

Numerical Heat Transfer

(数值传热学)

Chapter 5 Discretized Schemes of Diffusion and Convection Equation (2)



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数值传热学

第五章 对流扩散方程的离散格式(2)



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Chapter 5 Discretized diffusion—convection equation

5.1 Two ways of discretizing convection term

5.2 CD and UD of the convection term

5.3 Hybrid and power-law schemes

5.4 Characteristics of five three-point schemes

5.5 Discussion on false diffusion

5.6 Methods for overcoming or alleviating effects of false diffusion

5.7 Stability analysis of discretized diffusion-convection equation

5.8 Discretization of multi-dimensional problem and B.C. treatment

5.5 Discussion on false diffusion

5.5.1 Meaning and reasons of false diffusion

1. Original meaning

2. Extended meaning

3. Taylor expansion analysis

5.5.2 Examples of severe false diffusion caused by 1st-order scheme

5.5.3 Errors caused by oblique intersection (倾斜交叉) of grid lines

5.5.4 Other two famous examples

Appendix: False diffusion caused by non-constant source term

5.5 Discussion on false diffusion

5.5.1 Meaning and reasons of false diffusion

False diffusion (假扩散), also called numerical viscosity (数值黏性), is an important character of discretized convective scheme.

1. Original meaning

Numerical errors caused by discretized scheme of 1st order accuracy is called false diffusion;

The 1st term in the TE of such scheme contains 2nd order derivative, thus the role of diffusion is somewhat magnified, hence the numerical error is called “false diffusion” (假扩散).

**Taking 1-D unsteady advection eq. as an example.
The two 1st-order derivatives are discretized by 1st-order accuracy schemes.**

$$\frac{\partial \phi}{\partial t} = -u \frac{\partial \phi}{\partial x} \xrightarrow[\mathbf{u > 0}]{\mathbf{1^{st}\text{-order scheme}}} \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = -u \frac{\phi_i^n - \phi_{i-1}^n}{\Delta x}$$

Expanding $\phi_{i-1}^n, \phi_i^{n+1}$ at (i,n) by Taylor series, and substituting into the above equation:

$$\frac{\phi_i^n + \Delta t \left(\frac{\partial \phi}{\partial t} \right)_{i,n} + \frac{1}{2} \Delta t^2 \left(\frac{\partial^2 \phi}{\partial t^2} \right)_{i,n} + \dots - \phi_i^n}{-u \frac{\phi_i^n - \left[\phi_i^n - \Delta x \left(\frac{\partial \phi}{\partial x} \right)_{i,n} + \frac{1}{2} \Delta x^2 \left(\frac{\partial^2 \phi}{\partial x^2} \right)_{i,n} + \dots \right]} =$$

$$\left(\frac{\partial \phi}{\partial t}\right)_{i,n} = -u \left(\frac{\partial \phi}{\partial x}\right)_{i,n} - \frac{\Delta t}{2} \left(\frac{\partial^2 \phi}{\partial t^2}\right)_{i,n} + \frac{u \Delta x}{2} \left(\frac{\partial^2 \phi}{\partial x^2}\right)_{i,n} + O(\Delta x^2, \Delta t^2)$$

The 2nd term at right side is re-written as follows:

$$\frac{\partial^2 \phi}{\partial t^2} = \frac{\partial}{\partial t} \left(\frac{\partial \phi}{\partial t}\right) \cong \frac{\partial}{\partial t} \left(-u \frac{\partial \phi}{\partial x}\right) = -u \frac{\partial}{\partial x} \left(\frac{\partial \phi}{\partial t}\right) \cong -u \frac{\partial}{\partial x} \left(-u \frac{\partial \phi}{\partial x}\right) = u^2 \frac{\partial^2 \phi}{\partial x^2}$$

substituting into above equation

$$\left(\frac{\partial \phi}{\partial t}\right)_{i,n} = -u \left(\frac{\partial \phi}{\partial x}\right)_{i,n} + \left[\frac{u \Delta x}{2} \left(1 - \frac{u \Delta t}{\Delta x}\right) \right] \left(\frac{\partial^2 \phi}{\partial x^2}\right)_{i,n} + O(\Delta x^2, \Delta t^2)$$

Thus at the sense of 2nd-order accuracy above discretized equation simulates **a convective-diffusive process**, rather than (而不是) an advection process.

Only when $1 - \frac{u\Delta t}{\Delta x} = 0$ this error disappears(消失).

$\frac{u\Delta t}{\Delta x}$ is called Courant number, in memory of (纪念) a German mathematician Courant.

$$\frac{\partial \phi}{\partial t} \Big|_{i,n} = -u \frac{\partial \phi}{\partial x} \Big|_{i,n} + \left[\frac{u\Delta x}{2} \left(1 - \frac{u\Delta t}{\Delta x} \right) \right] \frac{\partial^2 \phi}{\partial x^2} \Big|_{i,n} + O(\Delta x^2, \Delta t^2)$$

Remark: We only study the false diffusion at the sense of 2nd-order accuracy; i.e., inspecting (审视) at the 2nd-order accuracy the above discretized equation actually simulates a convection-diffusion process. For most engineering problems 2nd-order accuracy solutions are satisfied.

2. Extended meaning (扩展的含义)

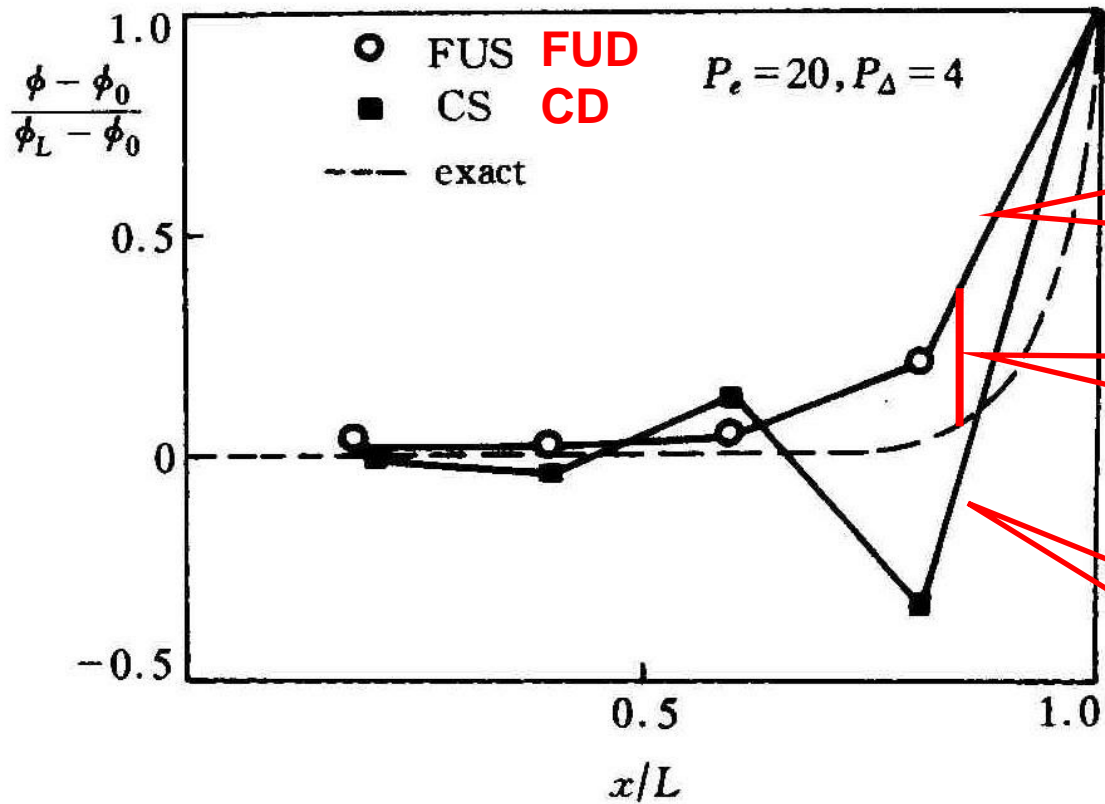
In most existing literatures almost all numerical errors are called false diffusion, which includes:

- (1) 1st-order accuracy schemes of the 1st order derivatives;
- (2) Oblique intersection(倾斜交叉) of flow direction with grid lines;
- (3) The effects of non-constant source term which are not considered in the discretized schemes.

5.5.2 Examples caused by 1st-order accuracy schemes

1. 1-D steady convection-diffusion problem

When convection term is discretized by FUD, diffusion term by CD, numerical solutions will severely deviate (偏离) from analytical solutions:



FUD Physically plausible solution

FUS severe error

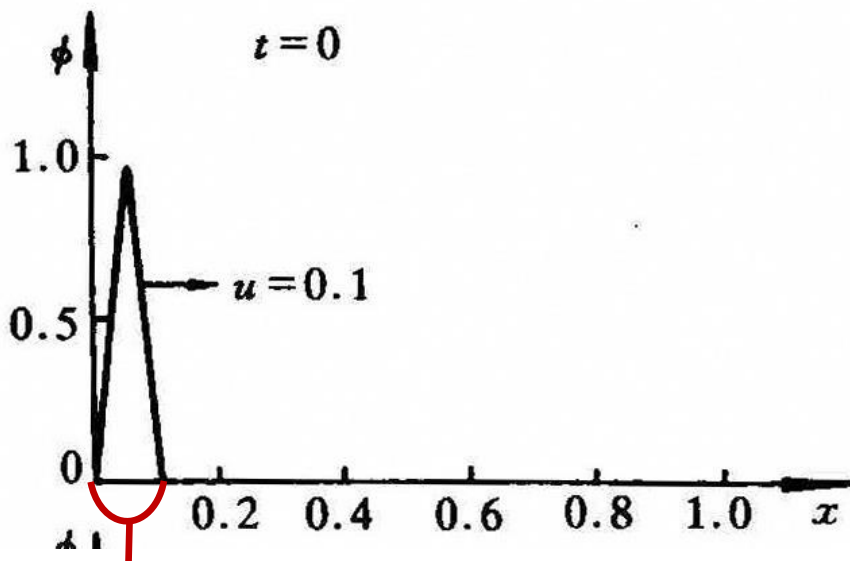
CD oscillating solution

2. 1-D unsteady advection problem (Noye, 1976)

$$\frac{\partial \phi}{\partial t} = -u \frac{\partial \phi}{\partial x}, \quad 0 \leq x \leq 1, \quad u = 0.1, \quad \phi(0, t) = \phi(1, t) = 0$$

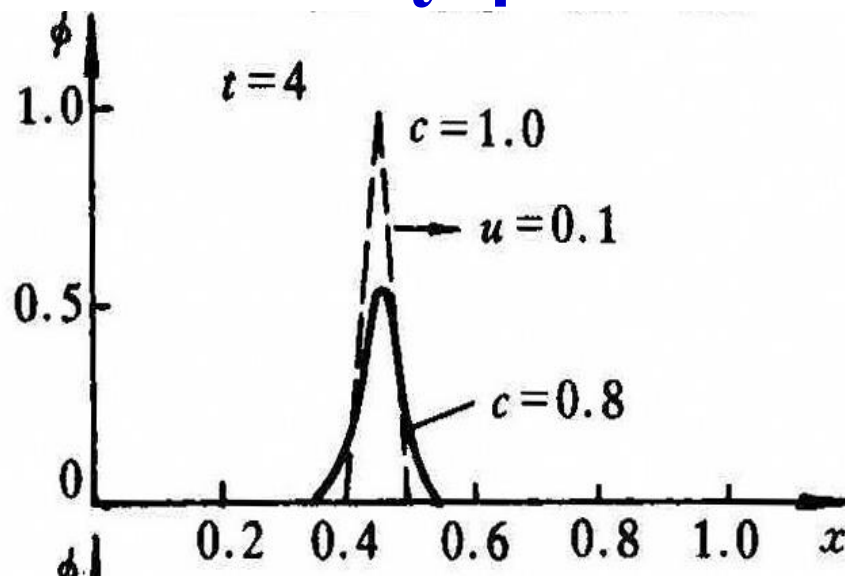
In the range of $x \in [0, 0.1]$ initial distribution is a triangle, others are zero.

