PDE

general non linear equation (FIRST order)

$$F\left(z, x, y, \frac{\partial z}{\partial x}, \frac{\partial z}{\partial y}\right) = 0$$

example

$$\underbrace{P(x,y)\frac{\partial z}{\partial x} + Q(x,y)\frac{\partial z}{\partial y} + S(x,y)\, z = R(x,y)}_{\text{linear}}$$

$$\underbrace{P(z,x,y)\frac{\partial z}{\partial x} + Q(z,x,y)\frac{\partial z}{\partial y} \mp R(z,x,y)}_{\text{Quasilinear}}$$

<u>Second order</u>

$$F(z, x, y, z_x, z_y, z_{xx}, z_{yy}, z_{xy}) = 0$$

linear $A(x,y) z_{xx} + B(x,y)\, z_{xy} + C(x,y)\, z_{yy} + D(x,y)\, z_x$

$$+ E(x,y)\, z_y + F(x,y)\, z = R(x,y)$$

Quasilinear

$$A z_{xx} + B z_{xy} + C z_{yy} + D z_x + E z_y = R$$

A, B, C, D, E, R functions of z, x, y

FIRST ORDER SYSTEMS

Linear cases

examples
$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = -Bu$$

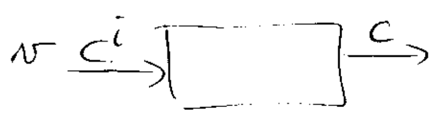
Tubular PFR

$u = u^0(x), \; t = 0 \quad 0 \le x \le 1$

$u = u^i(t), \; x = 0 \quad t > 0$

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

Chromatography equation



Γ = concentration of species in solid fixed phase

If $\Gamma = F(C)$

$$\Rightarrow \left[V\frac{\partial C}{\partial z} + \frac{\partial C}{\partial t} = 0 \right] \qquad V = \frac{v}{\epsilon + (1-\epsilon)\frac{dF}{dC}}$$

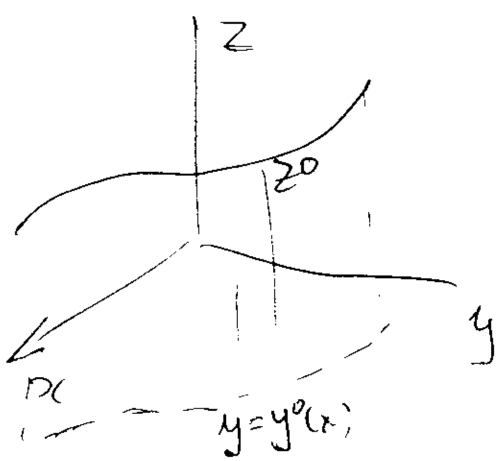
Quasilinear

Characteristic Curves

Consider the quasilinear 1st order PDE

$$P(z,x,y)\frac{\partial z}{\partial x} + Q(z,x,y)\frac{\partial z}{\partial y} = R(z,x,y)$$

with IC $z = z^0(x,y)$ along the curve $y = y^0(x)$



Now assume

$$\left.\begin{aligned} x &= x(s) \\ y &= y(s) \end{aligned}\right\} \Rightarrow \begin{aligned} x(0) &= \xi \\ y(0) &= y^0 \end{aligned}$$

$$\Rightarrow z = z(x,y) = z(s$$

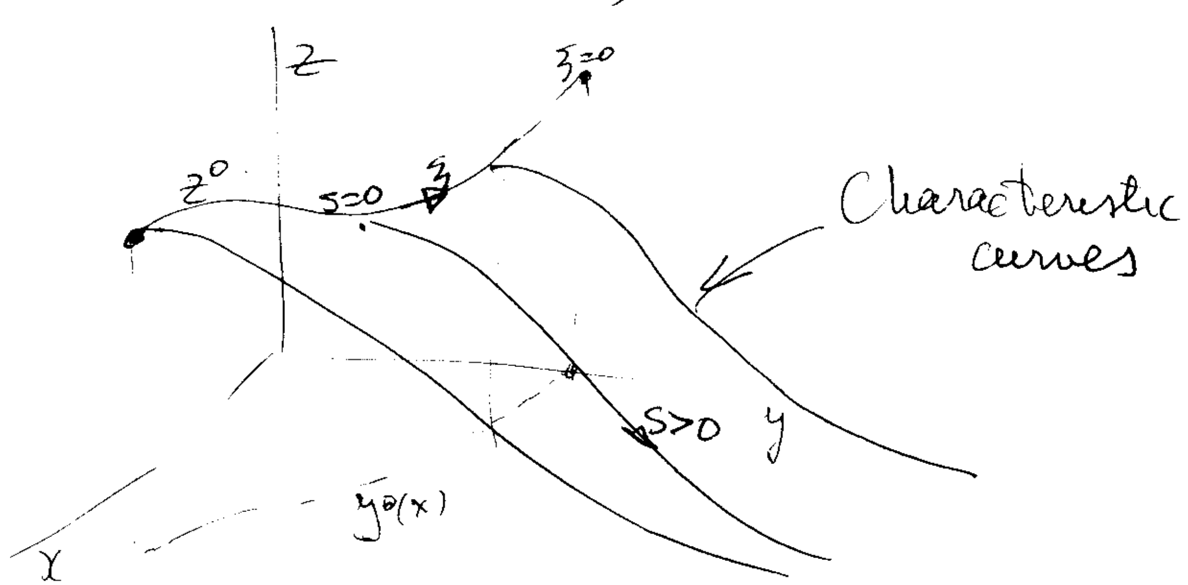
and $$\frac{dz}{ds} = \frac{\partial z}{\partial x}\frac{dx}{ds} + \frac{\partial z}{\partial y}\frac{dy}{ds}$$

