Chromatographic column

$$\frac{\partial}{\partial t}\left(\varepsilon c + (1-\varepsilon) f(c)\right) + \frac{\partial}{\partial z}\left(\varepsilon v c\right) = 0$$

→ (1) $f(c) = Hc$

→ (2) $f(c)$ is non-linear

adsorption isotherm

$$\varepsilon \frac{\partial c}{\partial t} + (1-\varepsilon)\frac{\partial f}{\partial t} + \varepsilon v \frac{\partial c}{\partial z} = 0$$

$$\boxed{\left(\varepsilon + (1-\varepsilon) f'(c)\right)\frac{\partial c}{\partial t} + \varepsilon v \frac{\partial c}{\partial z} = 0} \leftarrow \text{PDE}$$

$$M'(c)\frac{\partial c}{\partial t} + F'(c)\frac{\partial c}{\partial z} = 0$$

(1) $f(c) = Hc$

$f'(c) = H$

$R = 0$

homogeneous PDE

$$\Rightarrow \underbrace{\left(\varepsilon + (1-\varepsilon) H\right)}\frac{\partial c}{\partial t} + \underbrace{\varepsilon v}\frac{\partial c}{\partial z} = 0$$

constant

$$\begin{cases} \dfrac{dt}{ds} = \varepsilon + (1-\varepsilon) H \\[2mm] \dfrac{dz}{ds} = \varepsilon v \\[2mm] \dfrac{dc}{ds} = 0 \end{cases}$$

$$\frac{dt}{dz} = \frac{\varepsilon + (1-\varepsilon) H}{\varepsilon v} = \boxed{\frac{1}{v}\left(1 + \nu H\right) = \sigma}$$

$\nu = \dfrac{1-\varepsilon}{\varepsilon}$: phase ratio

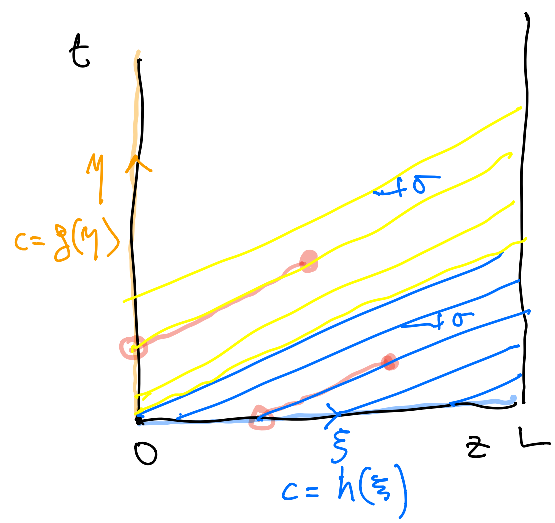
$$\begin{cases} t = 0 \\ z = \xi \\ c = h(\xi) \end{cases} \qquad \boxed{\begin{aligned} t &= \left(\varepsilon + (1-\varepsilon) H\right) s \\ z &= \varepsilon v s + \xi \end{aligned}}$$

$$\boxed{c = h(\xi) = h\left(z - \frac{t}{\sigma}\right)}$$

$$s = \frac{t}{\varepsilon + (1-\varepsilon) H}$$

$$\xi = z - \varepsilon v s = z - \frac{\varepsilon v}{\varepsilon + (1-\varepsilon) H}\, t$$

$$t \leq \sigma z$$



$$\begin{cases} t = \eta \\ z = 0 \\ c = g(\eta) \end{cases} \qquad \boxed{\begin{array}{l} t = (\varepsilon + (1-\varepsilon)H)s + \eta \\ z = \varepsilon \nu s \end{array}} \qquad \begin{cases} \eta = t - [\varepsilon + (1-\varepsilon)H]\dfrac{z}{\varepsilon\nu} \\ s = z/\varepsilon\nu \end{cases}$$

