Numerical Heat Transfer
(数值传热学)
Chapter 5 Discretized Schemes of Diffusion and Convection Equation (1)

Instructor Tao, Wen-Quan

CFD-NHT-EHT Center
Key Laboratory of Thermo-Fluid Science & Engineering
Xi’an Jiaotong University

Xi’an, 2017-Oct-16

数值传热学

第五章 对流扩散方程的离散格式(1)

主讲 陶文铨

西安交通大学能源与动力工程学院
热流科学与工程教育部重点实验室

2017年10月16日, 西安

Chapter 5 Discretized diffusion－convection equation

5.1 Two ways of discretizing convection term

5.2 CD and FUD of the convection term

5.3 Hybrid and power-law schemes

5.4 Characteristics of five three-point schemes

5.5 Discussion on false diffusion

5.6 Methods for overcoming or alleviating effects of false diffusion

5.7 Stability analysis of discretized diffusion-convection equation

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

5.1 Two ways of discretizing convection term

5.1.1 Importance of discretization scheme

1. Accuracy

2. Stability

3. Economics

5.1.2 Two ways for constructing discretization schemes of convective term

5.1.3 Relationship between the two ways

5.1 Two ways of discretizing convection term

5.1.1 Importance of discretization(离散) scheme

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

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

Scheme with 1st-order TE involves severe numerical error.

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

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

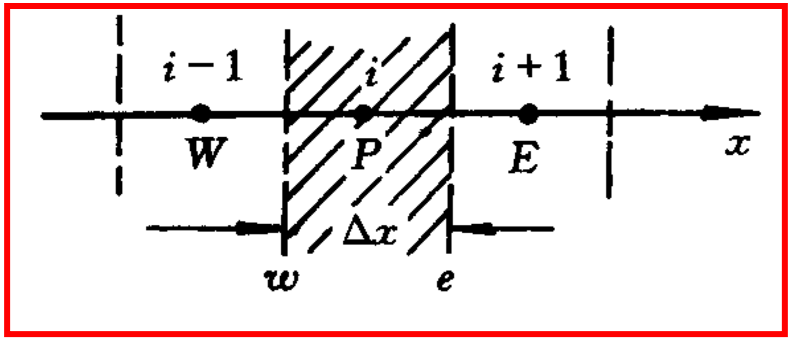
3. It affects numerical economics (经济性).

5.1.2 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 interpolation (插值) for the interface variable

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

Piecewise linear

Unifrom grids

$$=\frac{(\phi_E+\phi_P)/2-(\phi_P+\phi_W)/2}{\Delta x}=\frac{\phi_E-\phi_W}{2\Delta x}$$

5.1.3 Relationship between the two ways

1. For the same scheme they have the same T.E.
2. For the same scheme, the coefficients of the 1st term in T.E. are different
3. Taylor expansion provides the FD form at a point while CV integration gives the value of integral average (积分均值) within the domain

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

5.2 CD and FUD of the convection term

5.2.1 Analytical solution of 1-D model equation

5.2.2 CD discretization of 1-D diffusion-convection equation

5.2.3 Up wind scheme of convection term

1. Definition of CV integration

2. Compact form

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

5.2 CD and FUD of convection term

5.2.1 Analytical solution of 1-D diffusion and convection equation

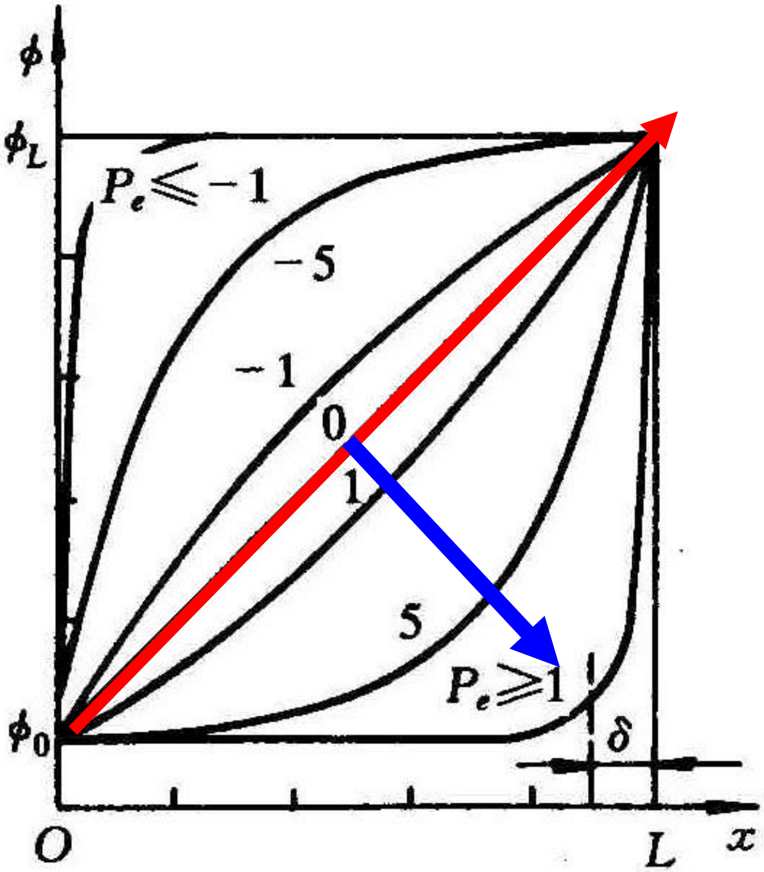
$$\begin{cases} \dfrac{d(\rho u\phi)}{dx} = \dfrac{d}{dx}\left(\Gamma\dfrac{d\phi}{dx}\right), \\ x=0,\ \phi=\phi_0;\ \ x=L,\ \phi=\phi_L \end{cases}$$

Physical properties and velocity are known constants

The analytical solution of this ODE:

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

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 close to L, ϕ increases dramatically (显著的) 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

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

$$\frac{\boxed{\text{Convection}}}{\boxed{\text{Diffusion}}}$$

When Pe is small－Diffusion dominated(占优)，linear distribution；

When Pe is large－Convection dominated，i.e., upwind effect is dominated，upwind information is transported downstream, and when Pe $\geq$ 100, streamwise (流向) conduction can be neglected.

