Spring 2015: part A:

Problem 1

a) i) $\partial_t(\phi S_w \rho_w) + \partial_x(\rho_w U_w) = 0$

$\partial_t(\phi S_o \rho_o) + \partial_x(\rho_o U_o) = 0$

$U_i = -K\frac{k_{ri}}{\mu_i}\partial_x P_i \quad , \quad i = w, o \qquad P_c = P_o - P_w$

$= -\lambda_i K \partial_x P_i \quad , \quad \lambda_i = \text{mobility} = \frac{k_{ri}}{\mu_i}$

ii) $U_w = -U_o$

$\lambda_w \partial_x P_w = -\lambda_o \partial_x P_o = -\lambda_o(\partial_x P_c + \partial_x P_w)$

$\Rightarrow [\lambda_w + \lambda_o]\partial_x P_w = -\lambda_o \partial_x P_c$

$\partial_x P_w = -\frac{\lambda_o}{\lambda_T}\partial_x P_c \quad , \quad \lambda_T = \lambda_w + \lambda_o$

iii) incompressible fluids, constant ϕ

$\Downarrow$

$\phi\,\partial_t S_w + \partial_x U_w = 0 \quad , \quad U_w = -K\lambda_w P_{wx} = K\frac{\lambda_w\lambda_o}{\lambda_T}\partial_x P_c$

$\phi\,\partial_t S_w = -\partial_x U_w = \partial_x\left(-\left[K\frac{\lambda_w\lambda_o}{\lambda_T}\right]\partial_x P_c\right)$

b) $U_i = -K\lambda_i(\partial_x P_i + \rho_w g)$ (positive direction is upward)

$U_w = -U_o$

$\lambda_w(P_{wx} + \rho_w g) = -\lambda_o(P_{ox} + \rho_o g) = -\lambda_o(P_{cx} + P_{wx} + \rho_o g)$

$P_{wx}\left(1 + \frac{\lambda_o}{\lambda_w}\right) = -\frac{\lambda_o}{\lambda_w}P_{cx} - g\left[\frac{\lambda_o}{\lambda_w}\rho_o + \rho_w\right]$

$P_{wx} = -\frac{\lambda_o}{\lambda_T}P_{cx} - g\frac{[\lambda_o\rho_o + \lambda_w\rho_w]}{\lambda_T}$

$\Rightarrow \quad U_w = -K\lambda_w(P_{wx} + \rho_w g)$

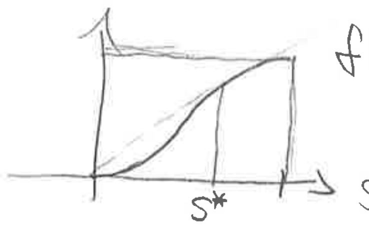
$= -K\lambda_w\left(-\frac{\lambda_o}{\lambda_T}P_{cx} - g\frac{[\lambda_o\rho_o + \lambda_w\rho_w]}{\lambda_T} + \rho_w g\right)$

$\vdots$

$= K\frac{\lambda_w\lambda_o}{\lambda_T}P_{cx} - K\frac{\lambda_w\lambda_o}{\lambda_T}g\,\Delta\rho \quad , \quad \Delta\rho = \rho_w - \rho_o$

$\Rightarrow \phi\,\partial_t S_w + \partial_x\left(-K\frac{\lambda_w\lambda_o}{\lambda_T}g\Delta\rho\right) = \partial_x\left(-\left[K\frac{\lambda_w\lambda_o}{\lambda_T}\right]\partial_x P_c\right)$

Problem 2: $S_t + f(S)_x = 0$ ②



fractional flow function

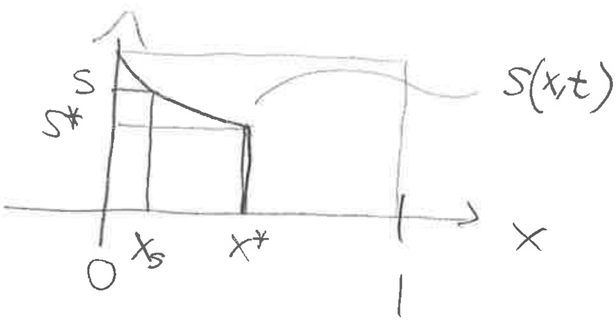
a) step 1:

compute front height s^* given by

$$f'(s^*) = \frac{f(s^*)}{s^*} \quad \text{(see figure)}$$

Step 2:

