Advection - Diffusion

Conservation law: for $u(x,t)$: $u_t + F_x = S$ in $a<x<b$
$t_0 < t < t_{end}$

Constitutive law for flux: $F = F_{adv} + F_{diff}$

$= vu - Du_x$, v = given vel. , D = diffusivity

so PDE for $u(x,t)$: $\boxed{u_t + (vu - Du_x)_x = S}$
advection-diffusion-reaction equ.

(As long as $D \neq 0$) this is a parabolic equ, so
needs IC: $u(x,0) = u_{init}(x)$ = given
and BCs: some BC at each boundary pt. for all time.

standard BCs: at $x=a$, $t_0 < t < t_{end}$

I. Dirichlet BC: $u(a,t) = u_a(t)$ given

II. Neumann BC: $F(a,t) = F_a(t)$ given
so $vu - Du_x \big|_{x=a} = F_a(t)$
In particular, insulated (impermeable) bry: $F(a,t) \equiv 0$

III. Convective BC: $F(a,t) = h \cdot [u_{amb}(t) - u(a,t)]$, h = film coeff.
heat transfer coeff

IV. Periodic BCs: $u(a,t) = u(b,t)$ and $F(a,t) = F(b,t)$

<u>Undimensionalization</u>: make all variables dimensionless

Simplest case: $v \equiv V = \text{const.}$, $D = \text{const.}$

$$u_t + V u_x = D u_{xx}$$

Choose a length scale L, a u-scale $\hat{u}$, a reference u_{ref}

[redacted] , a time-scale τ

Set: $\xi = \frac{x}{L}$, $W(\xi,\tau) = \dfrac{u(x,t) - u_{ref}}{\hat{u}} \Rightarrow u(x,t) = \hat{u}\cdot W(\xi,\tau) + u_{ref}$

$\tau = \frac{D}{L^2} t$: diffusion time-scale : <u>Fourier Number</u>

$$\Rightarrow u_t = \hat{u}\cdot W_\tau \cdot \tau_t = \hat{u}\cdot W_\tau \cdot \frac{D}{L^2}$$

$$u_x = \hat{u}\cdot W_\xi \cdot \xi_x = \hat{u}\cdot W_\xi \cdot \frac{1}{L}$$

$$u_{xx} = \hat{u}\cdot W_{\xi\xi}\cdot \frac{1}{L^2}$$

$$\overset{PDE}{\Longrightarrow} \cancel{\hat{u}}\cdot W_\tau \cdot \frac{D}{L^2} + \frac{V}{L}\cdot \cancel{\hat{u}}\cdot W_\xi = \frac{D}{L^2}\cdot \cancel{\hat{u}}\cdot W_{\xi\xi}$$

$\Rightarrow W_\tau + \frac{VL}{D} W_\xi = W_{\xi\xi}$ only one coeff. $\boxed{Pe = \frac{VL}{D} : \text{Peclet Number}}$

strength of $\frac{\text{advection}}{\text{diffusion}}$

Dimensionless advection-diffusion equ:

$$W_\tau + Pe \cdot W_\xi = W_{\xi\xi} \qquad \text{for} \quad 0 \lneqq Pe \lneqq \infty$$

$Pe = 0 \Leftrightarrow V = 0$: pure diffusion : $W_\tau = W_{\xi\xi}$

$Pe = \infty \Leftrightarrow D = 0$: pure advection : $W_\tau + W_\xi = 0$

choose $\tau = \frac{V}{L} t$: advection time-scale

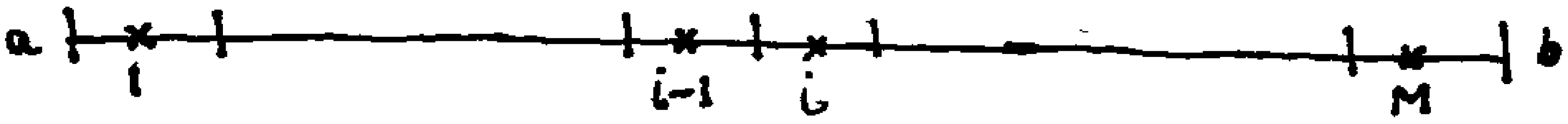
$$\Rightarrow W_\tau + W_\xi = \frac{1}{Pe} W_{\xi\xi}$$

scanned

Finite Volume discretization of $u_t + (vu - Du_x)_x = S$

It is a conservation law $u_t + F_x = S$, $a<x<b$, $t_0<t<t_{end}$
with flux $F = vu - Du_x = F_{adv} + F_{diff}$