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

5.2.2 CD discretization of 1-D diffusion-convection equation

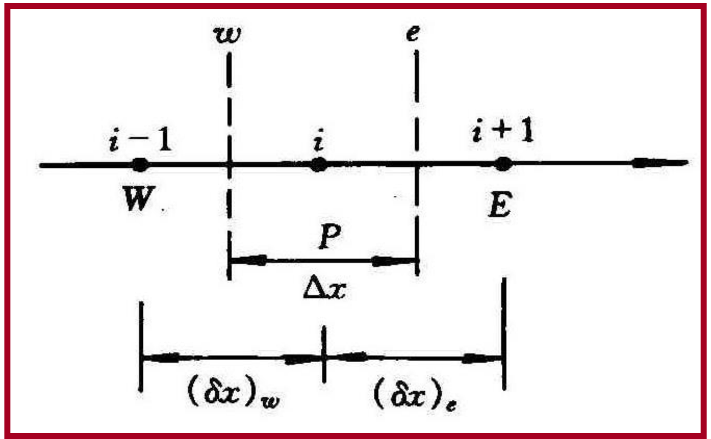
1. Integration of 1-D model equation

Adopting the linear profile, integration of 1-D molel equation over a CV , yields:

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

Thus:

$$\boxed{a_P\phi_P=a_E\phi_E+a_W\phi_W}$$



2. Relationship between coefficients

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

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

$$a_W = \frac{1}{2}(\rho u)_w + \frac{\Gamma_w}{(\delta x)_{wW}}$$

Rewriting a_P **as follows:**

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

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

Defining diffusion conductance(扩导): $D = \frac{\Gamma}{\delta x}$,

Interface flow rate: $F = \rho u$

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

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

$$a_E = D_e - \frac{1}{2}F_e \qquad a_W = D_w + \frac{1}{2}F_w$$

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

If in the iterative process the mass conservation is satisfied then

$$F_e - F_w = 0$$

In order to guarantee (保证) the convergence of iterative process, it is required:

$$a_P = a_E + a_W$$

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:**

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

Uniform grid

Cont property

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

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

With the given $\phi_E\,,\phi_W\,,\,\phi_P$ **can be determined.**

Given $\phi_W = 100, \phi_E = 200$

for $P_\Delta = 0,1,2,4$

the calculated results are shown as follows.

