

(数值传热学)

Chapter 4 Discretized Schemes of Diffusion and Convection Equation (2)



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### Chapter 4 Discretized diffusion-convection equation

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- 4.2 CD and UD of the convection term
- 4.3 Hybrid and power-law schemes
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### 4.5 Discussion on false diffusion

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### 4.5 Discussion on false diffusion

### 4.5.1 Meaning and reasons of false diffusion

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

### 1. Original meaning

Numerical errors caused by discretized scheme with 1<sup>st</sup> order accuracy is called false diffusion;

By Taylor expension, the equation of such scheme at the second-order sense contains  $2^{nd}$  order derivative, thus the diffusion action is somewhat magnified (放大) at the sense of (在…意义上) second-order accuracy, hence the numerical error is called "false diffusion".

Taking 1-D unsteady advection (black) equation as an example. The two 1<sup>st</sup>-order derivatives are discretized by 1<sup>st</sup>-order accuracy schemes.

1<sup>st</sup>-order derivatives

$$\frac{\partial \phi}{\partial t} = -u \frac{\partial \phi}{\partial x} \xrightarrow{\text{1st-oder scheme}} \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = -u \frac{\phi_i^n - \phi_{i-1}^n}{\Delta x}$$

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

$$\frac{\phi_{i}^{h} + \lambda_{t} \frac{\partial \phi}{\partial t})_{i,n} + \frac{1}{2} \lambda_{t}^{2} \frac{\partial^{2} \phi}{\partial t^{2}})_{i,n} + \frac{1}{6} \lambda_{t}^{3} \frac{\partial^{3} \phi}{\partial t^{3}})_{i,n} \dots - \phi_{i}^{h}}{\lambda_{t}^{h}} = \frac{\lambda_{t}^{h} - \left[\phi_{i}^{h} - \lambda_{t} \frac{\partial \phi}{\partial x}\right]_{i,n} + \frac{1}{2} \lambda_{t}^{2} \frac{\partial^{2} \phi}{\partial x^{2}})_{i,n} - \frac{1}{6} \lambda_{t}^{3} \frac{\partial^{3} \phi}{\partial x^{3}})_{i,n} \dots}{\lambda_{t}^{h}} = \frac{\lambda_{t}^{h} - \left[\phi_{i}^{h} - \lambda_{t} \frac{\partial \phi}{\partial x}\right]_{i,n} + \frac{1}{2} \lambda_{t}^{2} \frac{\partial^{2} \phi}{\partial x^{2}})_{i,n} - \frac{1}{6} \lambda_{t}^{3} \frac{\partial^{3} \phi}{\partial x^{3}})_{i,n} \dots}{\lambda_{t}^{h}} = \frac{\lambda_{t}^{h} - \left[\phi_{i}^{h} - \lambda_{t} \frac{\partial \phi}{\partial x}\right]_{i,n} + \frac{1}{2} \lambda_{t}^{2} \frac{\partial^{2} \phi}{\partial x^{2}})_{i,n} - \frac{1}{6} \lambda_{t}^{3} \frac{\partial^{3} \phi}{\partial x^{3}})_{i,n} \dots}{\lambda_{t}^{h}} = \frac{\lambda_{t}^{h} - \lambda_{t}^{h} - \lambda_{t}^{h} \frac{\partial \phi}{\partial x}}{\lambda_{t}^{h}} + \frac{1}{2} \lambda_{t}^{h} \frac{\partial^{2} \phi}{\partial x^{2}})_{i,n} - \frac{1}{6} \lambda_{t}^{h} \frac{\partial^{3} \phi}{\partial x^{3}})_{i,n} \dots}{\lambda_{t}^{h}} = \frac{\lambda_{t}^{h} - \lambda_{t}^{h} \frac{\partial^{2} \phi}{\partial x}}{\lambda_{t}^{h}} + \frac{1}{2} \lambda_{t}^{h} \frac{\partial^{2} \phi}{\partial x^{2}})_{i,n} - \frac{1}{6} \lambda_{t}^{h} \frac{\partial^{3} \phi}{\partial x^{3}})_{i,n} \dots}{\lambda_{t}^{h}} = \frac{\lambda_{t}^{h} - \lambda_{t}^{h} \frac{\partial^{2} \phi}{\partial x}}{\lambda_{t}^{h}} + \frac{1}{2} \lambda_{t}^{h} \frac{\partial^{2} \phi}{\partial x^{2}} + \frac{1}{2} \lambda_{t}^{h} \frac{\partial^{3} \phi}{\partial x^{3}} + \frac{1}$$



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

where the transient  $2^{nd}$  derivative can be re-written as follows:

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

$$\frac{\Delta t}{2} \frac{\partial^{2}\phi}{\partial t^{2}} \Big|_{i,n} = \frac{\Delta t}{2} u^{2} \frac{\partial^{2}\phi}{\partial x^{2}}; \quad \text{Substituting into Equation (1):}$$

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

Thus at the sense of  $2^{nd}$ -order accuracy above discretized equation simulates a convective-diffusive process,rather than an advection process(平流,纯对流).





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.

