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Numerical Heat Transfer

(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

4.1 Two ways of discretization of convection term

4.2 CD and UD of the convection term

4.3 Hybrid and power-law schemes

4.4 Characteristics of five three-point schemes

4.5 Discussion on false diffusion

4.6 Methods for overcoming or alleviating effects of false diffusion

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



4.5 Discussion on false diffusion

4.5.1 Meaning and reasons of false diffusion

1.Original meaning

2.Extended meaning

3.Taylor expansion analysis

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

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

4.5.4 False diffusion caused by non-constant source term

4.5.5 Two famous examples



4.5 Discussion on false diffusion

4.5.1 Meaning and reasons of false diffusion

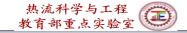
False diffusion (假扩散), also called numerical viscosity (数值黏性), is an important numerical character of the discretized convective scheme.

1. Original meaning

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

The 1st term in the TE of such scheme contains 2nd order derivative, thus the diffusion action is somewhat magnified at the sense of second-order accuracy, hence the numerical error is called "false diffusion".

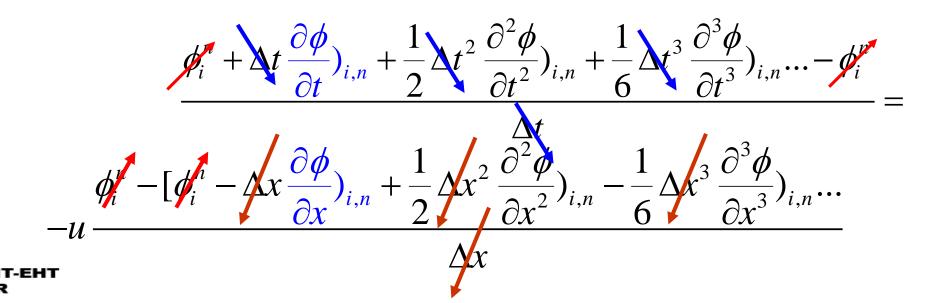
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> Taking 1-D unsteady advection equation as an example. The two 1st-order derivatives are discretized by 1st-order accuracy schemes.

 $\frac{\partial \phi}{\partial t} = -u \frac{\partial \phi}{\partial x} \xrightarrow{\text{1st-oder scheme}} \underbrace{\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t}}_{\text{L}} = -u \frac{\phi_i^n - \phi_{i-1}^n}{\Delta x}$ Expanding $\phi_{i-1}^n, \phi_i^{n+1}$ at (i,n) by Taylor series, and substituting into the above equation:





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

where the transient 2nd derivative can be re-written as follows:

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

substituting into above equation

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

Thus at the sense of 2nd-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.
 $\frac{u\Delta t}{\Delta x}$ is called **Courant** number, in memory of a
German mathematician Courant.
 $\frac{\partial \phi}{\partial t}_{i,n} = -u \frac{\partial \phi}{\partial x}_{i,n} + \left[\frac{u\Delta x}{2} \left(1 - \frac{u\Delta t}{\Delta x}\right)\right] \left(\frac{\partial^2 \phi}{\partial x^2}\right)_{i,n} + O(\Delta x^2, \Delta t^2)$

Remark: We only study the false diffusion at the sense of 2^{nd} -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^{nd} -oder accuracy solutions are satisfied.



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2. Extended meaning

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

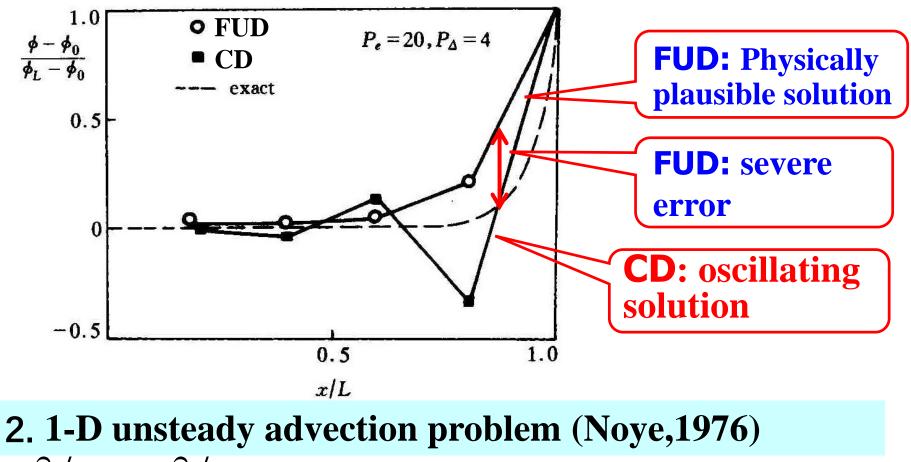
- (1) 1^{st} -order accuracy schemes of the 1^{st} order derivatives (original meaning);
- (2) Oblique intersection(倾斜交叉) of flow direction with grid lines;
- (3) The effects of non-constant source term which are not considered in the discretized schemes.

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 CFD-NHT-EHT deviate from analytical solutions:

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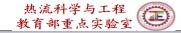
 $\frac{\partial \phi}{\partial t} = -u \frac{\partial \phi}{\partial x}, \ 0 \le x \le 1, u = 0.1, \ \phi(0,t) = \phi(1,t) = 0$ In the range of $x \in [0,0.1]$ initial distribution is an triangle, others are zero. The two derivatives are discretized