Initial condition

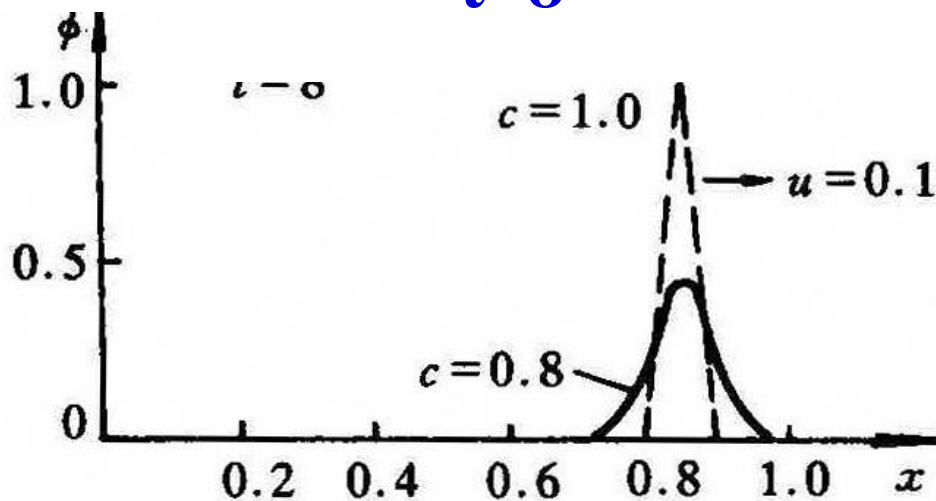


triangle

$t=4$



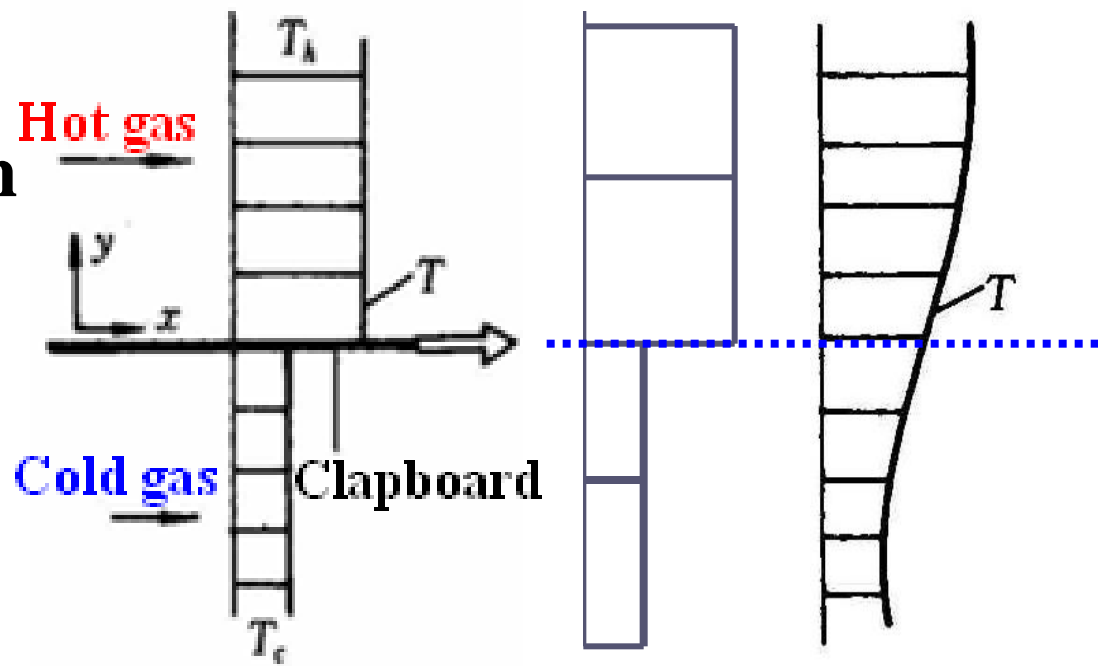
$t=8$



When Courant number is less than 1 ,severe error occurs, which erases (抹平) the sharp peak (尖峰) gradually. Such error is called **streamwise false diffusion** (流向假扩散).

5.5.3 Errors caused by oblique intersection(倾斜交叉)

Two gas streams with different temperatures meet each other. Assuming zero gas diffusivities. If the flow direction is oblique with respect to the grid lines, big numerical errors will be introduced.



$$\Gamma = 0 \quad \Gamma \neq 0$$

1. Case 1: with x-y coordinates either parallel or perpendicular to flow direction

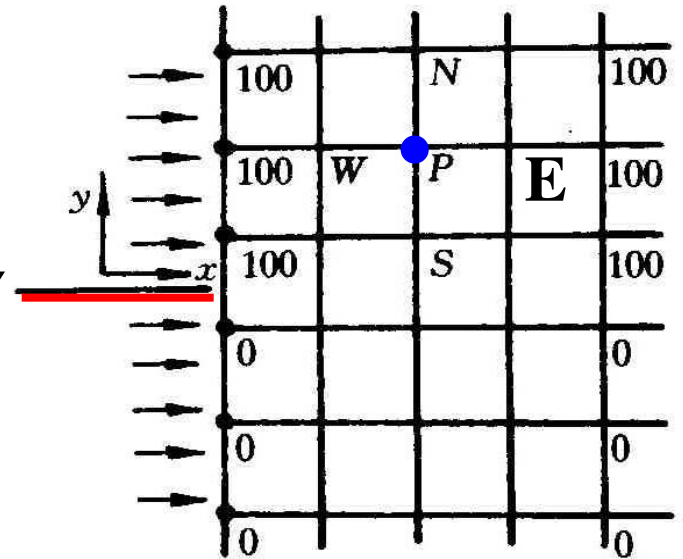
Adopting FUD, then $A(|P_\Delta|) = 1$; For CV. P:

$$a_E = D_e + \|-F_e, 0\| \xrightarrow{U > 0, \Gamma = 0} \mathbf{0}$$

$$a_W = D_W + \|F_w, 0\| \xrightarrow{U > 0, \Gamma = 0} \mathbf{F}_W$$

$$a_N = D_n + \|-F_n, 0\| \xrightarrow{V = 0, \Gamma = 0} \mathbf{0}$$

$$a_S = D_s + \|F_s, 0\| \xrightarrow{V = 0, \Gamma = 0} \mathbf{0}$$



Upstream velocity U

Thus : $a_P = \cancel{a_E} + a_W + \cancel{a_N} + \cancel{a_S} = a_W \quad \phi_P = \phi_W !$

The upstream temperature is kept downstream!

2. Case 2: x-y coordinates intersect the on coming flow with 45 degree

From upstream velocity U $u = v = \frac{\sqrt{2}}{2}U$,

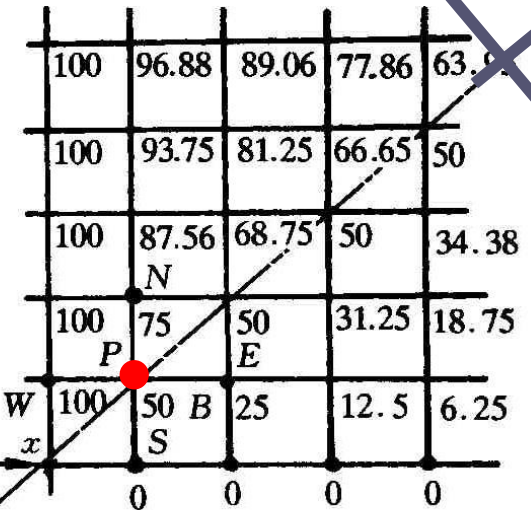
Again FUD is adopted, then for CV. P:

$$a_E = D_e + \|-F_e, 0\| \quad \underline{u > 0, \Gamma = 0} \quad \mathbf{0}$$

$$a_W = D_W + \|F_w, 0\| \quad \underline{u > 0, \Gamma = 0} \quad \mathbf{F_w}$$

$$a_N = D_n + \|-F_n, 0\| \quad \underline{v > 0, \Gamma = 0} \quad \mathbf{0}$$

$$a_S = D_s + \|F_s, 0\| \quad \underline{v > 0, \Gamma = 0} \quad \mathbf{F_s}$$



(b)

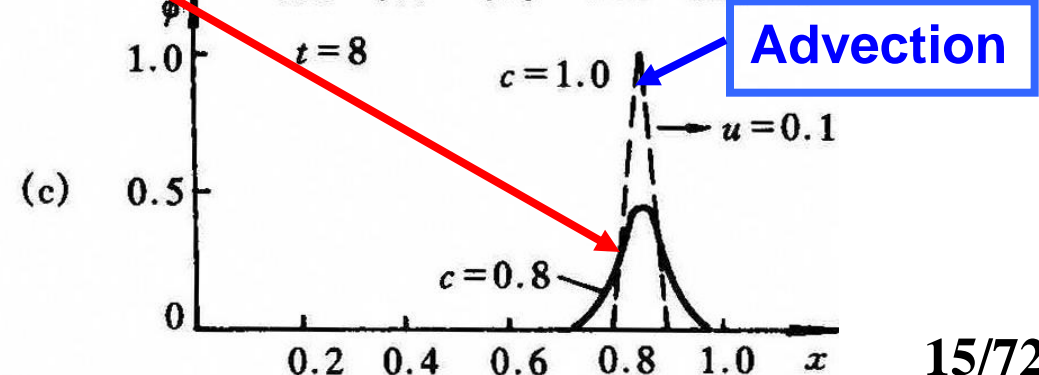
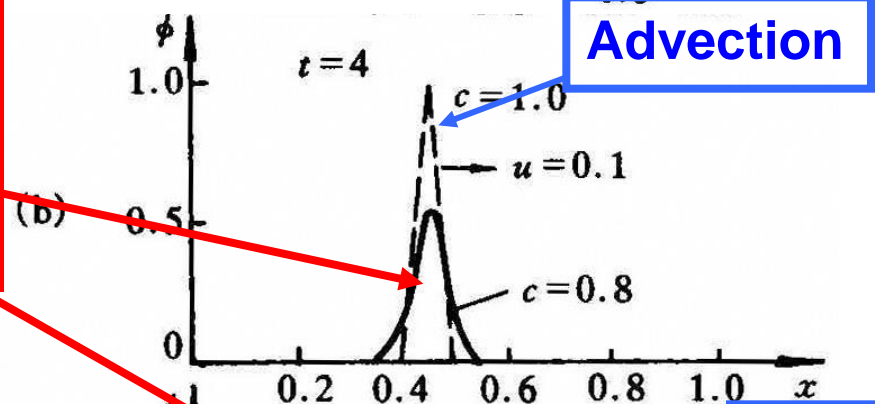
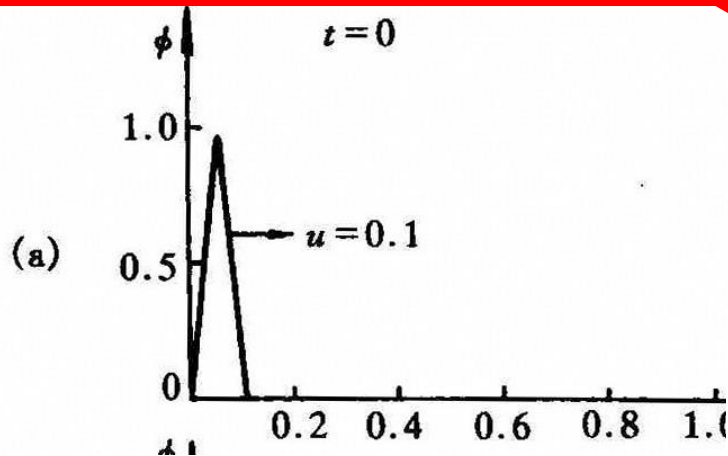
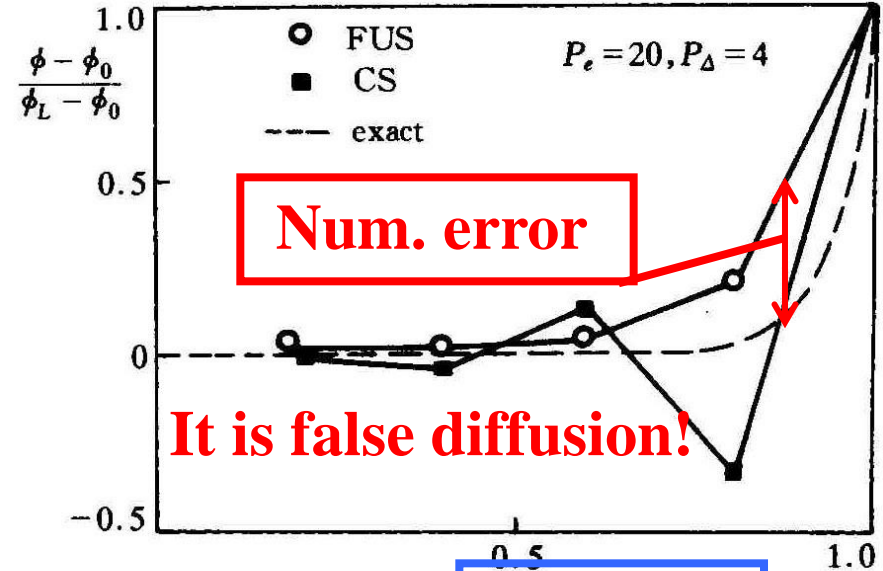
$$F_w = F_s, a_P \phi_P = a_W \phi_W + a_S \phi_S + 0 + 0, a_P = a_W + a_S, \phi_P = \frac{\phi_W + \phi_S}{2}!$$

Summary for three convective problems

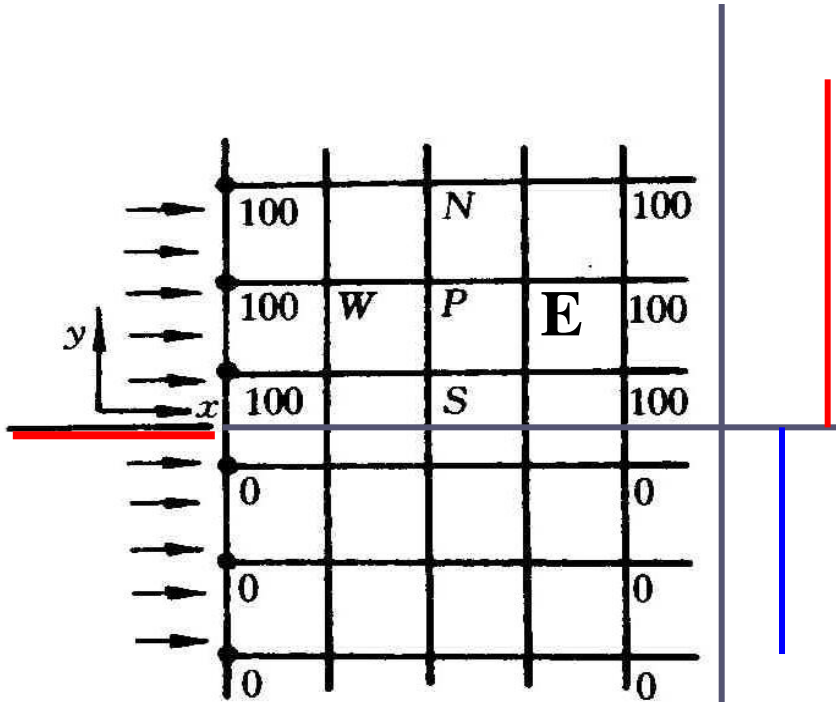
1) 1-D steady D-C problem

2) 1-D unsteady advection problem (Noye,1976)