Comparing

$$\left.\begin{aligned} \frac{dx}{ds} &= P(z,x,y) \\ \frac{dy}{ds} &= Q(z,x,y) \\ \frac{dz}{ds} &= R(z,x,y) \end{aligned}\right\} \text{ FIRST ORDER } \underline{\text{ODE}} \text{ system}$$

The solution needs some IC.

$$\Rightarrow \begin{aligned} x(0) &= \xi \\ y(0) &= y^0(\xi) \\ z(0) &= z^0(\xi) \end{aligned}$$



Thus, the solution is

$$x = x(s, \xi)$$
$$y = y(s, \xi)$$
$$z = z(s, \xi)$$

One can now solve for s, ξ the first two equations (provided the Jacobian does not vanish), and obtain

$$\left.\begin{aligned} s &= s(x, y) \\ \xi &= \xi(x, y) \end{aligned}\right\} \Rightarrow$$ plug in the third to get $z = z(x, y)$

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Example

PFR.

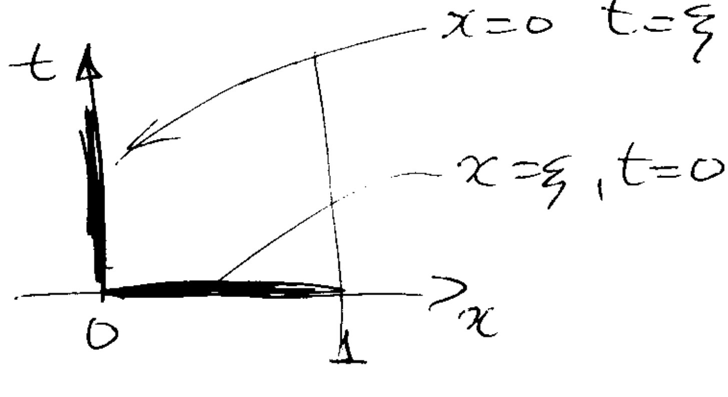
$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = -Bu$$

$$\Rightarrow \left.\begin{aligned} \frac{dx}{ds} &= 1 \\ \frac{dt}{ds} &= 1 \\ \frac{du}{ds} &= -Bu \end{aligned}\right\} \Rightarrow \begin{aligned} x &= s + c_1 \\ t &= s + c_2 \\ u &= c_3 e^{-Bs} \end{aligned}$$

IC: $u = u^0(x), \quad t = 0$

$u = u^i(t) \quad x = 0$

IC curve



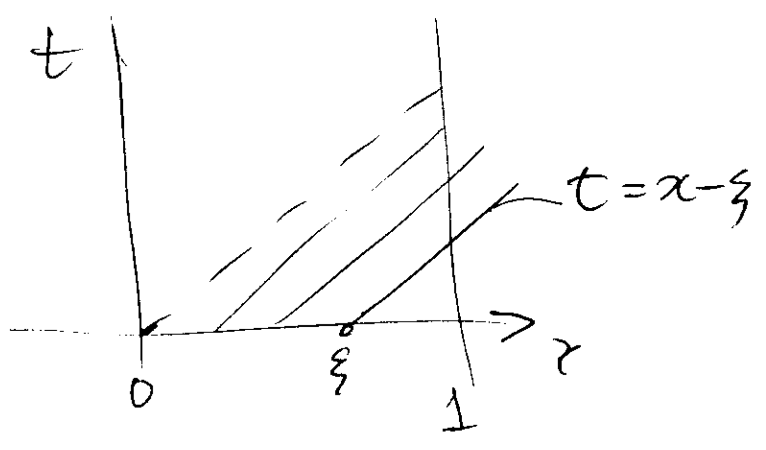
Thus the horizontal branch is

$$\left.\begin{aligned} x(0,\xi) &= c_1 = \xi \\ t(0,\xi) &= c_2 = 0 \end{aligned}\right\} \Rightarrow \begin{aligned} x &= s+\xi \\ t &= s \end{aligned}$$