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

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



### 2. Extended meaning (扩展的意义)

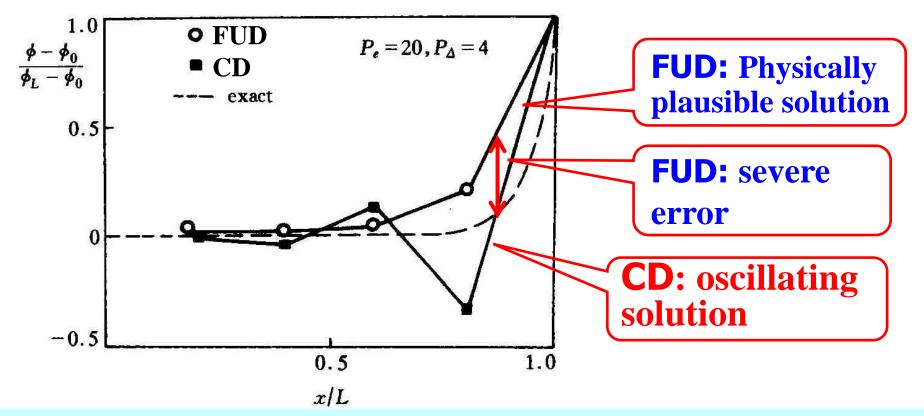
In most existing (现存) literatures almost all numerical errors are called false diffusion, which includes:

- (1) 1<sup>st</sup>-order accuracy schemes of the 1<sup>st</sup> order derivatives (original meaning);
- (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.
- 4.5.2 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)



EFD-NHT-EHT from analytical solutions:



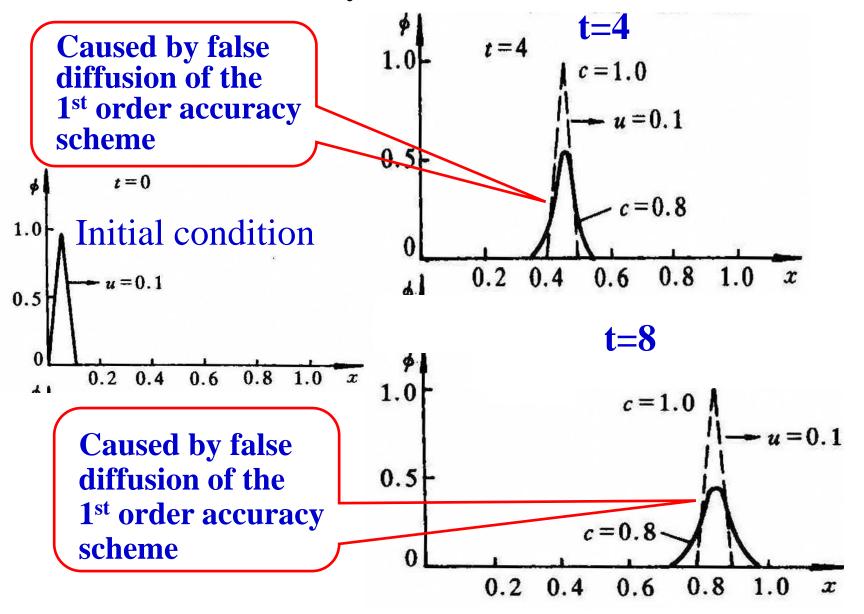
## 2. 1-D unsteady advection problem (Noye,1976) (20241008)

$$\frac{\partial \phi}{\partial t} = -u \frac{\partial \phi}{\partial x}, \quad 0 \le x \le 1, u = 0.1 \text{ (Linear problem)} \quad \phi(0, t) = \phi(1, t) = 0$$

In the range of  $x \in [0,0.1]$  initial distribution is an triangle, others are zero. The two derivatives are discretized by



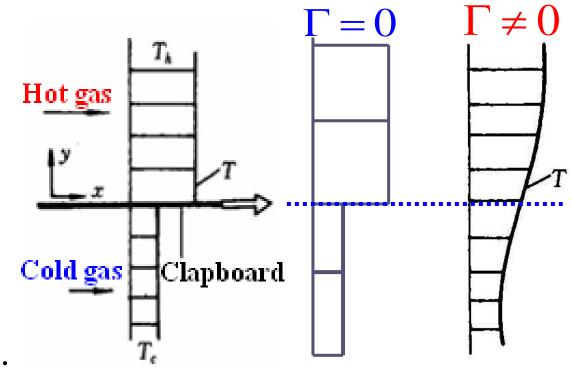
the 1<sup>st</sup> –order accuracy schemes. The results are as follows.



When Courant number is less than 1, severe (严重的) error occurs, which erases (抹平) the sharp peak (抹平尖峰) and magnify the base (放大基底) gradually. Such error is called streamwise false diffusion (流向假扩散).

## 4.5.3 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 obliquely with respect to the grid lines, big numerical errors will be introduced.



Gas flow with 0 and non-0 Gamma



## 1. Case 1: with x-y coordinates either parallel or perpendicular (垂直的) to flow direction

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

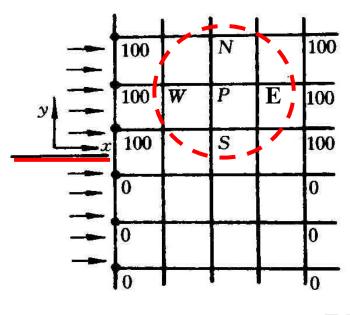
$$a_E = D_e + \llbracket -F, 0 \quad U > 0, \Gamma = 0$$

$$a_{W} = D_{W} + [F_{W}, 0] \quad U > 0, \Gamma = 0$$

Similar expressions can be written for north and south nodes:

$$a_N = D_n + [-F, 0] \quad V = 0, \Gamma = 0$$

$$a_S = D_s + [F, 0]$$
  $V = 0, \Gamma = 0$  Upstream velocity  $U$ 



Thus we have: 
$$a_P = \alpha_E + a_W + \alpha_N + \alpha_S = a_W \text{ so } \phi_P = \phi_W !$$

The upstream temperature is kept downstream!