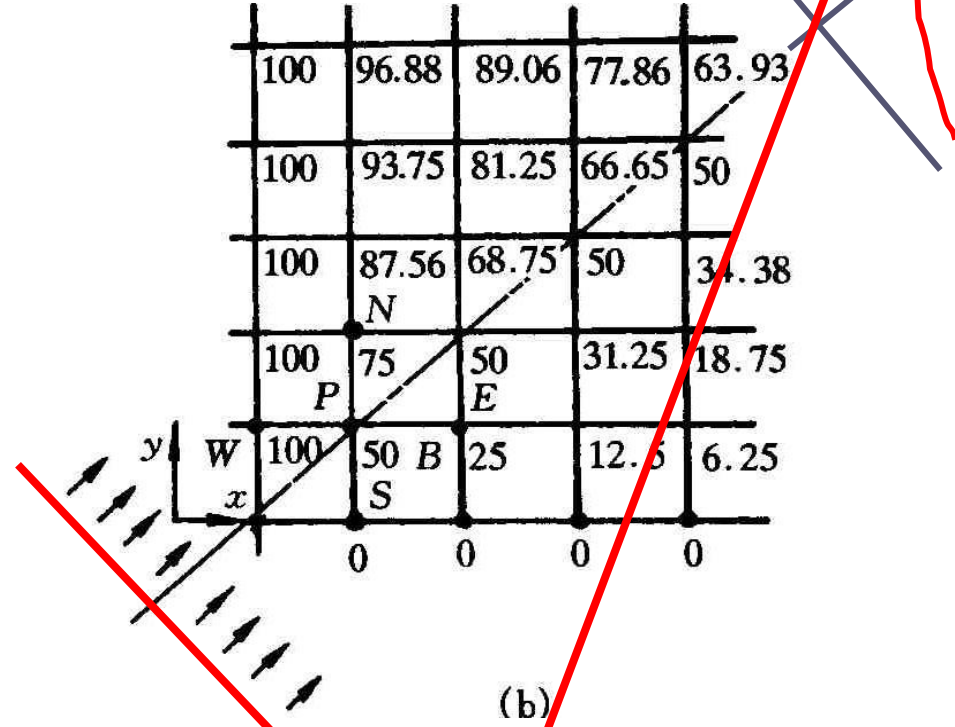
Such false diffusion is called **Streamwise false diffusion** (流向假扩散)。



3) Numerical error caused by oblique grid lines with respect to flow direction



Case 1



Case 2

(交叉扩散)
Cross-diffusion

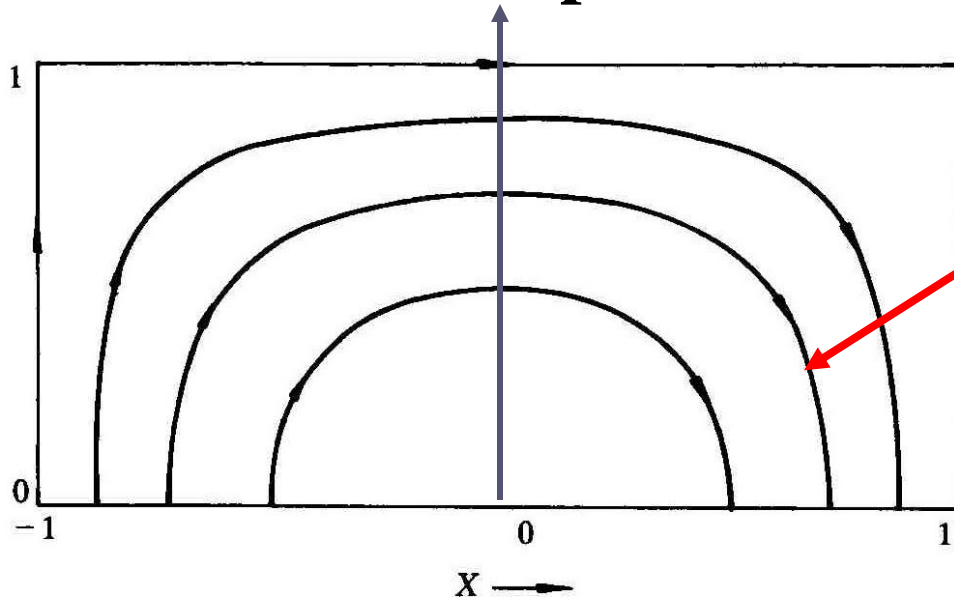
Fluid temperatures are unified between hot and cold fluids. That is caused by the **cross-diffusion**。

Discussion: For case 1 of Problem 3 where velocity is parallel to x coordinate, the FUD scheme also produces false diffusion, but compared with convection it can not be exhibited(展现): the zero diffusivity corresponds to an extremely large Peclet number, i.e., convection is so strong that false diffusion can not be exhibited. When chances come it will take action. Example 1 of this section is such a situation.

5.5.4 Other two famous examples

1. Smith-Hutton problems (1982)

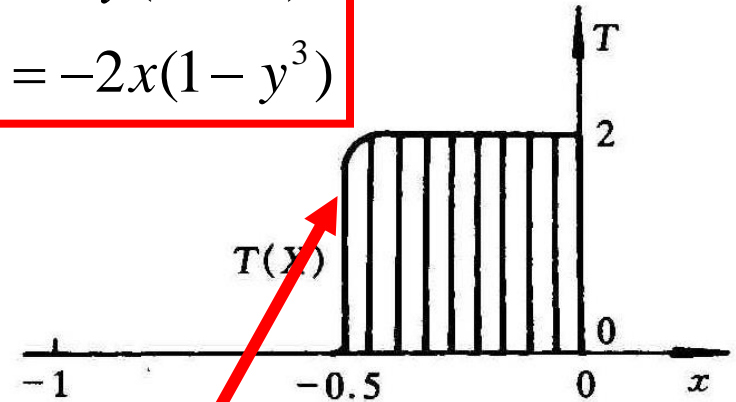
Solution for temp. distribution with a known flow field



Known flow field

$$u = 2y(1 - x^2),$$

$$v = -2x(1 - y^3)$$

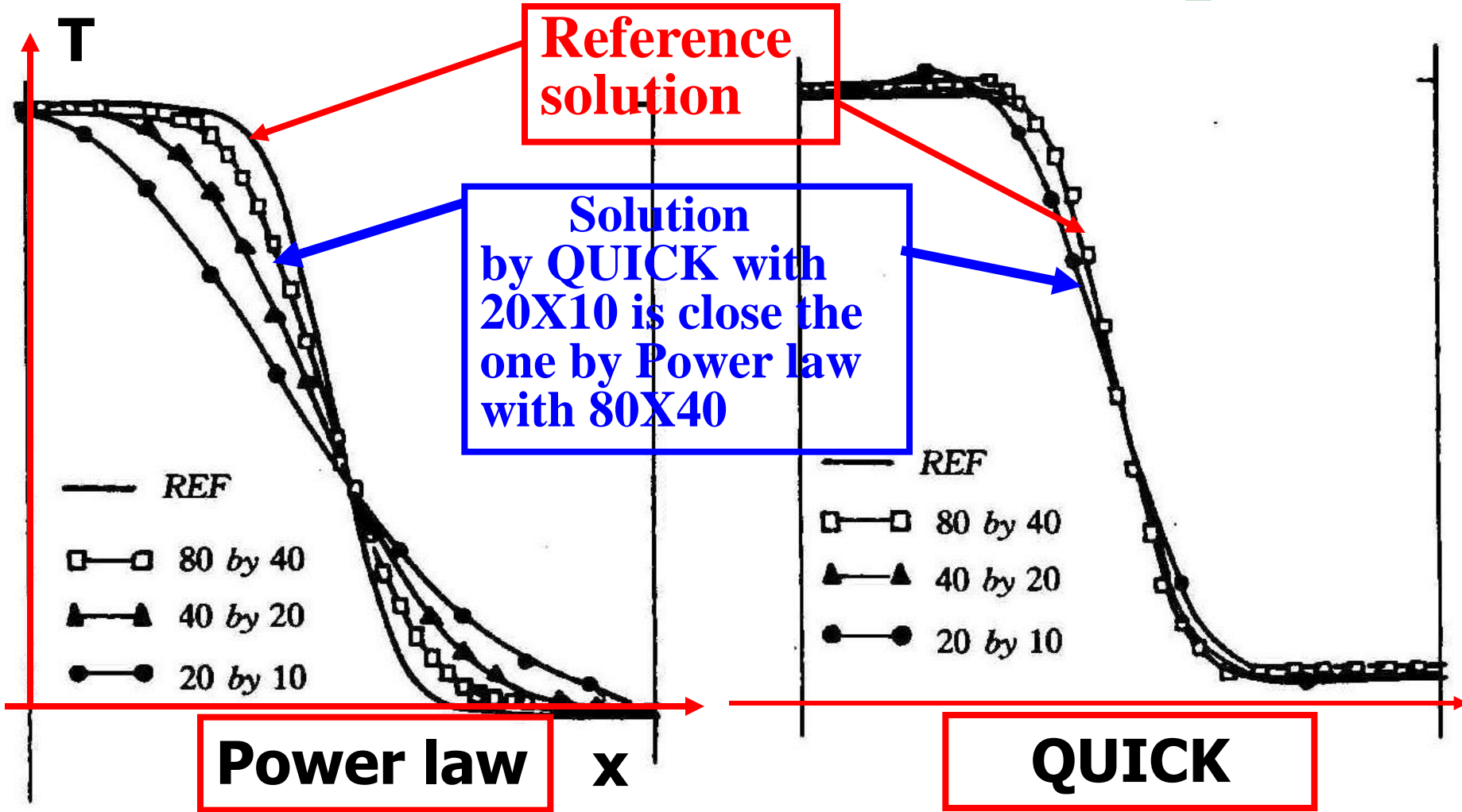


Specified inlet distribution^(b)

$$T_{in}(x) = 1 + \tanh[\alpha(1 + 2x)]$$

The larger the coefficient the sharper the profile.

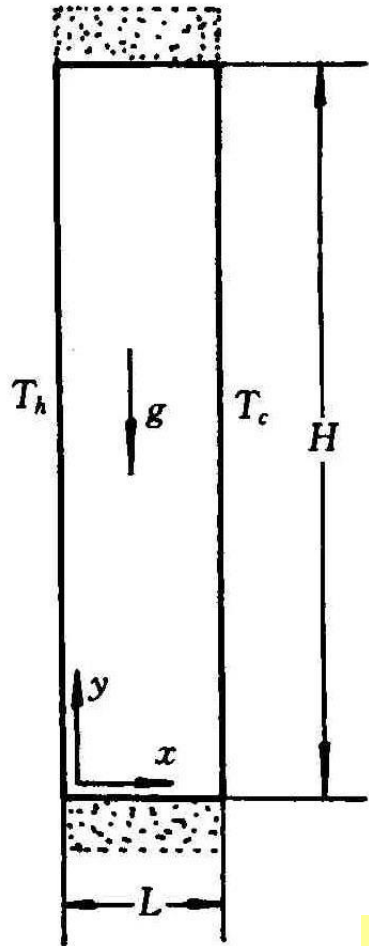
Solved by 2-D D-C eq., convection term is discretized by the scheme studied.



Solution from QUICK by 20X10 grids has the same accuracy as that from power law by 80X40 grids.

2) Leonard problem (1996)

Natural convection in a tall cavity

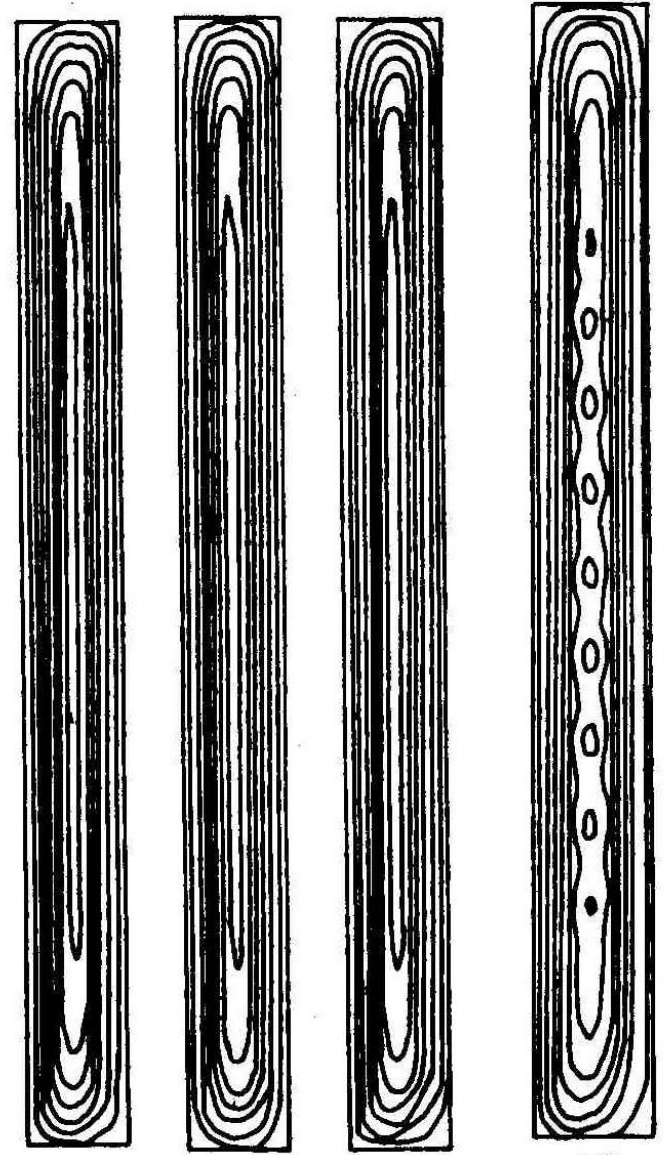


$$H / L = 33$$

$$Gr = \frac{gL^3\alpha\Delta T}{\nu^2} = 9500,$$

$$Pr = 0.71$$

$$32 \times 129 = 4128$$



(a)
FUS

(b)
HS

(c)
PLS

(d)
QUICK
20/72

PWL scheme

QUICK scheme

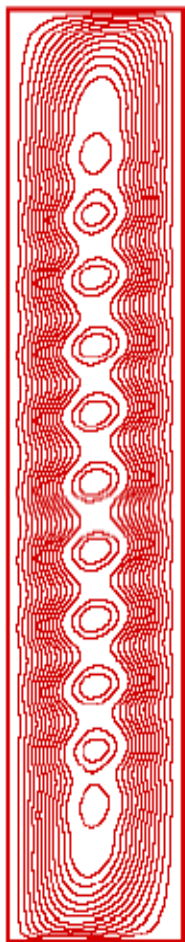


Table 5 Dimensionless cell coordinate
calculated with PWL

	X	Y
1	0.498515248326	27.8179321847
2	0.498515248326	25.7841071708
3	0.498515248326	23.4863048689
4	0.498515248326	21.1045097935
5	0.498515248326	18.6927172991
6	0.498515248326	16.2869242885
7	0.498515248326	13.8871307617
8	0.498515248326	11.4933367187
9	0.498515248326	9.1415390625
10	0.498515248326	6.89773211496
11	0.498515248326	4.92390193917

Note: $Nu = 39.0$

Grid number 102×3102



Table 8 Dimensionless cell coordinate
calculated with QUICK

	x	y
1	0.518501419014	29.1039634016
2	0.490007077493	27.4006482603
3	0.499915660431	24.67564866
4	0.499997148246	21.9077572869
5	0.499991534052	19.1825723813
6	0.499886807287	16.4151439754
7	0.499878758708	13.6898093029
8	0.499990193278	10.9220760437
9	0.50007191963	8.19718832227
10	0.500120639936	5.47165901886
11	0.479889934259	3.81172796021

Note: $Nu = 42.61$

Grid number 102×3102

Grids=316404

Solutions from lower-order scheme can not resolute small vortices if mesh is not fine enough.

