

Numerical Heat Transfer

(数值传热学)

Chapter 4 Discretized Schemes of Diffusion and Convection Equation (1)



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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

4.1 Two ways of discretization of convection term

4.1.1 Importance of discretized scheme of convection term

1. Accuracy

2. Stability

3. Economics

4.1.2 Two ways for constructing discretization schemes of convective term

4.1.3 Relationship between the two ways

4.1 Two ways of discretization of convection term

4.1.1 Importance of discretization scheme (离散格式)

Mathematically convective term is only of 1st order derivative, while its physical meaning (strong directional) makes its discretization one of the hot spots (热点) of numerical simulation:

1. It affects the numerical accuracy(精确性).

When a scheme with 1st-order is used the solution involves severe numerical error.

2. It affects the numerical stability(稳定性).

The schemes of CD, TUD and QUICK are only conditionally stable.

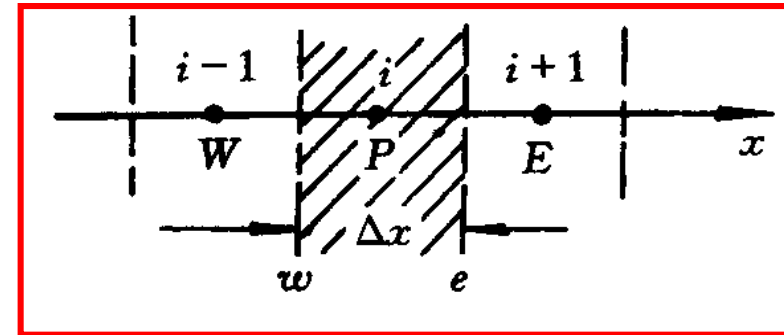
3. It affects numerical economics (经济性).

4.1.2 Two ways for constructing(构建) schemes

1. Taylor expansion – providing the FD form at a point

Taking CD as an example:

$$\left(\frac{\partial \phi}{\partial x}\right)_P = \frac{\phi_E - \phi_W}{2\Delta x} = \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x}$$



2. CV integration – providing average value within the domain

By assuming a profile for the interface variable

$$\frac{1}{\Delta x} \int_w^e \frac{\partial \phi}{\partial x} dx = \frac{\phi_e - \phi_w}{\Delta x} \xrightarrow{\text{Piecewise linear, Uniform grids}} \frac{(\phi_E + \phi_P)/2 - (\phi_P + \phi_W)/2}{\Delta x} = \frac{\phi_E - \phi_W}{2\Delta x}$$

4.1.3 Relationship between the two ways

1. For the same scheme they have the same order of the T.E.
2. For the same scheme, the coefficients of the 1st term in T.E. are different. The absolute value of FVM is usually less than that of FD.
3. Taylor expansion provides the FD form at a point while CV integration gives the average value by integration within the domain

$$\frac{1}{\Delta x} \int_w^e \frac{\partial \phi}{\partial x} dx = \frac{\phi_e - \phi_w}{\Delta x}$$

4.2 CD and UD of the convection term

4.2.1 Analytical solution of 1-D model equation

4.2.2 CD discretization of 1-D diffusion-convection equation

4.2.3 Up wind scheme of convection term

1. Definition of CV integration

2. Compact form

3. Discretization equation with UD of convection and CD of diffusion

4.2 CD and UD of convection term

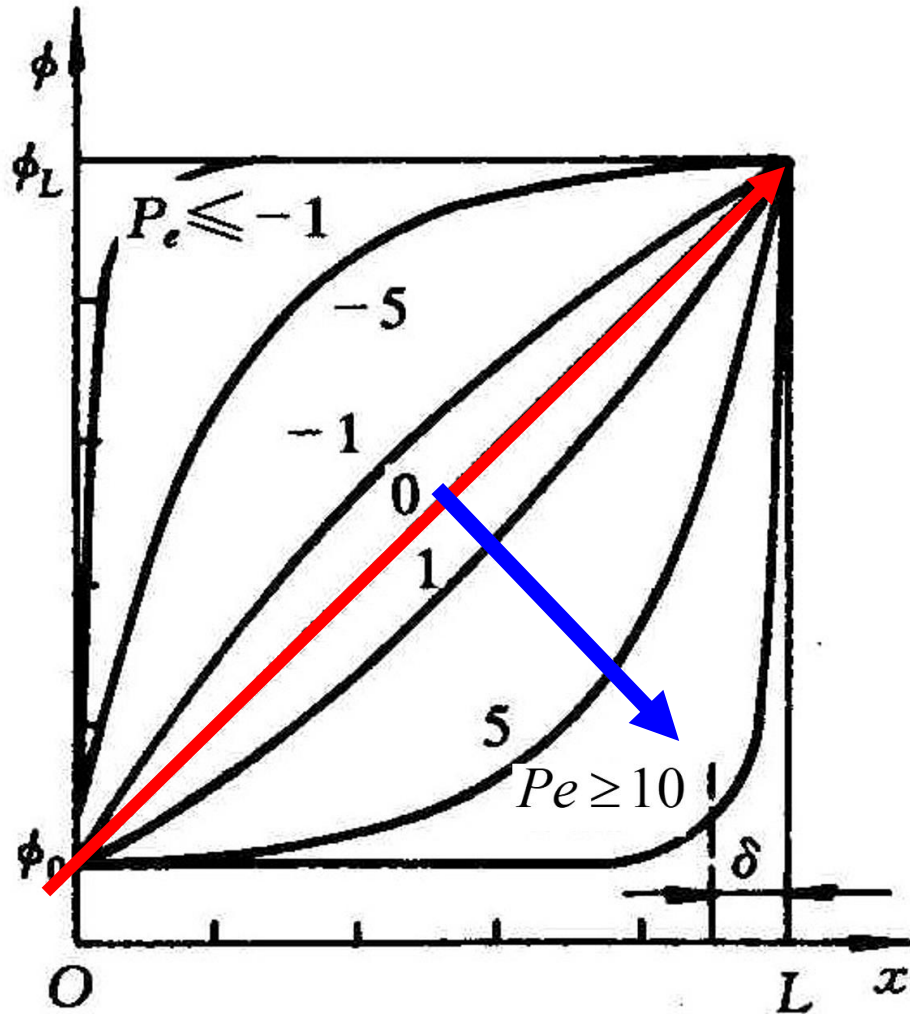
4.2.1 Analytical solution of 1-D model eq. without source term (diffusion and convection eq.)

$$\left\{ \begin{array}{l} \frac{d(\rho u \phi)}{dx} = \frac{d}{dx} \left(\Gamma \frac{d\phi}{dx} \right), \\ x = 0, \phi = \phi_0; \quad x = L, \phi = \phi_L \end{array} \right. \quad \begin{array}{l} \text{Physical properties and} \\ \text{velocity are known constants} \end{array}$$

The analytical solution of this ordinary differential equation:

$$\frac{\phi - \phi_0}{\phi_L - \phi_0} = \frac{\exp(\rho u x / \Gamma) - 1}{\exp(\rho u L / \Gamma) - 1} = \frac{\exp\left(\frac{\rho u L}{\Gamma} \frac{x}{L}\right) - 1}{\exp(\rho u L / \Gamma) - 1} = \frac{\exp(Pe \frac{x}{L}) - 1}{\exp(Pe) - 1}$$

Solution Analysis



$Pe = 0$, pure diffusion, linear Distribution;

With increasing Pe , distribution curve becomes more and more convex downward (下凸);

When $Pe = 10$, in the most region from $x=0-L$

$$\phi = \phi_0$$

Only when x is very close to L , ϕ increases dramatically and

when $x=L$, $\phi = \phi_L$.