$$\boxed{c = g(\eta) = g(t - \sigma z)} \qquad t \geq \sigma z$$

2

$$n = f(c) = \frac{Hc}{1+Kc}$$

H, K: positive constants

Langmuir isotherm

$$f'(c) = \frac{H}{(1+Kc)^2} > 0$$

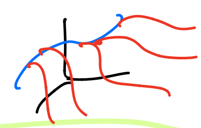
$$f''(c) < 0$$

$$\boxed{\left(\varepsilon + (1-\varepsilon)f'(c)\right)\frac{\partial c}{\partial t} + \varepsilon\nu\frac{\partial c}{\partial z} = 0}$$

first order homogeneous quasi-linear (reducible) PDE

↓ generalize

$$\boxed{M'(w)\frac{\partial w}{\partial t} + F'(w)\frac{\partial w}{\partial z} = 0}$$



$$\begin{cases} \dfrac{dt}{ds} = M'(w) \\ \dfrac{dz}{ds} = F'(w) \\ \dfrac{dw}{ds} = 0 \end{cases}$$

$$\sigma = \frac{dt}{dz} = \frac{M'(w)}{F'(w)} = \sigma(w) \qquad (\mathrm{I})$$

$w =$ constant along the characteristic (II)

characteristics are straight lines (III)

$$\mathrm{I} \begin{cases} t = \varphi(\xi) \\ z = \psi(\xi) \\ w = \omega(\xi) \end{cases} \qquad \text{on } \mathrm{I}$$

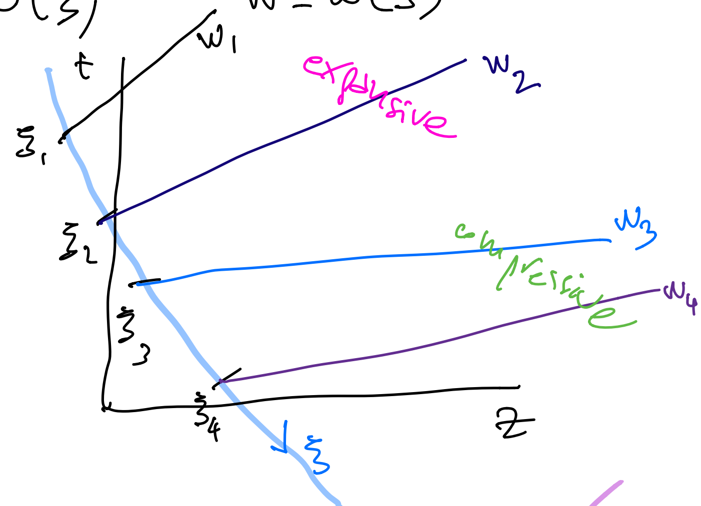
$$M'(\omega(\xi))\,\psi'(\xi) \neq F'(\omega(\xi))\,\varphi'(\xi)$$

this condition must be fulfilled

$$\begin{cases} \dfrac{dt}{ds} = M'(w) \\ \dfrac{dz}{ds} = F'(w) \\ \dfrac{dw}{ds} = 0 \end{cases} \qquad \begin{cases} t = \varphi(\xi) \\ z = \psi(\xi) \\ w = \omega(\xi) \end{cases} \qquad \begin{cases} t = M'(\omega(\xi))s + \varphi(\xi) \\ z = F'(\omega(\xi))s + \psi(\xi) \end{cases}$$