$$u(0,\xi) = u^0(\xi) \qquad \Rightarrow u = u^0(\xi)\, e^{-\beta s}$$

From $\left.\begin{aligned} x &= s+\xi \\ t &= s \end{aligned}\right\} \Rightarrow \begin{aligned} \xi &= x-t \\ s &= t \end{aligned}$

Characteristic curves



$$u = u^0(x-t)\, e^{-\beta t}$$

Valid only for

$t \le x$

Vertical branch IC.

$$\left.\begin{aligned} x(0,\xi) &= c_1 = 0 \\ t(0,\xi) &= c_2 = \xi \\ u(0,\xi) &= u^i(\xi) \end{aligned}\right\} \Rightarrow \begin{aligned} x &= s \\ t &= s+\xi \\ u &= u^i(\xi)e^{-Bs} \end{aligned}$$

$$\Rightarrow \boxed{u = u^i(t-x)\, e^{-Bx}} \qquad t > x$$

(8)

SHOCKS

Consider the chromatographic case

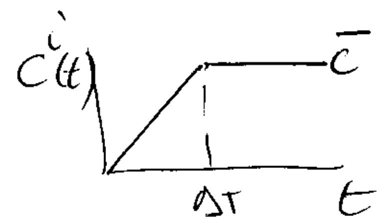
$$V\frac{\partial c}{\partial z}+\frac{\partial c}{\partial t}=0 \quad \left[V=\frac{v}{\varepsilon+(1-\varepsilon)\frac{dF}{dc}} \right]$$

with the following ic.

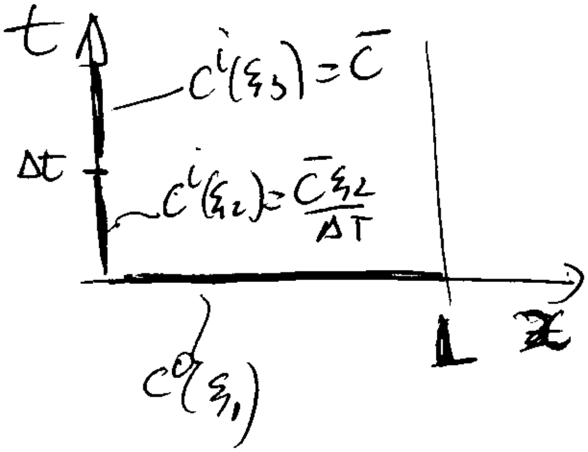
$$c=c^{o}(z)=0 \quad t=0$$

$$c=\begin{cases} c^{i}(t)=\frac{\bar{c}\,t}{\Delta t} & x=0 \quad t<\Delta t \\ c^{i}(t)=\bar{c} & x=0 \quad t\geq\Delta T \end{cases}$$

That is



or



Now let $F(C) = \dfrac{KC}{1+KC}\Gamma^{\infty}$ (Langmuir isotherm)

$$\Rightarrow \frac{dF}{dC} = \frac{\Gamma^{\infty} K}{(1+KC)^2}$$

Nondimensionalize

$$z = \frac{x}{L} \quad \tau = \frac{t}{\Delta t} \quad u = \frac{C}{\bar{C}} \quad \alpha = \frac{L\varepsilon}{v\Delta t}$$

$$\beta = \frac{(1-\varepsilon)\Gamma^{\infty} K}{\varepsilon} \quad \sigma = K\bar{C}$$

$$\Rightarrow \begin{cases} \dfrac{\partial u}{\partial z} + \varphi(u)\dfrac{\partial u}{\partial z} = 0 & 0 < z < 1,\ \tau > 0 \\ \varphi(u) = \alpha\left[1 + \dfrac{\beta}{(1+\sigma u)^2}\right] \end{cases}$$