The above variation trend with Peclet number is consistent(**协调的**) with the physical meaning of **Pe**

$$Pe = \frac{\rho u L}{\Gamma} = \frac{\rho u}{\Gamma / L} \quad \frac{\text{Convection}}{\text{Diffusion}}$$

When Pe is small – Diffusion dominated, linear distribution ;

When Pe is large – Convection dominated, i.e., upwind(**上游**) effect dominated, upwind information is transported downstream, and when $Pe \geq 100$, axial conduction can be neglected.

It is required in some sense that the discretized scheme of the convective term has some similar physical characteristics.

4.2.2 CD discretization of 1-D diffusion-convection equation

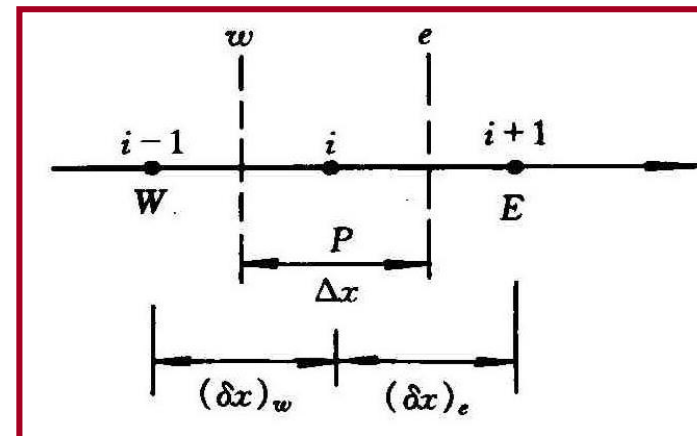
1. Integration of 1-D model equation

Adopting the linear profile, integration over a CV yields:

$$\phi_P \left[\underbrace{\frac{1}{2}(\rho u)_e + \frac{\Gamma_e}{(\delta x)_e}}_{a_P} - \underbrace{\frac{1}{2}(\rho u)_w + \frac{\Gamma_w}{(\delta x)_w}}_{a_W} \right] = \underbrace{\phi_E \left[\frac{\Gamma_e}{(\delta x)_e} - \frac{1}{2}(\rho u)_e \right]}_{a_E} + \underbrace{\phi_W \left[\frac{\Gamma_w}{(\delta x)_w} + \frac{1}{2}(\rho u)_w \right]}_{a_W}$$

Thus:

$$a_P \phi_P = a_E \phi_E + a_W \phi_W$$



2. Relationship between coefficients

Rewriting a_P as follows:

$$a_P = \frac{1}{2}(\rho u)_e + \frac{\Gamma_e}{(\delta x)_e} - \frac{1}{2}(\rho u)_w + \frac{\Gamma_w}{(\delta x)_w} =$$

$$\frac{\frac{1}{2}(\rho u)_e - (\rho u)_e + (\rho u)_e}{2} + \frac{\Gamma_e}{(\delta x)_e} - \frac{\frac{1}{2}(\rho u)_w + (\rho u)_w - (\rho u)_w}{2} + \frac{\Gamma_w}{(\delta x)_w} =$$

$$-\frac{1}{2}(\rho u)_e + \frac{\Gamma_e}{(\delta x)_e} + \frac{1}{2}(\rho u)_w + \frac{\Gamma_w}{(\delta x)_w} + [(\rho u)_e - (\rho u)_w] = a_E + a_W + [(\rho u)_e - (\rho u)_w]$$

a_E

a_W

Defining diffusion
Conductance:

$$\frac{\Gamma}{\delta x} = D,$$

Interface flow rate:

$$\rho u = F$$

The discretized form of 1-D steady diffusion and convection equation is:

$$a_P \phi_P = a_E \phi_E + a_W \phi_W \quad a_E = D_e - \frac{1}{2} F_e \quad a_W = D_w + \frac{1}{2} F_w$$
$$a_P = a_E + a_W + \underline{(F_e - F_w)}$$

If in the iterative process the mass conservation is satisfied then

$$F_e - F_w = 0$$

In order to guarantee the convergence of iterative process, it is always required:

$$a_P = a_E + a_W$$

Hence, it is demanded that at any iteration level mass must be conserved!

3. Analysis of discretized diffu-conv. eq. by CD

From $a_P \phi_P = a_E \phi_E + a_W \phi_W$ it can be obtained:

$$\phi_P = \frac{a_E \phi_E + a_W \phi_W}{a_E + a_W} = \frac{(D_e - \frac{1}{2} F_e) \phi_E + (D_w + \frac{1}{2} F_w) \phi_W}{(D_e - \frac{1}{2} F_e) + (D_w + \frac{1}{2} F_w)}$$

Uni.grid

Const property

$$\phi_P = \frac{(1 - \frac{1}{2} \frac{F}{D}) \phi_E + (1 + \frac{1}{2} \frac{F}{D}) \phi_W}{(D + D) / D} \longrightarrow \frac{(1 - \frac{1}{2} P_\Delta) \phi_E + (1 + \frac{1}{2} P_\Delta) \phi_W}{2}$$

P_Δ is the grid Peclet, $P_\Delta = \frac{\rho u (\delta x)}{\Gamma}$

With the given ϕ_E, ϕ_W ϕ_P can be determined.

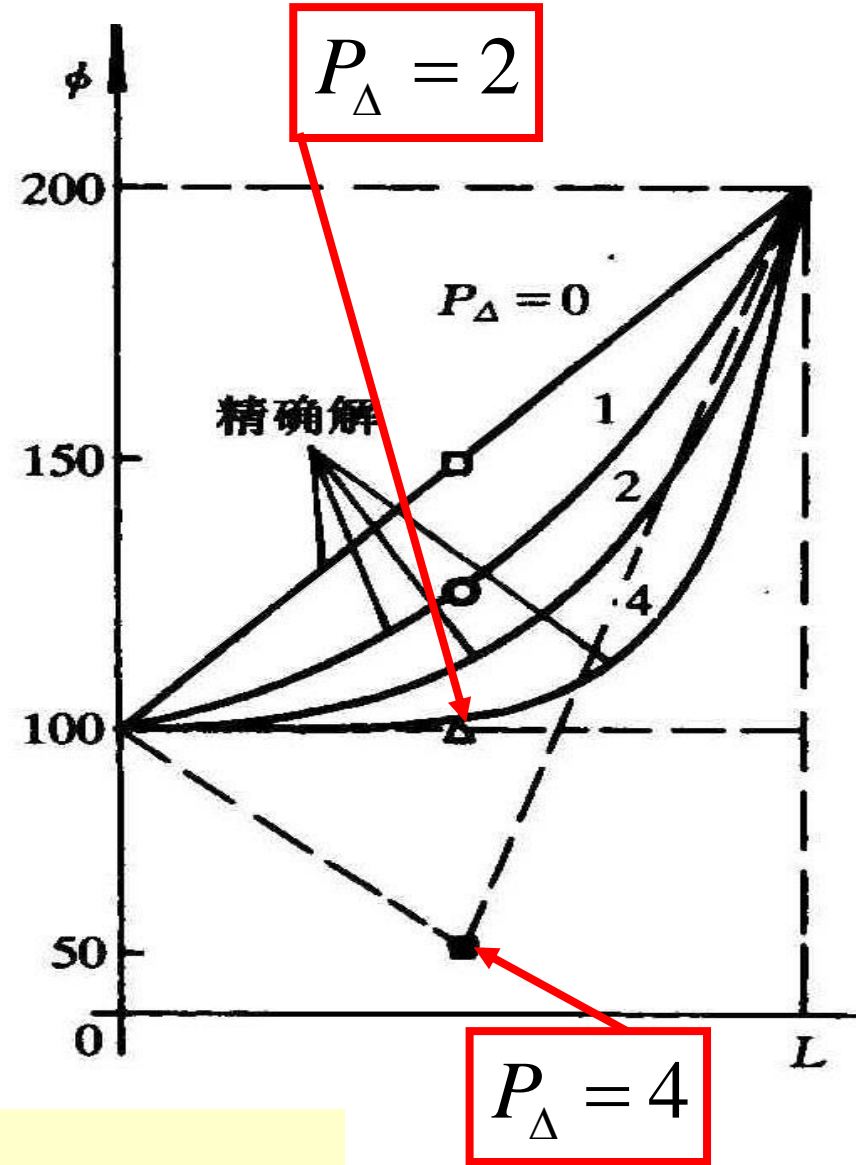
Given $\phi_W = 100, \phi_E = 200$
for $P_\Delta = 0, 1, 2, 4$
the calculated results are
shown in the figure.

