water saturation S.

b) 1) Determine the front saturation height. It can be done graphically as shown in the figure below.

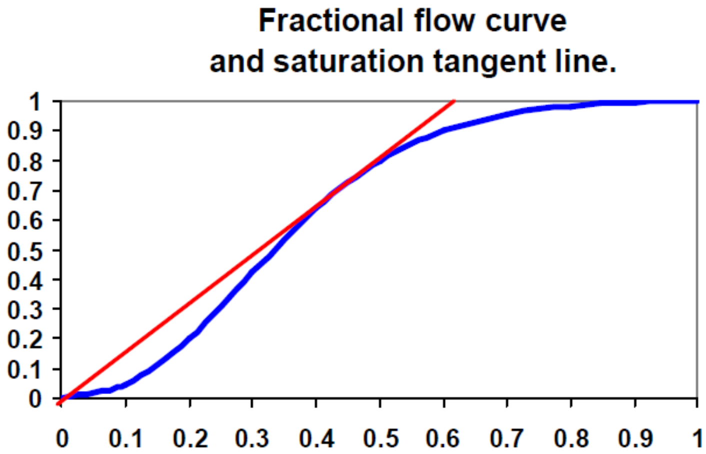
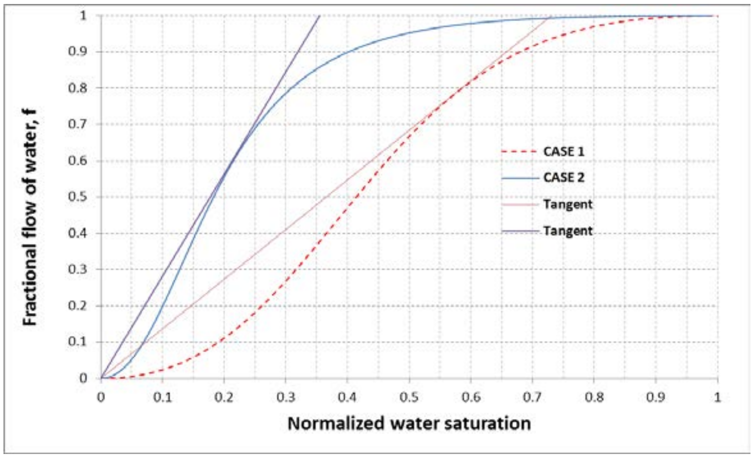


Figure 1 Graphical determination of front saturation

Draw the fractional flow curve and the tangent line passing through the origin. The front height saturation S_f corresponds to the tangent point saturation, 0.45 in the figure.

1) The speed of the saturation front is equal to the steepness of the tangent line used to determine front saturation, i.e. $f'(S_f)$. Hence, after time *T* the front has moved a distance $f'(S_f)T$.
2) The position of saturations $S > S_f$ after time T is given by $f'(S)T$.

c) At water breakthrough: $f'(S_f)\cdot T_b = 1$, $f'(S_f)$ is shock front velocity and T_b dimensionless breakthrough time.



From figure above:

CASE 1 has shock front saturation height ≈ 0.57 corresponding to a velocity of $f'(S_f) \approx 1.4$.

CASE 2 has shock front saturation height ≈ 0.22 corresponding to a velocity of $f'(S_f) \approx 2.6$.

$f'(S_f)\cdot TB1 = 1 \rightarrow TB1 = 1/1.4 = \underline{0.71}$

$f'(S_f)\cdot TB2 = 1 \rightarrow TB2 = 1/2.6 = \underline{0.38}$

d) Water-cut at breakthrough corresponds to the fractional flow of water at the shock front saturation S_f.
Hence, WCT (CASE 1) $\underline{\approx 0.78}$ and WCT (CASE 2) $\underline{\approx 0.61}$

e) Oil recovery up to breakthrough is given by dimensionless time TB. CASE 1 has the most stable displacement process with water breaking through at TB1 = 0.71. RF CASE 1 at breakthrough is therefore 0.71. The water front for CASE 2 broke through at TB2 = 0.38.
The water saturation at the outlet of the core for CASE 2 at time 0.71 is called S*.
$f'(S^*)\cdot 0.71 = 1 \rightarrow f'(S^*) = 1/0.71 \approx 1.41$. From the derivative plot it can be found that $df/dS = 1.41$ corresponds to $S^* \approx 0.3$. Corresponding $f(S^*)$ is then ≈ 0.78. Hence, recovery for CASE 2 at TB1 = 0.71 is:

$R = S^* + T\cdot(1 - f(S^*)) = 0.3 + 0.71(1 - 0.78) = \underline{0.46}$

Exercise 3. A brine contains 0.15 mol/L Na_2SO_4 consisting of the ions Na^+ and SO_4^{2-}.

a) Calculate the ionic strength.

In the following we consider dissolution of calcite $CaCO_3$ in this brine, according to

$$\mathrm{CaCO_3} \quad \rightleftharpoons \quad \mathrm{Ca^{2+}} + \mathrm{CO_3^{2-}}, \qquad K_{calcite} = 10^{-8.5} \tag{1}$$

The dissolved species are assumed not to affect the ionic strength. The carbon content is assumed to be mainly in form of CO_3^{2-}.

b) Calculate activity coefficients of Na^+, Ca^{2+}, CO_3^{2-} and SO_4^{2-}.

c) Without accounting for complexes, how many moles $CaCO_3$ per L can be dissolved in this brine?