## 2. Case 2: x-y coordinates intersect (与…交叉) 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:

$$a_{E} = D_{e} + \begin{bmatrix} -F_{e}, 0 \\ 0 \end{bmatrix} \xrightarrow{100} 96.88 \xrightarrow{89.06} 77.86 \xrightarrow{63.06} 0$$

$$a_{W} = D_{W} + \begin{bmatrix} F_{w}, 0 \\ 0 \end{bmatrix} \xrightarrow{100} 96.88 \xrightarrow{89.06} 77.86 \xrightarrow{63.06} 0$$

$$a_{W} = D_{W} + \begin{bmatrix} F_{w}, 0 \\ 0 \end{bmatrix} \xrightarrow{100} 75 \xrightarrow{50} 34.38$$

$$a_{N} = D_{n} + \begin{bmatrix} -F_{n}, 0 \end{bmatrix} \xrightarrow{V > 0, \Gamma = 0} 0$$

$$v > 0, \Gamma = 0$$

$$a_S = D_s + \llbracket F_s, 0 \qquad v > 0, \Gamma = 0$$

$$F_{_W} = F_{_S}, \, a_P \phi_P = a_W \phi_W + a_S \phi_S + 0 + 0, \quad a_P = a_W + a_S, \phi_P = \frac{\phi_W + \phi_S}{2}!$$



Fluid temperatures across the diagonal become smooth and continuous. This is caused by the cross-diffusion (交叉扩散).

**Discussion:** For case 1 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 (有机会时) it will take action. Example 1 of this section is such a situation.

### 4.5.4 Errors caused by non-constant source term

Given: 
$$\begin{cases} \frac{d(\rho u\phi)}{dx} = \frac{d}{dx}(\Gamma \frac{d\phi}{dx}) + S, & S \text{ non-constant,} \\ x = 0, \phi = \phi_0; x = L, \phi = \phi_L & \text{specified (规定了).} \end{cases}$$





# For cases with such non-constant source term neither one of the five 3-point schemes can get accurate solution.

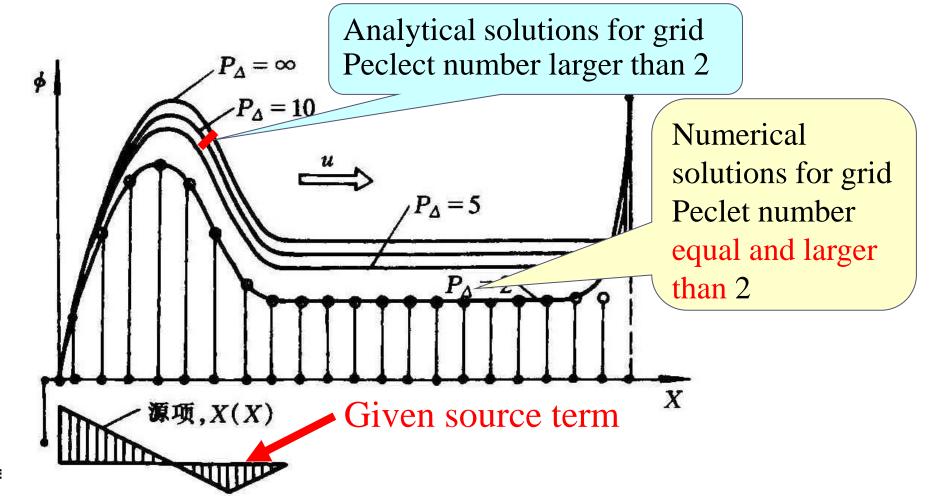
Taking hybrid scheme as an example. When grid Peclet number is less than 2, numerical results agree with analytical solution quite well; However, when grid Peclet number is larger than 2, deviations become large. Its coefficient is defined by:

$$a_E = D_e A(|P_{\Delta e}|) + [-F, 0, a_W = D_w A(|P_{\Delta w}|) + F_w, 0, A(|P_{\Delta e}|) = [0, 1 - 0.5|P_{\Delta e}|]$$

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



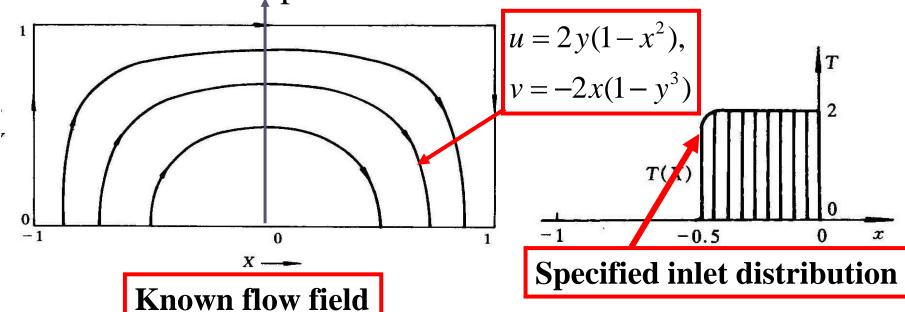
 $P_{\Delta e} \ge 2$ , hybrid:  $a_E = D_e A(|P_{\Delta e}|) + [-F, 0, A(|P_{\Delta e}|) = [0, 1 - 0.5|P_{\Delta e}|] = 0$  thus  $a_E = 0$  but  $a_W = D_w A(|P_{\Delta w}|) + F_w, 0$  remain the same, leading to the same numerical solutions for all cases with  $P_{\Delta e} \ge 2$ .



