



Numerical Heat Transfer

(数值传热学)

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



Instructor Chen, Li

Key Laboratory of Thermo-Fluid Science & Engineering Int. Joint Research Laboratory of Thermal Science & Engineering Xi'an Jiaotong University

Xi'an, 2018-Sept-26



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 discretization scheme
 - 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

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).



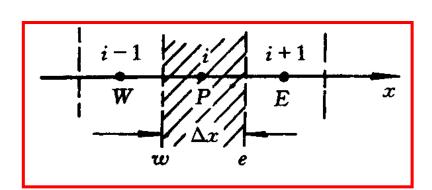


4.1.2 Two ways for constructing(构建) schemes

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

Taking CD as an example:

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



2. CV integration—providing interpolation 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

Uniform grids

$$= \frac{(\phi_{E} + \phi_{P})/2 - (\phi_{P} + \phi_{W})/2}{(\phi_{P} + \phi_{W})/2} = \frac{\phi_{E} - \phi_{W}}{(\phi_{E} - \phi_{W})}$$

4.1.3 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 mean value by integration average 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 diffusionconvection 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 diffusion and convection equation

$$\begin{cases} \frac{d(\rho u\phi)}{dx} = \frac{d}{dx} (\Gamma \frac{d\phi}{dx}), & \text{Physical and we know } \\ x = 0, \ \phi = \phi_0; \ x = L, \ \phi = \phi_L \end{cases}$$

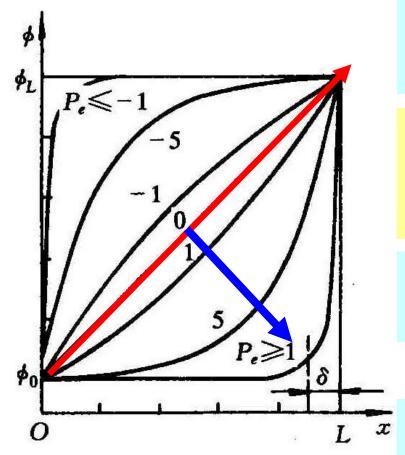
Physical properties and velocity are known constants

$$x = 0, \ \phi = \phi_0; \ x = L, \ \phi = \phi_L$$

The analytical solution of this ordinary DFE:

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

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 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

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

When Pe is small—Diffusion dominated, linear distribution;

When Pe is large—Convection dominated, i.e., upwind 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

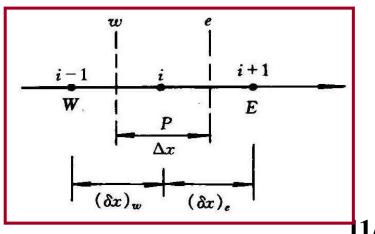
Adopting the linear profile, integration over a CV yields:

$$\frac{\phi_{P}\left[\frac{1}{2}(\rho u)_{e} + \frac{\Gamma_{e}}{(\delta x)_{e}} - \frac{1}{2}(\rho u)_{w} + \frac{\Gamma_{w}}{(\delta x)_{w}}\right] = \phi_{E}\left[\frac{\Gamma_{e}}{(\delta x)_{e}} - \frac{1}{2}(\rho u)_{e}\right] + \phi_{W}\left[\frac{\Gamma_{w}}{(\delta x)_{w}} + \frac{1}{2}(\rho u)_{w}\right]$$

 a_{P}

Thus:

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



2. Relationship between coefficients

Rewriting a_p as follows:

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

$$\frac{1}{2}(\rho u)_{e} - (\rho u)_{e} + (\rho u)_{e} + \frac{\Gamma_{e}}{(\delta x)_{e}} - \frac{1}{2}(\rho u)_{w} + (\rho u)_{w} - (\rho u)_{w} + \frac{\Gamma_{w}}{(\delta x)_{w}} =$$

$$-\frac{1}{2}(\rho u)_{e} + \frac{\Gamma_{e}}{(\delta x)_{e}} + \frac{1}{2}(\rho u)_{w} + \frac{\Gamma_{w}}{(\delta x)_{w}} + [(\rho u)_{e} - (\rho u)_{w}] = a_{E} + a_{W} + [(\rho u)_{e} - (\rho u)_{w}]$$

 a_{W}

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

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

Interface flow rate: $F = \rho u$



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

$$a_{P}\phi_{P} = a_{E}\phi_{E} + a_{W}\phi_{W}$$

$$a_{E} = D_{e} - \frac{1}{2}F_{e} \quad a_{W} = D_{w} + \frac{1}{2}F_{w}$$

$$a_{P} = a_{E} + a_{W} + (F_{e} - F_{w})$$

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 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:

$$\phi_{P} = \frac{a_{E}\phi_{E} + a_{W}\phi_{W}}{a_{E} + a_{W}} = \frac{(D_{e} - \frac{1}{2}F_{e})\phi_{E} + (D_{w} + \frac{1}{2}F_{w})\phi_{W}}{(D_{e} - \frac{1}{2}F_{e}) + (D_{w} + \frac{1}{2}F_{w})} \underbrace{\text{Uni.grid}}_{\text{Cons proper}}$$

$$\phi_{P} = \frac{(1 - \frac{1}{2} \frac{F}{D})\phi_{E} + (1 + \frac{1}{2} \frac{F}{D})\phi_{W}}{(D + D)/D} \longrightarrow \frac{(1 - \frac{1}{2} P_{\Delta})\phi_{E} + (1 + \frac{1}{2} P_{\Delta})\phi_{W}}{2}$$