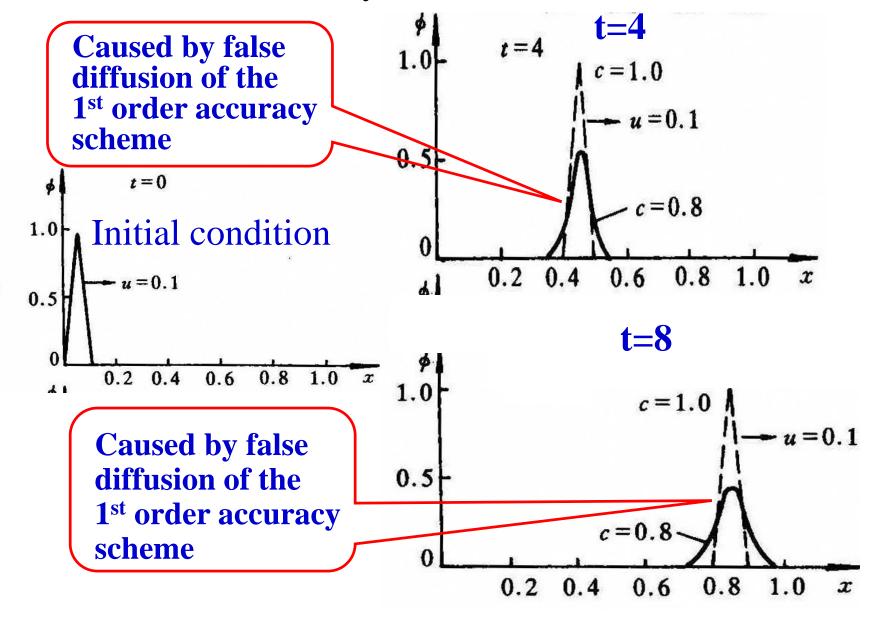
CFD-NHT-EHT

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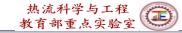


the 1st –order accuracy schemes. The results are as follows.



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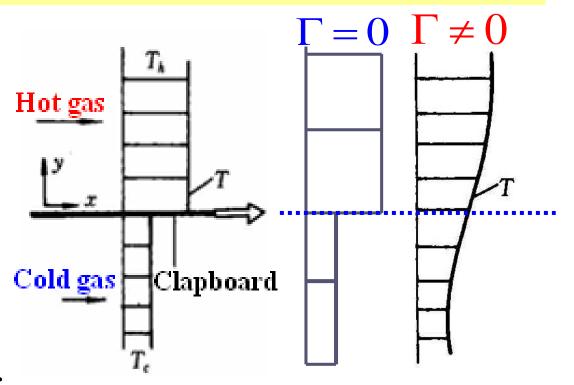




When Courant number is less than 1, severe error occurs, which erases (抹平) the sharp peak(抹平尖 峰) and magnify the base (放大基底) gradually. Such error is called streamwise false diffusion (流向假扩散).

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.



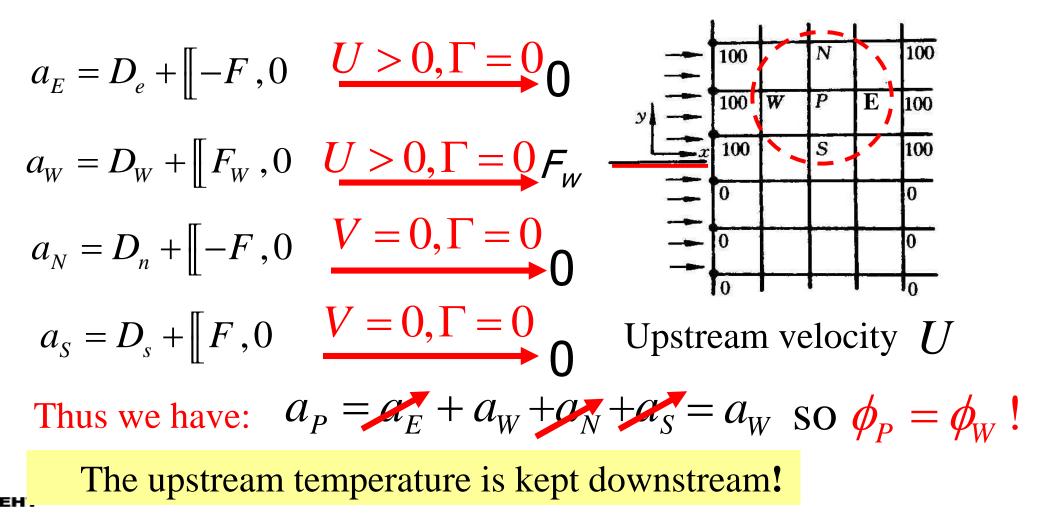
Gas flow with 0 and non-0 Gamma





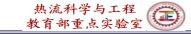
1. Case 1: with x-y coordinates either parallel or perpendicular to flow direction

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

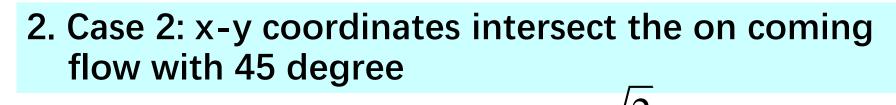


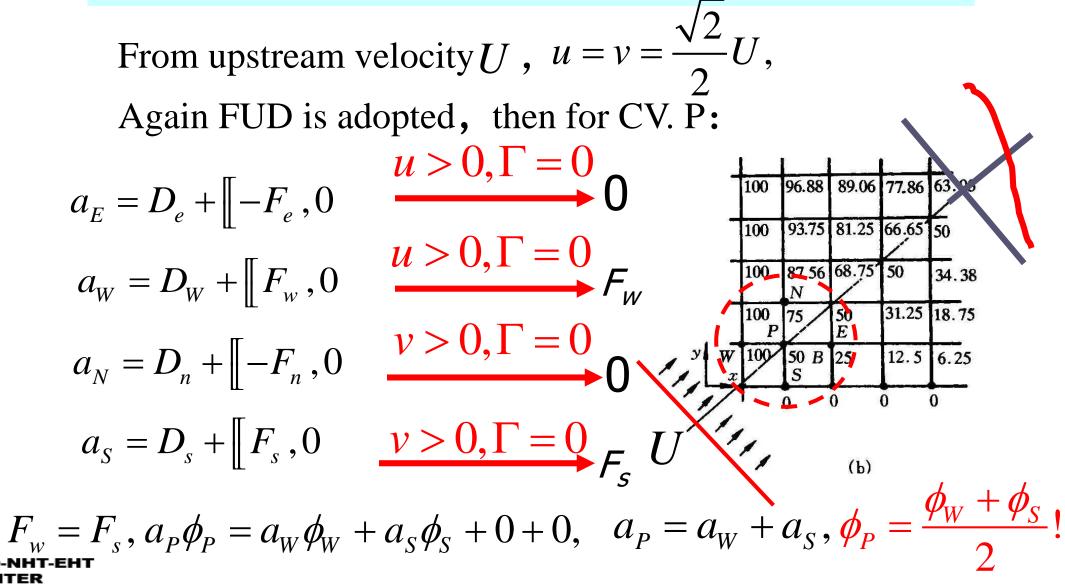
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13/52