## 4.5.5 Two famous examples

## 1. Smith-Hutton problems (1982)

Solution for temp. distribution with a known flow field

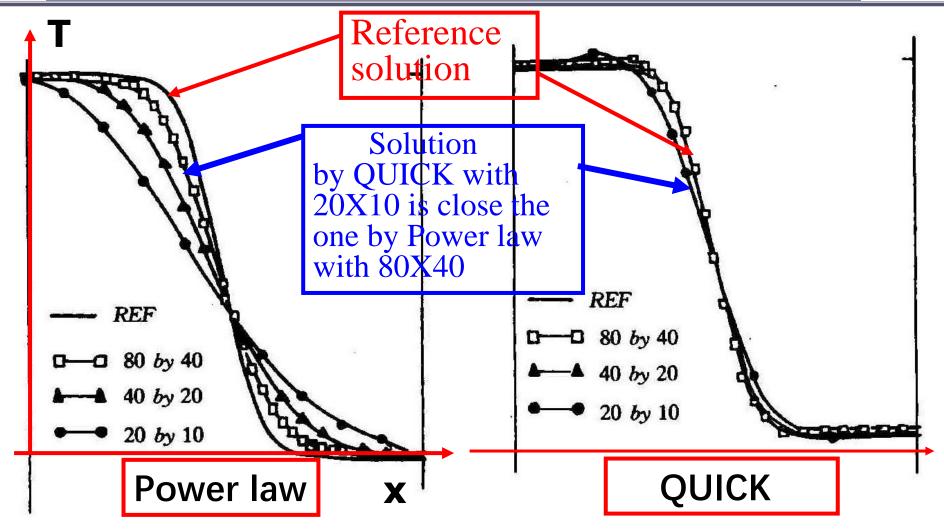


Eq. of  $T_{in}$ :  $T_{in}(x) = 1 + \tanh[\alpha(1+2x)]$ 

The larger the coefficient  $\alpha$  the sharper (更陡削) the profile.

Solved by 2-D D-C eq., convection term is discretized by different schemes studied.



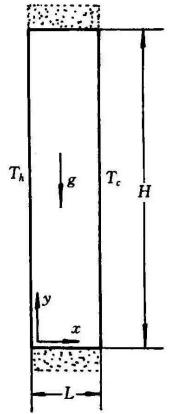


Solution from QUICK by 20X10 grids has the same accuracy as that from power law by 80X40 grids. PL has a larger false diffusion error.



### 2) Leonard problem (1996)

Natural convection in a tall cavity

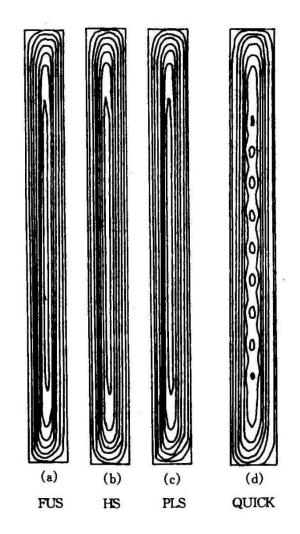


$$H/L=33$$

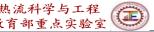
$$Gr = \frac{gL^3\alpha\Delta T}{v^2}$$
$$= 9500,$$
$$Pr = 0.71$$

$$32 \times 129 = 4128$$

When grid numbers are not large enough



FUS(FUD), HS and PLS have severe numerical error!



### PWL scheme Grids=316404

### **QUICK scheme**

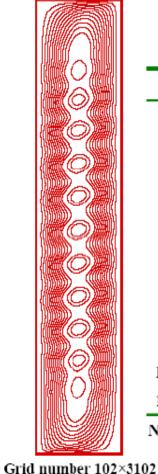


Table 5 Dimensionless cell coordinate calculated with PWL

	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



Table 8 Dimensionless cell coordinate calculated with QUICK

	Х	у
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

When grid numbers are large enough FUS(FUD), HS and PLS can resolute small vortex in the computational domain.



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

At coarse (粗) 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 resolute 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



## 4.6 Methods for overcoming or alleviating(减轻) effects of false diffusion

- 4.6.1 Higher order schemes to overcome streamwise false diffusion
  - 1. Second order upwind scheme (SUD)
  - 2. Third order upwind scheme (TUD)
  - 3. QUICK
  - 4. SGSD
- 4.6.2 Methods for alleviating cross false diffusion
- 1. Effective diffusivity method
- 2. Self-adaptive grid method

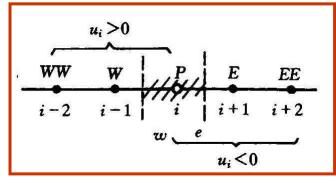


## 4.6 Methods for overcoming or alleviating effects of false diffusion

- 4.6.1 Higher order schemes to overcome or alleviate(減 轻) stream-wise false diffusion
- 1. SUD Taking two upstream points for scheme
- (1) Taylor expansion definition  $-2^{nd}$  order one side UD

$$u\frac{\partial \phi}{\partial x})_{i} = \frac{u_{i}}{2\Delta x}(3\phi_{i} - 4\phi_{i-1} + \phi_{i-2}), u > 0$$

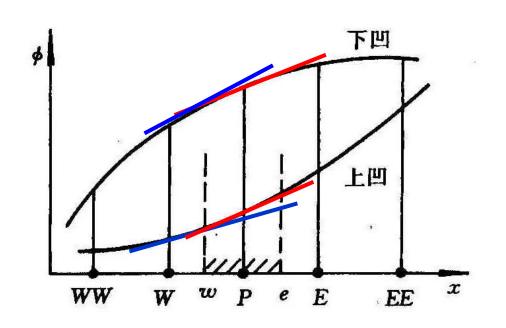
Rewriting it into the form of interface CD + an additional term:



$$u\frac{\partial\phi}{\partial x})_{P} = u_{P}\left(\frac{\phi_{P} - \phi_{W}}{\Delta x} + \frac{\phi_{P} - 2\phi_{W} + \phi_{WW}}{2\Delta x}\right)$$



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



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

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

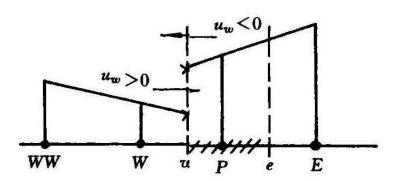
Concave upward(上凹),

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

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

$$\frac{1}{\Delta x} \int_{w}^{e} \frac{\partial \phi}{\partial x} dx = \frac{\phi_e - \phi_w}{\Delta x} = \frac{(1.5\phi_P - 0.5\phi_W) - (1.5\phi_W - 0.5\phi_{WW})}{\Delta x}$$

$$=\frac{3\phi_P - 4\phi_W + \phi_{WW}}{2\Delta x}$$

The same as FD

FVM: Integral averaged value

over a CV;

**FDM:** Discretized value at a node

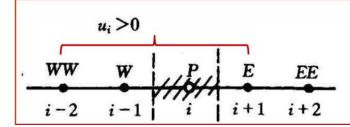




## 2. TUD (三阶迎风)

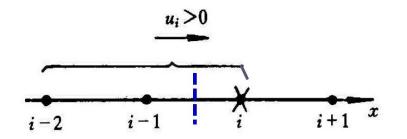
(1) Taylor expansion—3<sup>rd</sup>-order scheme of 1<sup>st</sup> derivative with biased positions of nodes (节点偏置).