Position of front: $\left\langle \begin{array}{l} \text{Speed: } V = f'(s^*) \\ \text{Position: } x^* = Vt = f'(s^*)t \end{array} \right.$

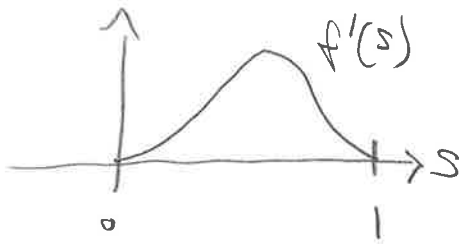


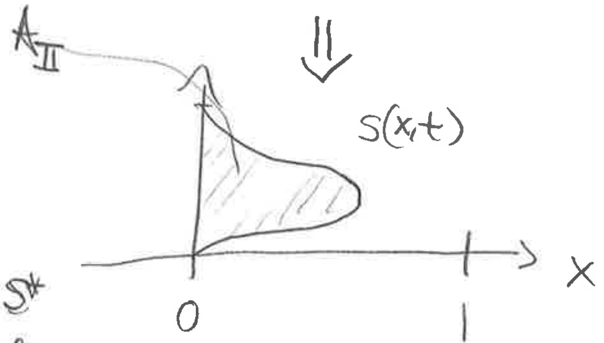
Step 3:

behind front: $s \in (s^*, 1] \Rightarrow x_s = f'(s)t$

b)

Method of characteristics: $x_s = f'(S)t$ for $S \in [0,1]$

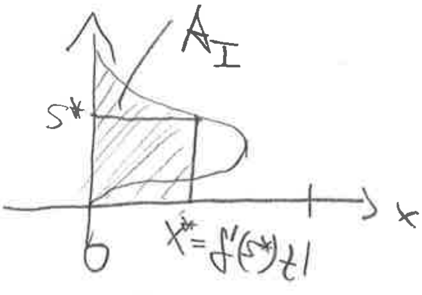




unphysical solution is obtained based on MOC

Physical correct solution:

Introduce a shock/front S^* such that mass conservation is ensured.



$\Rightarrow A_I = A_{II}$:

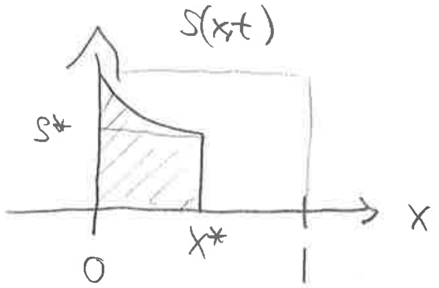
$$\int_0^1 f'(S)t\,dS = S^* x_s + \int_{S^*}^1 f'(S)t\,dS$$

$$t\cdot(f(1)-f(0)) = S^*\cdot f'(S^*)t + t\,[f(1)-f(S^*)]$$

i.e. $t = S^* f'(S^*) t + t(1 - f(S^*))$

$$1 = S^* f'(S^*) + 1 - f(S^*)$$

$$f'(S^*) = \frac{f(S^*)}{S^*}$$



c) <u>Oil recovery</u>

i) Before breakthrough:

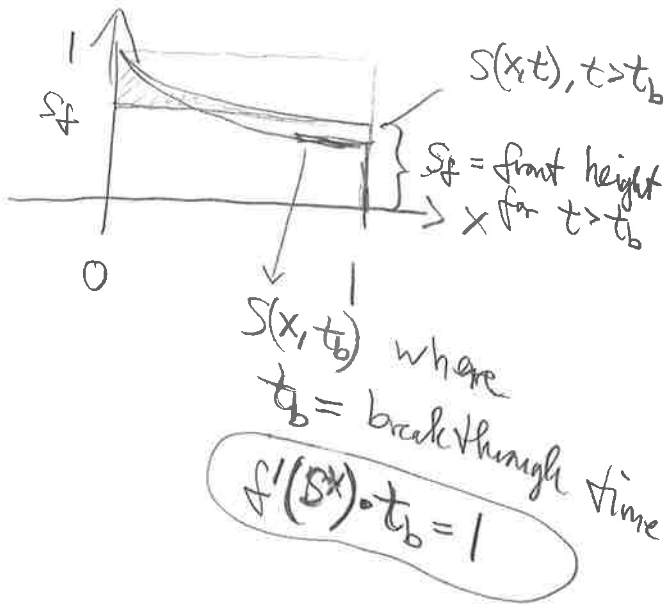
$R(t)$ = "area of injected water"

$$= x^* \cdot S^* + \int_{S^*}^{1} f'(S) t \, dS$$

$$= f'(S^*) t S^* + t(1 - f(S^*))$$

$$= [f'(S^*) S^* - f(S^*)] t + t$$

$$= t$$



ii) after breakthrough:

S_f (varying front height) given by

$$f'(S_f) t = 1$$

$$R(t) = S_f \cdot 1 + \int_{S_f}^{1} f'(S) t \, dS$$

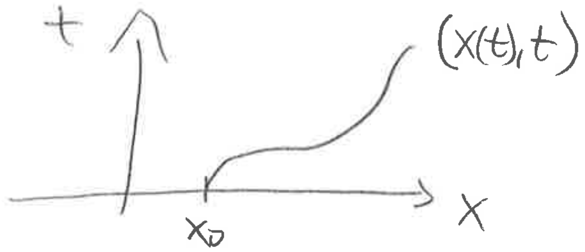
$$= S_f + t(1 - f(S_f))$$

Problem 3: (*) $U_t + f(U)_x = 0 \quad , x \in \mathbb{R}$

$$U(x, t=0) = \phi(x)$$

a)

Characteristics: $\dfrac{dX(t)}{dt} = f'(U(X(t),t)) \quad , \quad X(t=0) = X_0$



Consider U from (*) along $(X(t),t)$:

$$\tilde{U}(t) = U(X(t),t)$$

$$\Rightarrow \frac{d}{dt}\tilde{U}(t) = U_x \frac{dX(t)}{dt} + U_t \frac{dt}{dt} = U_x f'(U(X(t),t)) + U_t = 0$$

$$\Rightarrow \tilde{U}(t) = U(X(t),t) \text{ is constant}$$

$$\Rightarrow U(X(t),t) = U(X(t=0), t=0) = \phi(X_0) \qquad (**)$$

Now we can use this information to compute characteristic:

$$\frac{dX}{dt} = f'(\phi(X_0)) \quad , \quad X(t=0) = X_0$$

$$\Rightarrow X(t) = f'(\phi(X_0))t + X_0$$

$$\Rightarrow X_0 = X(t) - f'(\phi(X_0))t$$

Plugging back in (**), we get

$$U(X(t),t) = \phi\left(X(t) - f'(U(X(t),t))t\right)$$

$$\Rightarrow U(X,t) = \phi\left(X - f'(U(X,t))t\right)$$

b)

$$U_x = \phi'(\cdot)\frac{\partial}{\partial x}\left(X - f'(U)t\right)$$

$$= \phi'(\cdot)\left(1 - f''(U)U_x t\right)$$

$$= \phi' - \phi' \cdot f''(U)U_x t$$

$$\Downarrow$$

$$U_x\left(1 + \phi' \cdot f''(U)t\right) = \phi'$$

$$U_x = \frac{\phi'(X_0)}{1 + \phi'(X_0)f''(U)t}$$

Blow-up: $f''(U) > 0$ (convex f)

$$\Downarrow$$

if $\phi'(X_0) < 0$, then blowup for $1 + \phi'(X_0)f''(U)t = 0$

b) $U(x,t) = \phi(x - f'(U)t) = \phi(x_0)$

$$U_t = \phi'(\cdot)\frac{\partial}{\partial t}(x - f'(U)t) = \phi'(\cdot)(-1)\left(f''(U)U_t t + f'(U)\right)$$

$$U_x = \phi'(\cdot)\frac{\partial}{\partial x}(x - f'(U)t) = \phi'(\cdot)\left(1 - f''(U)U_x t\right)$$

$$U_t + f'(U)U_x = -\phi'(\cdot)f''(U)U_t t - \underline{\phi'(\cdot)f'(U)} + \underline{f'(U)\phi'(\cdot)} - \phi'(\cdot)f''(U)f'(U)U_x t$$

$$= U_t\left(-\phi'(\cdot)f''(U)t\right) - \phi'(\cdot)f''(U)t\, f(U)_x$$

$$= \left[U_t + f(U)_x\right](-1)\phi'(\cdot)f''(U)t$$

$$\left(U_t + f(U)_x\right)\left(1 + \phi'(\cdot)f''(U)t\right) = 0$$

$$U_t + f(U)_x = 0$$

if and only if

$$1 + \phi'(x_0)f''(\phi(x_0))t \neq 0$$

c) Weak solutions:

i) $$\int_0^{t_a}\int_{-\infty}^{\infty}\left(U_t + f(U)_x\right)\phi(x,t)\,dx\,dt = 0$$

$$\Downarrow$$

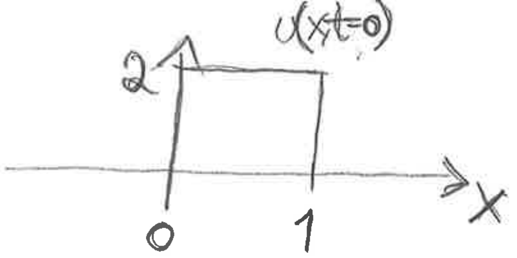
by integration by parts

$$-\int_0^{+\infty}\int_{-\infty}^{\infty}\left[U\phi_t + f(U)\phi_x\right]dx\,dt - \int_{-\infty}^{\infty}U(x,t=0)\,\phi(x,t=0)\,dx = 0$$

ii) We need weak solutions to ... include jumps in the solution

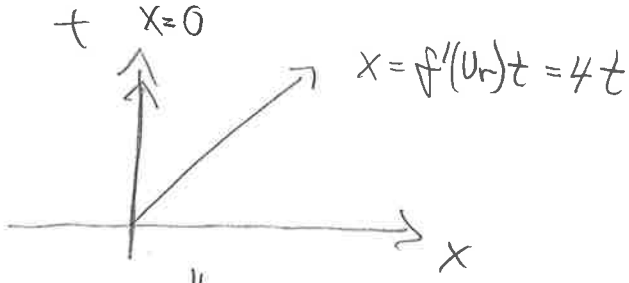
d) $u_t + f(u)_x = 0$, $f(u) = u^2$

$$\phi(x) = \begin{cases} 2 , & 0 \le x \le 1 \\ 0 , & \text{otherwise} \end{cases}$$



RP-1 at $x=0$:

- Increasing jump: $(u_l, u_r) = (0, 2)$
- $f'(u) = 2u \Rightarrow f'(u_l) = 2u_l = 0$
  $f'(u_r) = 2u_r = 4$



$\Downarrow$

spreading characteristics

$\Downarrow$

rarefaction wave solution

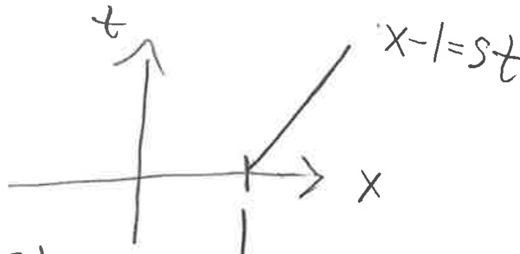
$$f'(u) = 2u$$
$$\Downarrow$$
$$(f')^{-1} = \frac{1}{2}u$$

$$u(x,t) = \begin{cases} u_l , & x < 0 \\ (f')^{-1}\left(\frac{x}{t}\right) , & 0 \le \frac{x}{t} \le 4 \\ u_r , & \frac{x}{t} > 4 \end{cases}$$

$$= \begin{cases} 0 , & x < 0 \\ \frac{1}{2}\frac{x}{t} , & 0 \le x \le 4t \\ 2 , & x > 4t \end{cases}$$

RP-2 at $x=1$:

- decreasing jump: $(u_l, u_r) = (2, 0)$
- $\left.\begin{array}{l} f'(u_l) = 2u_l = 4 \\ f'(u_r) = 2u_r = 0 \end{array}\right\}$ crossing characteristics



$$f'(u_l) = 4 > 0 = f'(u_r)$$

$\Rightarrow$ shock solution $u(x,t) = \begin{cases} u_l , & x < 1+st \\ u_r , & x \geq 1+st \end{cases} = \begin{cases} 2 , & x < 1+2t \\ 0 , & x \geq 1+2t \end{cases}$

when $s = \dfrac{f(u_l) - f(u_r)}{u_l - u_r} = \dfrac{4-0}{2-0} = 2$ is the Rankine-Hug speed

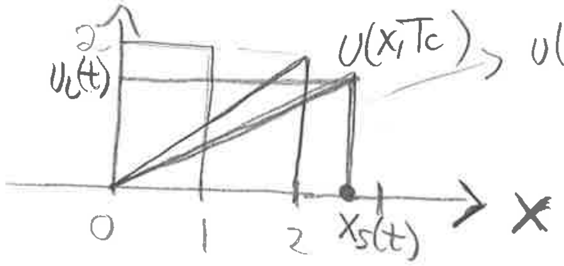
Lax entropy condition is satisfied since $f'(u_l) > s > f'(u_r)$