$w = \omega(\xi)$

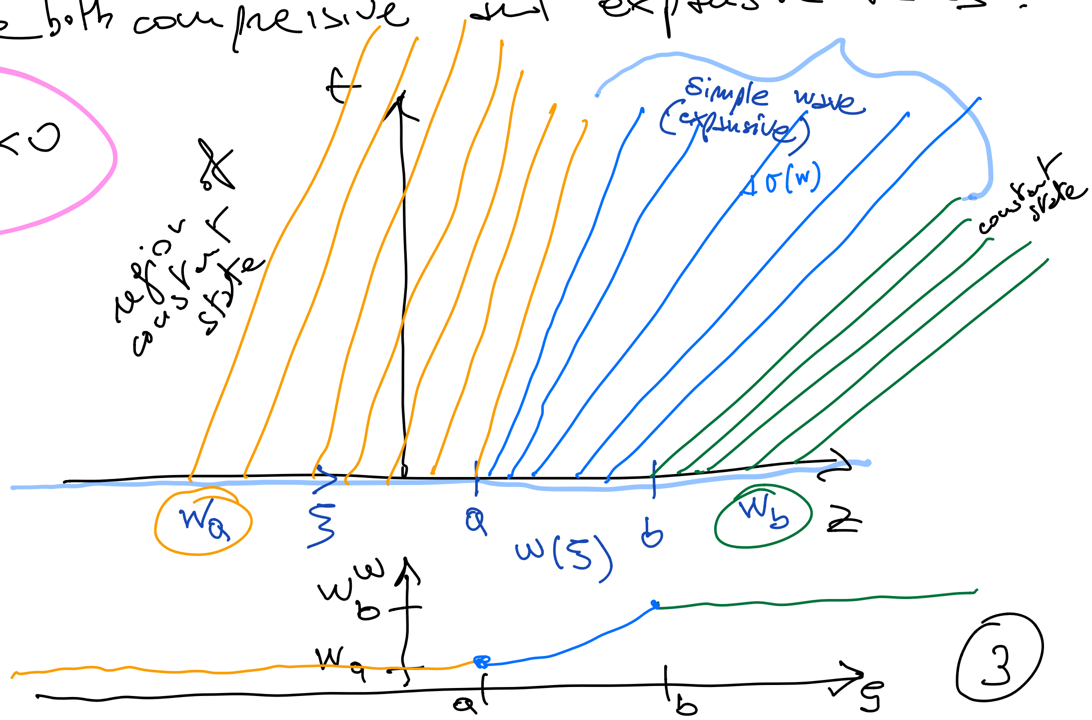
$$\xi_j \to w_j = \omega(\xi_j)$$
$$\downarrow$$
$$\sigma_j = \sigma(w_j)$$



for the same PDE (the same $\sigma(w)$), depending on the initial line, we can have both compressive and expansive waves.

$$\frac{d\sigma}{dw} < 0$$

$w_a < w_b$
$\sigma_a > \sigma_b$



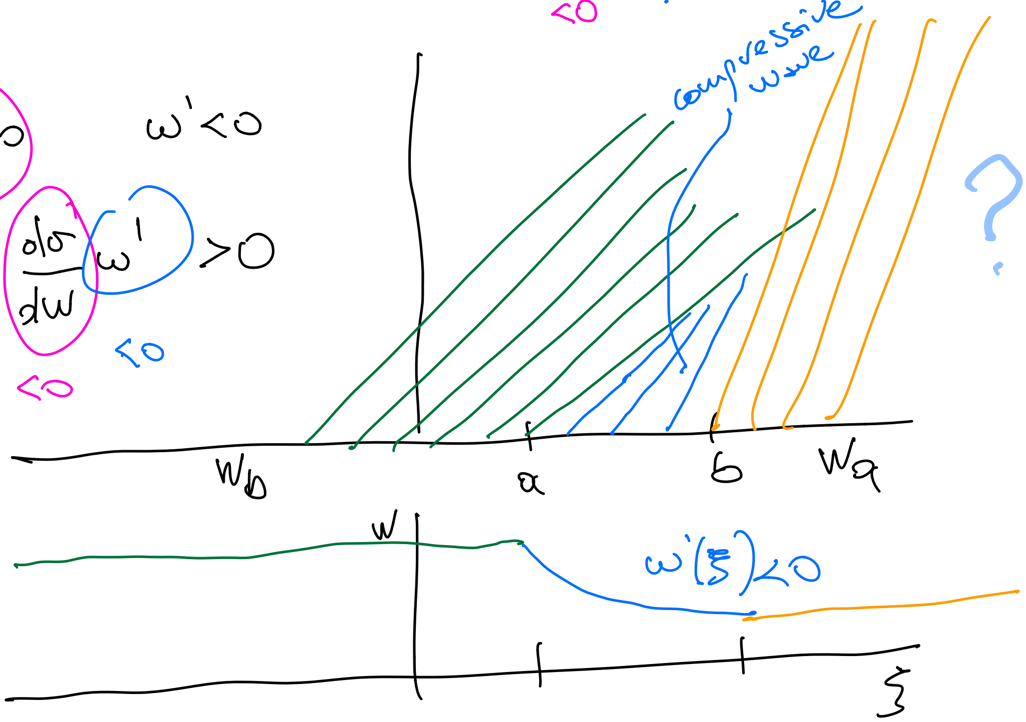
$$\mathrm{I}\ \begin{cases} t=0 \\ z=\xi \\ w = \begin{cases} w_a & \xi<a \\ \omega(w) & a\le\xi\le b \\ w_b & \xi>b \end{cases}\end{cases}$$