Fluid temperatures across the diagonal become smooth and continuous. This is caused by the **cross-diffusion**.

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:
$$\begin{cases} \frac{d(\rho u\phi)}{dx} = \frac{d}{dx}(\Gamma \frac{d\phi}{dx}) + S, \\ x = 0, \phi = \phi_0; x = L, \phi = \end{cases}$$

S non-constant, distribuiton is specified.



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

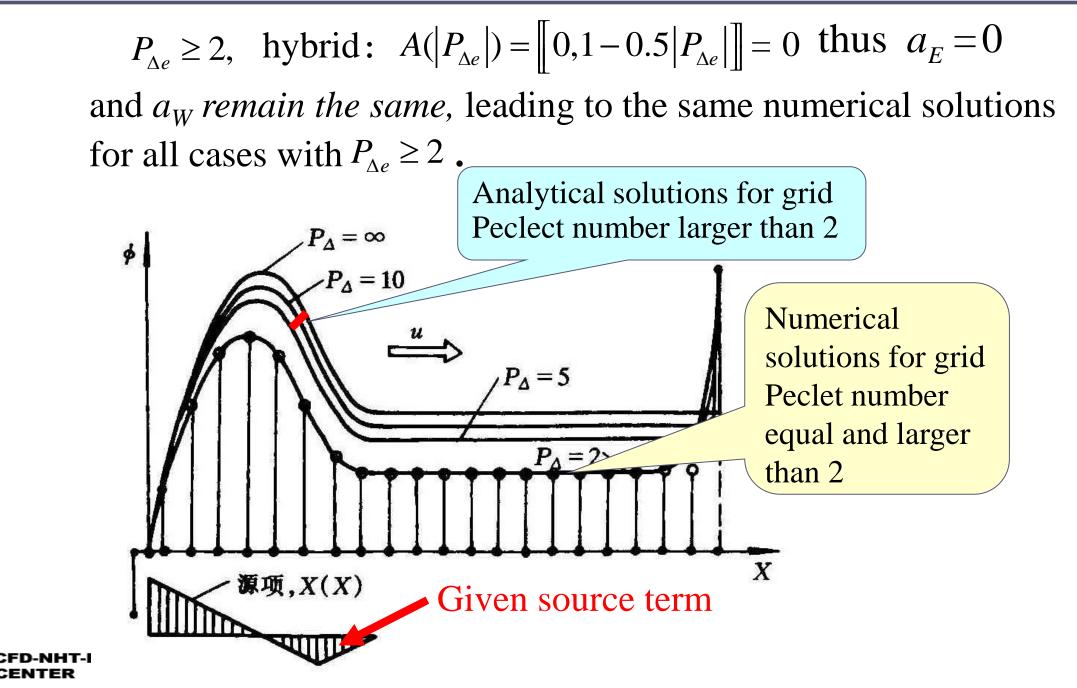
Taking hybrid scheme as an example. When grid Peclet number is less than 2, numerical results agree with analytical solution quite well; However, when grid Peclet number is larger than 2, deviations become large. Its coefficient is defined by:

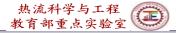
$$a_{E} = D_{e}A(|P_{\Delta e}|) + \left[-F, 0, a_{W} = D_{W}A(|P_{\Delta w}|) + F_{W}, 0 - A(|P_{\Delta e}|) = \left[0, 1 - 0.5 |P_{\Delta e}| \right] \right]$$