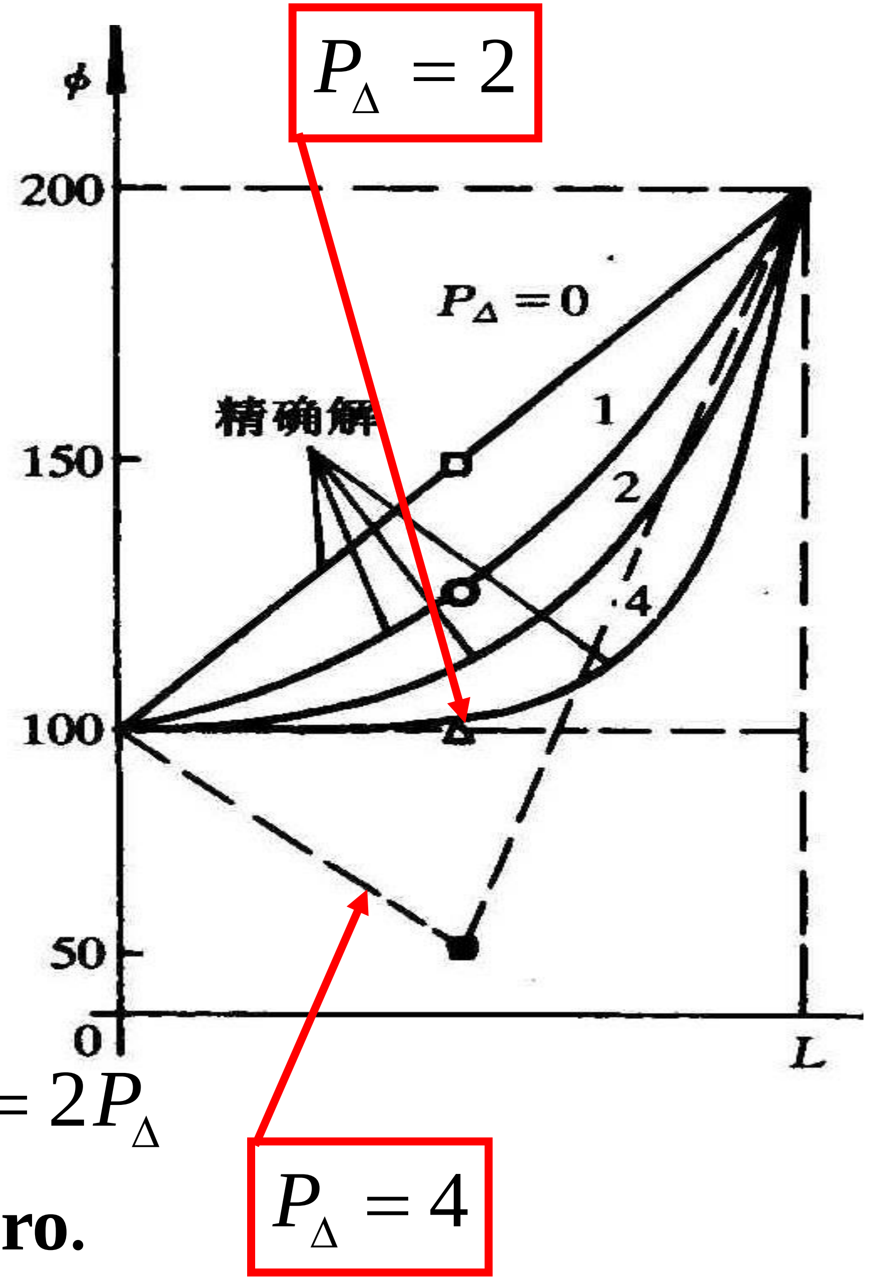
According to the analytical solution

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

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

based on whole length $Pe = 2P_\Delta$

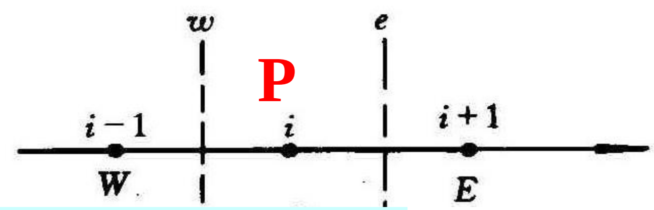
ϕ **should be larger than zero.**



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.**

5.2.3 FUD of convection term



1. Definition in CV－interpolation of interface always takes upstream grid value

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

$$O(\Delta x)$$

2. Compact form(紧凑形式)

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

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

Patankar proposed a special symbol as follows

MAX: $[\![X, Y]\!]$, then:

$$\boxed{(\rho u\phi)_e = \phi_P [\![F_e,0]\!] - \phi_E [\![-F_e,0]\!]}$$

Similarly:

$$\boxed{(\rho u\phi)_w = \phi_W [\![F_w,0]\!] - \phi_P [\![-F_w,0]\!]}$$

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

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

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

$$a_P = a_E + a_W + (\cancelto{0}{F_e - F_w})$$

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**).

FUD 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.

Chapter 5 Discretized diffusion－convection equation

5.1 Two ways of discretization of convection term

5.2 CD and UD of the convection term

5.3 Hybrid and power-law schemes

5.4 Characteristics of five three-point schemes

5.5 Discussion on false diffusion

5.6 Methods for overcoming or alleviating effects of false diffusion

5.7 Stability analysis of discretized diffusion-convection equation

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

5.3 Hybrid and Power-Law Schemes

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

5.3.2. Hybrid scheme

5.3.3. Exponential scheme

5.3.4. Power-law scheme

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

5.3 Hybrid and Power-Law Schemes

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

1. **3-point scheme**—interface interpolation is conducted by using two points at the two sides of the interface

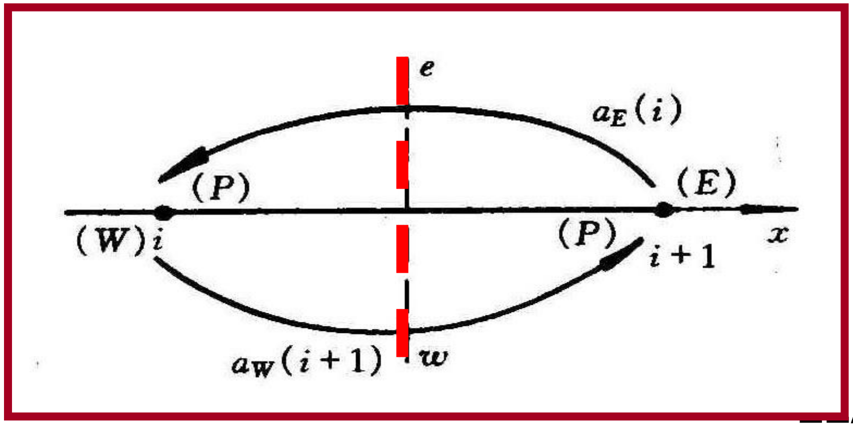
   With such scheme 1-D problem leads to tri-diagonal matrix, and 2-D penta-diagonal (五对角)matrix

2. **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 (**内部关系**).

For **CD**: $a_E = D_e(1-\frac{1}{2}P_{\Delta e})$ $\quad a_W = D_w(1+\frac{1}{2}P_{\Delta w})$

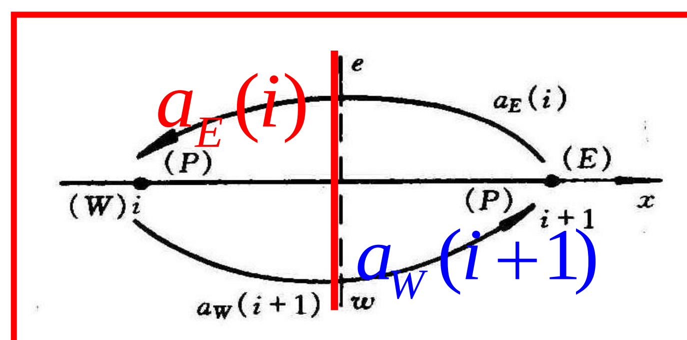
At the same interface $P_{\Delta e} = P_{\Delta w} = P_\Delta \quad D_e = D_w = D$

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

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

For convection if (u>0), node i has effect on (i+1), while (i+1) has no effect on i

Compared with $a_E(i)$, $a_W(i+1)$ has convection effect on grid i+1



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

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

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

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

Thus defining a scheme can be conducted by defining one coefficient. We will define the east coefficient.