**Physically and according
to the analytical solution**

$$\frac{\phi - \phi_0}{\phi_L - \phi_0} = \frac{\exp\left(\frac{\rho u L}{\Gamma} \frac{x}{L}\right) - 1}{\exp\left(\frac{\rho u L}{\Gamma}\right) - 1}$$

**the value of ϕ should be
larger than zero.**

$$\frac{\rho u L}{\Gamma} = Pe = 2 P_\Delta$$

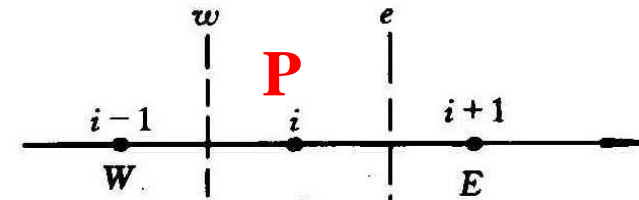


Thus when P_Δ is larger than 2, numerical solutions are unrealistic; ϕ_P is less than its two neighboring grid values, which is not possible for the case without source.

The reason is $a_E = \frac{1}{2}(1 - \frac{1}{2}P_\Delta) < 0$, i.e. the east influencing coefficient is negative, which is physically meaningless.

4.2.3 FUD of convection term

1. Definition in FDM—



$$\left(\frac{\partial \phi}{\partial x}\right)_i = \frac{\phi_i - \phi_{i-1}}{\Delta x}, u > 0; \left(\frac{\partial \phi}{\partial x}\right)_i = \frac{\phi_{i+1} - \phi_i}{\Delta x}, u < 0$$

2. Definition in FVM— interpolation of interface always takes upstream grid value

$$\phi_e = \begin{cases} \phi_P, u_e > 0 \\ \phi_E, u_e < 0 \end{cases} O(\Delta x) \quad \phi_w = \begin{cases} \phi_W, u_w > 0 \\ \phi_P, u_w < 0 \end{cases}$$

2. Compact form (紧凑形式)

For the convenience of discussion, **combining interface value ϕ_e with flow rate**

$$(\rho u \phi)_e = F_e \phi_e = \phi_P \max(F_e, 0) - \phi_E \max(-F_e, 0)$$

Patankar proposed a special symbol as follows

$$\text{MAX: } \llbracket X, Y \rrbracket, \text{ then: } (\rho u \phi)_e = \phi_P \llbracket F_e, 0 \rrbracket - \phi_E \llbracket -F_e, 0 \rrbracket$$

Similarly:

$$(\rho u \phi)_w = \phi_W \llbracket F_w, 0 \rrbracket - \phi_P \llbracket -F_w, 0 \rrbracket$$

3. Discretized form of 1-D model equation with FUD for convection and CD for diffusion

$$a_P \phi_P = a_E \phi_E + a_W \phi_W$$

$$a_E = D_e + \|-F_e, 0\| \quad a_W = D_w + \|F_w, 0\|$$

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

Because $a_E \geq 0, a_W \geq 0$ **FUD can always obtained physically plausible solution** (物理上看起来合理的解).

It was widely used in the past decades since its proposal in 1950s.

However, because of its severe **numerical errors** (severe false diffusion, **严重的假扩散**), it is not recommended for the final solution.

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4.3 Hybrid and Power-Law Schemes

4.3.1. Relationship between a_E, a_W of 3-point schemes

4.3.2. Hybrid scheme

4.3.3. Exponential scheme

4.3.4. Power-law scheme

4.3.5. Expressions of coefficients of five 3-point schemes and their plots

4.3 Hybrid and Power-Law Schemes

4.3.1. Relationship between coefficients a_E, a_W of 3-point schemes

- 3-point scheme** — interface interpolation is conducted by using two points at the two sides of the interface

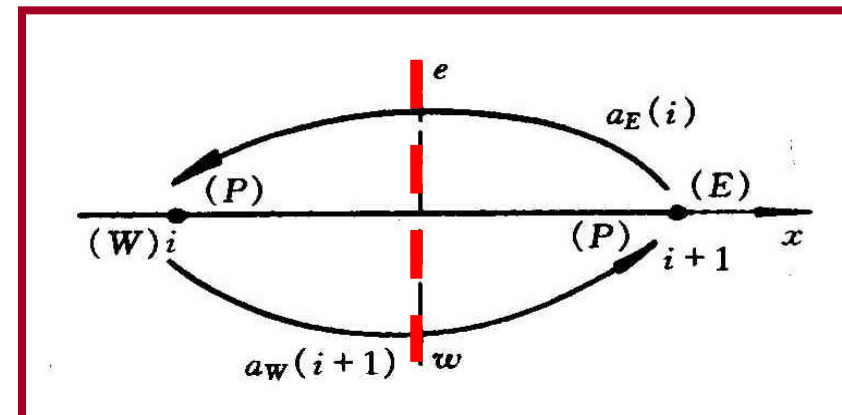
With such scheme 1-D problem leads to tri-diagonal matrix, and 2-D penta-diagonal (五对角) matrix.

- Relationship between a_E, a_W**

East or West interfaces are relative to the grid position.

For the same interface shown by the red line:

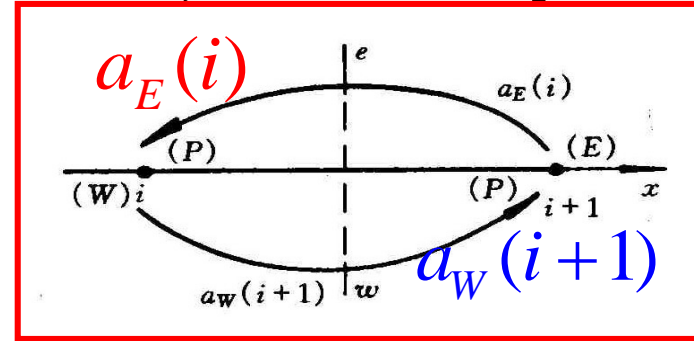
it is East for point P,
while West for E.



$a_E(i)$ and $a_W(i+1)$ share the same interface, the same conductivity and the same absolute flow rate, hence they must have some interrelationship.

For **CD**:

$$a_E = D_e \left(1 - \frac{1}{2} P_{\Delta e}\right) a_W = D_w \left(1 + \frac{1}{2} P_{\Delta w}\right)$$



At the same interface $P_{\Delta e} = P_{\Delta w} = P_{\Delta}$ $D_e = D_w = D$

$$\frac{a_W(i+1)}{D} - \frac{a_E(i)}{D} = 1 + \frac{1}{2} P_{\Delta} - \left(1 - \frac{1}{2} P_{\Delta}\right) = P_{\Delta}$$

Meaning: for diffusion problem, $a_E(i) = a_W(i+1)$

For convection if $(u > 0)$, node i has effect on $(i+1)$, while $(i+1)$ has no convection effect on i ; $a_E(i)$ has no convection effect on grid i , while $a_W(i+1)$ has some convection effect on grid $(i+1)$.