At coarse grid system, solution differences by different schemes are often significant!

Solution from higher order scheme with a less grid number can reach the same accuracy as that from lower order scheme with a larger grid number.

With increased grid number power law can also predict (预测) small vortices.

The differences between different schemes are gradually reduced with increasing grid number.

Jin WW, He YL, TaoWQ. How many secondary flows are in Leonard's vertical slot?
Progress in Computational Fluid Dynamics, 2009, 9(3/4):283-291

Appendix of Section 5-1

Errors caused by non-constant source term

Given:
$$\left\{ \begin{array}{l} \frac{d(\rho u \phi)}{dx} = \frac{d}{dx} \left(\Gamma \frac{d\phi}{dx} \right) + S, \\ x = 0, \phi = \phi_0; x = L, \phi = \phi_L \end{array} \right. \quad \begin{array}{l} S \text{ non-constant,} \\ \text{distribuiton is} \\ \text{specified.} \end{array}$$

Taking hybrid scheme as an example. When grid Peclet number is less than 2, numerical results agree with analytical solution quite well; However, when grid Peclet number is larger than 2, deviations become large. Its coefficient is defined by:

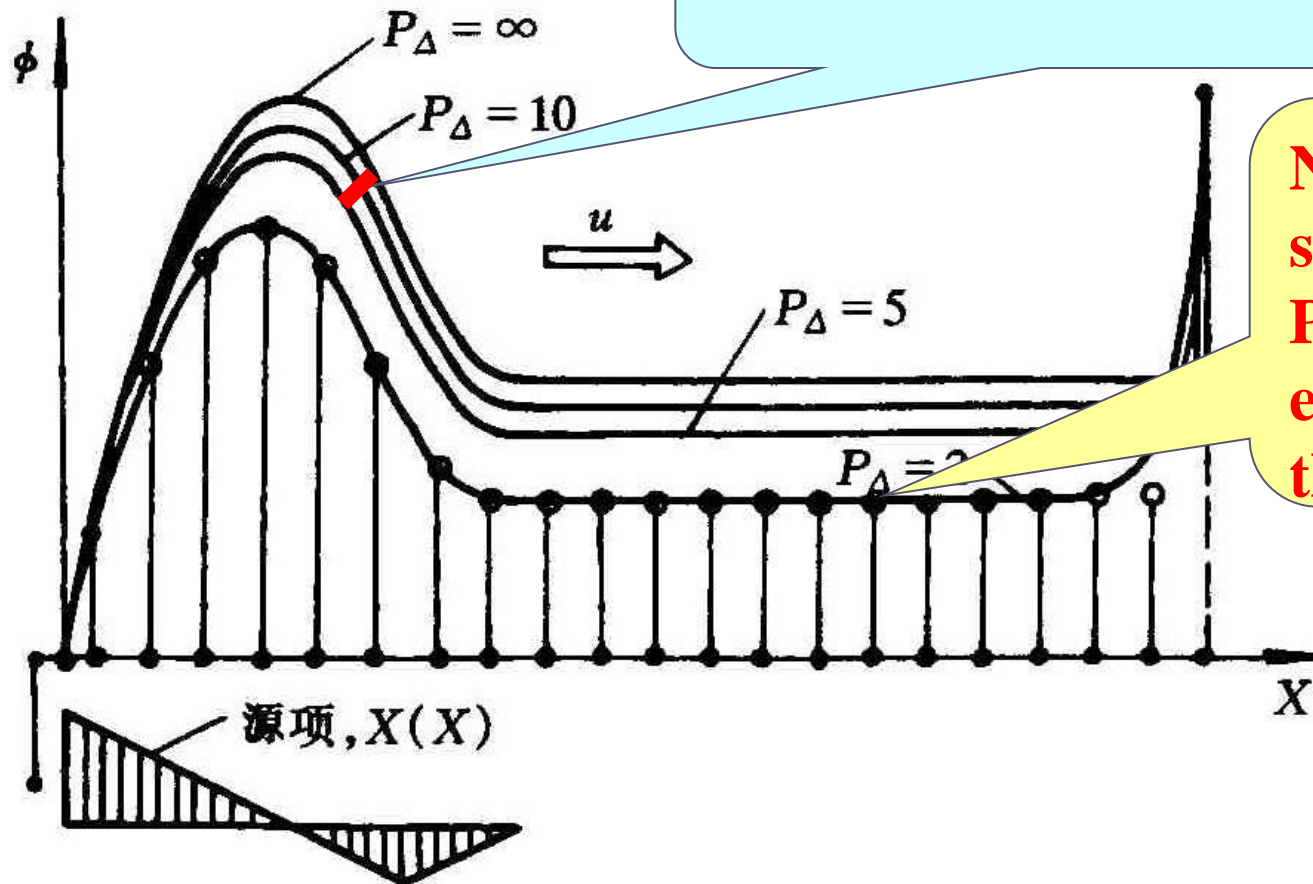
$$a_E = D_e A(|P_{\Delta e}|) + \|-F_e, 0\| ; A(|P_{\Delta e}|) = \|0, 1 - 0.5|P_{\Delta e}|\|$$

Assuming that variation of Peclet number is implemented via changing diffusion coefficient while flow rate is remained unchanged then when

$P_{\Delta e} \geq 2$, because $A(|P_{\Delta}|) = 0$ coefficient a_E is remained unchanged, leading to the same numerical solutions for all cases with $P_{\Delta e} \geq 2$.

Analytical solutions for grid Peclet number larger than 2

Numerical solutions for grid Peclet number equal and larger than 2



5.6 Methods for overcoming or alleviating effects of false diffusion

5.6.1 Higher order schemes to overcome streamwise false diffusion

1. Second order upwind scheme (SUD)
2. Third order upwind scheme (TUD)
3. QUICK
4. SGSD

5.2.2 Methods for alleviating (减轻) cross false diffusion

1. Effective diffusivity method
2. Self-adaptive grid method

5.6 Methods for overcoming or alleviating effects of false diffusion

5.6.1 Higher order schemes to overcome streamwise false diffusion

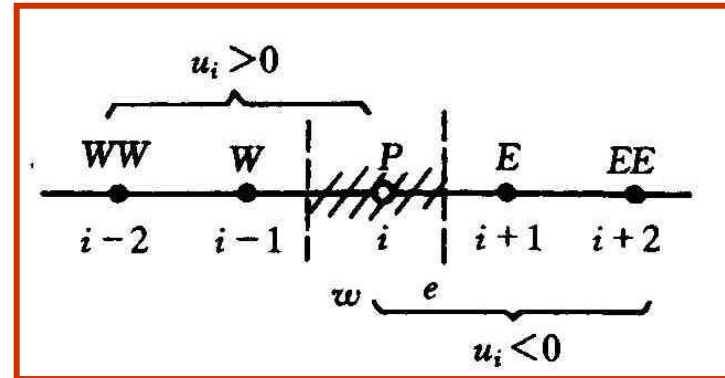
1. SUD(2nd-order upwind difference)---Taking two upstream points for scheme construction

(1) Taylor expansion definition — 2nd order one side diff.

$$u \frac{\partial \phi}{\partial x} \Big|_i = \frac{u_i}{2\Delta x} (3\phi_i - 4\phi_{i-1} + \phi_{i-2}), u > 0$$

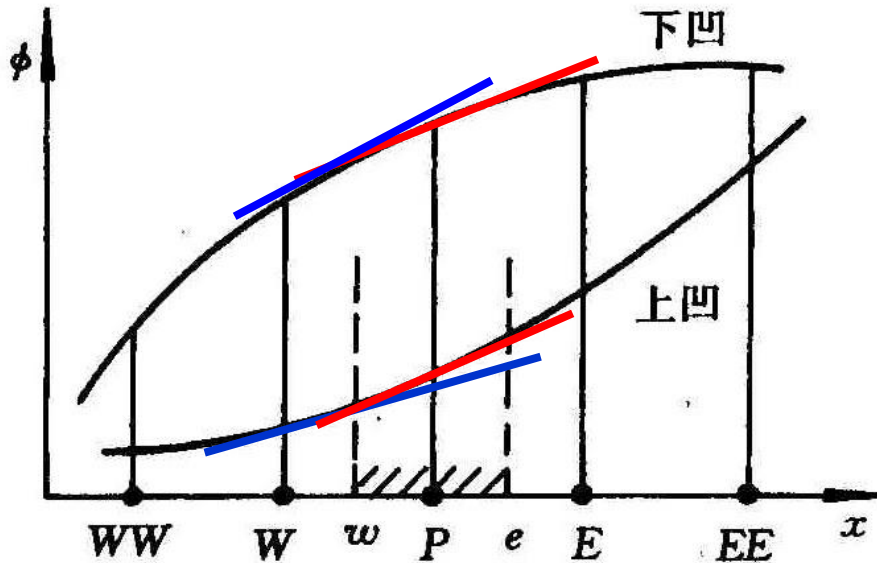
Rewriting it into the form of interface CD + an additional term:

$$u \frac{\partial \phi}{\partial x} \Big|_P = u_P \left(\frac{\phi_P - \phi_W}{\Delta x} + \frac{\phi_P - 2\phi_W + \phi_{WW}}{2\Delta x} \right)$$



This is equivalent to CD + curvature correction: slope at grid P = slope at w-interface + a correction term:

$$\left(\frac{\phi_P - 2\phi_W + \phi_{WW}}{2\Delta x} \right)$$



Check the sign (plus or minus) of the correction term to see if it is consistent with the curvature.

Concave upward(上凹),

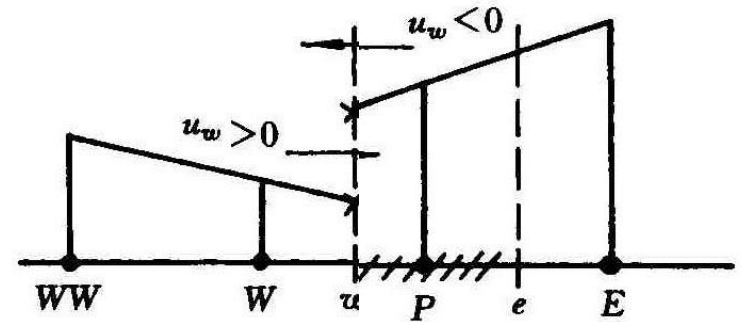
$$(\phi_P - 2\phi_W + \phi_{WW}) > 0 \text{ Correction} > 0 ;$$

Concave Downward(下凹)

$$(\phi_P - 2\phi_W + \phi_{WW}) < 0 \text{ Correction} < 0$$

(2) FVM – Interface interpolation takes two upstream points.

$$\phi_w = \begin{cases} 1.5\phi_w - 0.5\phi_{ww}, & u > 0 \\ 1.5\phi_p - 0.5\phi_e, & u < 0 \end{cases}$$



Equivalence of the two definitions:

$$\begin{aligned} \frac{1}{\Delta x} \int_w^e \frac{\partial \phi}{\partial x} dx &= \frac{\phi_e - \phi_w}{\Delta x} = \frac{(1.5\phi_p - 0.5\phi_w) - (1.5\phi_w - 0.5\phi_{ww})}{\Delta x} \\ &= \frac{3\phi_p - 4\phi_w + \phi_{ww}}{2\Delta x} \end{aligned}$$

FVM: Integral averaged value over a CV;

FDM: Discretized value at a node

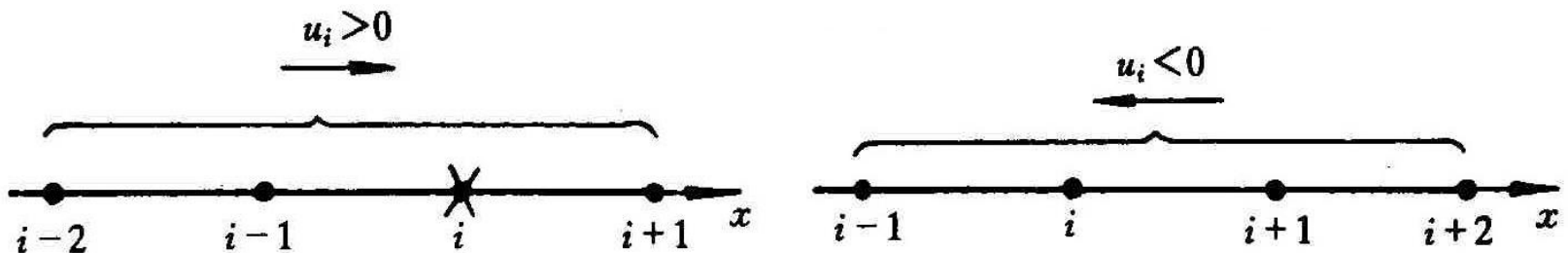
2. TUD (三阶迎风)

(1) Taylor expansion — 3rd-order scheme of 1st derivative with biased positions of nodes (节点偏置).

$$u \left(\frac{\partial \phi}{\partial x} \right)_i = \frac{u_i}{6\Delta x} (2\phi_{i+1} + 3\phi_i - 6\phi_{i-1} + \phi_{i-2}), \quad u > 0$$

Remark: one downstream node is adopted, which improves the accuracy but weakens(削弱) the stability.