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

15/52







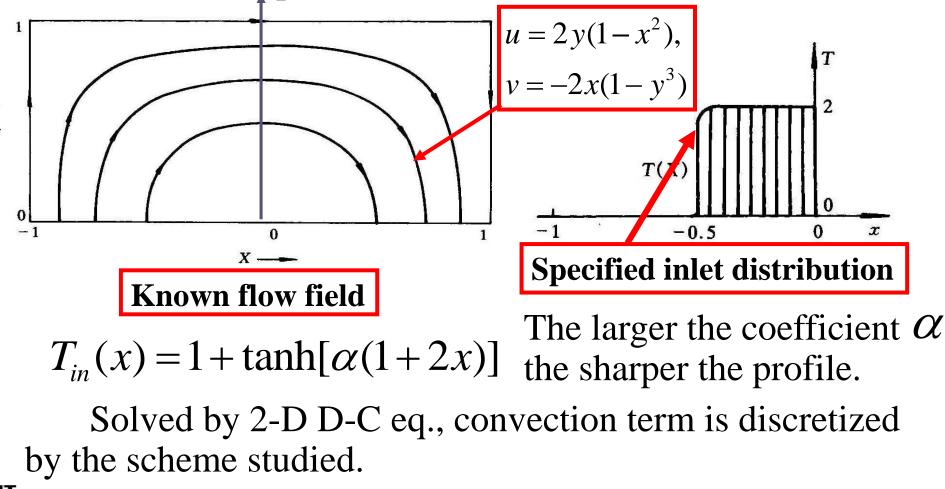
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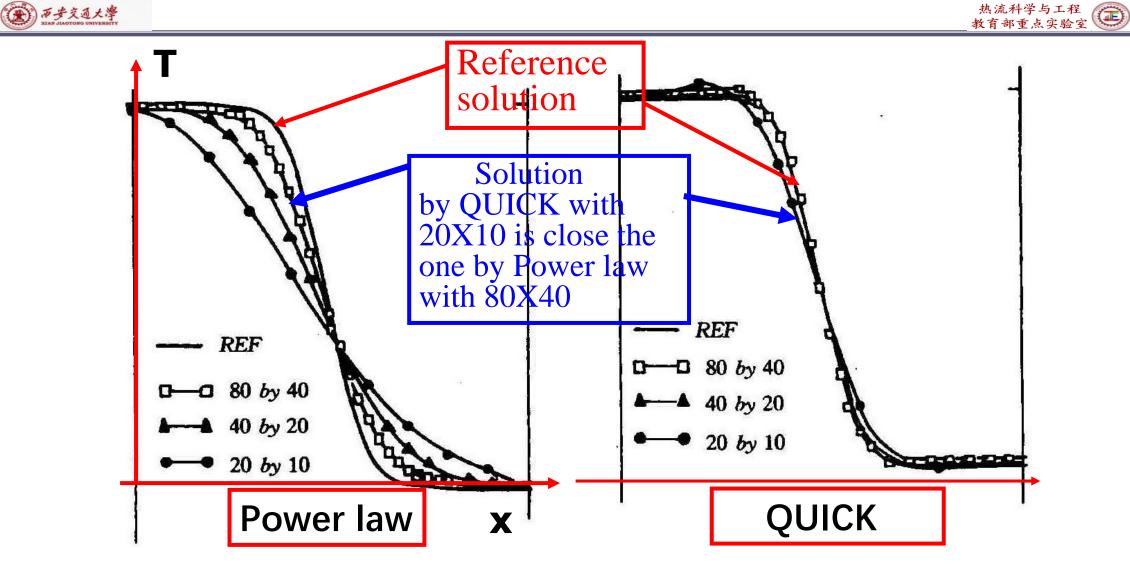
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4.5.5 Two famous examples

1. Smith-Hutton problems (1982)

Solution for temp. distribution with a known flow field





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



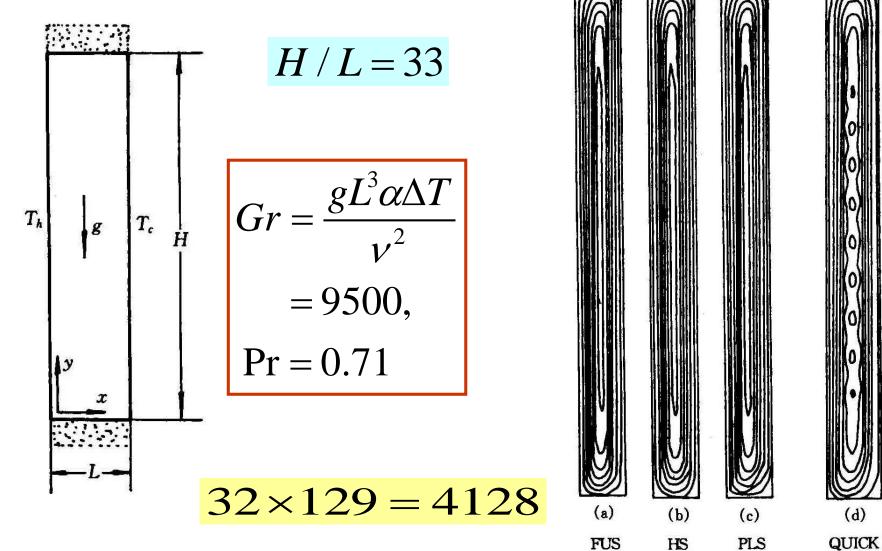
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2) Leonard problem (1996)





19/52



PWL scheme

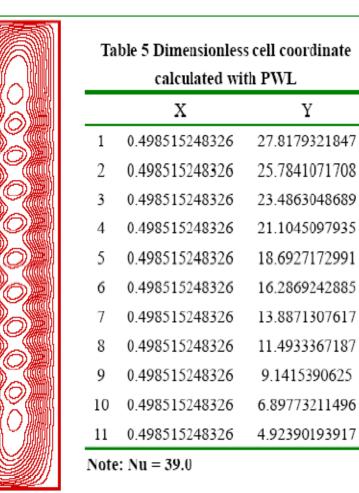




Table 8 Dimensionless cell coordinate

QUICK scheme

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

Grids=316404

Grid number 102×3102





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!

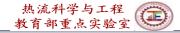
Solution from higher order scheme with a less grid number can reach the same accuracy as that from lower order scheme with a larger grid number.

With increased grid number power law can also 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

CFD-NH1





4.6 Methods for overcoming or alleviating 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

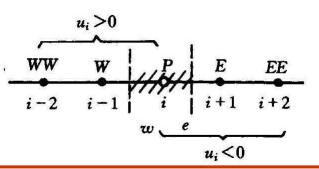
4.6.1 Higher order schemes to overcome or alleviate(減 轻) stream-wise false diffusion

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:



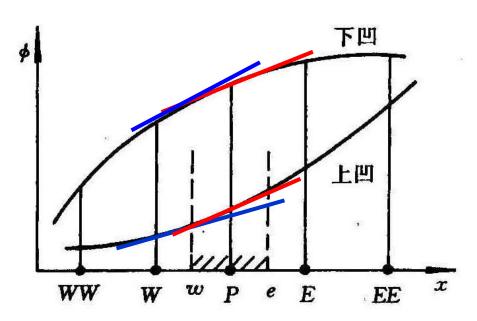
$$u\frac{\partial\phi}{\partial x})_{P} = u_{P}\left(\frac{\phi_{P} - \phi_{W}}{\Delta x} + \frac{\phi_{P} - 2\phi_{W} + \phi_{WW}}{2\Delta x}\right)$$