Answer.

a)

$$I = 0.5(2 \cdot 0.15 \cdot 1^2 + 0.15 \cdot (-2)^2) = 0.5(0.3 + 0.6) = 0.45 \tag{2}$$

b) Using Davies formula we obtain:

$$\log_{10} \gamma_i \quad = \quad -0.51 Z_i^2 \Big(\frac{\sqrt{0.45}}{1 + \sqrt{0.45} - 0.3 \cdot 0.45} \Big) = -0.136 Z_i^2 \tag{3}$$

$$\gamma_{na} \quad = \quad 10^{-0.136} = 0.73 \tag{4}$$

$$\gamma_{ca} \quad = \quad \gamma_{co3} = \gamma_{so4} = 10^{-0.136 \cdot 4} = 10^{-0.136 \cdot 4} = 0.28 \tag{5}$$

c) We have that $m_{calcite} = m_{ca} = m_{co3} = m$

$$K = \gamma^2 m^2 \tag{6}$$

$$m = \sqrt{K}/\gamma = \sqrt{10^{-8.5}}/0.28 = 0.20 \text{ mmol/L} \tag{7}$$

Exercise 4. This is a continuation of Task 1, considering how the formation of complexes influences the solubility of calcite in the given brine. The complex $CaSO_4^0$ can form according to

$$\mathrm{CaSO_4^0} \quad \rightleftharpoons \quad \mathrm{Ca^{2+}} + \mathrm{SO_4^{2-}}, \qquad K_{caso} = 10^{-2.5} \tag{8}$$

a) Write down the following 5 equations:
   - Equilibrium of the aqueous complex reaction (8) according to the law of mass action
   - 2 mass balance equations for Ca^{2+} and SO_4^{2-} species
   - Equilibrium of the calcite dissolution reaction (1)
   - The relation between the concentrations of CO_3^{2-} and Ca^{2+}

   Specify which variables are unknown.

PS: Express the equations using total concentrations C_i, concentrations of free species m_i and concentrations of complexes n_{ij}. You do NOT have to solve the equations.

Answer.

a)

$$\frac{m_{\mathrm{Ca^{2+}}} m_{\mathrm{SO_4^{2-}}}}{n_{\mathrm{CaSO_4^0}}} \frac{\gamma_{\mathrm{Ca^{2+}}} \gamma_{\mathrm{SO_4^{2-}}}}{\gamma_{\mathrm{CaSO_4^0}}} \quad = \quad K_{caso} \tag{9}$$

$$C_{\mathrm{Ca^{2+}}} \quad = \quad m_{\mathrm{Ca^{2+}}} + n_{\mathrm{CaSO_4^0}} \tag{10}$$

$$C_{\mathrm{SO_4^{2-}}} \quad = \quad m_{\mathrm{SO_4^{2-}}} + n_{\mathrm{CaSO_4^0}} \tag{11}$$

$$m_{\mathrm{Ca^{2+}}} m_{\mathrm{CO_3^{2-}}} \gamma_{\mathrm{Ca^{2+}}} \gamma_{\mathrm{CO_3^{2-}}} \quad = \quad K_{calcite} \tag{12}$$

$$m_{\mathrm{CO_3^{2-}}} \quad = \quad C_{\mathrm{Ca^{2+}}} \tag{13}$$

Unknowns: $m_{\mathrm{Ca^{2+}}}, m_{\mathrm{SO_4^{2-}}}, n_{\mathrm{CaSO_4^0}}, C_{\mathrm{Ca^{2+}}}, m_{\mathrm{CO_3^{2-}}}$

Exercise 5. A core contains c=0 mol/L of a species initially and is then injected with a brine containing c=1 mol/L. The species adsorbs according to an isotherm $q(c) = c^3$. Assume a retardation model can be applied.

a) Sketch the concentration profile along the core after flooding 1 pore volume.
b) How many pore volumes must be flooded before the core stops adsorbing more species?
c) After the core is flooded sufficiently with the 1 mol/L brine, the core is cleaned by flooding a brine with $c = 0$ mol/L. How many pore volumes of the new brine must be injected to remove all the species from the core?

Answer.

c	$dq/dc = 3c^2$	$R = 1 + dq/dc$	$x_c/x_w = 1/R$
0	0	1	1
0.5	0.75	1.75	0.57
1	3	4	0.25

a) See table.
b) The slowest concentration must have reached the outlet. R is largest for the highest concentration, $c = 1$. $x_{c=1} = 1$ when $x_w/R_{c=1} = 1$ which is $x_w = R_{c=1} = 4$, i.e. 4 PV.
c) The sorbant is displaced in a frontlike manner where $R_f = 1 + \frac{1^3-0^3}{1-0} = 2$. The front has reached the outlet after 2 PV.

FORMULAS

$$I = 1/2 \sum_i m_i Z_i^2 \tag{14}$$

$$\log_{10} \gamma_i = -0.51 Z_i^2 \Big(\frac{\sqrt{I}}{1 + \sqrt{I} - 0.3I} \Big) \tag{15}$$

$$R_c = 1 + \frac{dq}{dc}, \qquad \text{(broadening front)} \tag{16}$$

$$R_f = 1 + \frac{\Delta q}{\Delta c}, \qquad \text{(sharpening front)} \tag{17}$$