For **FUD**: $a_E = D_e (1 + \|-P_{\Delta e}, 0\|)$ $a_W = D_w (1 + \|P_{\Delta w}, 0\|)$

$$\frac{a_W(i+1)}{D} - \frac{a_E(i)}{D} = \underbrace{1 + \|P_{\Delta}, 0\|} - \underbrace{(1 + \|-P_{\Delta}, 0\|)} \longrightarrow$$

$$\|P_{\Delta}, 0\| - \|-P_{\Delta}, 0\| = P_{\Delta}$$

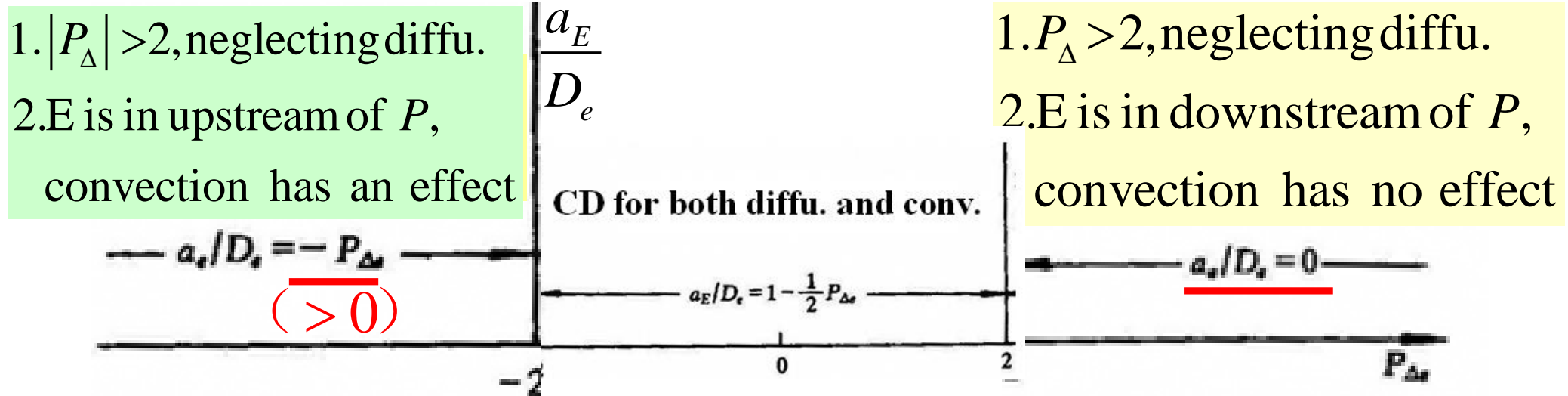
For a_E or a_W once one of them is known, the other can be obtained.

Thus defining a scheme can be conducted just by defining one coefficient. We will define the E-coeff.

4.3.2 Hybrid scheme (混合格式)

1. Graph definition

Spalding proposed: taking P_Δ as abscissa (横坐标)
and a_E / D_e as ordinate (纵坐标)



$$\frac{a_E}{D_e} = \left\{ \begin{array}{l} 0, P_\Delta > 2 \\ 1 - \frac{1}{2} P_\Delta, |P_\Delta| \leq 2 \\ -P_\Delta, P_\Delta < -2 \end{array} \right\} \text{ Hybrid scheme of Spalding}$$

2. Compact definition

$$\frac{a_E}{D_e} = \left\| -P_{\Delta e}, 1 - \frac{1}{2} P_{\Delta e}, 0 \right\|$$

4.3.3. Exponential scheme (指数格式)

Definition: the discretized form identical to the analytical solution of the 1-D model equation.

Method: rewriting the analytical solution in the form of algebraic equation of ϕ at three neighboring grid points.

1. Total flux J (总通量) of diffusion and convection

Define $J = \rho u \phi - \Gamma \frac{d\phi}{dx}$, then 1-D model eq. can be rewritten as $\frac{dJ}{dx} = 0$, or $J = const$

For CV. P: $J_e = J_w$

2. Analytical expression for total flux of diffu. and conv.

Substituting the analytical solution of ϕ into J :

$$\phi = \phi_0 + (\phi_L - \phi_0) \frac{\exp(Pe \frac{x}{L}) - 1}{\exp(Pe) - 1}$$

$$J = \rho u \phi - \Gamma \frac{d\phi}{dx} = \rho u \left[\phi_0 + (\phi_L - \phi_0) \frac{\exp(Pe \frac{x}{L}) - 1}{\exp(Pe) - 1} \right] - \Gamma \left[(\phi_L - \phi_0) \frac{\frac{Pe}{L} \exp(Pe \frac{x}{L})}{\exp(Pe) - 1} \right]$$

$Pe = \frac{\rho u L}{\Gamma}$

$\rho u \phi$
 $\Gamma d\phi / dx$

Hence: $J = F \left[\phi_0 + \frac{\phi_0 - \phi_L}{\exp(Pe) - 1} \right]$

$$\frac{\Gamma}{L} Pe = \frac{\Gamma}{L} \frac{\rho u L}{\Gamma} = \rho u$$

2. Expressions of total flux for e,w interfaces

For e: $\phi_0 = \phi_P, \phi_L = \phi_E, L = (\delta x)_e : J_e = F_e \left[\phi_P + \frac{\phi_P - \phi_E}{\exp(P_{\Delta e}) - 1} \right]$

For w: $\phi_0 = \phi_W, \phi_L = \phi_P, L = (\delta x)_w : J_w = F_w \left[\phi_W + \frac{\phi_W - \phi_P}{\exp(P_{\Delta w}) - 1} \right]$

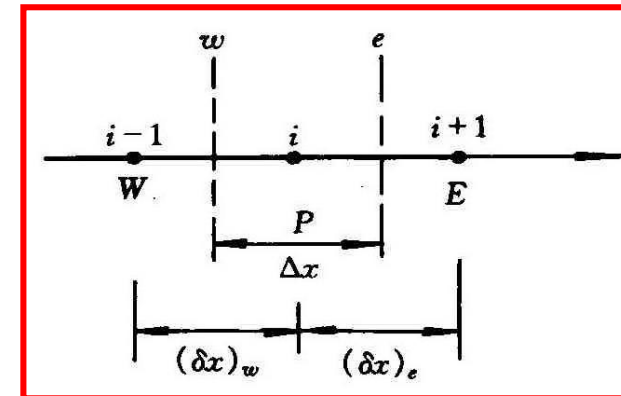
Substituting the two expressions into $J_e = J_w$ and