IC :

$$u = 0 \quad z = \xi_1 \quad \tau = 0 \quad 0 \le \xi_1 \le 1$$

$$u = \begin{cases} \xi_2 & z = 0 \quad \tau = \xi_2 \quad 0 < \xi_2 < 1 \\ 1 & z = 0 \quad \tau = \xi_3 \quad 1 < \xi_3 < \alpha \end{cases}$$

$$\frac{dz}{ds} = 1$$

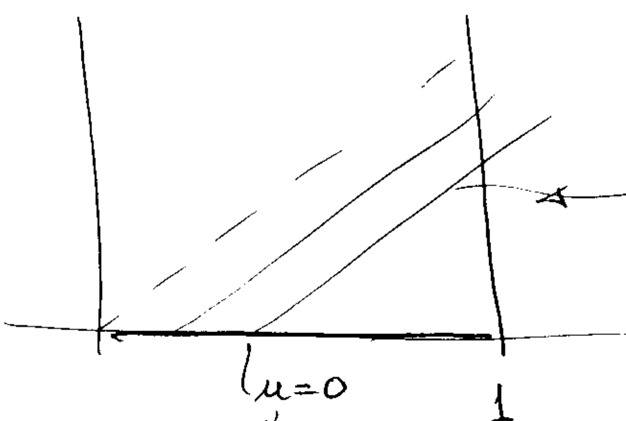
$$\frac{d\sigma}{ds} = \psi(u)$$

$$\frac{du}{ds} = 0 \implies u = \text{constant on a char. line!}$$

$\implies \psi(u)$ is constant on a characteristic line.

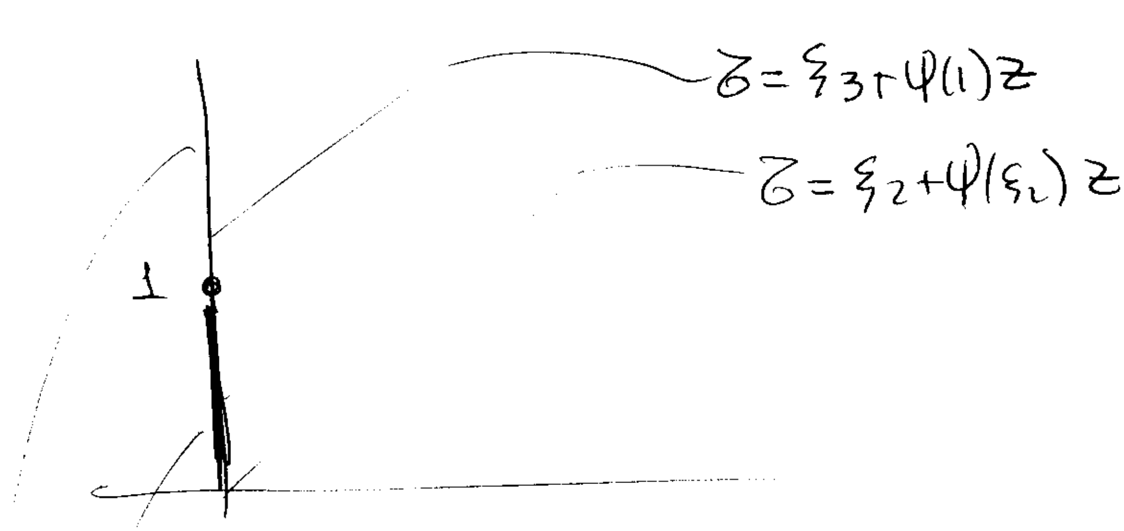
$$\implies \begin{cases} z = c_1 + s \\ \sigma = \psi(0)\, s + c_2 \\ u = u(0) \end{cases}$$

$= \alpha(1+\beta)$



$\sigma = \psi(0)(z - \xi_1)$

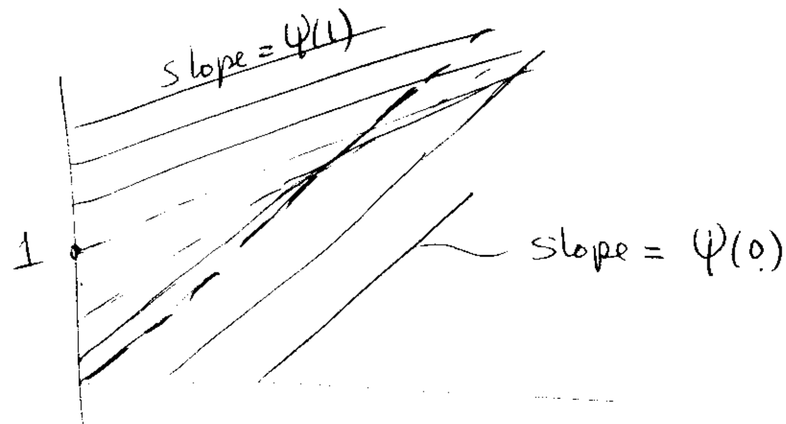
$$\left.\begin{array}{l} \sigma(0) = c_2 = 0 \\ z(0) = \xi_1 = c_1 \end{array}\right\} \implies \left.\begin{array}{l} z = \xi_1 + s \\ \sigma = \psi(0)s \\ u = 0 \end{array}\right\} \implies z = \psi(0)(z - \xi_1)$$