Solution

$$U(x,t) = \begin{cases} 0 , & x<0 \\ \frac{1}{2}\frac{x}{t} , & 0 \le x \le 4t \\ 2 , & x \geq 4t \text{ and } x < 2t+1 \\ 0 , & x \geq 2t+1 \end{cases}$$

T^c: $4T_c = 2T_c + 1 \Rightarrow 2T_c = 1 \Rightarrow T_c = \frac{1}{2}$

e) Solution for $t > T_c = \frac{1}{2}$



We must find $U_L(t)$ and $X_s(t)$

i) $X_s(t)$ is determined from eq. for characteristics:

$$\frac{dX_s}{dt} = f'(U_L(t)) \quad , \quad X_s(t=T_c) = 2$$

$$X_s(t) = 2U_L(t)t \quad , \quad t \geq T_c = \tfrac{1}{2}$$

ii) Rankine-Hugoniot condition: $S = \frac{f(U_L(t)) - f(0)}{U_L(t) - 0} = \frac{U_L(t)^2}{U_L(t)} = U_L(t)$

However, $S = \frac{dX_s}{dt} \Rightarrow U_L(t) = 2\left(\frac{dU_L}{dt}\cdot t + U_L(t)\right)$

$$U_L(t) = 2U_L(t) + 2t\frac{dU_L}{dt}$$

$$-U_L(t) = 2t\frac{dU_L}{dt}$$

$$\int_{T_c}^{t} -\frac{1}{2t}\,dt = \int_{2}^{U_L} \frac{dU_L}{U_L}$$

$$-\frac{1}{2}\ln t\Big|_{\frac{1}{2}}^{t} = \ln U_L\Big|_2^{U_L} = \ln U_L - \ln 2$$

$$-\frac{1}{2}\ln\frac{t}{\frac{1}{2}} = \ln\frac{U_L}{2}$$

$$e^{\ln(2t)^{-\frac{1}{2}}} = e^{\ln\frac{U_L}{2}}$$

$$\frac{1}{\sqrt{2t}} = \frac{U_L}{2} \Rightarrow U_L(t) = \frac{2}{\sqrt{2t}} \,,\; t \geq T_c = \tfrac{1}{2}$$

$$= \sqrt{\frac{2}{t}}$$

$$\boxed{\begin{aligned} U_L(t) &= \sqrt{\tfrac{2}{t}} \,, \quad t \geq T_c = \tfrac{1}{2} \\ X_s(t) &= 2\cdot U_L(t)\cdot t \\ &= 2t\cdot\frac{\sqrt{2}}{\sqrt{t}} = 2\sqrt{2}\sqrt{t} \end{aligned}}$$

Solution:

$$U(x,t) = \begin{cases} 0 , & x \le 0 \\ \frac{1}{2}\frac{x}{t} , & 0 < x \le X_s(t) \\ 0 , & x > X_s(t) \end{cases}$$

Task 4

Assume activity coefficients are 1 in this task. Halite, NaCl, dissolves according to the reaction

$$\text{NaCl}(s) \rightleftharpoons \text{Na}^+(aq) + \text{Cl}^-(aq), \qquad K_s = 10^{1.56} \tag{1}$$

- Write the equilibrium condition for this reaction. Calculate the number of moles NaCl that can dissolve in 1 L of water. In a similar way complexes can form according to

$$\text{NaCl}(aq) \rightleftharpoons \text{Na}^+(aq) + \text{Cl}^-(aq), \qquad K_c = 10^{0.76} \tag{2}$$

- Write the equilibrium conditions for this system and the mass balances for Na and Cl.
- Calculate the number of moles NaCl that can dissolve in 1 L of water when accounting for the formation of complexes.

solution.

-

$$C_{na}C_{cl} = K_s \tag{3}$$

$$C_{na} = C_{cl} = K_s^{1/2} = 6.03\text{mol} \tag{4}$$

-

$$\frac{m_{na}m_{cl}}{n_{nacl}} = K_c \tag{5}$$

$$m_{na}m_{cl} = K_s \tag{6}$$

$$C_{na} = m_{na} + n_{nacl} \tag{7}$$

$$C_{cl} = m_{cl} + n_{nacl} \tag{8}$$

-

$$m^2 = K_s \tag{9}$$

$$n = m^2/K_c = K_s/K_c = 6.31 \tag{10}$$

$$m = 6.03 \tag{11}$$

$$m + n = 12.34\text{mol} \tag{12}$$

Task 5

- Explain how adsorption tests can be used to measure wettability properties

A species adsorbs according to $q = c^3$ where c is concentration and q(mol/L pore) is the adsorption isotherm (amount adsorbed species as function of brine concentration).