rewrite into algebraic equation among ϕ_W, ϕ_P, ϕ_E

yields: $a_P \phi_P = a_W \phi_W + a_E \phi_E$

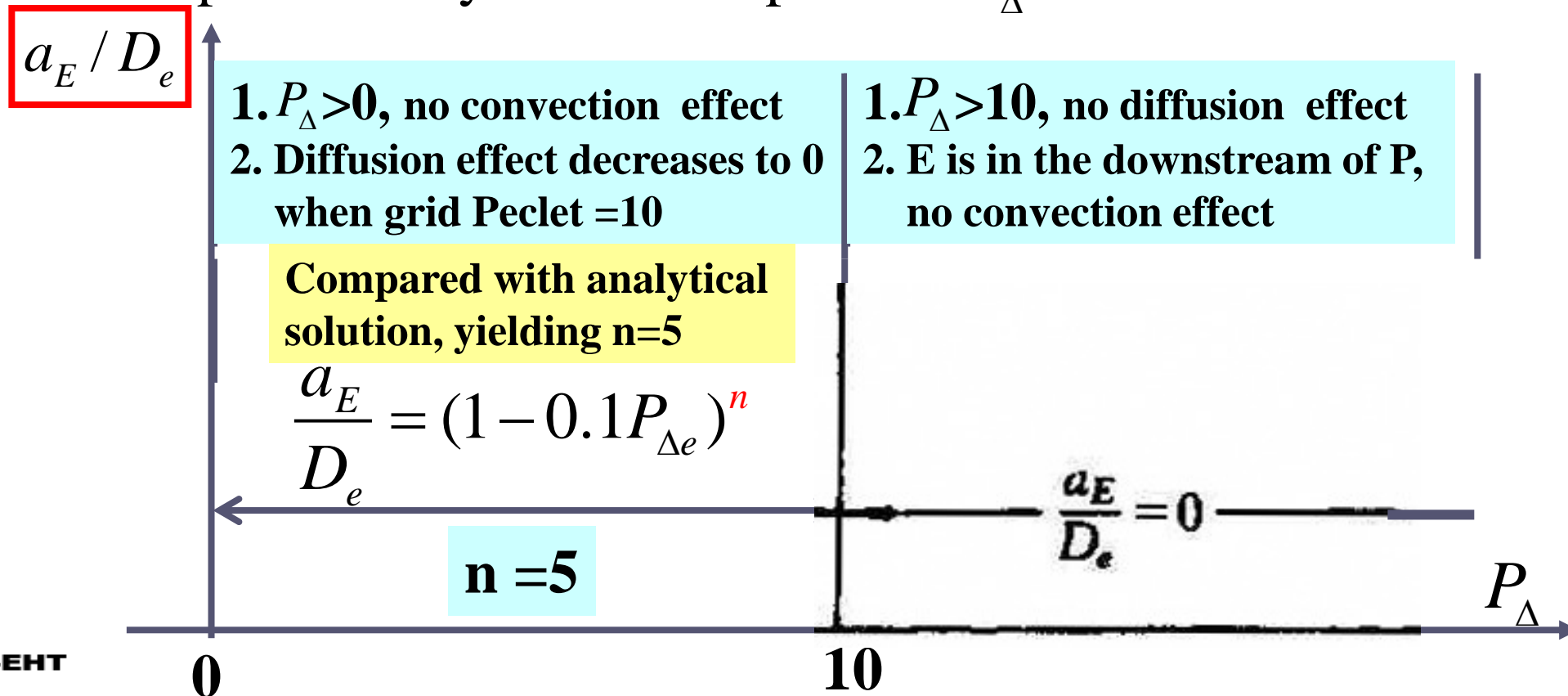
$$a_E = \frac{F_e}{\exp(P_{\Delta e}) - 1}, a_W = \frac{F_w \exp(P_{\Delta w})}{\exp(P_{\Delta w}) - 1}$$

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



4.3.4. Power-law scheme (乘方格式)

Exponential scheme is computationally very expensive. Patankar proposed the power-law scheme, which is very close to the exponential scheme and computationally much cheaper. For $P_{\Delta} > 0$:



For $P_{\Delta} < 0$

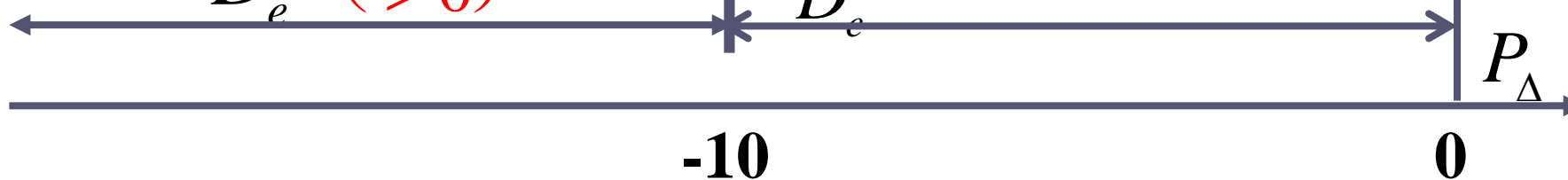
$$\frac{a_E}{D_e}$$

1. $P_{\Delta} < 0$, E is in the upstream of P, convection has effect
2. $P_{\Delta} > 10$ diffusion has no effect

1. $P_{\Delta} < 0$, E is in the upstream of P, convection has effect
2. $P_{\Delta} < 10$ diffusion has effect
3. Diffusion effect has the same expression as for $P_{\Delta} > 0$

$$\frac{a_E}{D_e} = -P_{\Delta} \quad (> 0)$$

$$\frac{a_E}{D_e} = (1 + 0.1P_{\Delta e})^5 - P_{\Delta e}$$



Compact form of the power-law scheme

$$\frac{a_E}{D_e} = \left\| 0, (1 - 0.1|P_{\Delta e}|)^5 \right\| + \left\| 0, -P_{\Delta e} \right\|$$