(2) FVM — interface interpolation is implemented by two upstream nodes and one downstream node



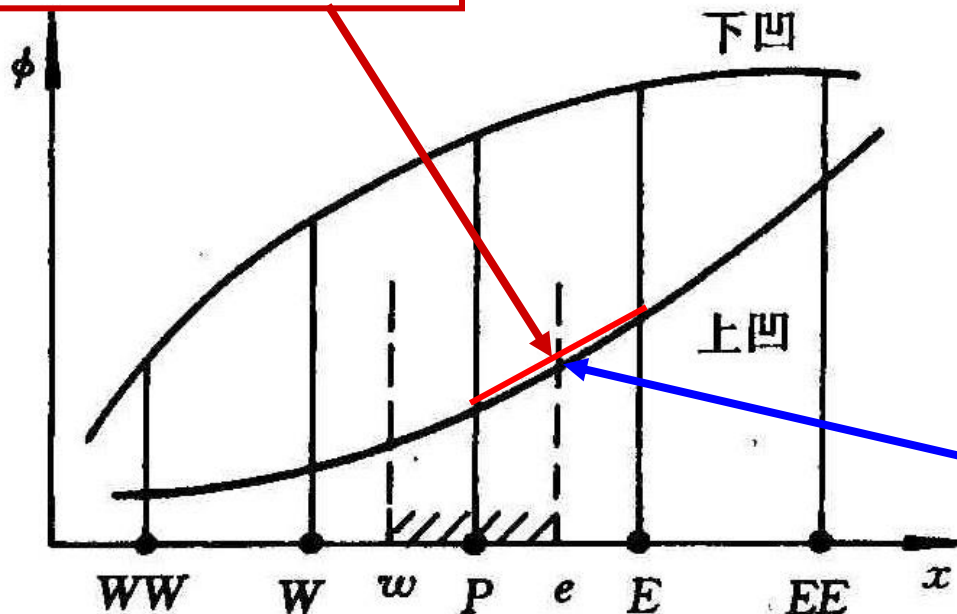
3. QUICK scheme (FVM definition)

1) Position definition – CD at interface with a curvature correction (曲率修正)

$$\phi_e = \frac{\phi_E + \phi_P}{2} - \frac{1}{8} Cur$$

CD at interface

curvature correction



Actual interface value

How to determine CUR? There are two conditions:

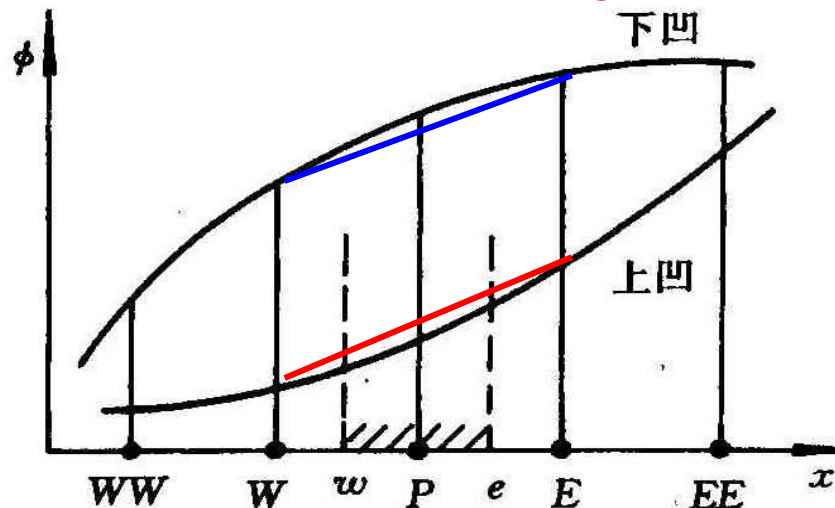
(1) reflecting concave (凹) or convex (凸) curvature automatically

Concave upward

$$(\phi_W - 2\phi_P + \phi_E) > 0, \quad -\frac{1}{8}Cur \quad \text{Decreasing the inf. value a bit!}$$

Concave downward

$$(\phi_W - 2\phi_P + \phi_E) < 0 \quad -\frac{1}{8}Cur \quad \text{Increasing the inf. value a bit!}$$



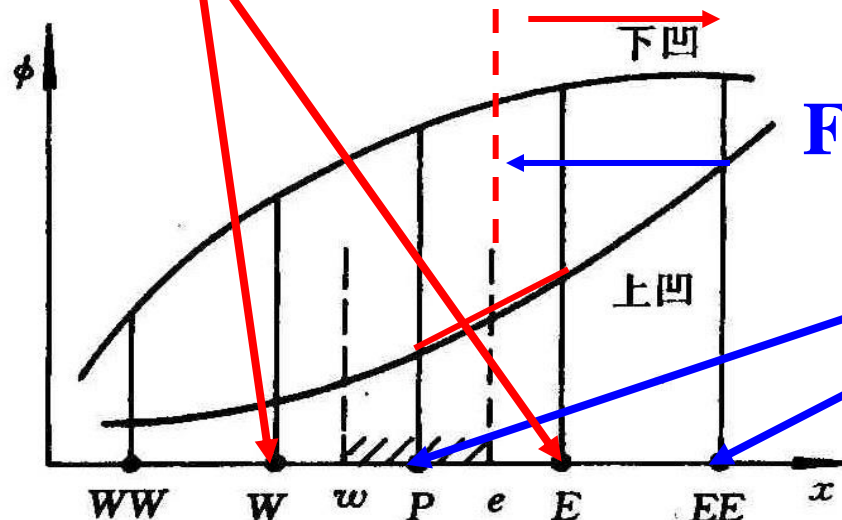
How to select three neighboring points?

(2) Adopting upwind idea for enhancing stability: for Interface e

When $u_e > 0$, taking ϕ_W, ϕ_P, ϕ_E

When $u_e < 0$, taking $\phi_P, \phi_E, \phi_{EE}$

For $u_e > 0$, taking ϕ_W, ϕ_P, ϕ_E



For $u_e < 0$, taking $\phi_P, \phi_E, \phi_{WW}$

Curvature correction for QUICK:

$$\text{Cur} = \begin{cases} \phi_W - 2\phi_P + \phi_E, u > 0 \\ \phi_P - 2\phi_E + \phi_{EE}, u < 0 \end{cases} \quad \phi_e = \frac{\phi_E + \phi_P}{2} - \frac{1}{8} \text{Cur}$$

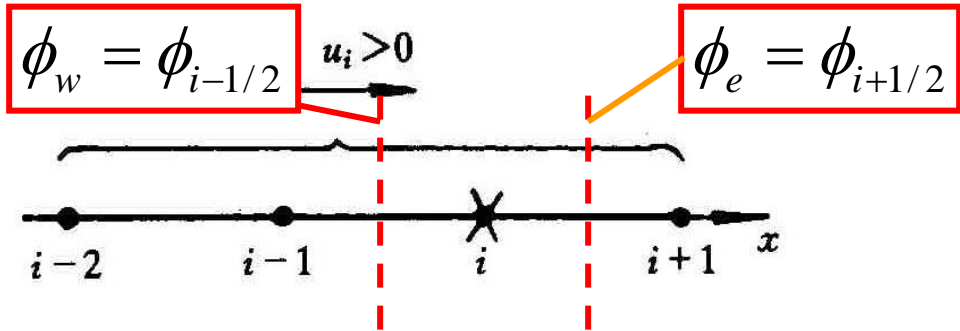
QUICK = quadratic interpolation of convective kinematics

2) QUICK –subscript definition

For $u > 0$:

$$\begin{cases} \phi_e = \phi_{i+1/2} = \frac{1}{8} (3\phi_{i+1} + 6\phi_i - \phi_{i-1}) \\ \phi_w = \phi_{i-1/2} = \frac{1}{8} (3\phi_i + 6\phi_{i-1} - \phi_{i-2}) \end{cases}$$

8 → 6 → 3



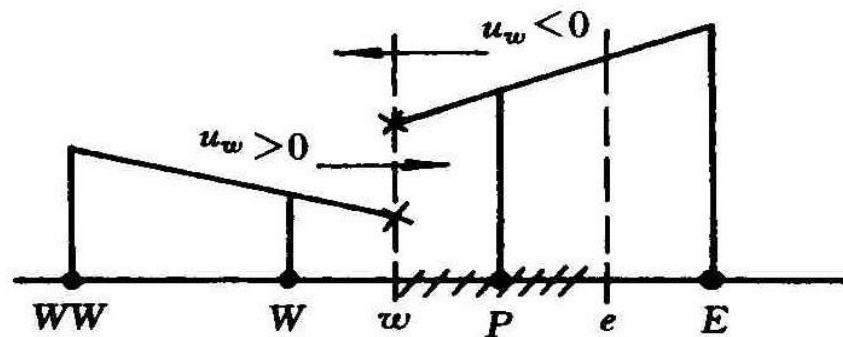
4. SGSD – A kind of composite (组合) scheme

1) SCSD scheme (1999)

CD: $\phi_e = 0.5(\phi_P + \phi_E)$ **No false diffusion (2nd order), but only conditionally stable!**

SUD: $\phi_e = \begin{cases} 1.5\phi_W - 0.5\phi_{WW}, & u > 0 \\ 1.5\phi_P - 0.5\phi_E, & u < 0 \end{cases}$

Absolutely stable (discussed later) , but has appreciable(显著的) numerical errors.



Thus combining the two schemes in such a way maybe useful:

When Pe number is small, CD predominates;

When Pe number is large, SUD predominates:

$$\phi_e^{SCSD} = \beta \phi_e^{CD} + (1 - \beta) \phi_e^{SUD}, \quad 0 \leq \beta \leq 1$$

$$\beta = 1, \phi^{SCSD} \equiv \phi^{CD}; \quad \beta = 0, \phi^{SCSD} \equiv \phi^{SUD}; \quad \beta = 3/4, \phi^{SCSD} \equiv \phi^{QUICK}$$

It can be shown:

$$P_{\Delta,cr} = \left(\frac{\rho u \delta x}{\Gamma} \right)_{cr} = \frac{2}{\beta}$$

By adjusting Beta value its critical Peclet number can vary from 0 to infinite! Thus it is called:

stability-controllable second-order difference – SCSD
(倪明玖, 1999) .

Question: how to determine Beta? Especially how to calculate beta based on the flow field automatically?

2) SGSD scheme (2002)

From $P_{\Delta,cr} = \frac{2}{\beta} \rightarrow \beta = \frac{2}{P_{\Delta,cr}}$, replace $P_{\Delta,cr}$ in denominator

by $(2 + P_{\Delta})$:

$$\beta = \frac{2}{2 + P_{\Delta}} \begin{cases} P_{\Delta} \rightarrow 0, \beta \rightarrow 1, \text{ CD dominates;} \\ P_{\Delta} \rightarrow \infty, \beta \rightarrow 0, \text{ SUD dominates} \end{cases}$$

1) It can be determined from flow field with different effects of diffusion and convection being considered automatically!

2) Three coordinates can have their own Peclet numbers!

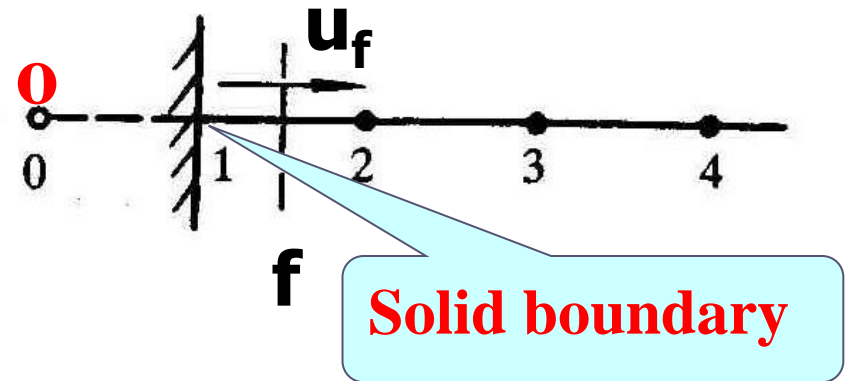
Li ZY, Tao WQ. A new stability-guaranteed second-order difference scheme.

Numerical Heat Transfer-Part B, 2002, 42 (4): 349-365

5. Discussion on implementing higher-order schemes

1) Near boundary point:

Taking practice A as an example: For the interface between nodes 1 and 2, if $u_f > 0$, how to implement higher order schemes?



Two ways can be adopted:

(1) Fictitious point method (虚拟点法): Introducing a fictitious point O and assuming:

$$\phi_o + \phi_2 = 2\phi_1 \longrightarrow \phi_o = 2\phi_1 - \phi_2$$

(2) Order reduction method (降阶法): $\phi_f = \phi_1, u_f > 0$

2) Solution of ABEqs.:

When QUICK, TUD etc. are used, the matrix of 2-D problem is nine-diagonal and the ABEqs. may be solved by

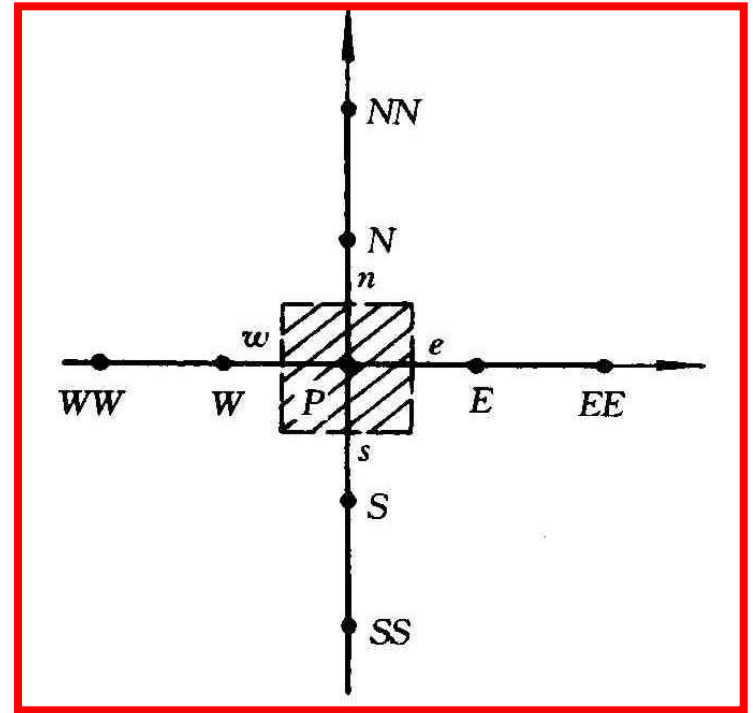
(1) **Penta-diagonal matrix**

(五对角阵算法) **PDMA;**

(2) **Deferred correction**(延迟修正)。

$$\phi_e^H = \phi_e^L + (\phi_e^H - \phi_e^L)^* \quad * - \text{previous iteration}$$

The lower-order part ϕ_e^L forms ABEqs.; those with “*” go to source part, and ADI method is used. The converged solution is the one of higher-order scheme.