$$\left.\begin{array}{l} \zeta(0) = \xi_2 = c_2 \\ z(0) = 0 = c_1 \end{array}\right\} \Rightarrow \left.\begin{array}{l} z = s \\ \zeta = \psi(\xi_2) s + \xi_2 \end{array}\right\} \Rightarrow \zeta = \xi_2 + \psi(\xi_2) z$$

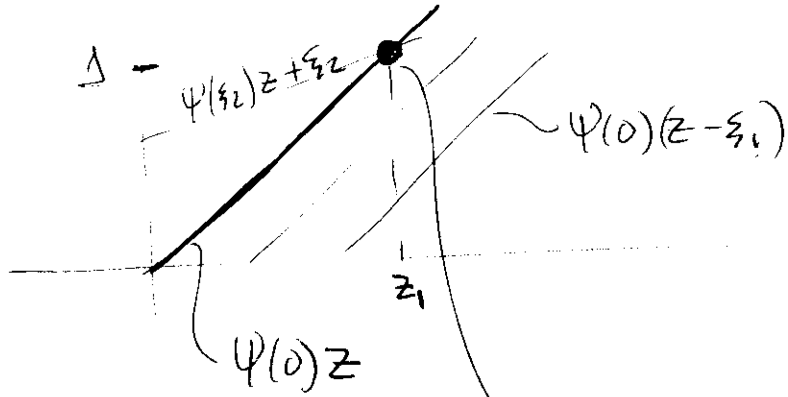
$$\left.\begin{array}{l} \zeta(0) = \xi_3 = c_2 \\ z(0) = 0 = c_1 \end{array}\right\} \Rightarrow \zeta = \xi_3 + \psi(1) z$$

Now $\psi(0) = \alpha(1+\beta) \geq \psi(\xi_2) \geq \psi(1) =$
$= \alpha\left[1 + \frac{\beta}{(1+\sigma)^2}\right.$



<u>Characteristic lines cross!</u>

Where they cross?



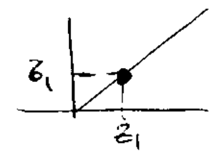
here we have $\psi(0)z_1=\psi(\xi_2)z_1+\xi_2$

$$\Rightarrow z_1=\frac{\xi_2}{\psi(0)-\psi(\xi_2)} \qquad 0<\xi_2<1$$

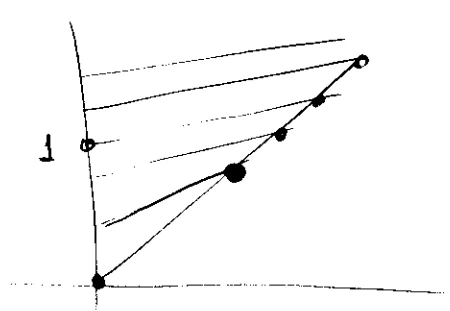
$$z_1=\frac{(1+\sigma\xi_2)^2}{\alpha\beta\sigma(2+\sigma\xi_2)}$$

$$\boxed{\underset{\forall \xi_2}{\text{Min}}\ z_1=\frac{1}{2\alpha\beta\sigma} \quad \text{at } \xi_2=0}$$