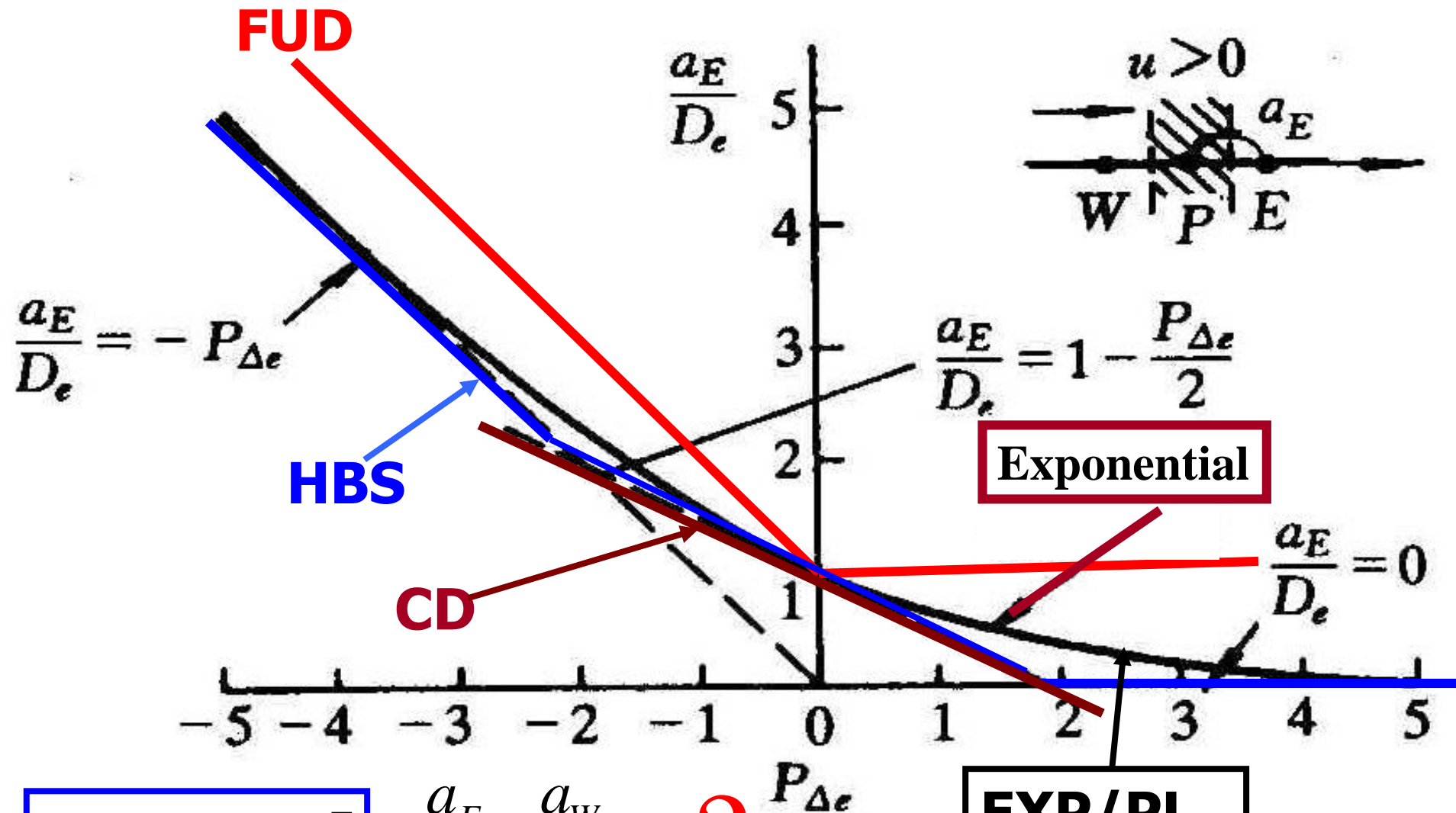
Diffusion effect

Convection effect

4.3.5. a_E / D_e coefficient expressions of five schemes and their graph illustration

Scheme	Central difference	Upwind difference
Definition	$1 - 0.5 P_{\Delta e}$	$1 + \left\ -P_{\Delta e}, 0 \right\ $
Hybrid	Power-law	Exponential
$\left\ -P_{\Delta e}, 1 - \frac{1}{2} P_{\Delta e}, 0 \right\ $	$\left\ 0, (1 - 0.1 P_{\Delta e})^5 \right\ + \left\ 0, -P_{\Delta e} \right\ $	$\frac{P_{\Delta e}}{\exp(P_{\Delta e}) - 1}$

$$a_E / D_e = 1 + \parallel -P_{\Delta e}, 0 \parallel$$



$$a_E, a_W \dots J$$

$$\frac{a_E}{D_E}, \frac{a_W}{D_W} \dots ?$$

EXP/PL

4.4 Characteristics of five three-point schemes

4.4.1 J^* flux definition and its discretized form

4.4.2 Relationship between coefficients A and B

4.4.3 Important conclusions from coefficient characters

4.4.4 General expression for coefficients a_E, a_W

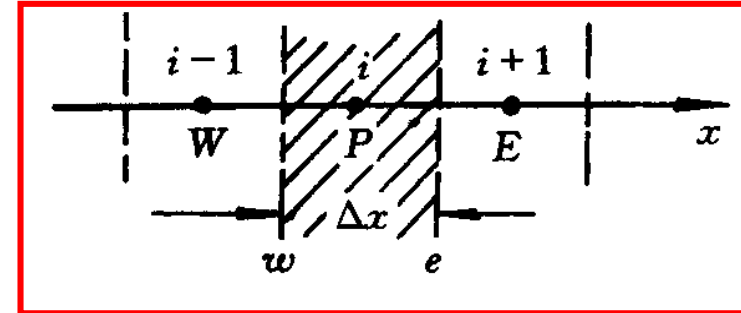
4.4.5 Discussion

Key Points of Last lecture(10-13)

1. Two ways of defining a scheme for convection term

(1) By FDM – providing the finite difference form for the 1st order derivative

$$\text{CD: } \left. \frac{\partial \phi}{\partial x} \right)_i = \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x}$$



(2) By FVM – providing average value within the domain.
Different interface interpolation method leads to different scheme.

2. Basic idea of upwind (upstream) scheme

Taking the value(s) of upstream grids to construct the scheme.

$$\left. \frac{\partial \phi}{\partial x} \right)_i \stackrel{u \geq 0}{=} \frac{\phi_i - \phi_{i-1}}{\Delta x} ; \left. \frac{\partial \phi}{\partial x} \right)_i \stackrel{u < 0}{=} \frac{\phi_{i+1} - \phi_i}{\Delta x}$$

$$\phi_e = \begin{cases} \phi_P, u_e > 0 \\ \phi_E, u_e < 0 \end{cases}$$

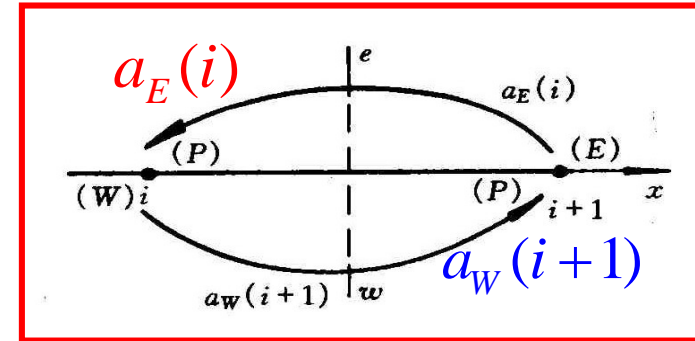
FUD in FDM

FUD in FVM

3. Relationship between a_E and a_W of three-point scheme

$$\frac{a_W(i+1)}{D} - \frac{a_E(i)}{D} = P_\Delta$$

$$P_\Delta = \frac{\rho u \delta x}{\Gamma}$$



4. Compact form of the definition of a scheme

$$\text{Hybrid scheme } \frac{a_E}{D_e} = \left\{ \begin{array}{l} 0, P_\Delta > 2 \\ 1 - \frac{1}{2} P_\Delta, |P_\Delta| \leq 2 \\ -P_\Delta, P_\Delta < -2 \end{array} \right\} \frac{a_E}{D_e} = \left\| -P_{\Delta e}, 1 - \frac{1}{2} P_{\Delta e}, 0 \right\|$$

$$\text{Power-law } \frac{a_E}{D_e} = \left\| 0, (1 - 0.1 |P_{\Delta e}|)^5 \right\| + \left\| 0, -P_{\Delta e} \right\|$$

Diffusion effect Convection effect

4.4 Characteristics of five three-point schemes

4.4.1 J^* flux definition and its discretized form

1. J^* definition (analytical expression)

J flux is correspondent to the discretized equation $a_P \phi_P = a_W \phi_W + a_E \phi_E$, while flux correspondent to coefficient a_E / D_e is called J^* , which is defined by:

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

$$J^* = P_{\Delta} \phi - \frac{d\phi}{dX} \quad P_{\Delta} = \frac{\rho u \delta x}{\Gamma} \quad X = \frac{x}{\delta x}$$

2. Discretized form of J^*

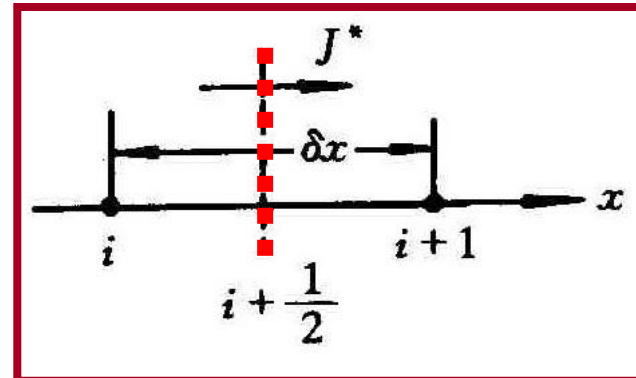
For the three-point scheme J^* at interface can be expressed by a combination of variables at nearby two grids.

For interface $(i+1/2)$,

Let $J^* = B\phi_i - A\phi_{i+1}$

Ahead of the interface

Behind of the interface



Viewed from positive direction of coordinate

Coefficients A , B are dependent on grid Peclet, P_{Δ}

4.4.2 Analysis of relationship between A and B

Analysis is based on fundamental physical and mathematical concepts.