with
$\omega(a) = w_a$
$\omega(b) = w$
$\omega' > 0$

$$\frac{d\sigma}{d\xi}<0 \qquad \frac{d\sigma}{dw}\frac{dw}{d\xi} = \underbrace{\frac{d\sigma}{dw}}_{<0}\,\underbrace{\omega'(\xi)}_{>0} < 0 \Rightarrow$$ simple wave

$$\frac{d\sigma}{dw}<0 \qquad \omega'<0$$

$$\frac{d\sigma}{d\xi} = \underbrace{\frac{d\sigma}{dw}}_{<0}\,\underbrace{\omega'}_{<0} > 0$$



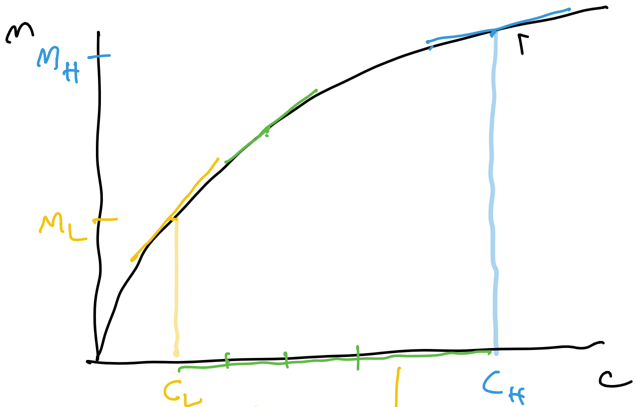
$$\boxed{\left(\varepsilon + (1-\varepsilon) f'(c)\right)\frac{\partial c}{\partial t} + \varepsilon v \frac{\partial c}{\partial z} = 0}$$