Accordingly $\tau_1=\dfrac{(1+\beta)}{2\beta\sigma}$



If you do the same for $\tau>1$

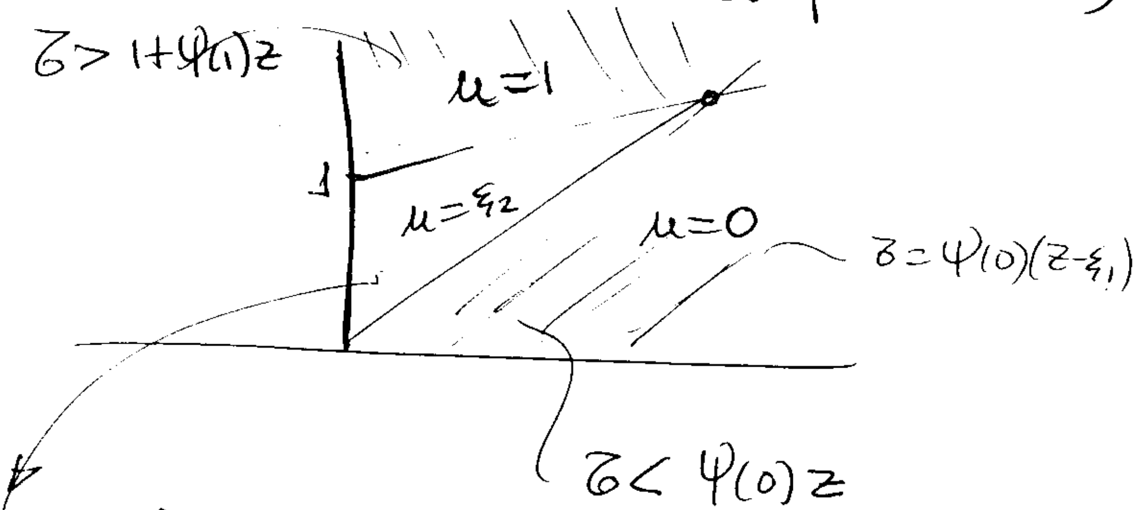


we can find that $z_2>z_1$

$\Rightarrow$ we are not interested in those intersections anymore.

Thus if $z_1 < 1$ we are in trouble, ($z_1 < 1 \Rightarrow \alpha\beta\sigma > 1/2$)

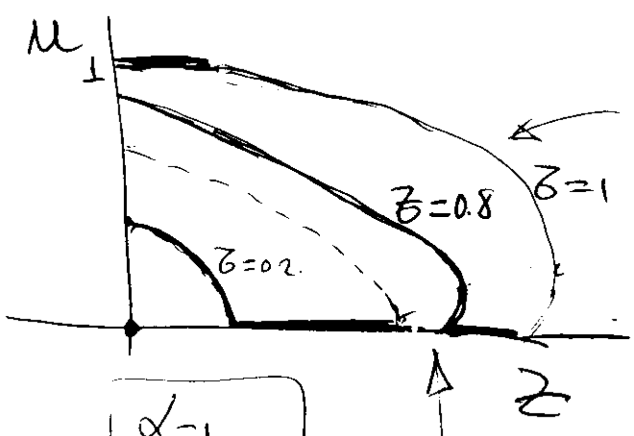
Consider the case $z_1 > 1$ (no shock or compressed wave)



$$\left.\begin{aligned} &\zeta = \xi_2 + \psi(\xi_2) z \\ &u = \xi_2 \end{aligned}\right\} \Rightarrow \boxed{\zeta = u + \psi(u) z}$$

$$\Rightarrow \quad z = \frac{\zeta - u}{\psi(u)} = \frac{(\zeta-u)(1+\sigma u)^2}{\alpha[\beta + (1+\sigma u)^2]}$$

$0 < u < 1$



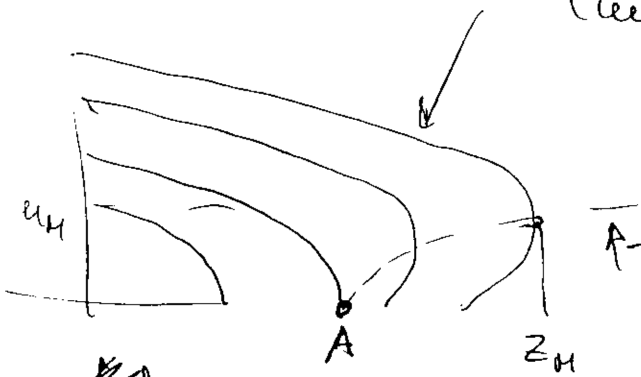
wave travels faster at higher u

Speed of wave is $\frac{1}{\psi(u)}$

$\alpha = 1$
$\beta = 1$
$\sigma = 2$

At some point there are 2 values of u!

Can this be true (14)



Trajectory of Maximum

We can find maximum by setting

$$\frac{\partial z}{\partial u} = 0 \qquad \frac{\partial}{\partial u}\left[\frac{\tau - u}{\psi(u)}\right] = \frac{-\psi(u) - (\tau - u)\psi'(u)}{\psi(u)^2} =$$

$$\Rightarrow 2\sigma\beta(\tau - u_H) - (1+\sigma u_H)\left[\beta + (1+\sigma u_H)^2\right] = 0$$