- Assume a core contains $c = 0$ initially and is flooded with $c = 1$. Consider the time when 1 pore volume (PV) has been flooded. Sketch the concentration profile along the core.
- Assume a core contains $c = 1$ initially and is flooded with $c = 0$. Consider the time when 1 PV has been flooded. Sketch the concentration profile along the core.
- In the last situation, how many mols of species are still stored on the surface after injecting 1PV? Assume the pore volume is 0.04 L.

solution.

- More adsorption on water-wet cores.
- Broadening profile

$$x(c=0) \;=\; 1, \quad x(c=0.25) = 0.842, \quad x(c=0.5) = 0.571, \tag{13}$$

$$x(c=0.75) \;=\; 0.372, \quad x(c=1) = 0.25, \tag{14}$$

- Sharpening front profile

$$x_f/x_w = \frac{1}{1 + \frac{0^3 - 1^3}{0-1}} = 0.5 \tag{15}$$

$$c(x > 0.5) = 1, \qquad c(x < 0.5) = 0 \tag{16}$$

- $$q(x < 0.5) = 0, \qquad q(x > 0.5) = 1^3 = 1 \tag{17}$$
  $$N = 1 \cdot 0.5 \cdot 0.04 = 0.02mol \tag{18}$$

Task 6

A chalk core is flooded with 1 mol/L $MgCl_2$ brine. It is assumed that calcite $CaCO_3$ can dissolve, while magnesite $MgCO_3$ precipitates in a substitution-like manner and that ion exchange of Ca and Mg occurs at the surface. The formation water contains Ca in the brine and on the surface, but not Mg or Cl.

- Write down relevant reactions, rates and equilibrium conditions for the mentioned chemistry.
- Write down transport partial differential equations for the species in the brine (Ca, Mg, Cl), on the surface (Ca, Mg) and the minerals (calcite, magnesite). Also write down initial conditions and boundary conditions.
- Sketch the expected concentration profiles for Ca, Mg, Cl as measured at the outlet vs injected pore volumes. What is the role of the different mechanisms you have included in the system?

solution.

- $$\begin{aligned} \mathrm{CaCO_3}(s) + \mathrm{Mg^{2+}}(aq) &\rightleftharpoons \mathrm{MgCO_3}(s) + \mathrm{Ca^{2+}}(aq) && (19) \\ \mathrm{CaX_2} + \mathrm{Mg^{2+}}(aq) &\rightleftharpoons \mathrm{MgX_2} + \mathrm{Ca^{2+}}(aq) && (20) \\ r &= k_1 C_{ca} - k_2 C_{mg} && (21) \\ K &= \frac{C_{ca}\beta_{mg}}{C_{mg}\beta_{ca}} && (22) \end{aligned}$$
- $$\begin{aligned} \partial_t(C_{ca} + \rho^s_{ca}) &= -v\partial_x C_{ca} + D\partial_{xx} C_{ca} + r && (23) \\ \partial_t(C_{mg} + \rho^s_{mg}) &= -v\partial_x C_{mg} + D\partial_{xx} C_{mg} - r && (24) \\ \partial_t C_{cl} &= -v\partial_x C_{cl} + D\partial_{xx} C_{cl} && (25) \\ \partial_t \rho_c &= -r && (26) \\ \partial_t \rho_m &= r && (27) \end{aligned}$$
- Cl: from 0 to injected concentration with middle value after 1 PV.
  Ca: peak from ion exchange, stable effluent from dissolution.
  Mg: delay from ion exchange, stable effluent below injected concentration due to precipitation.

Appendix A. Formulas

Davies formula (at 25°C):

$$\log_{10}\gamma_i = -0.5085 Z_i^2 \Big(\frac{\sqrt{I}}{1 + \sqrt{I} - 0.3I} \Big) \tag{28}$$

Retardation formula

$$R_c = 1 + \frac{dq}{dc}, \qquad \text{(broadening front)} \tag{29}$$

$$R_f = 1 + \frac{\Delta q}{\Delta c}, \qquad \text{(sharpening front)} \tag{30}$$

pH

$$pH = -log_{10}([H^+]) \tag{31}$$