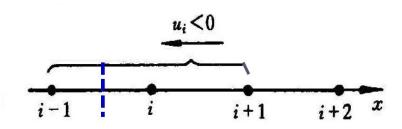
$$u \frac{\partial \phi}{\partial x}\Big|_{i}^{u} = \frac{0}{6\Delta x} u_{i} (2\phi_{i+1} + 3\phi_{i} - 6\phi_{i-1} + \phi_{i-2})$$
www w



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

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

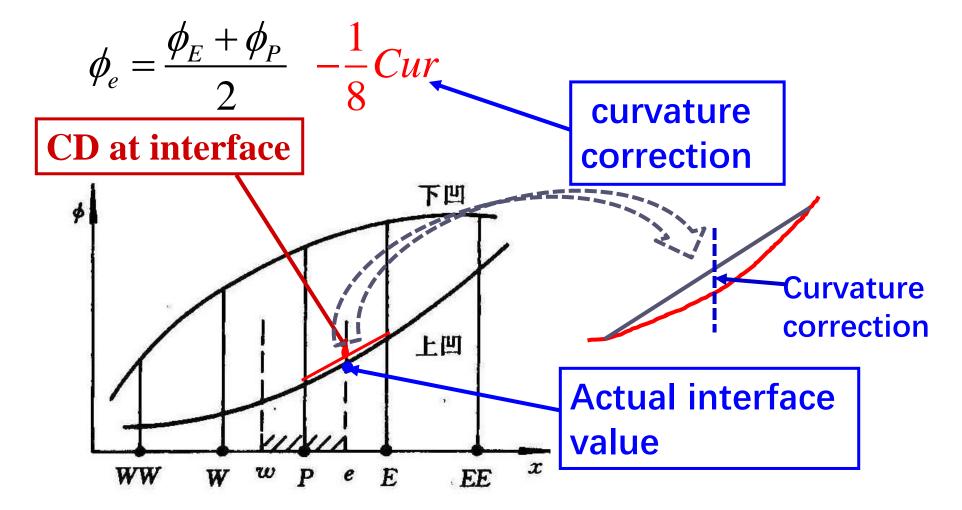






### 3.QUICK scheme---Interface interpolation method in FVM

1) Position definition (W-P-W)—CD at interface with a curvature correction (曲率修正)



#### **How to determine CUR?** Two considerations:

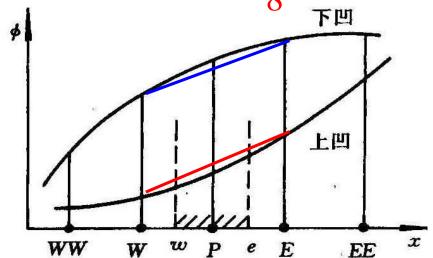
(1) Reflecting concave (凹) upward (向上凸) or concave downward (向下凹) curvature automatically

Concave upward

$$(\phi_W - 2\phi_P + \phi_E) > 0, -\frac{1}{8}Cur < 0;$$

Concave downward

$$(\phi_W - 2\phi_P + \phi_E) < 0 - \frac{1}{8}Cur > 0;$$



Decreasing the
Interface value a bit!
Increasing the
Interface value a bit!



### (2) Adopting upwind idea for enhancing stability:

For interface e

When u > 0, taking  $\phi_W, \phi_P, \phi_E, \phi_W$  is the upstream point!

When u < 0, taking  $\phi_P, \phi_E, \phi_{EE}$ ,  $\phi_{EE}$  is the upstream point!

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



Interface interpolation by QUICK:

$$\phi_e = (\phi_E + \phi_P)/2 - (1/8)Cur$$

$$Cur = \begin{cases} \phi_W - 2\phi_P + \phi_E, \ u > 0 \\ \phi_P - 2\phi_E + \phi_{EE}, \ u < 0 \end{cases}$$
QUICK=quadratic interpolation of convective kinematics

2) QUICK — Subscript definition (defined by subscripts i, i+1, i-1),

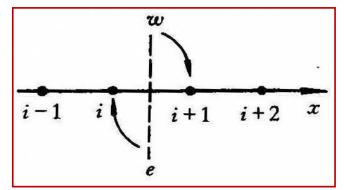
For 
$$u > 0$$
: 
$$\begin{cases} \phi_e = \phi_{i+1/2} = \frac{1}{8} (3\phi_{i+1} + 6\phi_i - \phi_{i-1}) & \phi_w = \phi_{i-1/2} & u_i > 0 \\ \phi_w = \phi_{i-1/2} = \frac{1}{8} (3\phi_i + 6\phi_{i-1} - \phi_{i-2}) & i-2 \end{cases}$$

How to verify schemes possessing conservative character? Taking QUICK+CD as an analysis example.



### 1) Interface interpolations from its two side are identical

For QUICK: (i+1/2) interface value only depends on flow direction, for both i and (i+1) is the same (this is termed as continuous);

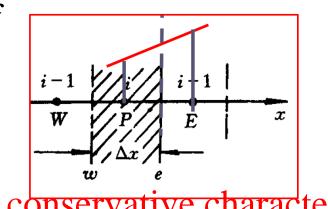


### 2) Interface flux from its two side are identical

If at interface linear profile is adopted, then interface diffusion flux is  $(\phi_E - \phi_P)/(\delta x)_e$ , which is the same for both P point or E point

(termed as continuous). Then QUICK with CD of diffusion term possesses conservative character.