Brief review of 2017-10-23 lecture key points

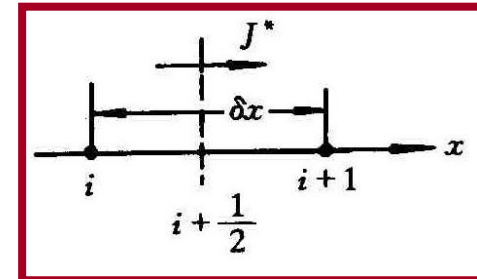
1. J^* flux discretized expression by A and B

$$J^* = \frac{J}{D} = \frac{1}{\Gamma / \delta x} (\rho u \phi - \Gamma \frac{d\phi}{dx}) = P_{\Delta} \phi - \frac{d\phi}{dX}$$

$$J^* = B(P_{\Delta})\phi_i - A(P_{\Delta})\phi_{i+1}$$

$$B(P_{\Delta}) - A(P_{\Delta}) = P_{\Delta} \quad \text{Summ/Subt}$$

$$B(P_{\Delta}) = A(-P_{\Delta}); A(P_{\Delta}) = B(-P_{\Delta}) \quad \text{Symmetry}$$



2. General expressions of coefficients of 1D model eq.

$$a_E = D_e A(|P_{\Delta e}|) + \|-F_e, 0\| \quad a_W = D_w A(|P_{\Delta w}|) + \|F_w, 0\|$$

$$a_P = a_E + a_W + (F_e - F_w)$$

3. Major concept of false diffusion

Numerical errors caused by discretized scheme of 1st order accuracy is called false diffusion;

Numerical errors caused by oblique intersection of flow direction with grid lines and non-constant source term.

4. Methods for alleviating false diffusion

TUD $u > 0, \frac{\partial \phi}{\partial x}_i = \frac{1}{6\Delta x} (2\phi_{i+1} + 3\phi_i - 6\phi_{i-1} + \phi_{i-2})$

QUICK $u > 0$

$$\phi_e = \phi_{i+1/2} = (1/8)(3\phi_{i+1} + 6\phi_i - \phi_{i-1})$$

$$\phi_w = \phi_{i-1/2} = (1/8)(3\phi_i + 6\phi_{i-1} - \phi_{i-2})$$

SGSD $\phi_e^{SCSD} = \beta \phi_e^{CD} + (1 - \beta) \phi_e^{SUD} \quad \beta = 2/(2 + P_\Delta)$

5.6.2 Methods for alleviating (减轻) effects of cross-diffusion

1. Adopting effective diffusivity for FUD

$$(\Gamma_{\phi,x})_{eff} = \left\| 0, (\Gamma_{\phi} - \Gamma_{cd,x}) \right\|$$

Γ_{ϕ} – diffusivity of physical problem;

$\Gamma_{cd,x}$ – diffusivity from cross false diffusion

By reducing diffusivity used in simulation the cross diffusion effect can be alleviated.

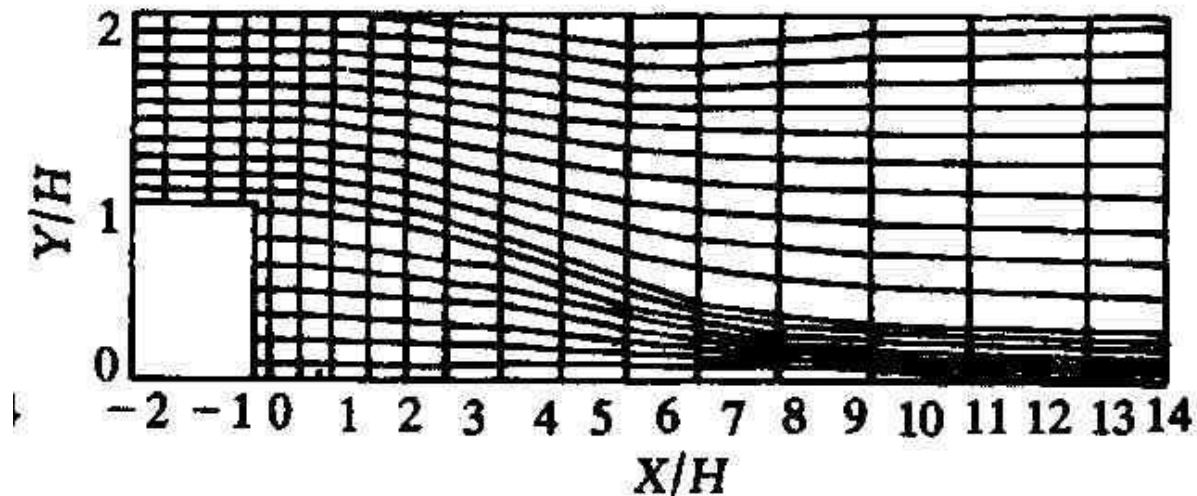
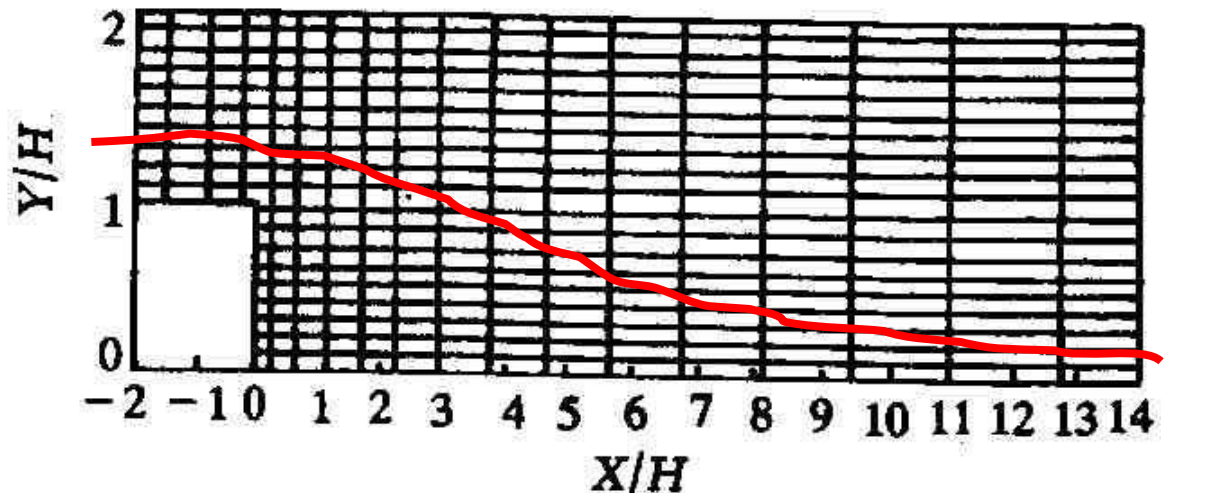
$$\Gamma_{cd,x} = u\Delta x \left(1 - \frac{u\delta t}{\Delta x}\right)$$

Inspired (得到启发) from
Noye problem

$$\delta t = \frac{1}{\frac{u}{\Delta x} + \frac{v}{\Delta y} + \frac{w}{\Delta z}}$$

2. Adopting self-adaptive grids (SAG-自适应网格)

SAG can alleviate (减轻) cross-diffusion caused by oblique intersection of streamline to grid line



5.7 Stability analysis of discretized diffusion-convection equation

5.7.1 Three kinds of instability in numerical simulation

5.7.2 Sign preservation principle for analyzing convective instability

1. Basic idea

2. Analysis method

3. Implementation procedure

4. Implementation example

5.7.3 Discussion on the stability analysis results

5.7.4 Summary of adopting convective scheme

5.7 Stability analysis of discretized diffusion-convection equation

5.7.1 Three kinds of instability in numerical simulation

1. Instability of explicit scheme for initial problem

Too large time step of explicit scheme will introduce oscillating results; Purpose of stability study is to find the allowed maximum time step; for 1-D diffusion problem:

$$\frac{a\Delta t}{\Delta x^2} \leq 0.5$$

2. Instability of iterative solution procedure of ABEqs.

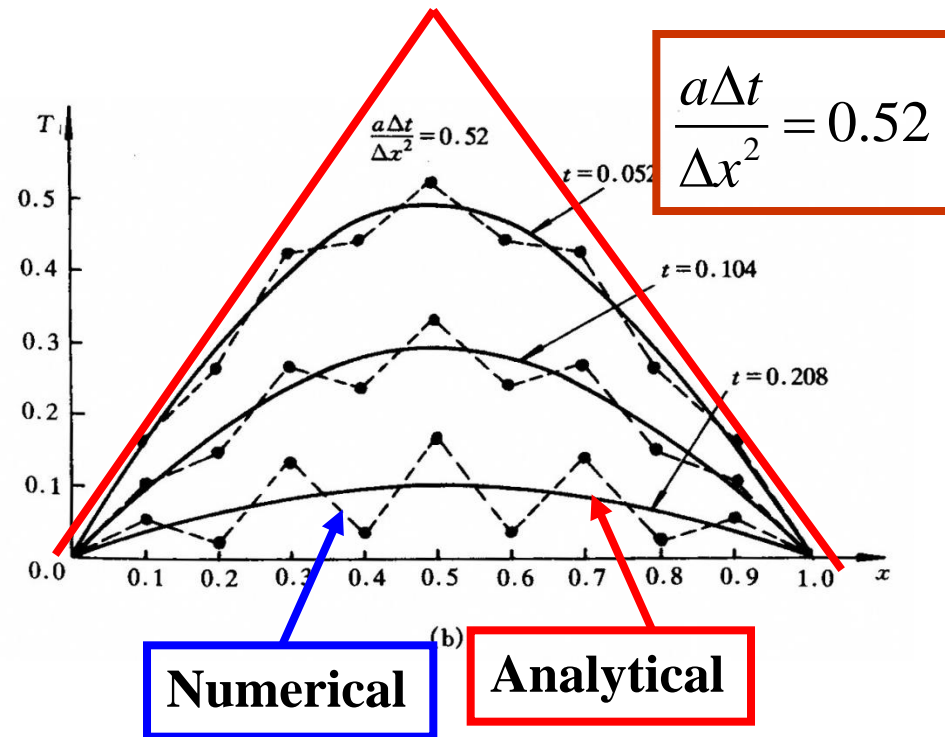
If iterative procedure can not converge, such procedure is called unstable! Unstable procedure can not get a solution!

3. Instability caused by discretized convective term

For CD, QUICK, TUD large space step, high velocity may cause to oscillating (wiggling) (振荡的) results. It is called convective instability. The purpose of stability study is to find the related critical Peclet number.

The consequence (后果) of the three instabilities:

1. Transient instability of explicit scheme: **oscillating solutions**, and these are the actual solutions of the ABEqs. solved.
2. Instability of solution procedure for ABEqs.: **no solution at all.**

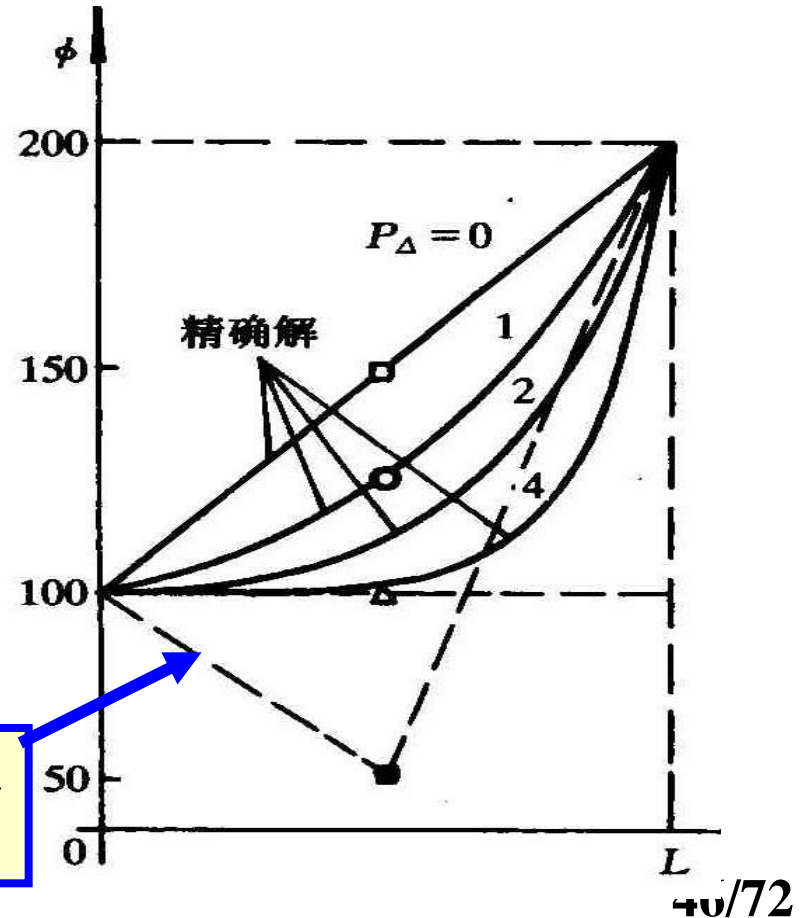


Von Neumann method can be adopted to analyze such instability, see

Ni MJ, Tao WQ, Wang SJ .Stability analysis for discretized steady convective-diffusion equation. Numerical Heat Transfer, Part B,1999, 35 (3): 369-388

3. **Convective instability** :
 leading to oscillating solutions and they are the actual solution of the ABEqs. solved.
 The problem is caused by unphysical coefficients of the discretized equations.