5.3.2 Hybrid scheme(HBS, 混合格式)

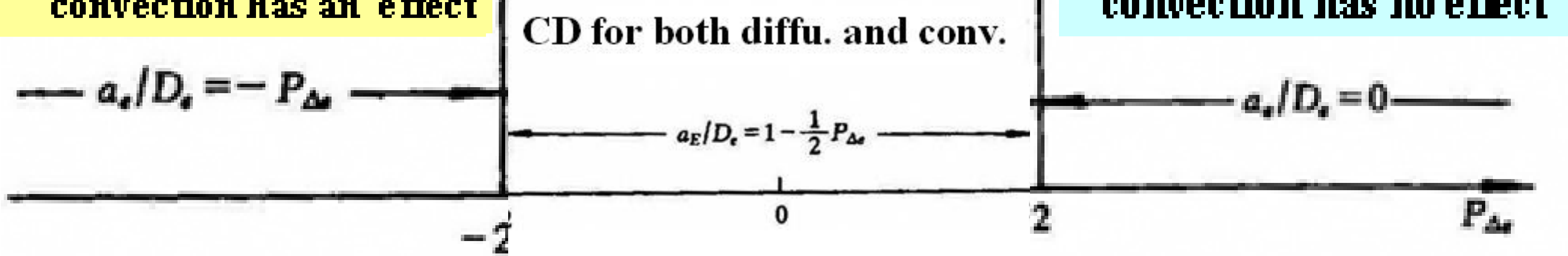
1.Graph definition

Taking P_Δ as abscissa (横坐标), $\dfrac{a_E}{D_e}$ as ordinate(纵坐标)

Proposed by Spalding

1 $|P_\Delta|$ >2, neglecting diffu.
2. E is in upstream of P, convection has an effect

1. P_Δ >2, neglecting diffu.
2. E is in downstream of P, convection has no effect



$$\frac{a_E}{D_e} = \begin{cases} 0, & P_\Delta > 2 \\ 1-\frac{1}{2}P_\Delta, & |P_\Delta| \le 2 \\ -P_\Delta, & P_\Delta < -2 \end{cases}$$

2.Compact definition

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

5.3.3. Exponential scheme （指数格式）

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

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

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

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

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

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

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

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

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

$F = \rho u$

2. Expressions of total flux for e,w interfaces

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

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

Substituting the two expressions into $J_e = J_w$ **and**

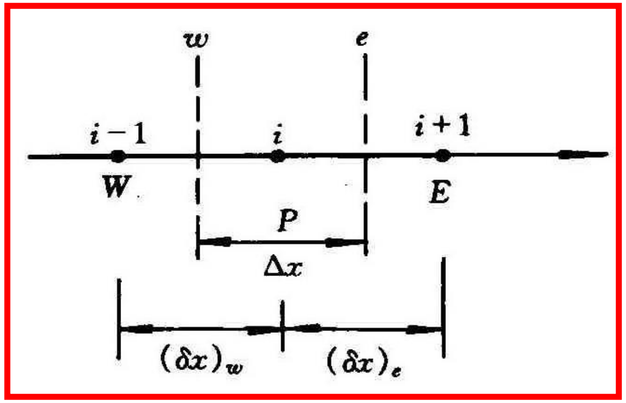
rewrite into algebraic equation among ϕ_W, ϕ_P, ϕ_E

yields:

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

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

$$a_P = a_E + a_W + \overbrace{(F_e - F_w)}^{0}$$



5.3.4. Power-law scheme (乘方格式)

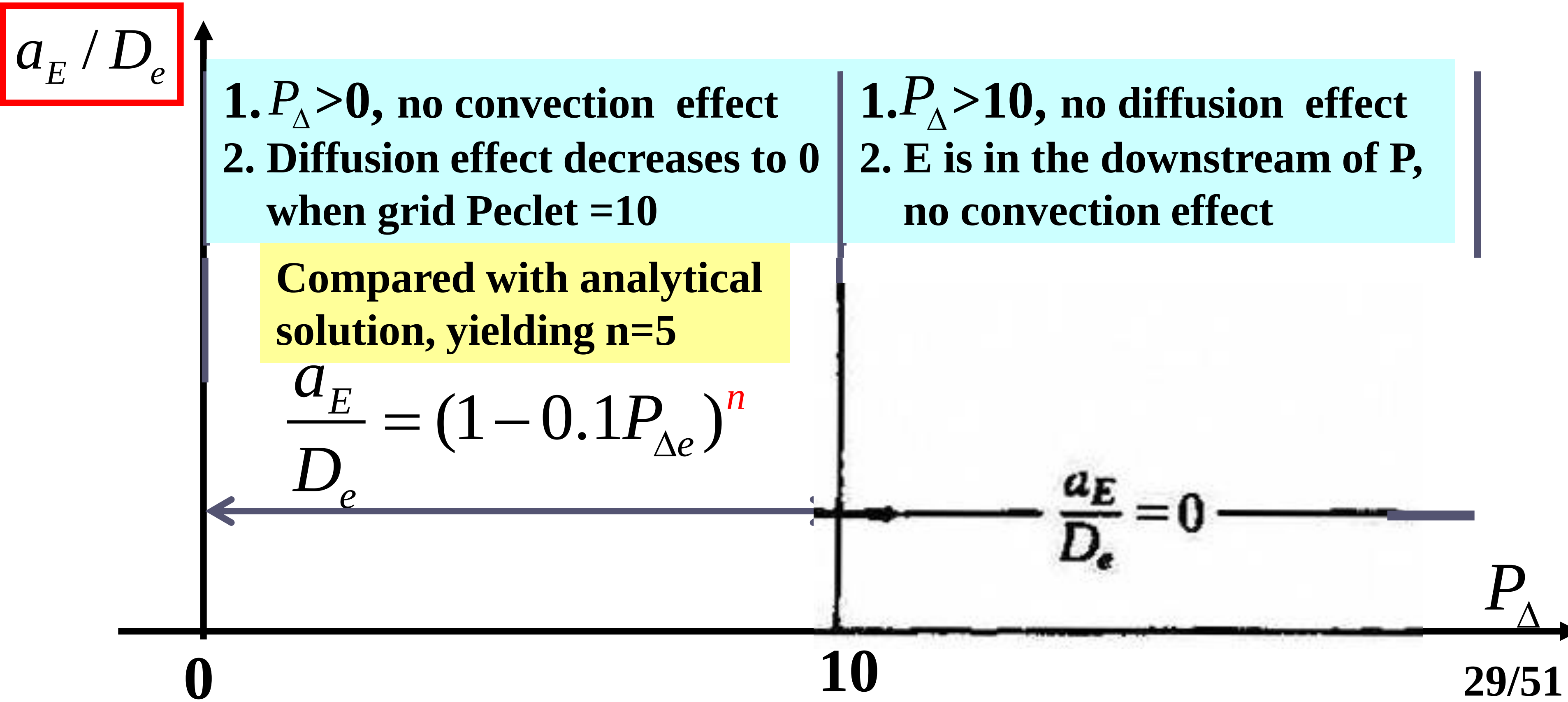
Exponential scheme is computationally very expensive. Patankar proposed the power-law scheme, which is very close to the exponential scheme and computationally much cheaper:

1. $P_\Delta > 0$, no convection effect
2. Diffusion effect decreases to 0 when grid Peclet =10

1. $P_\Delta > 10$, no diffusion effect
2. E is in the downstream of P, no convection effect

Compared with analytical solution, yielding n=5

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



a_E / D_e

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

$$\frac{a_E}{D_e} = -P_\Delta$$

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

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

P_Δ

-10 **0**

Brief review of 2017-10-16 lecture key points

1. Importance of discretization of convection term:

Accuracy, stability and economics

2. The discretized form of 1-D diffusion/ convection model equation :

$$a_P\phi_P = a_E\phi_E + a_W\phi_W \qquad a_P = a_E + a_W + (F_e - F_w)$$

a_E, a_W **depend on convection/diffusion scheme.**

To guarantee the convergence of iterative process, it is required:

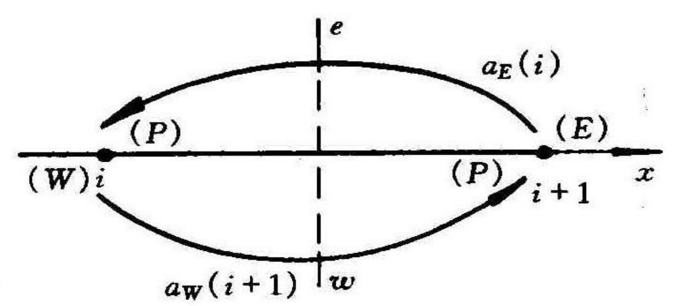
$$F_e - F_w = 0 \rightarrow a_P = a_E + a_W$$

3. FUD takes upstream information for scheme construction

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

It can always get physically plausible results with severe numerical error. Not recommended for final solution.

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



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

$$\rightarrow \|P_\Delta, 0\| - \|-P_\Delta, 0\| = P_\Delta$$

Compact form of the power-law scheme

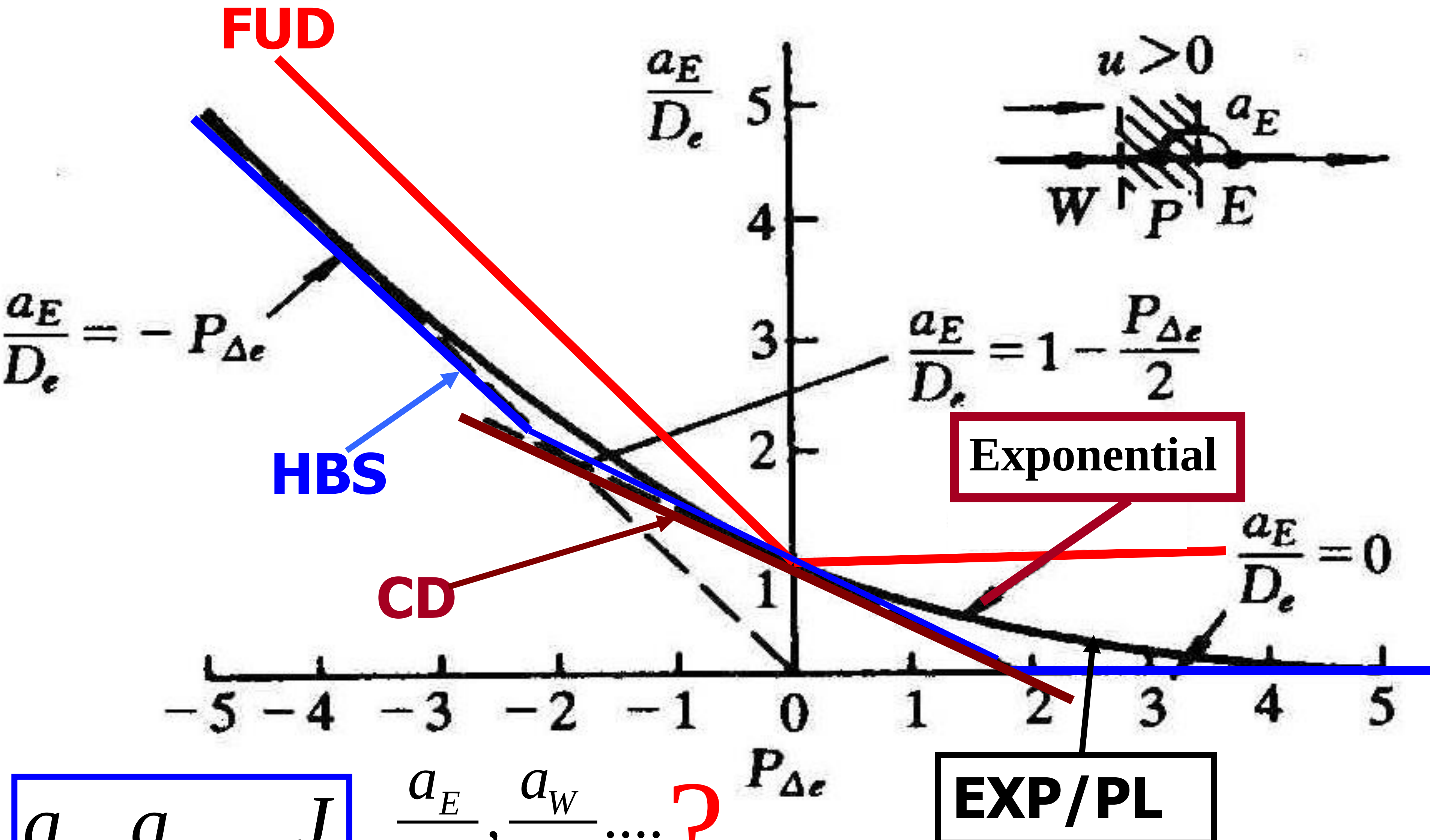
$$\frac{a_E}{D_e} = \left\| 0,\ (1-0.1|P_{\Delta e}|)^5 \right\| + \left\| 0,\ -P_{\Delta e} \right\|$$