In summary: if a combination of convection and diffusion schemes can ensure that the interface values and flux are continuous, then they possess conservative character.





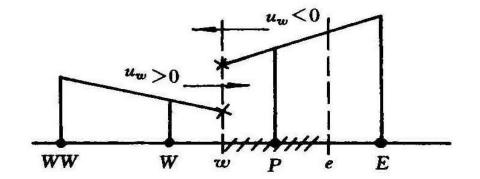
## 4. SGSD - A kind of composite (组合)scheme

## 1) SCSD scheme (1999) (Uniform grid)

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

$$\mathrm{SUD:} \ \phi_e = \ \left\{ \begin{array}{l} 1.5\phi_{\!\scriptscriptstyle W} - 0.5\phi_{\!\scriptscriptstyle WW}, \ \textit{u} > 0 \\ 1.5\phi_{\!\scriptscriptstyle P} - 0.5\phi_{\!\scriptscriptstyle E}, \ \textit{u} < 0 \end{array} \right.$$

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



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

When Pe number is small, CD predominates (占优); when Pe number is large, SUD predominates:

$$\phi_{e}^{SCSD} = \beta \phi_{e}^{CD} + (1 - \beta) \phi_{e}^{SUD}, \ 0 \le \beta \le 1$$

$$\beta = 1, \phi^{SCSD} \equiv \phi^{CD}; \ \beta = 0, \phi^{SCSD} \equiv \phi^{SUD}; \ \beta = 3/4, \phi^{SCSD} \equiv \phi^{QUICK}$$
It can be shown: 
$$P_{\Delta,cr} = (\frac{\rho u \delta x}{\Gamma})_{cr} = \frac{2}{\beta} \quad \text{Beyond which} (\Box \Box \Box \Box)$$
the scheme is unstable!

By adjusting Beta value its critical Peclet number can vary from 0 to infinite! Therefore 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格式 (2002)

From 
$$P_{\Delta,cr} = \frac{2}{\beta}$$
  $\rightarrow \beta = \frac{2}{P_{\Delta,cr}}$ , replace  $P_{\Delta,cr}$  in denominator by  $(2 + P_{\Delta})$ :
$$\beta = \frac{2}{2 + P_{\Delta}} \begin{cases} P_{\Delta} \to 0, \beta \to 1, \text{ CD dominates;} \\ P_{\Delta} \to \infty, \beta \to 0, \text{ SUD dominates} \end{cases}$$

- 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!

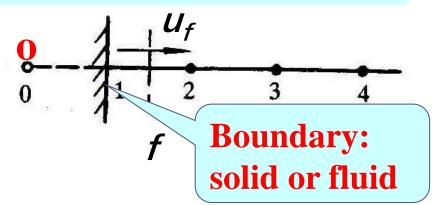
Li ZY, Tao WQ. A new stability-guaranteed second-order difference scheme. **NHT-Part B**, 2002, 42 (4): 349-365



### 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:

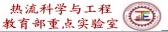
(1) Fictitious point method (虚拟点法): Introducing a fictitious point O and assuming:

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

Usually the fictitious point should be in the solid part.

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

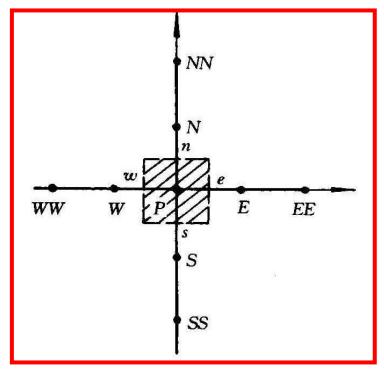




## 2) Solution of ABEqs.:

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)。

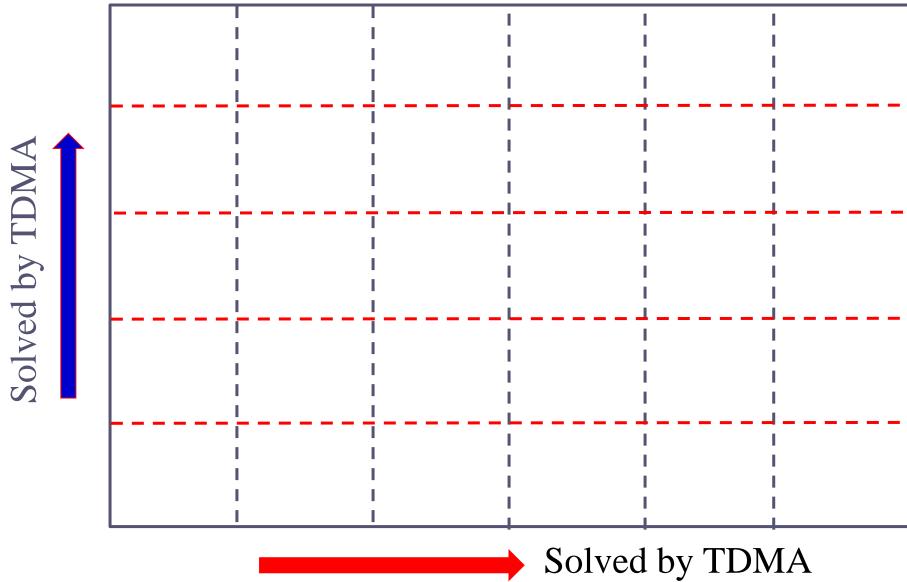
$$\phi_e^H = \phi_e^L + (\phi_e^H - \phi_e^L)^*$$
 \*-previous iteration

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





### **ADI ---Alternative Direction Iteration**





# 4.6.2 Methods for alleviating (减轻) effects of cross-diffusion

## 1. Adopting effective diffusivity for FUD

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

 $\Gamma_{\phi}$  —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.