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



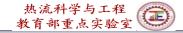
$$(rac{\phi_P - 2\phi_W + \phi_{WW}}{2\Delta x})$$

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

Concave upward(上凹), Concave Downward(下凹)

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

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





D-NHT-EH

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(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:

$$\frac{1}{\Delta x}\int_{w}^{e} \frac{\partial \phi}{\partial x} dx = \frac{\phi_{e} - \phi_{w}}{\Delta x} = \frac{(1.5\phi_{p} - 0.5\phi_{w}) - (1.5\phi_{w} - 0.5\phi_{ww})}{\Delta x}$$

$$= \frac{3\phi_{p} - 4\phi_{w} + \phi_{ww}}{2\Delta x}$$
FVM: Integral averaged value over a CV;
FDM: Discretized value at a node

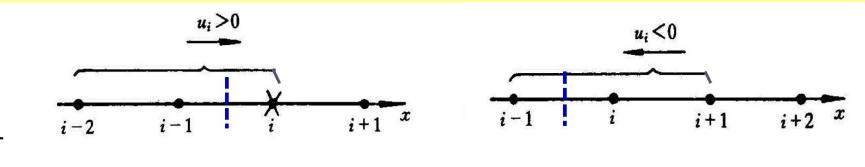


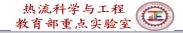
2. TUD (三<mark>阶迎风</mark>)

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

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

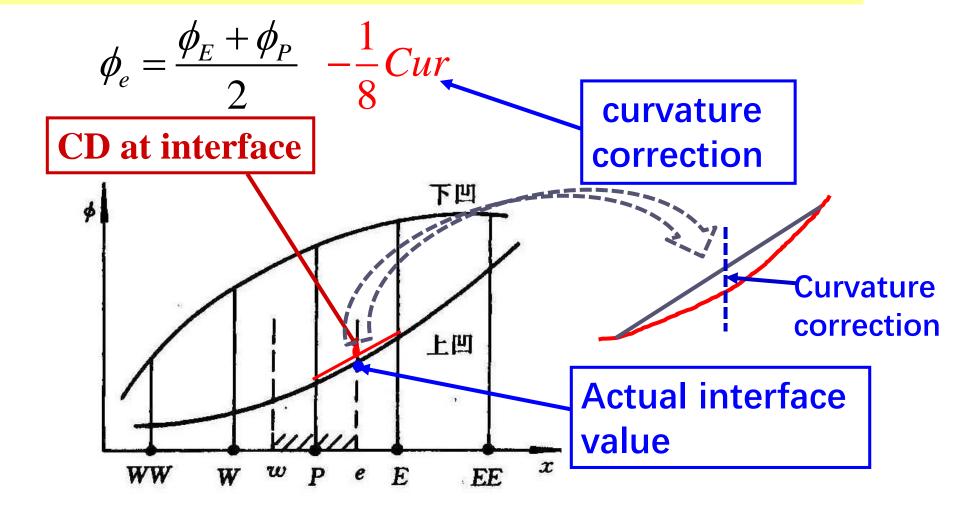




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3.QUICK scheme (FVM definition)

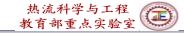
1) Position definition – CD at interface with a curvature correction







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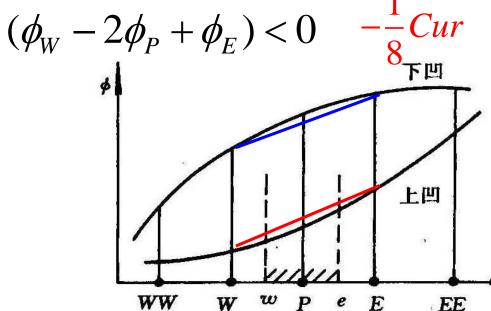


How to determine CUR? Two considerations: (1) Reflecting concave (凹) upward (向上凸) or concave downward (向下凹) curvature automatically

Concave upward

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

Concave downward

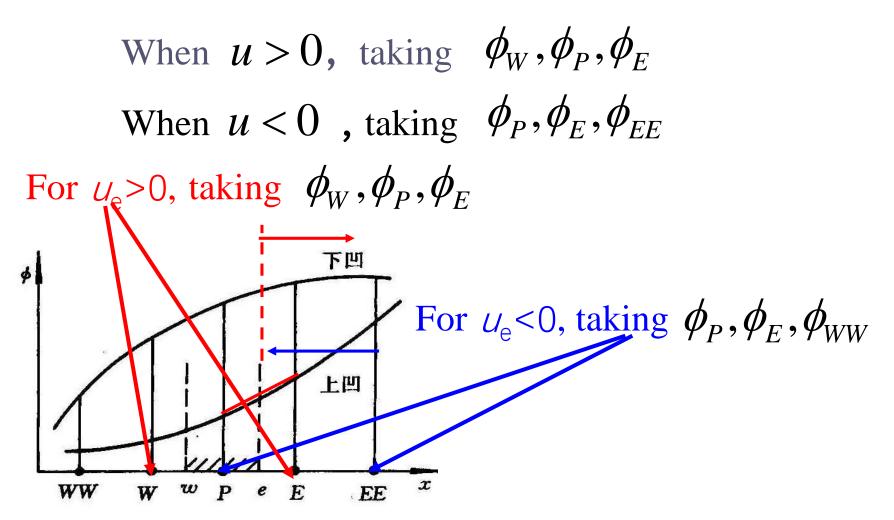


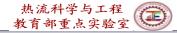
Decreasing the Interface value a bit! Increasing the Interface value a bit!

x



(2) Adopting upwind idea for enhancing stability:For interface e







Curvature correction for QUICK:

$$\operatorname{Cur} = \begin{cases} \phi_{W} - 2\phi_{P} + \phi_{E}, \ u > 0 \\ \phi_{P} - 2\phi_{E} + \phi_{EE}, \ u < 0 \end{cases}$$