Diffusion effect　　Convection effect

5.3.5. Coefficient expressions of five schemes and graph illustration（ a_E / D_e ）

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

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



$\boxed{a_E, a_W \ldots J}$ $\quad \frac{a_E}{D_E}, \frac{a_W}{D_W} \ldots ?$

5.4 Characteristics of five three-point schemes

5.4.1 J^* flux definition and its discretized form

5.4.2 Relationship between coefficients A and B

5.4.3 Important conclusions from coefficient characters

5.4.4 General expression for coefficients

$$a_E, a_W$$

5.4.5 Discussion

5.4 Characteristics of five three-point schemes

5.4.1 *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:

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

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

2. Discretized form of J^*

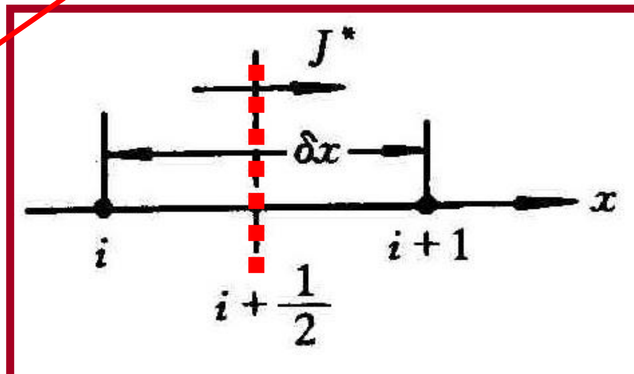
For the three-point scheme J^* at interface can be expressed by a combination of variables at nearby (附近) two grids.

For interface (i+1/2), let

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

Ahead of (在…之前) the interface

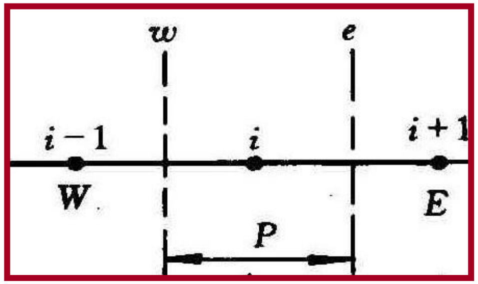
Behind of (在…之后) the interface



Viewed from positive direction of coordinate

Coefficients A, B are dependent on grid Peclet, P_Δ

$$J_e^* = B(P_{\Delta e})\phi_P - A(P_{\Delta e})\phi_E \qquad J_w^* = B(P_{\Delta w})\phi_W - A(P_{\Delta w})\phi_P$$



5.4.2 Two characters of *A* and *B*

1. **Summation-subtraction character (和差特性)**

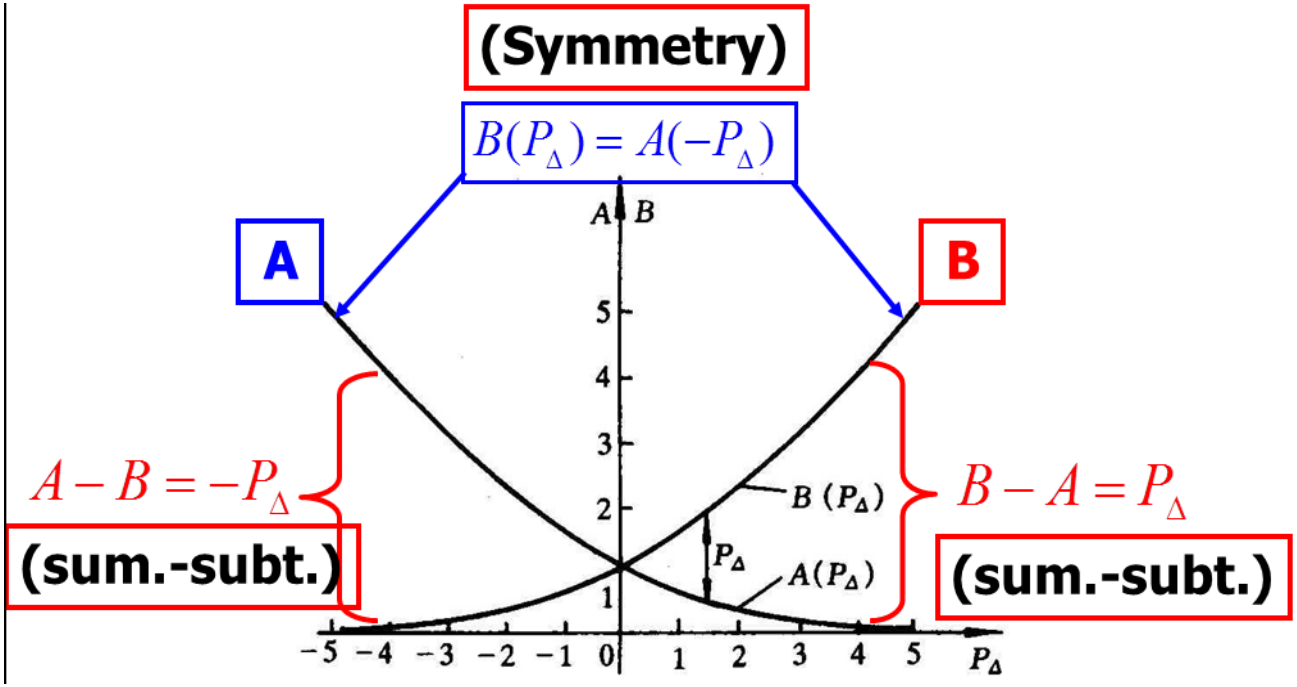
$$B - A = P_\Delta$$

2. **Symmetry character (对称特性)**

$$B(P_\Delta) = A(-P_\Delta);$$

$$A(P_\Delta) = B(-P_\Delta)$$

See appendix for detailed derivation.