Actual solution of the scheme



5.7.2 Sign preservation principle for analyzing convective instability

1. Basic idea:

An iterative solution procedure of the ABEqs. of diffusion-convection problem is a marching process (步进过程), from step to step, like the solution procedure of the explicit scheme of an initial problem;

If any disturbance (扰动) at a node is transported in such a way that its effect on the neighboring node is of the opposite sign (符号相反) then the final solution will be oscillating.

Thus to avoid oscillating results we should require that any disturbance at a node should be transported in such a way that its effect on the neighboring nodes must have the same sign as the original disturbance, i.e., **sign should be preserved**(符号不变).

2. Analysis method:

- (1) The iterative solution procedure of the discretized diffusion-convection equation is modeled by the **marching process** of the **explicit scheme** of an initial problem;
- (2) Stability is an inherent (**固有的**) character, which can be tested by adding any disturbance ;
- (3) The studied scheme is used to discretize the convection term of 1-D transient diffusion-convection

equation, and diffusion term is by CD; The transfer of a disturbance to the next time level is determined by the **discrete disturbance analysis method**.

(4) Stability of the scheme requires that the effect of any disturbance at any time level on the neighboring point at the next time level **must has the same sign**.

3. Implementation procedure

- (1) Applying the studied scheme to the explicit scheme of 1-D transient diffusion-convection equation ;
- (2) Adopting the discrete disturbance analysis method to determine the transportation of disturbance ε_i^n introduced at any time level n and node i ;

(3) Stability of the studied scheme requires:

$$\frac{\phi_{i\pm 1}^{n+1}}{\epsilon_i^n} \geq 0 \quad (\text{Sign preservation principle, SPP})$$

If above equation is unconditionally valid, the scheme is absolutely stable; Otherwise the condition that makes the above equation valid gives the critical Peclet number.

(4) We have shown that disturbance transportation by CD of diffusion term is $\frac{\Gamma \Delta t}{\rho \Delta x^2}$, discrete disturbance analysis can only be conducted for the studied convection scheme, and then adding the two effect terms together.

4. Implementation example

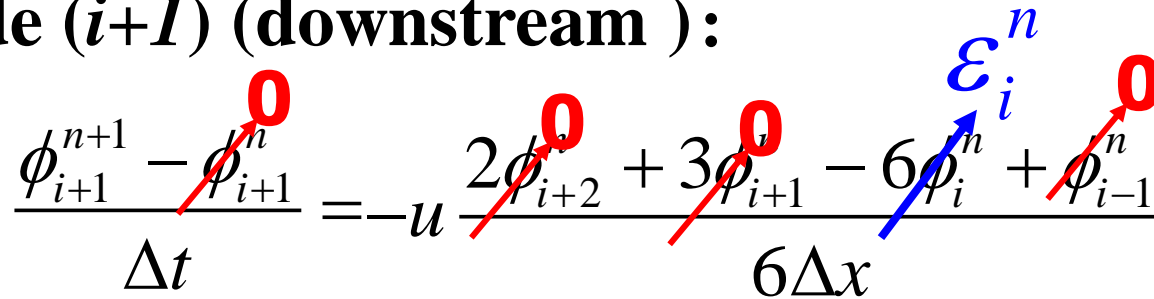
Stability analysis for TUD scheme:

Disturbance analysis for the convection term

$$\frac{\partial \phi}{\partial t} = -u \frac{\partial \phi}{\partial x} \quad \boxed{u \geq 0} \quad \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = -u \frac{2\phi_{i+1}^n + 3\phi_i^n - 6\phi_{i-1}^n + \phi_{i-2}^n}{6\Delta x}$$

For node $(i+1)$ (downstream):

$$\frac{\phi_{i+1}^{n+1} - \phi_{i+1}^n}{\Delta t} = -u \frac{2\phi_{i+2}^n + 3\phi_{i+1}^n - 6\phi_i^n + \phi_{i-1}^n}{6\Delta x}$$



Thus:
$$\phi_{i+1}^{n+1} = \left(\frac{u\Delta t}{\Delta x} \right) \varepsilon_i^n$$

Disturbance is transported by convection downstream!

For node $(i-1)$ (upstream):

$$\frac{\phi_{i-1}^{n+1} - \cancel{\phi_{i-1}^n}}{\Delta t} = -u \frac{2\phi_i^n + 3\cancel{\phi_{i-1}^n} - 6\cancel{\phi_{i-2}^n} + \cancel{\phi_{i-3}^n}}{6\Delta x} \implies \phi_{i-1}^{n+1} = -\frac{1}{3} \left(\frac{u\Delta t}{\Delta x} \right) \varepsilon_i^n$$

Disturbance is transported upstream with opposite sign!

For node (i+1):

$$\frac{\frac{\Gamma \Delta t}{\Delta x^2} + \left(\frac{u\Delta t}{\Delta x} \right) \varepsilon_i^n}{\varepsilon_i^n} > 0 \quad \text{Automatically}$$

For node (i-1):

$$\frac{\frac{\Gamma \Delta t}{\Delta x^2} - \frac{1}{3} \left(\frac{u\Delta t}{\Delta x} \right) \varepsilon_i^n}{\varepsilon_i^n} \geq 0 \quad \text{Only when} \quad \frac{\rho u \Delta x}{\Gamma} \leq 3 \implies P_{\Delta cr} = 3!$$

Leonard once analyzed the stability character of TUD and concluded that it is inherently stable.

However numerical practice shows it is only conditionally stable.

5.7.3 Discussion on the analysis results

- 1) For those schemes possessing transportive property the SPP is always satisfied, and the schemes are absolutely stable, such as **FUD**, **SUD**;
- 2) For those schemes containing downstream node they do not possess transportive property, and are **often conditionally stable**. Only when coefficients in the interpolation satisfy certain conditions they can be absolutely stable: **CD**, **TUD**, **QUICK**, **FROMM**;
- 3) For conditionally stable schemes, the larger the coefficients of the downstream nodes the smaller the critical Peclet number.

CD:
$$\phi_e = \frac{\phi_E + \phi_P}{2},$$

Coefficient of downstream node is 1/2, $P_{\Delta cr} = 2$

QUICK:
$$\phi_{i+1/2} = \frac{1}{8}(3\phi_{i+1} + 6\phi_i - \phi_{i-1})$$

Coefficient of downstream node is 3/8, $P_{\Delta cr} = 8/3$

TUD:
$$\left(\frac{\partial \phi}{\partial x}\right)_i = \frac{2\phi_{i+1} + 3\phi_i - 6\phi_{i-1} + \phi_{i-2}}{6\Delta x}$$

Coefficient of downstream node is 2/6,

$$P_{\Delta cr} = 6 / 2 = 3$$

FROMM:
$$\phi_e = \frac{1}{4}(\phi_{i+1} + 4\phi_i - \phi_{i-1})$$

Coefficient of downstream node is 1/4, $P_{\Delta cr} = 4$

There is some inherent relationship!

4) Derivation conditions (导出条件) for obtaining the above results:

- (1) 1-D problem;**
- (2) Linear problem (u, Γ are known constants) ;**
- (3) Two-point boundary problem (1st kind);**
- (4) No source term;**
- (5) Uniform grid system;**
- (6) Diffusion term is discretized by CD.**

**The resulted critical Peclet is the smallest one;
Violation(违反) of the any above condition will
enhance (强化) scheme stability.**

5.7.4 Summary of adopting convective scheme

1. For conventional fluid flow and heat transfer problems, in the debugging process(调试过程) FUD or PLS may be used; For the final computation QUICK or SGSD is recommended, and defer correction is used for solving the ABEqs.
2. For DNS (直接模拟)of turbulent flow, schemes of fourth order or more are often used;
3. When there exists a sharp variation of properties, higher order and bounded schemes (高阶有界格式) should be used.

Recent advances in scheme construction can be found in:

Jin W W, Tao W Q. Numerical Heat Transfer, Part B, 2007, 52(3): 131-254
Jin W W, Tao W Q. Numerical Heat Transfer, Part B, 2007, 52(3): 255-280

Appendix of Section 5-7

Summary of stability analysis results

Stability of seven schemes

No	Scheme	Definition of scheme	Transferred by convection		Stability condition
			Up	Down	
1	FUD	$\left. \frac{\partial \phi}{\partial x} \right _i \approx \frac{\phi_i - \phi_{i-1}}{\Delta x}, u > 0$ $\frac{\phi_{i+1} - \phi_i}{\Delta x}, u < 0$	0	$\left(\frac{u\Delta t}{\Delta x}\right)^\epsilon$	Abs. stable
2	CD	$\left. \frac{\partial \phi}{\partial x} \right _i \approx \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x}$	$-\frac{1}{2}$ $\left(\frac{u\Delta t}{\Delta x}\right)^\epsilon$	$\frac{1}{2}$ $\left(\frac{u\Delta t}{\Delta x}\right)^\epsilon$	$P_\Delta \leq 2$

No	Scheme	Definition of scheme	Transferred by convection		Stability condition
			Up	Down	
3	SUD	$\left. \frac{\partial \phi}{\partial x} \right _i \cong \frac{\phi_i - \phi_{i-1}}{\Delta x} + \frac{\phi_i - 2\phi_{i-1} + \phi_{i-2}}{2\Delta x}, u > 0$ $\frac{\phi_{i+1} - \phi_i}{\Delta x} + \frac{\phi_i - 2\phi_{i+1} + \phi_{i+2}}{2\Delta x}, u < 0$	0	$2\left(\frac{u\Delta t}{\Delta x}\right)\epsilon$	Abs. stable
4	TUD	$\left. \frac{\partial \phi}{\partial x} \right _i \cong \frac{2\phi_{i+1} + 3\phi_i - 6\phi_{i-1} + \phi_{i-2}}{6\Delta x}, u > 0$ $\frac{-\phi_{i+2} + 6\phi_{i+1} - 3\phi_i - 2\phi_{i-1}}{6\Delta x}, u < 0$	$-\frac{1}{3}$	$\left(\frac{u\Delta t}{\Delta x}\right)\epsilon$	$P_\Delta \leq 3$
5	Fromm	$\phi_{i+1/2} = \frac{1}{4}(\phi_{i+1} + 4\phi_i - \phi_{i-1})$	$-\frac{1}{4}$	$\frac{1}{4}$	$P_\Delta \leq 4$



No	Scheme	Definition of scheme	Transferred by convection		Stability condition
			Up	Down	
6	QUICK	$\phi_{i+1/2} = \frac{\phi_i + \phi_{i+1}}{2} - \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{8}, u > 0$ $\frac{\phi_i + \phi_{i+1}}{2} - \frac{\phi_{i+2} - 2\phi_{i+1} + \phi_i}{8}, u < 0$	$\frac{-3}{8}$ $\left(\frac{u\Delta t}{\Delta x}\right)_\epsilon$	$\frac{7}{8}$ $\left(\frac{u\Delta t}{\Delta x}\right)_\epsilon$	$P_\Delta \leq \frac{8}{3}$
7	Expon. scheme	<p>Discretized form of 1-D diffusion-convection eq.</p> $a_P \phi_P = a_E \phi_E + a_W \phi_W$ $a_E = \frac{\rho u}{\exp(P_\Delta) - 1}, a_W = \frac{\rho u \exp(P_\Delta)}{\exp(P_\Delta) - 1}$ $a_P = a_E + a_W + a_P^0, b = a_P^0 \phi_P^0, a_P^0 = \frac{\rho \Delta x}{\Delta t}$	<p>Total effects of Dif-Con</p> $\frac{a_E}{a_P} \epsilon (\geq 0) \quad \left \quad \frac{a_W}{a_P} \epsilon (\geq 0)$		<p>Abs. stable</p>

5.8 Discretization of multi-dimensional problem and B.C. treatment

5.8.1 Discretization of 2-D diffusion-convection equation

1. Governing equation expressed by J_x, J_y

2. Results of discretization

3. Ways for adopting other schemes

5.8.2 Treatment of boundary conditions

1. Inlet boundary

2. Solid boundary

3. Central line

4. Outlet boundary

5.8 Discretization of multi-dimensional problem and B.C. treatment

5.8.1 Discretization of 2-D diffusion-convection equation

1. Governing equation expressed J_x , J_y

$$\frac{\partial(\rho\phi)}{\partial t} + \frac{\partial(\rho u\phi)}{\partial x} + \frac{\partial(\rho v\phi)}{\partial y} = \frac{\partial}{\partial x} \left(\Gamma \frac{\partial\phi}{\partial x} \right) + \frac{\partial}{\partial y} \left(\Gamma \frac{\partial\phi}{\partial y} \right) + S$$

$$\frac{\partial(\rho\phi)}{\partial t} + \frac{\partial}{\partial x} \underbrace{(\rho u\phi - \Gamma \frac{\partial\phi}{\partial x})}_{J_x} + \frac{\partial}{\partial y} \underbrace{(\rho v\phi - \Gamma \frac{\partial\phi}{\partial y})}_{J_y} = S$$

$$\frac{\partial(\rho\phi)}{\partial t} + \frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} = S$$

2. Results of discretization

$$a_P \phi_P = a_E \phi_E + a_W \phi_W + a_S \phi_S + a_N \phi_N + b$$

$$a_P = a_E + a_W + a_N + a_S + a_P^0 - S_P \Delta V$$

$$b = S_C \Delta V + a_P^0 \phi_P^0 \quad a_P^0 = \frac{\rho_P \Delta V}{\Delta t}$$

$$a_E = D_e A(|P_{\Delta e}|) + \|-F_e, 0\| \quad a_W = D_w A(|P_{\Delta w}|) + \|F_w, 0\|$$

$$a_N = D_n A(|P_{\Delta n}|) + \|-F_n, 0\| \quad a_S = D_s A(|P_{\Delta s}|) + \|F_s, 0\|$$