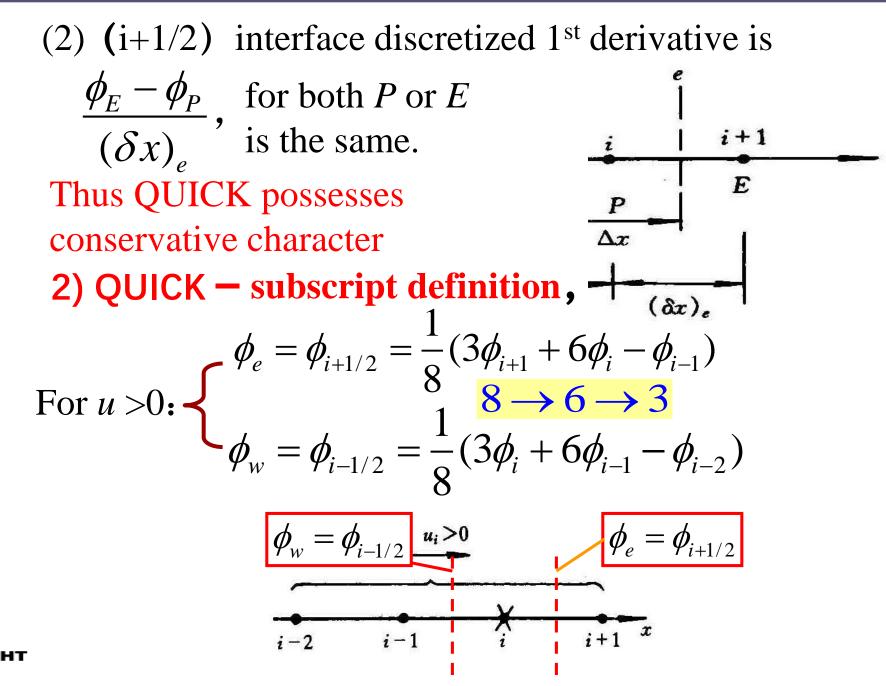
QUICK = quadratic interpolation of convective kinematics

Two remarks

1) QUICK possesses conservative character(守恒特性)— Interface interpolation and discretized 1st derivative are continuous at interface: (1) (i+1/2) interface value depends on flow direction, for both i and (i+1) is the same;



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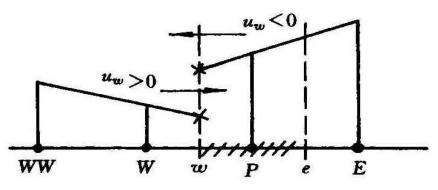
4. SGSD - A kind of composite (组合)scheme

1) SCSD scheme (1999) (Uniform grid)

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

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

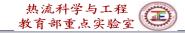
Absolutely stable (discussed later), but has appreciable(显著的) numerical errors.







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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:

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

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

It can be
shown:
$$P_{\Delta,cr} = (\frac{\rho u \delta x}{\Gamma})_{cr} = \frac{2}{\beta}$$
Beyond which the
scheme is unstable!

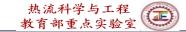
By adjusting Beta value its critical Peclet number can vary from 0 to infinite! Therefore it is called: stability-controllable second-order difference—SCSD (倪明玖, 1999) .

Ni M J, Tao W Q. J. Thermal Science, 1998, 7(2):119-130

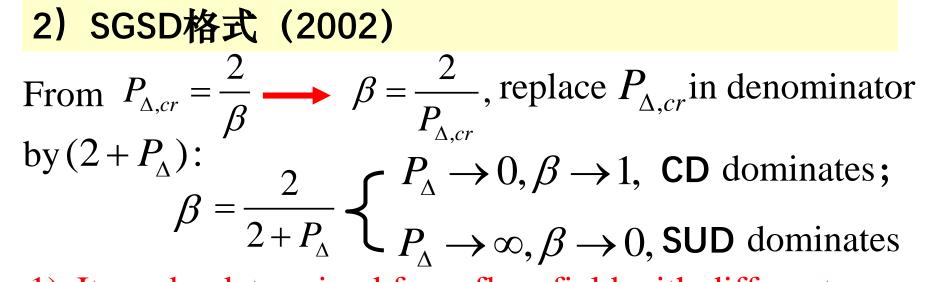




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Question: how to determine Beta? Especially how to calculate Beta based on the flow field automatically?



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



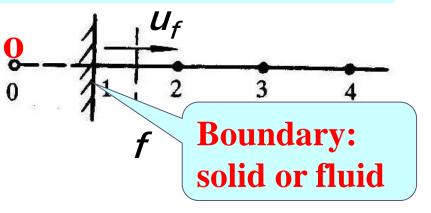


5. Discussion on implementing higher-order schemes

1) Near boundary point:

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Taking practice A as an example: For the interface between nodes 1 and 2,



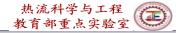
if $u_{\rm f} > 0$, how to implement higher order schemes?

Two ways can be adopted:

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

$$\phi_{o} + \phi_{2} = 2\phi_{1} \longrightarrow \phi_{o} = 2\phi_{1} - \phi_{2}$$

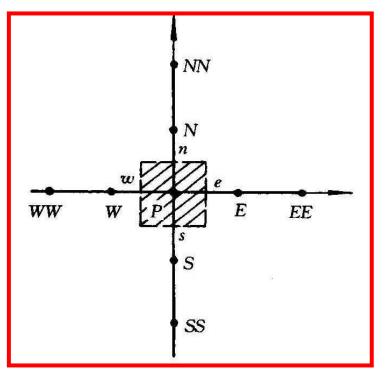
(2) Order reduction (降阶) method: $\phi_f = \phi_1, u_f > 0$





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)。

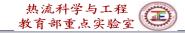
 $\phi_e^H = \phi_e^L + (\phi_e^H - \phi_e^L)^*$ *-previous iteration The lower-order part ϕ_e^L forms the ABEqs.; those with * go to the source part, and **ADI method** is used. The converged solution is the one of higher-order scheme.