Point A can be obtained by setting

$$u_H = 0 \quad \Rightarrow \quad 2\sigma\beta\tau_A - [\beta + 1] = 0$$

$$z_A = \frac{\tau_A}{\psi(0)}$$

$$\Rightarrow \tau_A = \frac{(\beta+1)}{2\sigma\beta} \quad \Rightarrow z_A = \frac{1}{2\alpha\beta\sigma}$$

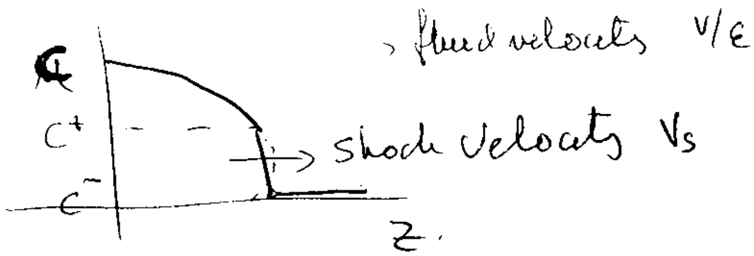
Coordinates of $(z_s \tau_s)$

point at which shock develops

$\Rightarrow$ Shock develops because wave travels faster at higher u.

We now assume that larger values of C do not overtake smaller ones

$\Rightarrow$ A discontinuity develops



Let us make a mass balance at the discontinuity.

$$\underbrace{\varepsilon C_+\left(\frac{v}{\varepsilon}-V_s\right)+(1-\varepsilon)\Gamma_- V_s}_{\text{Mass going in}} = \underbrace{\varepsilon C_-\left(\frac{v}{\varepsilon}-V_s\right)+(1-\varepsilon)\Gamma_+ V_s}_{\text{Mass going out}}$$

mobile phase)

stationary phase retaining material

$$\frac{v}{V_s}=\varepsilon+(1-\varepsilon)\frac{\Gamma_+-\Gamma_-}{C_+-C_-}$$

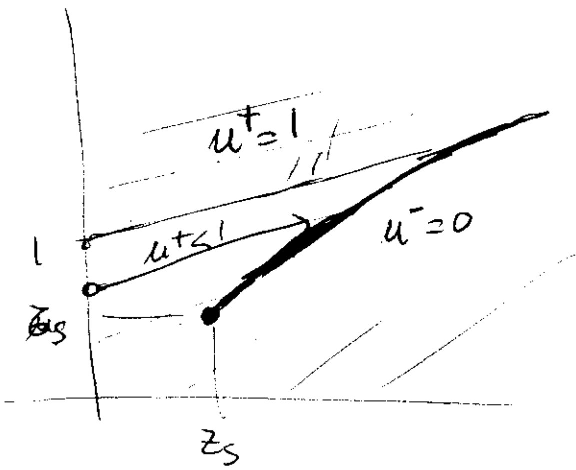
use equilibrium

$$\Rightarrow \frac{v}{\varepsilon V_s}=1+\frac{\beta}{(u_+-u_-)}\left[\frac{u_+}{(1+\sigma u_+)}-\frac{u_-}{(1+\sigma u_-)}\right]$$

Velocity of shock wave is V_s (16)

$$\left.\frac{d\tau}{dz}\right)_{shock} = \frac{1}{V_s/(L/\Delta t)} = \alpha\left[1 + \frac{T^2}{(1+\sigma u_+)(1+\sigma u_-)}\right]$$

characteristic velocity



Axial Dispersion

$$-\varepsilon E_a \frac{\partial^2 c}{\partial x^2} + v\frac{\partial c}{\partial x} + \varepsilon\frac{\partial c}{\partial t} + (1-\varepsilon)\frac{\partial \Gamma}{\partial t} = 0$$

$$\Gamma = F(c)$$

$$u = \frac{c}{c_r} \qquad f(u) = \frac{F(c)}{c_r} \qquad z = \frac{x}{L}$$

$$\tau = \frac{tv}{\varepsilon L} \qquad Pe = \frac{vL}{\varepsilon E_a} \qquad \nu = \frac{1-\varepsilon}{\varepsilon}$$

$$\Rightarrow -\frac{1}{Pe}\frac{\partial^2 u}{\partial z^2} + \frac{\partial u}{\partial z} + \frac{\partial u}{\partial \tau} + \nu\frac{\partial f}{\partial \tau} = 0$$

As $Pe \to \infty$ (Diffusion not important)

Outer is

$$\boxed{\frac{\partial u}{\partial z} + \psi(u)\frac{\partial u}{\partial \tau} = 0}$$