$$\sigma(c) = \frac{1}{v}\left(1 + \nu f'(c)\right)$$

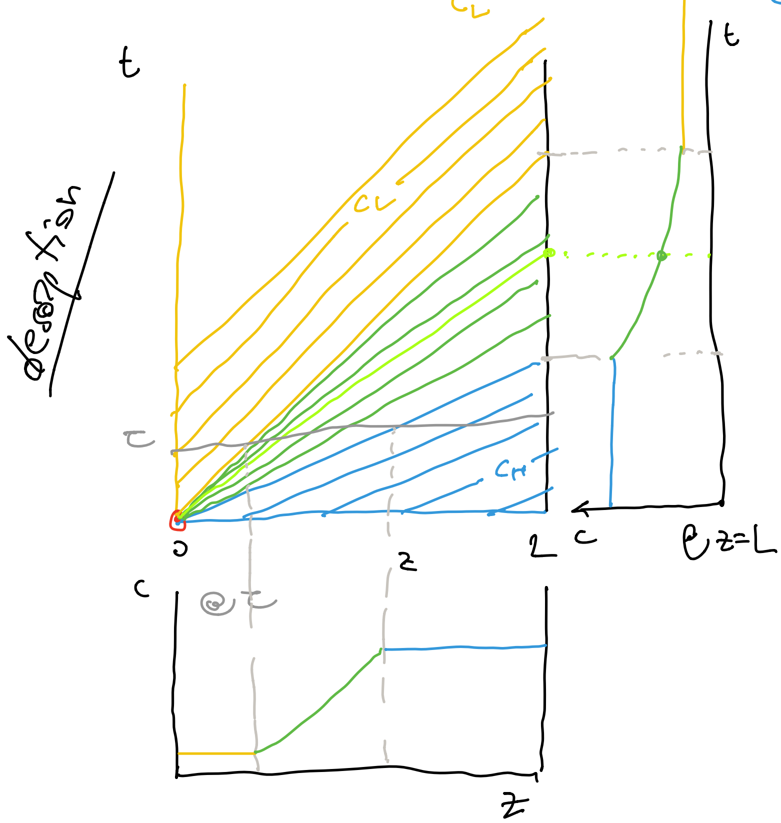
$$f(c) = \frac{Hc}{1+Kc} \qquad f'(c) = \frac{H}{(1+Kc)^2}$$

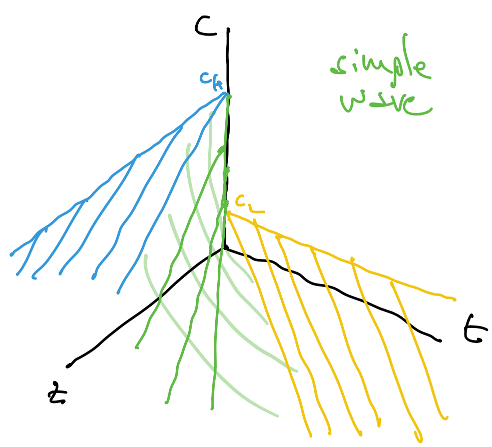
$$\sigma(c) = \frac{1}{v}\left(1 + \frac{\nu H}{(1+Kc)^2}\right)$$

$$\frac{d\sigma}{dc} = \frac{\nu}{v} f''(c) < 0$$

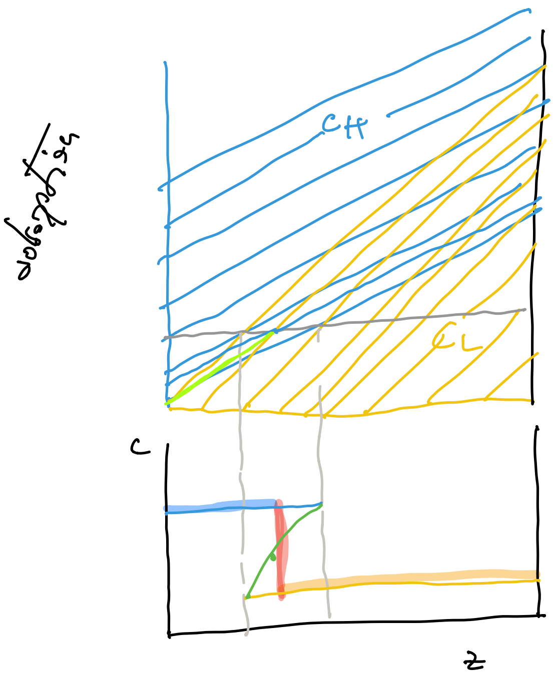


Riemann problems ≡ piecewise constant initial value problems





simple wave



discontinuity??

three-value solution, which is physically impossible

⇒ next week