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

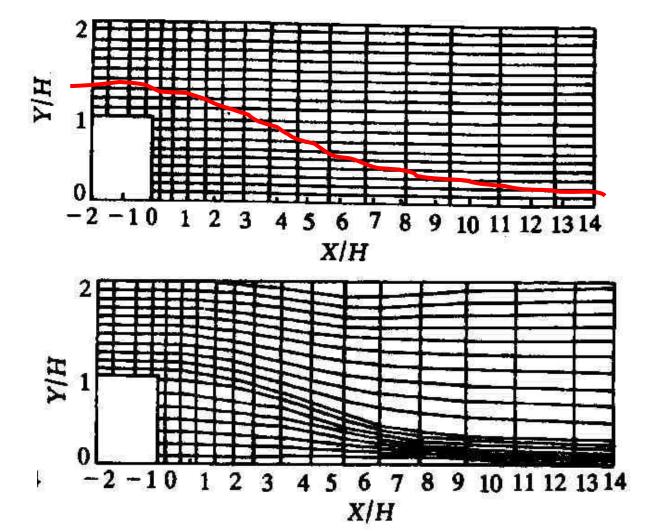
$$\delta t = \frac{1}{\frac{u}{\Delta x} + \frac{v}{\Delta y} + \frac{w}{\Delta z}}$$

(Inspired(启发) from Noye problem)



# 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



## 4.6.3 Summary of 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 direct numerical simulation (DNS) of turbulent flow, 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 can be found in:

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





# 4.7 Discretization of multi-dimensional problem and B.C. treatment

# 4.7.1 Discretization of 2-D diffusion-convection equation

- 1. Governing equation expressed by  $J_{x}$ ,  $J_{y}$
- 2. Results of disctretization
- 3. Ways for adopting other schemes
- 4.7.2 Treatment of boundary conditions
  - 1.Inlet boundary
  - 2. Solid boundary
  - 3.Central line
  - 4.Outlet boundary



## 4.7 Discretization of multi-dimensional problem and B.C. treatment

## 4.7.1 Discretization of 2-D diffusion-convection equation

# 1. Governing equation expressed by $J_x$ , $J_y$

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

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

## 2. Integration the GE over 2D CV

Integrating the GE over a 2D CV, and regarding every coordinate as 1-D problem :





Finally the general discretization equation for 2-D five-point scheme:

$$a_{P}\phi_{P} = a_{E}\phi_{E} + a_{W}\phi_{W} + a_{S}\phi_{S} + a_{N}\phi_{N} + b$$

$$a_{P} = a_{E} + a_{W} + a_{N} + a_{S} + a_{P}^{0} - S_{P}\Delta V$$

$$b = S_{C}\Delta V + a_{P}^{0}\phi_{P}^{0} \qquad a_{P}^{0} = \rho_{P}\Delta V/\Delta t$$

$$a_{E} = D_{e}A(|P_{\Delta e}|) + [-F_{e}, 0 \qquad a_{W} = D_{w}A(|P_{\Delta w}|) + [F_{w}, 0]$$

$$a_{N} = D_{n}A(|P_{\Delta n}|) + [-F_{n}, 0 \qquad a_{S} = D_{S}A(|P_{\Delta S}|) + [F_{S}, 0]$$

### 3. Ways for adopting other schemes

Adopting defer correction method, and putting the additional part of the other scheme into source term (b) of the algebraic equation. Thus a code developed from three-point schemes can also accept higher order schemes.



# 4.7.2 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;

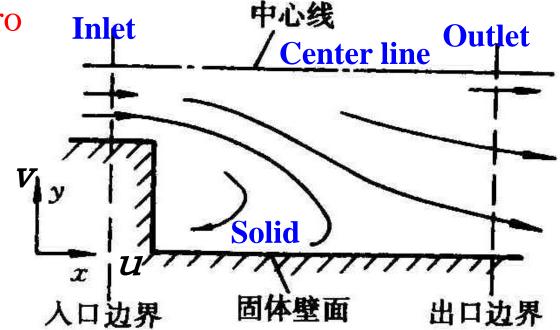
First derivative normal to the lcenter ine of other

variable is equal to zero

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

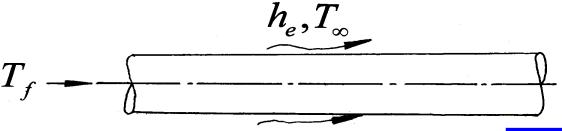
## 3. Solid boundary

No slip for u,v; Three types for T.



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

External convective heat transfer — 3;



For solving the inner convective heat transfer

# 4. Outlet boundary

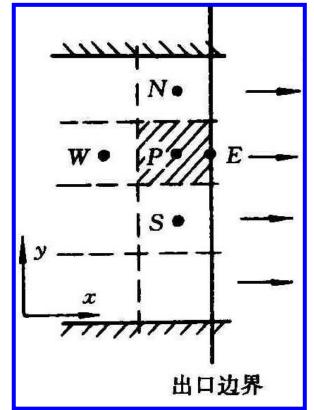
Conventional methods:

(1) Local one-way (局部单向化)

$$a_E = 0$$

(2) Fully developed (充分发展)

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





#### Home Work 4 (2024-2025)

Please finish your homework independently !!!

Please hand in on October 18,2022

#### **Problem 4-1**

For a one-dimensional steady state diffusion-convection problem without source term, at x=0,  $\phi=\phi_0$  and  $x=L, \phi=\phi_L$ . Take 20 nodes for x=0-1, and use 1<sup>st</sup>-order upwind difference, central difference, 3<sup>rd</sup>-order upwind difference and QUICK for the convective term and central difference for the diffusion term. Determine the grid values for three grid Peclet numbers: 1, 20 and 200. Draw the picture of  $(\phi-\phi_0)/(\phi_L-\phi_0)$  versus x/L, and compare the results of the exact solution.