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ADI ---Alternative Direction Iteration





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

1. Adopting effective diffusivity for FUD

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

$$\Gamma_{\phi}$$
 — 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.

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

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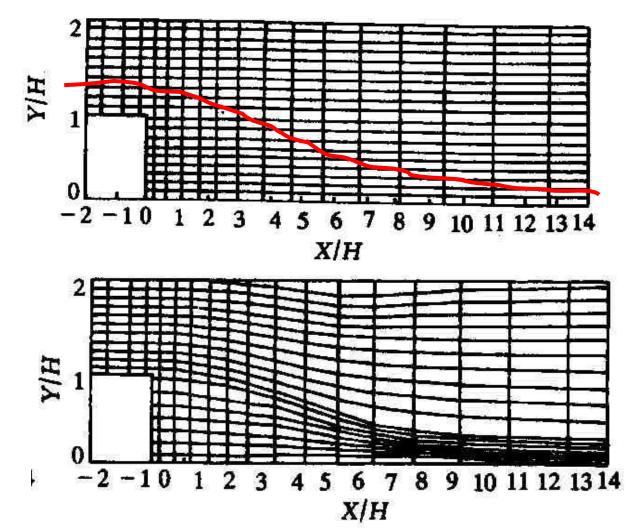
$$\delta t = \frac{1}{\frac{u}{\Delta x} + \frac{v}{\Delta y} + \frac{w}{\Delta z}}$$

(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

- 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

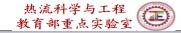
order and bounded schemes (高阶有界格式) should be used.

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



D-NHT-EHT NTER





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

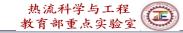
1.Inlet boundary

2.Solid boundary

3.Central line







4.7 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

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



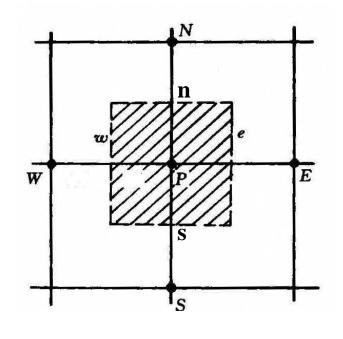
CENTER

2. Results of discretization

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

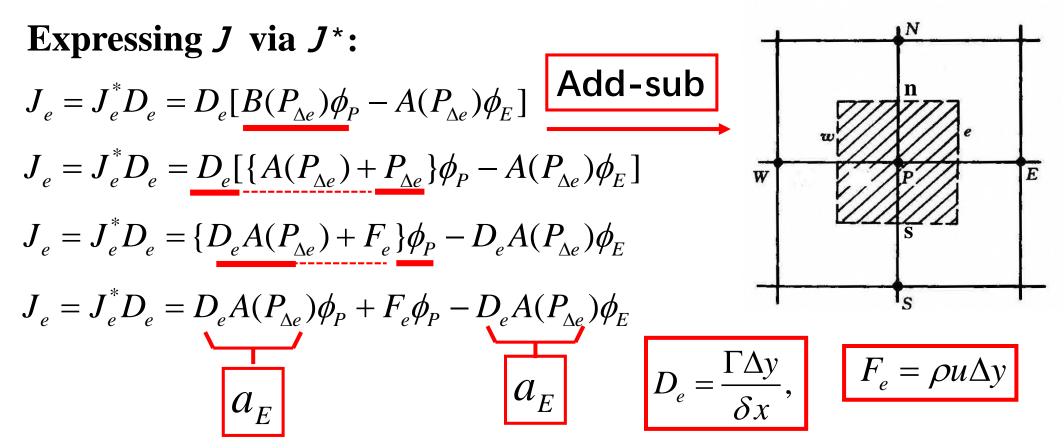
Integrating above equations for CV. P

$$\begin{split} & \iiint \frac{\partial (\rho \phi)}{\partial t} dt dx dy = [(\rho \phi)_P - (\rho \phi)_P^0] \Delta V \\ & \iiint \frac{e}{\partial x} \frac{\partial J_x}{\partial x} dx dy dt = \int_{t-\Delta t}^{t+\Delta t} \int_{t-\Delta t}^n (J_x^e - J_x^w) dy dt \\ & \iiint \frac{e}{\partial y} \frac{\partial J_y}{\partial y} dx dy dt = \int_{t-\Delta t}^t \int_{w}^s (J_y^n - J_y^s) dx dt \\ & \iiint S dx dy dt = (S_C + S_P \phi_P) \Delta V \Delta t \end{split}$$





Assuming that at the interface J_x^e, J_x^w are constant, then: $(J_x^e - J_x^w)\Delta y\Delta t = (\underline{J}_x^e \Delta y - \underline{J}_x^w \Delta y)\Delta t = (J_e - J_w)\Delta t$



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

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Finally the general discretization equation for 2-D five-point scheme: $a_{P}\phi_{P} = a_{F}\phi_{F} + a_{W}\phi_{W} + a_{S}\phi_{S} + a_{N}\phi_{N} + b$ $a_{P} = a_{E} + a_{W} + a_{N} + a_{S} + a_{P}^{0} - S_{P}\Delta V$ $b = S_C \Delta V + a_P^0 \phi_P^0$ $a_P^0 = \rho_P \Delta V / \Delta t$ $a_E = D_e A(|P_{\Delta e}|) + [-F_e, 0 \quad a_W = D_w A(|P_{\Delta w}|) + [F_w, 0]$ $a_N = D_n A(|P_{\Lambda n}|) + [-F_n, 0 \quad a_S = D_s A(|P_{\Lambda s}|) + [F_s, 0]$