1. Summation-subtraction character (和差特性)

For a uniform field, there is no diffusion at all. Then J^* is totally caused by convection

From the analytical expression of J^* :

$$J^* = \left(P_{\Delta} \phi - \frac{d\phi}{dX} \right)_i = \left(P_{\Delta} \phi - \frac{d\phi}{dX} \right)_{i+1} = P_{\Delta} \phi_i = P_{\Delta} \phi_{i+1}$$

From the discretized expression of J^* :

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

Analytical =
Discretized!

$$(B - A) \cancel{\phi_{i+1}} = P_{\Delta} \cancel{\phi_i} = P_{\Delta} \cancel{\phi_{i+1}} \longrightarrow$$

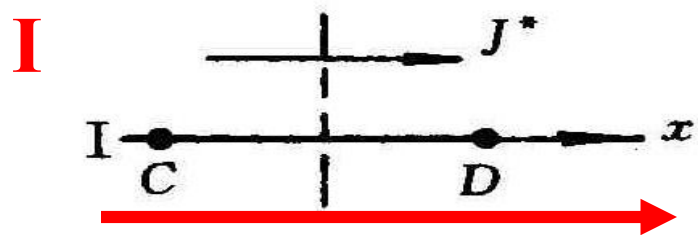
$$B - A = P_{\Delta} \quad \text{Summation-subtraction(和差特性)}$$

2. Symmetry character

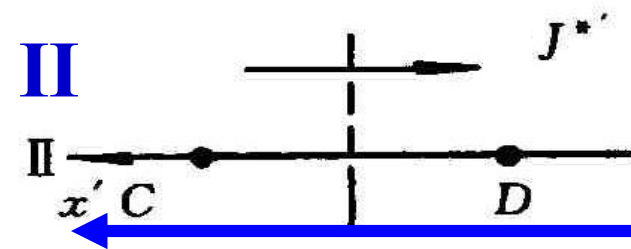
For the same process its mathematical formulation is expressed in two coordinates. The two coordinates are I, II, and their positive directions are opposite (相反的). Two points C, D are located at the two sides of an interface

Viewed from coordinate positive direction

C-behind/D-ahead



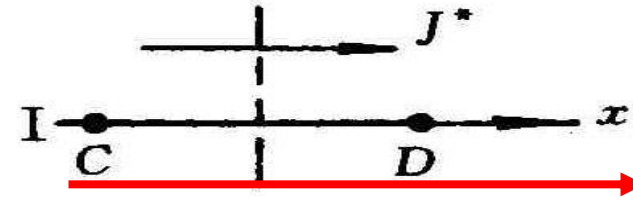
C-ahead/D-behind



For the same flux, in coordinate I it is denoted by J^* , while in II denoted by $J^{*'}$, then we have

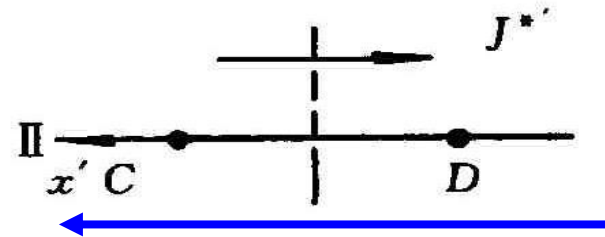
For I **C-behind/D-ahead**

$$J^* = B(P_\Delta) \phi_C - A(P_\Delta) \phi_D$$



For II **D-behind/C-ahead**

$$J^{*'} = B(-P_\Delta) \phi_D - A(-P_\Delta) \phi_C$$



The flux is the same so: $J^* = -J^{*'}$

$$B(P_{\Delta})\phi_C - A(P_{\Delta})\phi_D = -[B(-P_{\Delta})\phi_D - A(-P_{\Delta})\phi_C]$$

Merging (合并) the terms according to ϕ_D, ϕ_C

$$[B(P_{\Delta}) - A(-P_{\Delta})]\phi_C = [A(P_{\Delta}) - B(-P_{\Delta})]\phi_D$$

ϕ_D, ϕ_C can take any values. In order that above eq.

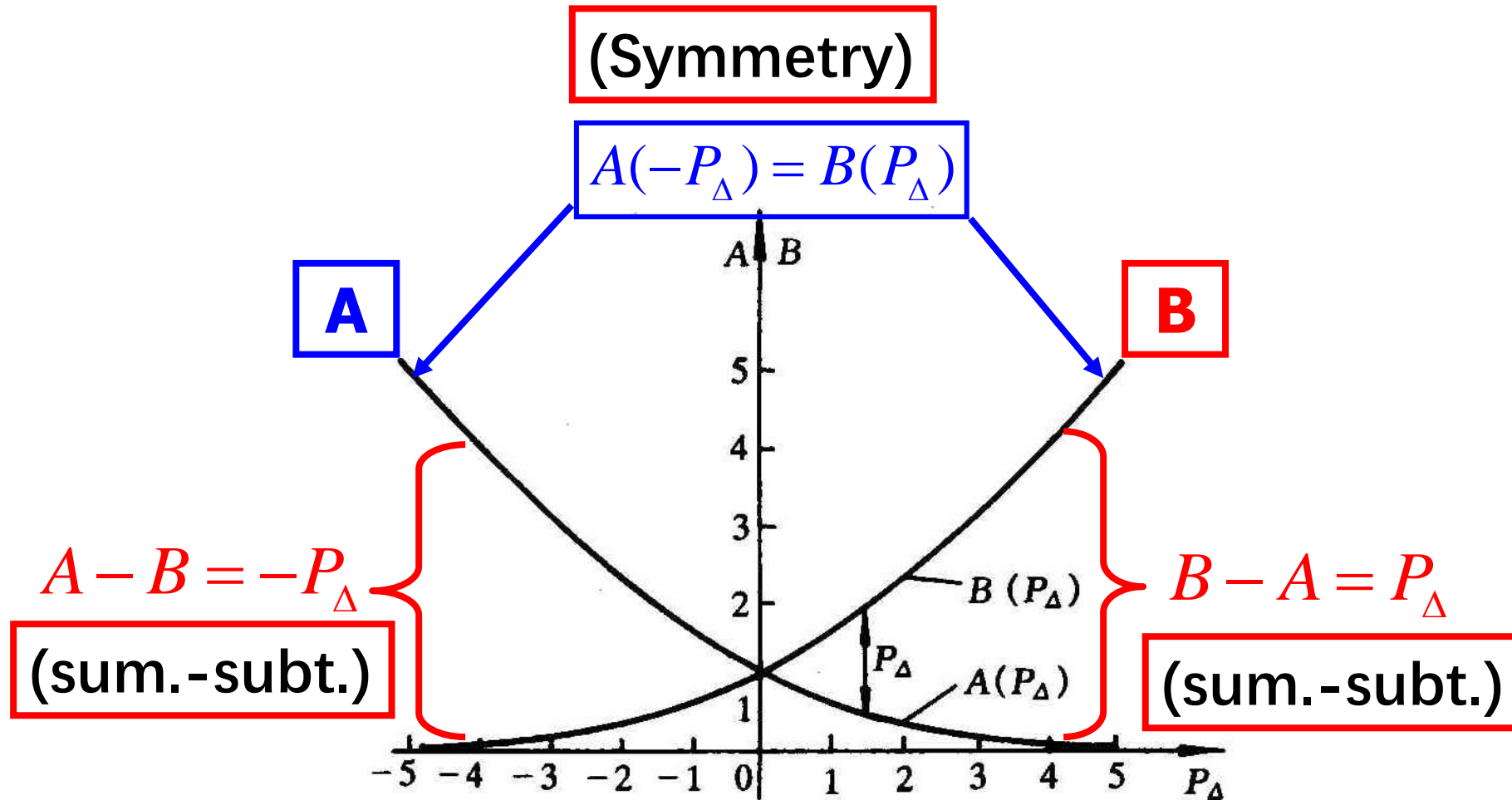
is valid for any ϕ_D, ϕ_C , **the only solution is:**

$$B(P_{\Delta}) - A(-P_{\Delta}) = 0 \quad A(P_{\Delta}) - B(-P_{\Delta}) = 0$$

i.e.,: $B(P_{\Delta}) = A(-P_{\Delta}); \quad A(P_{\Delta}) = B(-P_{\Delta})$

Symmetry character (对称特性)

Taking $P_{\Delta} = 0$ as the symmetric axis, their plots are:



These are basic features of A and B of the five 3-point schemes.