5.4.3 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 $P_\Delta \ge 0$ then in the entire range of $-|P_\Delta| \le P_\Delta \le |P_\Delta|$ the analytical expressions are known for both $A(P_\Delta)$ and $B(P_\Delta)$

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

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

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

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

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

Either $P_\Delta > 0$ or $P_\Delta < 0$

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

$$A(P_\Delta) = A(|P_\Delta|) + \|-P_\Delta, 0\|$$

2. Next for $B(P_\Delta)$ **above statement is also valid.**

Sum.-subt.

From *A* (*P*) expression

$$B(P_\Delta) \longrightarrow A(P_\Delta) + P_\Delta \longrightarrow$$

$$A(|P_\Delta|) + \underbrace{\|-P_\Delta, 0\| + P_\Delta} \longrightarrow A(|P_\Delta|) + \|P_\Delta, 0\|$$

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

Finished!

5.4.4 Derivation of general expression for a_E, a_W from coefficient charcaters

Basic idea：

(1) For CV. P writing down diffusion convection flux balance equation for its two interface:

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

(2) Expressing *J* *via A，B;

$$J_e^* = B(P_{\Delta e})\phi_P - A(P_{\Delta e})\phi_E \qquad J_w^* = B(P_{\Delta w})\phi_W - A(P_{\Delta w})\phi_P$$

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

$$A(|P_\Delta|) + \| -P_\Delta, 0 \|$$

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

Then the general expressions of coefficients via $A(|P_\Delta|)$ can be obtained.

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

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

$$a_P = a_E + a_W + \cancelto{0}{(F_e - F_w)}$$

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

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

See appendix for detailed derivation.

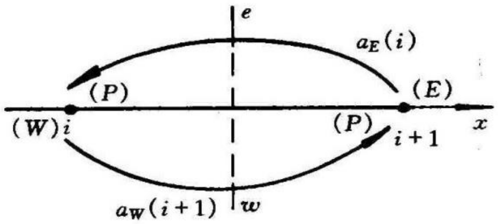
5.4.5 Discussion

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

For every coordinate constructing coefficients 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**



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

$$a_E(i)=\{D_e A(|P_{\Delta e}|)+\|-F_e,0\|\}_i \qquad (F_w)_{i+1}=(F_e)_i$$

$$\underline{a_W(i+1)-a_E(i)=\|F,0\|-\|-F,0\| = F} \qquad (P_{\Delta w})_{i+1}=(P_{\Delta e})_i$$

Appendix 1 of Section 5-4

Analysis of the relationship between A and B is based on fundamental physical and mathematical

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^*:

$$J^* = (P_\Delta \phi - \cancel{\frac{d\phi}{dX}}^{\,0})_i = (P_\Delta \phi - \cancel{\frac{d\phi}{dX}}^{\,0})_{i+1} = P_\Delta \phi_i = P_\Delta \phi_{i+1}$$

From the discretized expression of J^*:

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

Analytical= Discretized!

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

$$B - A = P_\Delta$$

Summation-subtraction (和差特性)

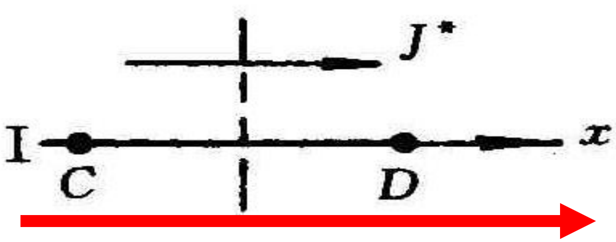
2. Symmetry character

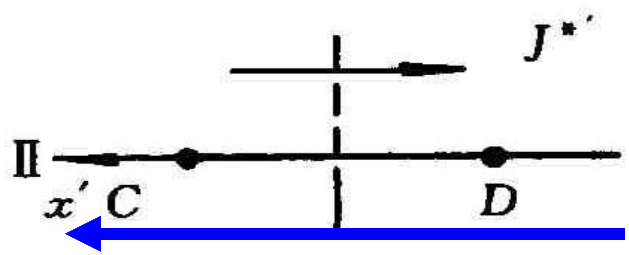
For the same process its mathematical formulation is expressed in two coordinates. The two coordinates are Ⅰ，Ⅱ, their positive directions are opposite（相反的）. Two points C,D are located at the two sides of an interface

Viewed from coordinate positive direction

C-behind/D-ahead

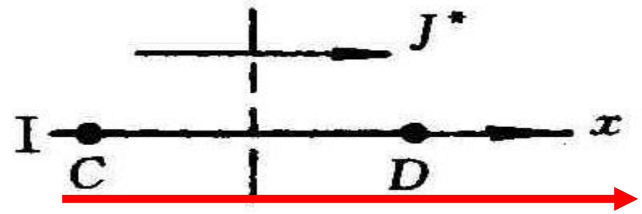
C-ahead/D-behind





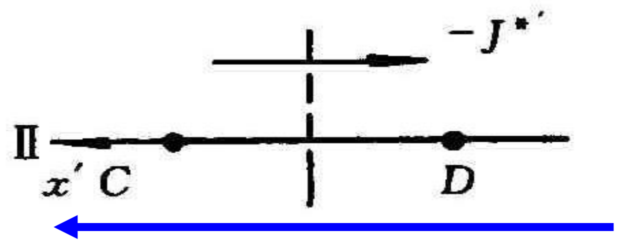
For the same flux, in coordinate Ⅰ it is denoted by J^*, while in Ⅱ denoted by $J^{*\prime}$, then