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_o

45/52



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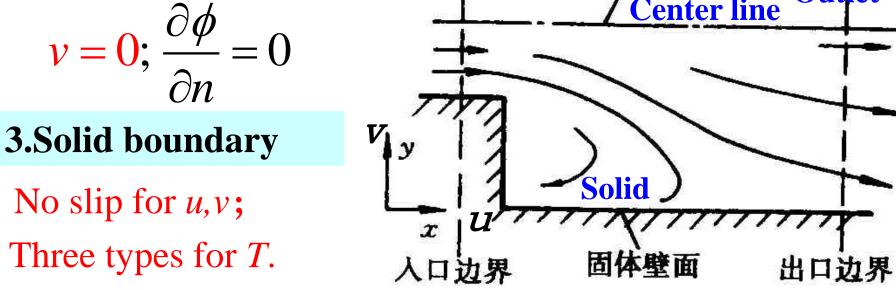
4.7.2 Treatment of boundary conditions

1.Inlet boundary – usually specified;

2.Center line – symmetric boundary:

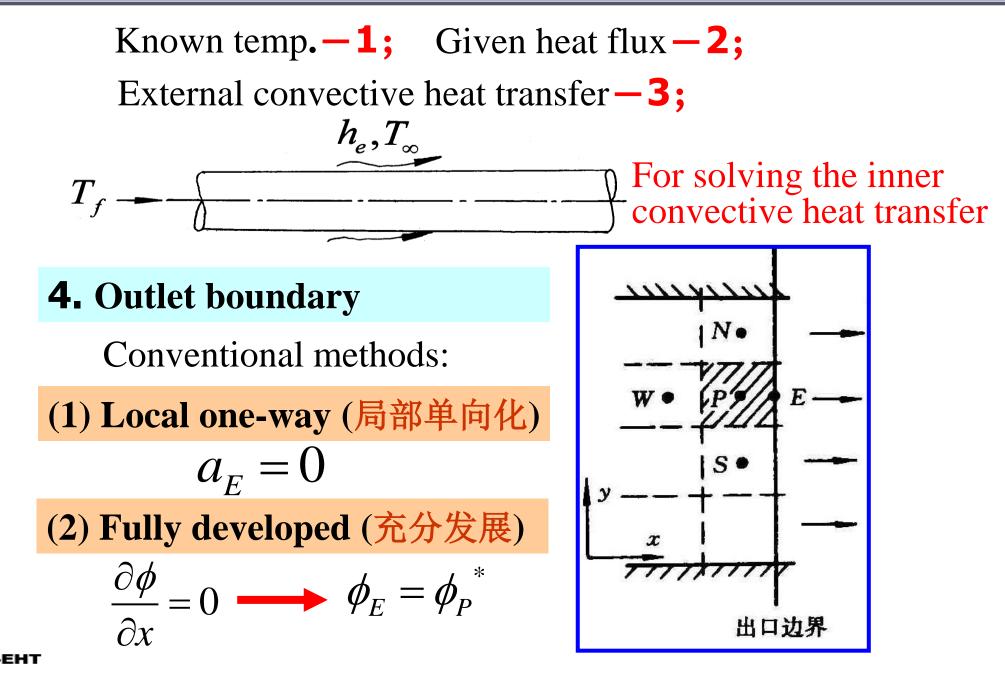
Velocity component normal to the center line is equal to zero;

First derivative normal to the lcenter ine of other variable is equal to zero Inlet $\frac{中心线}{/Center line}$ Outlet





CENTER





Home Work 4 (2022-2023)

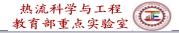
Please finish your homework independently !!!

Please hand in on October 19,2022

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 10 nodes for x=0-1, and use 1st-order upwind difference, central difference, 3rdorder 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, 10 and 100. Draw the picture of $(\phi - \phi_0)/(\phi_L - \phi_0)$ versus x/L, and compare the results of the exact solution.

48/52



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Problem 4-2

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

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

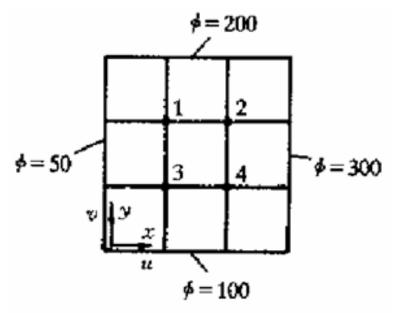
adopt the 1st-order upwind scheme for the convection term and central difference for the diffusion term, find the values of the four coefficients a_E, a_W, a_P, a_P^0 at following conditions: $\Delta t = 0.05, \rho u = 4, P_{\Delta} = 1$ and 5.

Problem 4-3

For a one-dimensional steady state diffusion-convection problem without a source term with boundary condition shown in the figure. Take $\rho u = 3$, $\rho v = 4$, $\Gamma = 7$, $\Delta x = \Delta y = 0.2$.

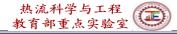


Take 1st-order upwind scheme, 2nd-order upwind scheme for the convection term and central scheme for the diffusion term. Determine the ϕ values at the four nodes 1,2,3 and 4.



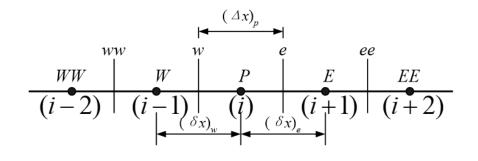
Problem 4-4

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





 $\begin{cases} \phi_e = a_i \phi_i + \left(\frac{1}{4} - \frac{a_i}{2}\right) \phi_{i-1} + \left(\frac{3}{4} - \frac{a_i}{2}\right) \phi_{i+1} \\ \phi_w = a_i \phi_{i-1} + \left(\frac{1}{4} - \frac{a_i}{2}\right) \phi_{i-2} + \left(\frac{3}{4} - \frac{a_i}{2}\right) \phi_i \end{cases}$

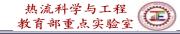


Determine the values of the constant a_i for : (1) central scheme; (2) 2nd-order upwind scheme; (3) QUICK scheme; (4) 3rd-order upwind scheme.

Problem 4-5

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





本组网页地址: <u>http://nht.xjtu.edu.cn</u> 欢迎访问! *Teaching PPT will be loaded on ou website*







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