4.4.3 Important conclusions from the two features

For the five 3-point schemes **if and only** if the function of $A(P_\Delta)$ is known for $P_\Delta \geq 0$, then in the entire range of $-|P_\Delta| \leq P_\Delta \leq |P_\Delta|$, the analytical expressions are known for both $A(P_\Delta)$ and $B(P_\Delta)$.

[Proving] 1. First we show that this is correct for $A(P_\Delta)$.

(1) For case of $P_\Delta \geq 0$ $A(|P_\Delta|)$ is given in the conditions.

(2) For case of $P_\Delta < 0$ We have

$$A(P_\Delta) \xrightarrow{\text{Sum-sub}} B(P_\Delta) - P_\Delta \xrightarrow{\text{Symmet}} A(-P_\Delta) - P_\Delta$$

$$\xrightarrow{P_\Delta \leq 0} A(|P_\Delta|) + |P_\Delta|$$

Therefore either $P_{\Delta} > 0$ or $P_{\Delta} < 0$

$$A(P) = \left\{ \begin{array}{l} A(P_{\Delta}), P \geq 0 \\ A(|P_{\Delta}|) + |P_{\Delta}|, P_{\Delta} < 0 \end{array} \right\} A(|P_{\Delta}|) + \|-P_{\Delta}, 0\|$$

2. Then we show that for $B(P_{\Delta})$ above statement is also valid.

$$B(P_{\Delta}) \xrightarrow{\text{Sum.-subt.}} A(P_{\Delta}) + P_{\Delta} \xrightarrow{\text{From } A(P) \text{ expression}} A(|P_{\Delta}|) + \|-P_{\Delta}, 0\| + P_{\Delta} \xrightarrow{\quad} A(|P_{\Delta}|) + \|P_{\Delta}, 0\|$$

Thus $B(P_{\Delta}) = A(|P_{\Delta}|) + \|P_{\Delta}, 0\|$

Verification is finished !

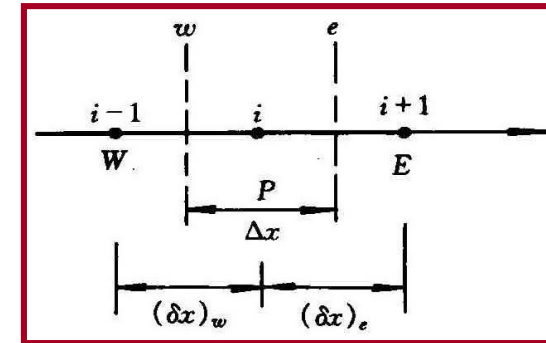
4.4.4 Derivation of general expression for a_E, a_W of three-point schemes from coefficient characters

Basic idea

- (1) For CV. P writing down diffusion/convection flux balance equation for its two interfaces;

$$J_e = J_w$$

$$J_e^* D_e = J_w^* D_w$$



- (2) Expressing J^* via **A, B** and the related grid value;
- (3) Expressing **A, B** via $A(|P_\Delta|)$;
- (4) Then rewrite above eq. in terms of ϕ_W, ϕ_P, ϕ_E ;

(5) Comparing the above-resulted eq. with the standard form

$$a_P \phi_P = a_E \phi_E + a_W \phi_W$$

The general expressions of coefficients of the discretized equation of five 3-point schemes can be obtained:

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

$$a_W = D_w A(|P_{\Delta w}|) + \|F_w, 0\|$$

$$a_P = a_E + a_W + (\cancel{F_e} - F_w)$$

See the appendix for the detailed derivation.

Expressions of $A(|P_{\Delta}|)$

Scheme	$A(P_{\Delta})$
CD	$1 - 0.5 P_{\Delta} $
FUD	1
Hybrid	$[0, 1 - 0.5 P_{\Delta}]$
Exponential	$ P_{\Delta} / (\exp(P_{\Delta}) - 1)$
Power-law	$[0, (1 - 0.1 P_{\Delta})^5]$

4.4.5 Discussion

1. Extend from 1-D to multi-D:

Regarding every coordinate as 1-D coordinate and constructing the influencing coefficients by the way as shown above;

2. For the five 3-point schemes, by selecting $A(|P_{\Delta}|)$ the scheme is set up.

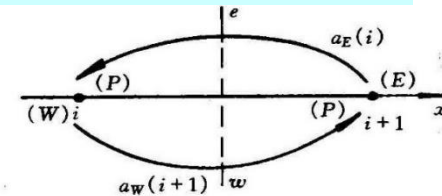
3. Relationship between $a_W(i+1), a_E(i)$

can be used to simplify computation

$$a_W(i+1) = \{D_w A(|P_{\Delta w}|) + \|F_w, 0\|\}_{i+1}$$

$$a_E(i) = \{D_e A(|P_{\Delta e}|) + \|-F_e, 0\|\}_i$$

$$a_W(i+1) - a_E(i) = \|F, 0\| - \|-F, 0\| = F$$



$$(D_w)_{i+1} = (D_e)_i$$

$$(F_w)_{i+1} = (F_e)_i$$

$$(P_{\Delta w})_{i+1} = (P_{\Delta e})_i$$

Appendix 1 of Section 5-4

$$J_e^* D_e = J_w^* D_w$$

$$D_e [B(P_{\Delta e}) \phi_P - A(P_{\Delta e}) \phi_E] = D_w [B(P_{\Delta w}) \phi_W - A(P_{\Delta w}) \phi_P]$$

$$\phi_P \underbrace{[D_e B(P_{\Delta e}) + D_w A(P_{\Delta w})]}_{a_P} = \underbrace{[D_e A(P_{\Delta e})]}_{a_E} \phi_E + \underbrace{[D_w B(P_{\Delta w})]}_{a_W} \phi_W$$

Expressing A, B via $A(|P_{\Delta}|)$

$$A(P_{\Delta w}) = A(|P_{\Delta w}|) + \|-P_{\Delta w}, 0\| \quad B(P_{\Delta w}) = A(|P_{\Delta w}|) + \|P_{\Delta w}, 0\|$$

$$A(P_{\Delta e}) = A(|P_{\Delta e}|) + \|-P_{\Delta e}, 0\| \quad B(P_{\Delta e}) = A(|P_{\Delta e}|) + \|P_{\Delta e}, 0\|$$

$$a_E = D_e A(P_{\Delta e}) = D_e \{A(|P_{\Delta e}|) + \|-P_{\Delta e}, 0\|\} \quad \longrightarrow$$

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

$a_P = D_e \underline{B(P_{\Delta e})} + D_w \underline{A(P_{\Delta w})}$ can be transformed as

$$D_e [A(|P_{\Delta e}|) + \|P_{\Delta e}, 0\|] + D_w [A(|P_{\Delta w}|) + \|-P_{\Delta w}, 0\|] =$$

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

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

$$a_E \quad \|-F_e, 0\|$$

$$a_W \quad \|F_w, 0\|$$

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

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cross to the other
bank, where....