For a two-dimensional unsteady state diffusion-convection problem without a source,

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

adopt the central scheme for both the convection term and the diffusion term, find the values of the four coefficients  $a_E, a_W, a_P, a_P^0$  of an inner point for the following conditions:

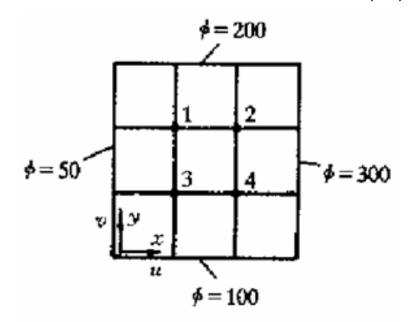
$$\Delta x = 0.1, \Delta t = 0.05, \rho = 1, \rho u = 4, P_{\Lambda} = 1 \text{ and } 5$$





For a two-dimensional steady state diffusion-convection problem without source term with boundary condition shown in the figure. Take  $\rho u = 3$ ,  $\rho v = 4$ ,  $\Gamma = 5$ ,  $\Delta x = \Delta y = 0.1$ .

Take 1<sup>st</sup>-order upwind scheme, 2<sup>nd</sup>-order upwind scheme for the convection term and central scheme for the diffusion term. Determine the  $\phi$  values at the four nodes 1,2,3 and 4.





From the following general interpolation expression for the schemes of the convection term with at least 2<sup>nd</sup>-order,

$$\begin{cases} \phi_{e} = a_{i}\phi_{i} + \left(\frac{1}{4} - \frac{a_{i}}{2}\right)\phi_{i-1} + \left(\frac{3}{4} - \frac{a_{i}}{2}\right)\phi_{i+1} \\ \phi_{w} = a_{i}\phi_{i-1} + \left(\frac{1}{4} - \frac{a_{i}}{2}\right)\phi_{i-2} + \left(\frac{3}{4} - \frac{a_{i}}{2}\right)\phi_{i} \end{cases}$$

$$\begin{cases} \phi_{e} = a_{i}\phi_{i} + \left(\frac{1}{4} - \frac{a_{i}}{2}\right)\phi_{i-1} + \left(\frac{3}{4} - \frac{a_{i}}{2}\right)\phi_{i} \\ \hline (i-2) + \left(\frac{1}{4} - \frac{1}{4}\right) + \left(\frac{1}{4} - \frac{1}{4}\right) + \left(\frac{3}{4} - \frac{1}{4}\right)\phi_{i} \end{cases}$$

Determine the values of the constant  $a_i$  for : (1) central scheme; (2) 2<sup>nd</sup>-order upwind scheme; (3) QUICK scheme; (4) 3<sup>rd</sup>-order upwind scheme; (5) SGSD scheme.



Show that when the diffusion term is discretized by the CD, the convective term is discretized by 3<sup>rd</sup>-order upwind difference, the discretized diffusion-convection equation by the control volume method has the conservative property.



# Appendix: Discretization of 2-D diffusion-convection equation

# 1. Governing equation expressed by $J_x$ , $J_y$

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

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

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

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



#### 2. Results of discretization

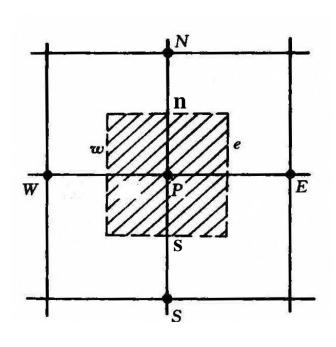
Integrating above equations for CV. P

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

$$\iiint_{w}^{e} \frac{\partial J_{x}}{\partial x} dx dy dt = \int_{t}^{t+\Delta t} \int_{s}^{n} (J_{x}^{e} - J_{x}^{w}) dy dt$$

$$\iiint_{s}^{n} \frac{\partial J_{y}}{\partial y} dxdydt = \int_{t}^{t+\Delta t} \int_{w}^{e} (J_{y}^{n} - J_{y}^{s}) dxdt$$

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



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

$$(J_x^e - J_x^w) \Delta y \Delta t = (\underline{J_x^e} \Delta y - \underline{J_x^w} \Delta y) \Delta t = (J_e - J_w) \Delta t$$

## Expressing J via $J^*$ :

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

$$J_{e} = J_{e}^{*}D_{e} = D_{e}[\{A(P_{\Delta e}) + P_{\Delta e}\}\phi_{P} - A(P_{\Delta e})\phi_{E}]$$

$$J_{e} = J_{e}^{*}D_{e} = \{D_{e}A(P_{\Delta e}) + F_{e}\} \underline{\phi_{P}} - D_{e}A(P_{\Delta e})\phi_{E}$$

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

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

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

The same derivation can be done for three other terms,  $J_w$ ,  $J_n$ ,  $J_s$ .



Finally the general discretization equation for 2-D five-point scheme:

$$a_{P}\phi_{P} = a_{E}\phi_{E} + a_{W}\phi_{W} + a_{S}\phi_{S} + a_{N}\phi_{N} + b$$

$$a_{P} = a_{E} + a_{W} + a_{N} + a_{S} + a_{P}^{0} - S_{P}\Delta V$$

$$b = S_{C}\Delta V + a_{P}^{0}\phi_{P}^{0} \qquad a_{P}^{0} = \rho_{P}\Delta V/\Delta t$$

$$a_{E} = D_{e}A(|P_{\Delta e}|) + [-F_{e}, 0 \qquad a_{W} = D_{W}A(|P_{\Delta w}|) + [F_{w}, 0]$$

$$a_{N} = D_{n}A(|P_{\Delta n}|) + [-F_{n}, 0 \qquad a_{S} = D_{S}A(|P_{\Delta S}|) + [F_{S}, 0]$$



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Teaching PPT will be loaded on ou website



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渡彼岸!

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