To make it simple, avoid end effects by putting $u = u_+ \quad z \to -\infty$

$u = u_- \quad z \to +\infty$

We know this has a shock solution

Let $\xi = z - \lambda\tau$

$$\Rightarrow \mu(z,\tau) = u(\xi)$$

$$\frac{\partial u}{\partial z} = \frac{du}{d\xi}\frac{\partial \xi}{\partial z} = \frac{du}{d\xi} \qquad \frac{\partial^2 u}{\partial z^2} = \frac{d^2 u}{d\xi^2}$$

$$\frac{\partial u}{\partial \tau} = \frac{du}{d\xi}\frac{\partial \xi}{\partial \tau} = -\lambda\frac{du}{d\xi} \qquad \frac{\partial f}{\partial \tau} = -\lambda\frac{df}{d\xi}$$

$$\Rightarrow \frac{1}{Pe} u'' - u' + \lambda u' + \lambda \nu f' = 0$$

Integrate from $-\infty$ to ξ

$$\frac{1}{Pe} u' - (1-\lambda)(u - u^+) + \lambda\nu\left[f(u) - f(u_+)\right] = 0$$

We assumed $u' \to 0$ as $\xi \to -\infty$

$\hookrightarrow$ Applying this at $+\infty$ (where $u' = 0$)

we get

$$-(1-\lambda)(u^- - u^+) + \lambda\nu\left[f(u) - f(u_+)\right] = 0$$

From which we get λ

Assume one wants

$$u = u_+ \quad \xi \to -\infty$$
$$u = u_- \quad \xi \to +\infty$$

$$\underbrace{\frac{1}{Pe} u' = (1-\lambda)(u-u_+) - \nu\lambda [f(u) - f(u_+)] = 0}$$

First order ODE

$\Rightarrow$ requires only one IC.

$$\frac{1}{Pe} u' = G(u, \nu, \lambda) = \lambda\nu \left\{ \frac{\Delta f}{\Delta u} (u - u_+) - [f(u) - f(u_+)] \right\}$$

$G(u^+) = G(u^-) = 0 \Rightarrow$ u^+ and u^- stationary points of the ODE ($u' = 0$)

$\Rightarrow$ one can do stability analyses on these zeros!

Structure of Shock.

Let $\theta = P_e^{m}(\xi)$

$$\Rightarrow P_e^{2m-1} \frac{d^2u}{d\theta^2} + (1-\lambda) P_e^{m} \frac{du}{d\theta} + \lambda \nu P_e^{m} \frac{df}{d\theta} = 0$$

$m = 1/2 \Rightarrow \dfrac{d^2u}{d\theta^2} = 0$ Valid in B.L.

$$m = 1 \Rightarrow \frac{d^2u}{d\theta^2} + (1-\lambda)\frac{du}{d\theta} + \lambda\nu \frac{df}{d\theta} = 0$$

$$\boxed{\hat{u}' + (1-\lambda)\hat{u} + \lambda\nu f(\hat{u}) = \mathbb{C}}$$

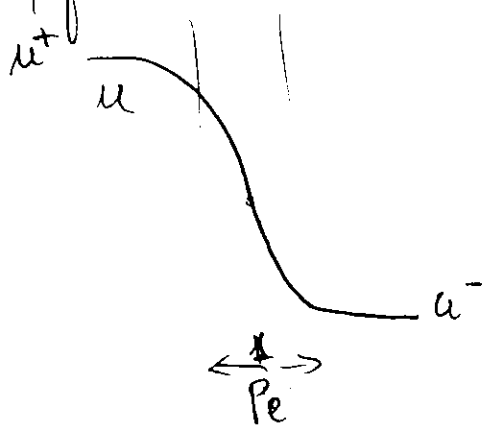
$$\int_{u^s}^{\hat{u}} \frac{d\hat{u}}{\mathbb{C} - (1-\lambda)\hat{u} + \lambda\nu f(\hat{u})} = \int_0^\theta d\theta$$

$$f(u) = \frac{\beta}{\nu} \frac{\hat{u}}{1+\sigma\hat{u}} \Rightarrow \frac{d\hat{u}}{c - (1-\lambda)\hat{u} + \lambda\nu f(\hat{u})} =$$

$$= \frac{(1+\sigma\hat{u})\, d\hat{u}}{A + B\hat{u} + C\hat{u}^2}$$

$\Rightarrow \boxed{G(\hat{u}) = \theta}$ solution $\Rightarrow \hat{u} = G^{-1}(\theta)$

Expect



$$\underbrace{\begin{aligned} G^{-1}(-\infty) &= u^+ = \begin{cases} 1 \\ <1 \end{cases} \\ G^{-1}(\infty) &= u^- = 0 \end{aligned}}_{\text{Matching with outer}}$$

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