For Ⅰ $\boxed{\text{C-behind/D-ahead}}$



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

For Ⅱ $\boxed{\text{D-behind/C-ahead}}$



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

The flux is the same, so: $J^* = -J^{*\prime}$

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

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 **, it is required:**

$$B(P_\Delta) - A(-P_\Delta) = 0 \qquad A(P_\Delta) - B(-P_\Delta) = 0$$

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

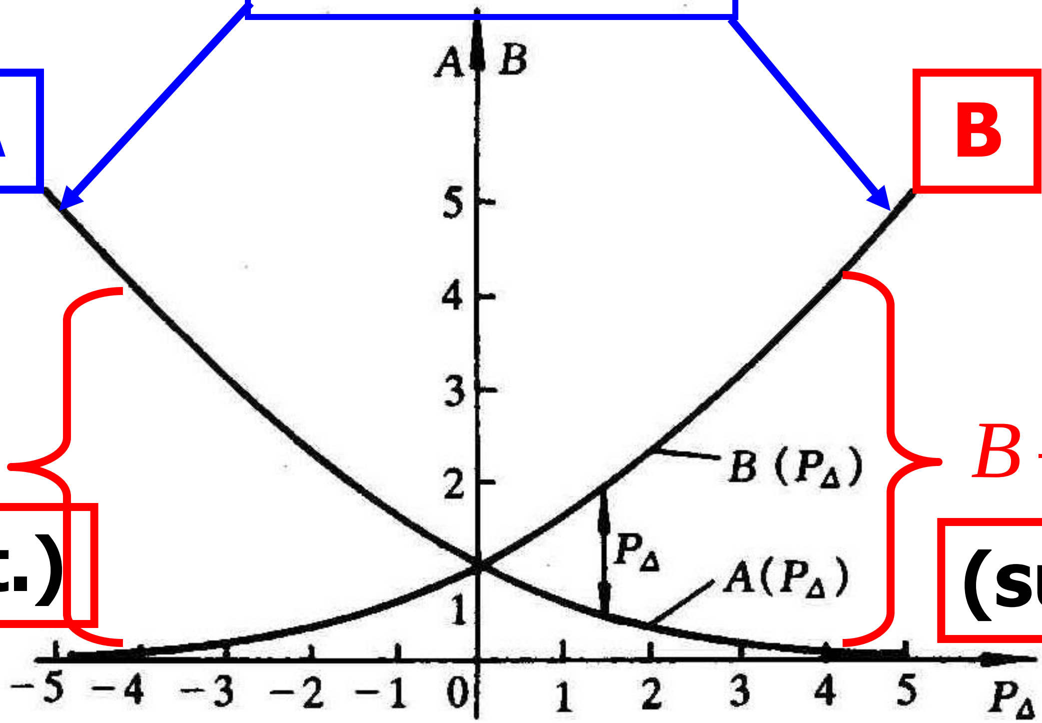
Symmetry character(对称特性)

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

(Symmetry)

$$B(P_\Delta) = A(-P_\Delta)$$

A **B**



$$A - B = -P_\Delta$$

(sum.-subt.)

$$B - A = P_\Delta$$

(sum.-subt.)

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

Appendix 2 of Section 5-4

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

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

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

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

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

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

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

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

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

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

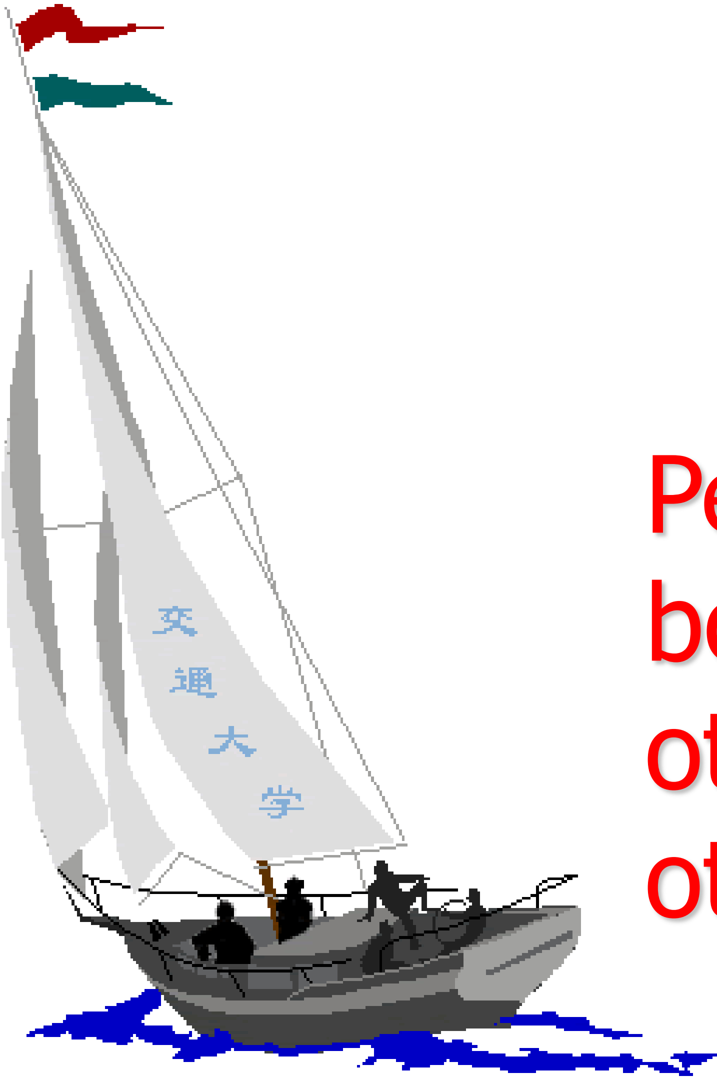
$$D_e A(|P_{\Delta e}|) + \|F_e, 0\| + D_w A(|P_{\Delta w}|) + \|-F_w, 0\| =$$

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

$$a_E \qquad \|-F_e, 0\| \qquad a_W \qquad \|F_w, 0\|$$

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

0



同舟共济
渡彼岸!

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