(Derivation process is shown in appendix):

3. Ways for adopting other schemes

- 1) Through source term for introducing the additional part of other scheme ;
- 2) The ABEqs. are solved by defer correction method

5.8.2 Treatment of boundary conditions

1. Inlet boundary – usually specified;

2. Center line – symmetric boundary:

Velocity component normal to the center line is equal to zero;

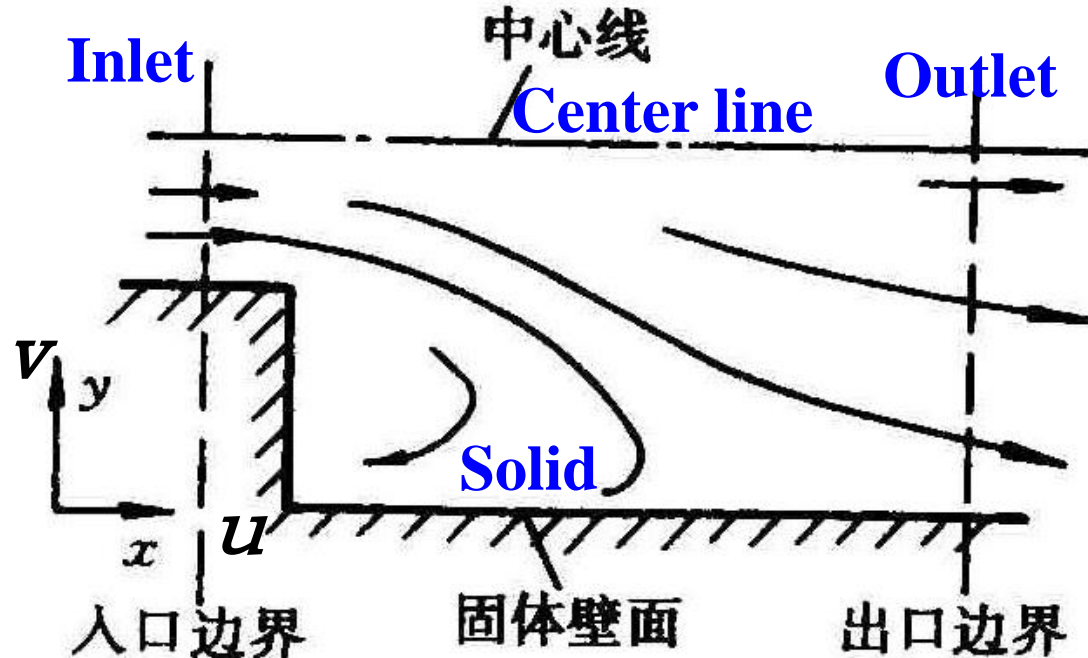
First derivative normal to the line of other variable is equal to zero.

$$v = 0; \frac{\partial \phi}{\partial n} = 0$$

3. Solid boundary

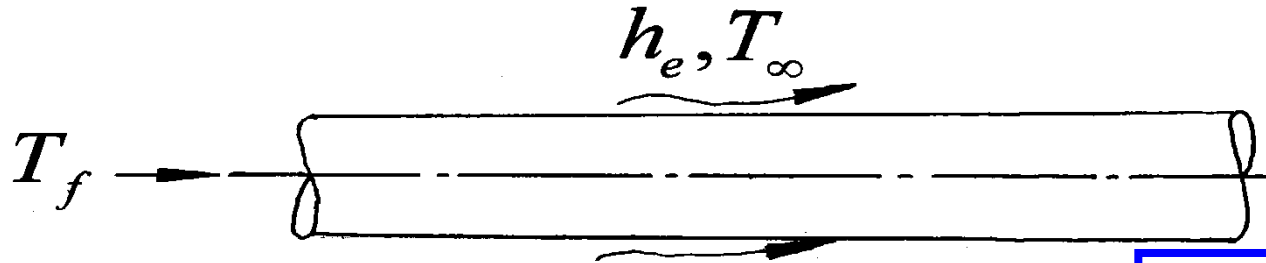
No slip for u, v ;

Three types for T.



Known temp. - 1; Given heat flux - 2;

External convection - 3;



4. Outlet boundary

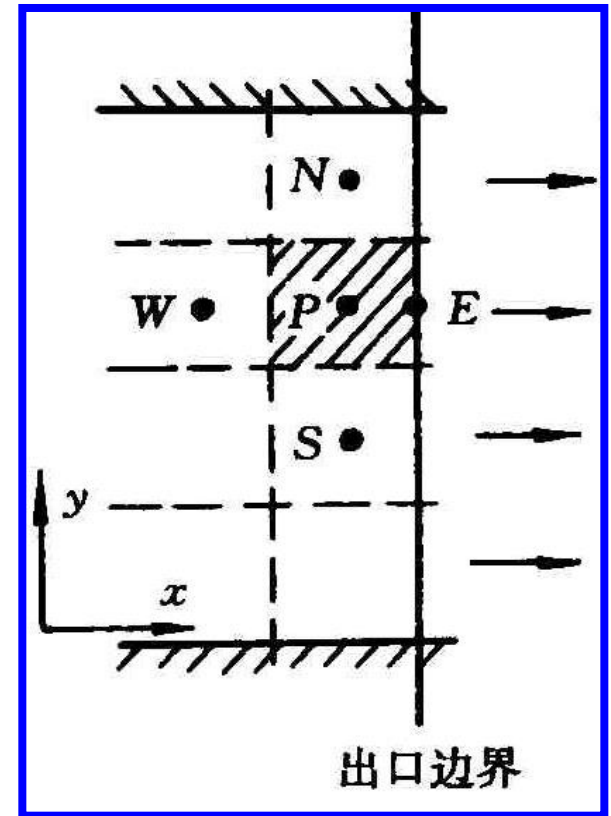
Conventional methods:

(1) Local one-way (局部单向化)

$$a_E = 0$$

(2) Fully developed (充分发展)

$$\frac{\partial \phi}{\partial x} = 0 \longrightarrow \phi_E = \phi_P^*$$



Appendix of Section 5-8

In order to extend the results of 1-D discussion,
introducing J_x , J_y to 2-D case

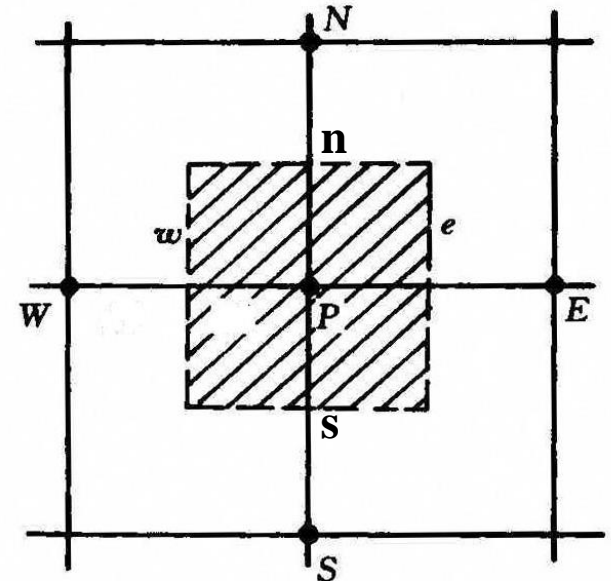
Integrating above equations
for CV. P

$$\iiint \frac{\partial(\rho\phi)}{\partial t} dt dx dy = [(\rho\phi)_P - (\rho\phi)_P^0] \Delta V$$

$$\iiint \frac{\partial J_x}{\partial x} dx dy dt = \int_{t+\Delta t}^t \int_n^s (J_x^e - J_x^w) dy dt$$

$$\iiint \frac{\partial J_x}{\partial x} dx dy dt = \int_{t+\Delta t}^t \int_n^s (J_x^e - J_x^w) dy dt$$

$$\iiint S dx dy dt = (S_C + S_P \phi_P) \Delta V \Delta t$$



Assuming that at the interface J_x^e, J_x^w are constant:

$$(J_x^e - J_x^w) \Delta y \Delta t = (J_e - J_w) \Delta t \quad J_e = J_x^e \Delta y, J_w = J_x^w \Delta y$$

Introducing J^* and adopting the characters of the coefficients

$$J_e = J_e^* D_e = D_e [B(P_{\Delta e}) \phi_P - A(P_{\Delta e}) \phi_E]$$

Add-sub

$$J_e = J_e^* D_e = D_e [\{A(P_{\Delta e}) + P_{\Delta e}\} \phi_P - A(P_{\Delta e}) \phi_E]$$

$$J_e = J_e^* D_e = \{D_e A(P_{\Delta e}) + F_e\} \phi_P - D_e A(P_{\Delta e}) \phi_E$$

$$J_e = J_e^* D_e = \underbrace{D_e A(P_{\Delta e})}_{a_E} \phi_P + F_e \phi_P - \underbrace{D_e A(P_{\Delta e})}_{a_E} \phi_E$$

a_E

a_E

$$D_e = \frac{\Gamma \Delta y}{\delta x},$$

$$F_e = \rho u \Delta y$$



Home work of Chapter 5

5-2 5-3 5-8 5-9 5-11

For Problem 5-8, only QUICK and FUD are adopted and compared.

Home work due on 11-01

Problem # 5-2

One-dimensional steady-state convection diffusion equation without source term, whereas boundary conditions are $x=0, \phi = \phi_0, x=L, \phi = \phi_L$. Taking 10 to 20 nodes for range $x/L = 0 \sim 1$, using the following 4 methods: Central difference, first order upwind, Hybrid scheme and QUICK scheme, then draw the plot between $(\phi - \phi_0)/(\phi_L - \phi_0)$ and x/L using three values of Peclet number i.e. $P_\Delta = 1, 5, 10$ and compare the results with exact values.

(Note: take care the difference between grid Peclet number, P_Δ , whole Peclet number

and $P_\Delta = \frac{\rho u L}{\Gamma}$).

Problem # 5-3

For one-dimensional unsteady convection - diffusion equation

$$\frac{\partial(\rho\phi)}{\partial(t)} = -\frac{\partial(\rho u\phi)}{\partial x} + \frac{\partial}{\partial x} \left(\Gamma \frac{\partial\phi}{\partial x} \right), \text{ using power law scheme for the discretization and find}$$

the values of followings constants a_E , a_W , a_P^0 and $a_P : \Delta t = 0.05$, where $\rho u = 1$,

$P_\Delta = 0.1, 10$. All units are the same.

Problem 5-8

For 1-D diffusion-convection problem with source term, following conditions are given: $x = 0, \phi = 0, x = 1, \phi = 1; S = 0.5 - x$

By adopting (1) FUD, (2) QUICK for the convection term and CD for the diffusion term, calculate the values of ϕ at 10-20 uniformly distributed grids. Compare the numerical results with the analytical solution.

Hint: The analytical solution is

$$T = \frac{\exp(PeX) - 1}{\exp(Pe) - 1} - \frac{X^2}{2Pe} + \frac{X}{2Pe} \quad 0 \leq X \leq 1$$

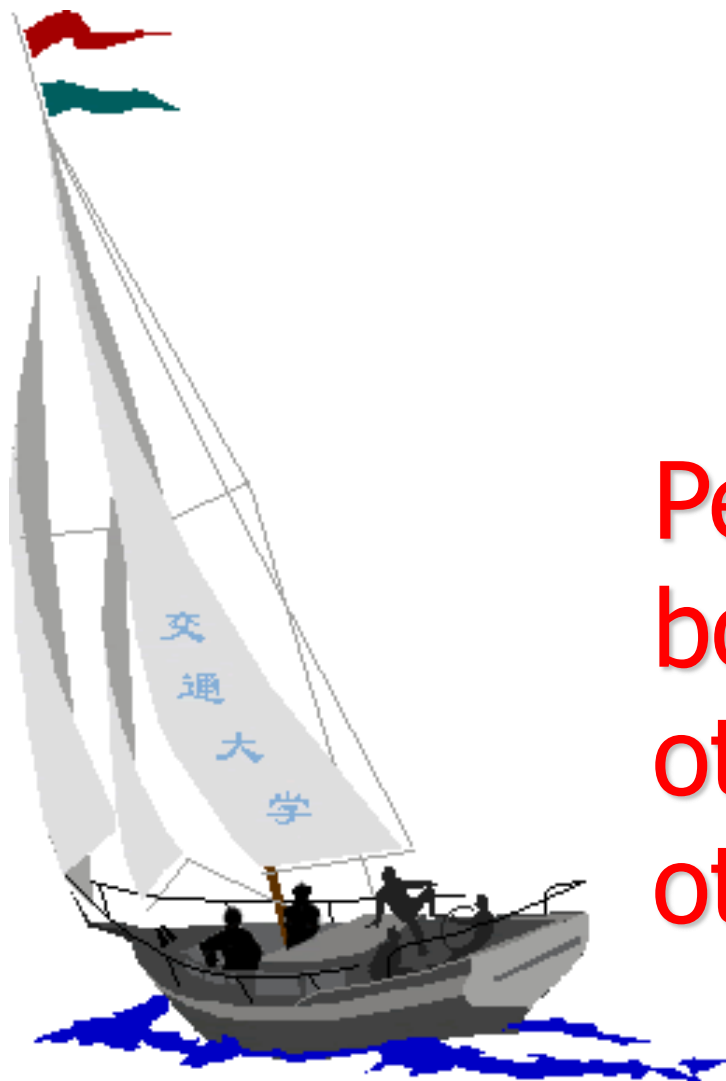
$$T = \frac{\phi - \phi_0}{\phi_L - \phi_0} \quad X = \frac{x}{L}$$

Problem # 5-9

Define the third-order upwind scheme using the interface function interpolation method and verify the consistence in form with the definition of derivative expression for given nodes.

Problem 5-11

Adopt the Fromm scheme for the convection term of 1-D diffusion-convection equation without source term . Analyze its stability by sign preservation principle and find its critical grid Peclet number.



同舟共济 渡彼岸!

People in the same
boat help each
other to cross to the
other bank, where....