We know how to discretize each piece.
Mesh of M control volumes: $x(0:M+1)$, $\Delta x = \frac{b-a}{M}$



Integrating $u_t + F_x = S$ over each $CV_i = [x_{i-\frac12}, x_{i+\frac12}]$
and each timestep $[t_n, t_{n+1}]$ and setting

$$U_i^n = \frac{1}{\Delta x}\int_{x_{i-\frac12}}^{x_{i+\frac12}} u(x,t_n)\,dx = \text{mean } u \text{ over } CV_i \text{ at time } t_n$$
$$\approx u(x_i, t_n)$$

$$\bar{F}_{i-\frac12}^{n+\theta} = \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} F(x_{i-\frac12}, t)\,dt = \text{mean } F \text{ over } [t_n, t_{n+1}] \text{ at face } x_{i-\frac12}$$

$$S_i^{n+\theta} = \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} \frac{1}{\Delta x}\int_{x_{i-\frac12}}^{x_{i+\frac12}} S(x,t)\,dx\,dt = \text{mean source}$$

we get, as before

$$U_i^{n+1} = U_i^n + \frac{\Delta t}{\Delta x}\left[\bar{F}_{i-\frac12}^{n+\theta} - \bar{F}_{i+\frac12}^{n+\theta}\right] + \Delta t\, S_i^{n+\theta}$$

$$i = 1:M, \quad n = 0:N, \quad 0 \le \theta \le 1$$

$$F_{i-\frac12} = (vu)_{i-\frac12} + (-Du_x)_{i-\frac12}, \quad i = 2:M, \quad F_{\frac12}, F_{M+\frac12} \text{ from BCs}$$

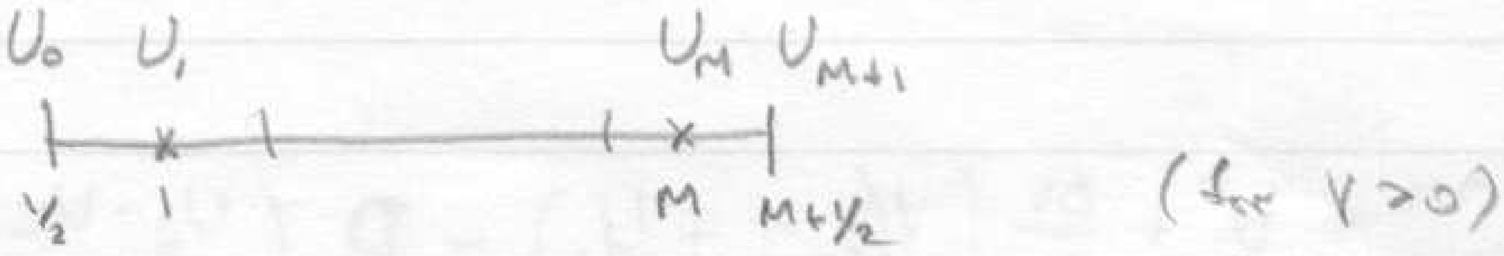
$$\approx \underset{\text{adv. flux}}{\text{upwind}} \; - D\,\frac{U_i - U_{i-1}}{\Delta x}$$

$$= \begin{cases} v_{i-\frac12} U_{i-1} & \text{if } v_{i-\frac12} > 0 \\ v_{i-\frac12} U_i & \text{if } v_{i-\frac12} < 0 \end{cases} \; - D\,\frac{U_i - U_{i-1}}{\Delta x}$$

Advection + Diffusion: Boundary Conditions

Total Flux is $F = F^{adv} + F^{diff}$
$$= Vu - Du_x$$

so boundary fluxes are (for $V>0$)



$$F_{1/2} = VU_0 - D\,\frac{U_1 - U_0}{\Delta x/2} \quad \text{and} \quad F_{M+1/2} = VU_M - D\,\frac{U_{M+1}-U_M}{\Delta x/2}$$

for $V<0$: $= VU_1 - D$ ——   for $V<0$: $= VU_{M+1} - D$ ——

1. Dirichlet: U_0 = given
   $F_{1/2}$ from the above formula
   If $D=0$: OK if $V>0$, no BC if $V<0$

   U_{M+1} = given
   $F_{M+1/2}$ from above formula
   If $D=0$: $F_{M+1/2} = VU_{M+1} - D\frac{U_{M+1}-U_M}{\Delta x/2}$ if $V<0$
   – no BC if $V>0$

2. Neuman: $F_{1/2} = q_a$ = given

   Solve for U_0:
   $$U_0 = \frac{q_a\frac{\Delta x}{2} + DU_1}{V\frac{\Delta x}{2} + D}$$

   If $D=0$: $V>0$, then $U_0 = \frac{q_a}{V}$
   $V<0$ no BC

   $F_{M+1/2} = q_b$ = given

   Solve for U_{M+1}:
   $$U_{M+1} = \frac{\left[V\frac{\Delta x}{2} + D\right]U_M - q_b\frac{\Delta x}{2}}{D} \quad \text{if } V>0$$
   $$U_{M+1} = \frac{-q_b\frac{\Delta x}{2} + DU_M}{-V\frac{\Delta x}{2} + D} \quad \text{if } V<0$$

   If $D=0$: $V>0$: no BC
   $V<0$: OK, $U_{M+1} = \frac{q_b}{V}$

3. Convective BC: $F_{1/2} = h\left[U_\infty - U_0\right]$
   $$VU_0 - D\frac{U_1-U_0}{\Delta x/2} = h\left[U_\infty - U_0\right]$$
   $$\Rightarrow U_0 = \frac{\frac{2D}{\Delta x}U_1 + hU_\infty}{V + \frac{2D}{\Delta x} + h}$$
   $$\Rightarrow F_{1/2} = \frac{VU_\infty - D\frac{U_1 - U_\infty}{\Delta x/2}}{1 + \frac{V}{h} + \frac{D}{h\Delta x/2}}$$

   as $h \to \infty$ we get $F_{1/2}$ for Dirichlet with U_∞ as U_0

   $F_{M+1/2} = -h\left[U_\infty - U_{M+1}\right]$
   $$VU_M - D\frac{U_{M+1}-U_M}{\Delta x/2} = hU_{M+1} - hU_\infty$$
   $$\Rightarrow U_{M+1} = \frac{\left(V + \frac{2D}{\Delta x}\right)U_M + hU_\infty}{\frac{2D}{\Delta x} + h}$$
   $$\Rightarrow F_{M+1/2} = \frac{VU_M + \frac{2D}{\Delta x}\left(U_M - U_\infty\right)}{1 + \frac{2D}{h\Delta x}}$$

   as $h \to \infty$, $F_{M+1/2} = VU_M - D\frac{U_\infty - U_M}{\Delta x/2}$ = Dirichlet with U_∞ as U_{M+1}

CFL condition

So, say for $V > 0$:

$$U_j^{n+1} = U_j^n + \frac{\Delta t}{\Delta x}\left[V U_{j-1}^n - V U_j^n - D_{j-1/2}\frac{U_j - U_{j-1}}{\Delta x} + D_{j+1/2}\frac{U_{j+1} - U_j}{\Delta x} \right]$$

and for $D \equiv$ const:

$$U_j^{n+1} = U_j^n \left[1 - V\frac{\Delta t}{\Delta x} - 2\frac{D\Delta t}{\Delta x^2} \right] + V\frac{\Delta t}{\Delta x}U_{j-1}^n + D\frac{\Delta t}{\Delta x^2}\left(U_{j-1}^n + U_{j+1}^n\right)$$

Stability via the "positive coefficient rule":

$$1 - V\frac{\Delta t}{\Delta x} - 2D\frac{\Delta t}{\Delta x^2} > 0$$

so $\boxed{0 < V\frac{\Delta t}{\Delta x} + 2D\frac{\Delta t}{\Delta x^2} \leq 1 \quad \text{is the CFL condition}}$

This restricts the time step to; $\Delta t \leq \dfrac{\Delta x^2}{|V|\Delta x + 2D} = \dfrac{1}{\frac{|V|}{\Delta x} + \frac{2D}{\Delta x^2}}$

Pure advection case ($D \equiv 0$): Courant number $|V|\frac{\Delta t}{\Delta x} \leq 1$, CFL: $\Delta t \leq \dfrac{\Delta x}{V_{max}}$

Pure diffusion case ($V \equiv 0$): Courant number $D\frac{\Delta t}{\Delta x^2} \leq \frac{1}{2}$, CFL: $\Delta t \leq \dfrac{\Delta x^2}{2D_{max}}$

Advection-diffusion: Courant number $|V|\frac{\Delta t}{\Delta x} + 2\frac{D\Delta t}{\Delta x^2} \leq 1 \implies \Delta t \leq \dfrac{\Delta x^2}{|V|\Delta x + 2D}$

Note: taking $\Delta t = \min(\Delta t_{ad}, \Delta t_{...})$ ...