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

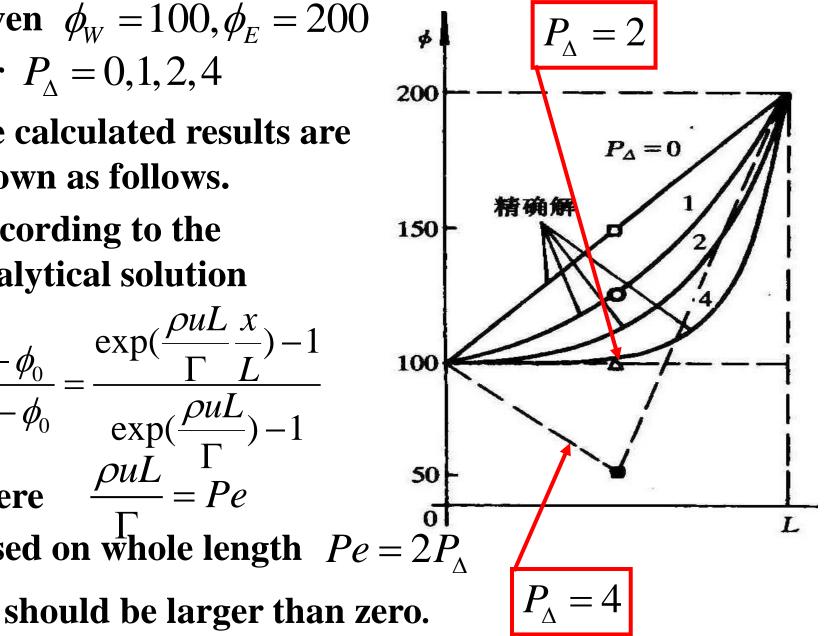
With the given ϕ_E, ϕ_W ϕ_P can be determined.

Given $\phi_W = 100, \phi_F = 200$ for $P_{\Lambda} = 0, 1, 2, 4$

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 $Pe = 2P_{\Delta}$







Brief review of 2018-09-26 lecture key points

1. Dimensionless G.Eq. of FDHT in straight tubes

Define
$$\Theta = \frac{T - T_{\infty}}{T_b - T_{\infty}} \leftarrow \frac{T - T}{T_b - T} \leftarrow \frac{T - T}{T - T}$$

$$\rho c_p u \frac{\partial T}{\partial x} = \frac{1}{r} \frac{\partial}{\partial r} (\lambda r \frac{\partial T}{\partial r})$$

$$\frac{1}{\eta} \frac{d}{d\eta} (\eta \frac{d\Theta}{d\eta}) = -\Lambda (\frac{1}{2} \Theta \frac{u}{u_m}) \qquad \begin{cases} \eta = 0, \frac{d\Theta}{d\eta} = 0; \\ \frac{d\Theta}{d\eta} \rangle_{\eta=1} = -Bi\Theta_w \end{cases}$$
Both eq. and boundary conditions are homogeneous!

Both eq. and boundary conditions are homogeneous!

2. Condition for unique solution

To find a non-homogeneous condition to fix(固定) Θ ! 16/51





$$\Theta_b = \left(\frac{T_b - T_\infty}{T_b - T_\infty}\right) = 1 \longrightarrow \int_0^1 \eta \frac{u}{u_m} \Theta d\eta = 1/2$$

3. Numerical method for homogeneous problem

By introducing $\Theta = \Lambda \Phi$ a non-homogeneous equation is obtained which can be used to iteratively determine the eigenvalue.

4. The eigenvalue can be used to get Nu

$$Nu = \frac{2Rh}{\lambda} = \frac{2R}{\lambda} \frac{h_e \Lambda \phi_w}{1 - \Lambda \phi_w} = \frac{2Bi \Lambda \phi_w}{1 - \Lambda \phi_w}$$

5. Importance of discretization of convection term:

Accuracy, stability and economics

6. Two ways of discretization of convection term:

Taylor expansion and CV integration have the same order of accuracy for the same scheme, but different coefficient of the 1st term in the T.E.; Taylor expansion is the FD form at a point while CV integration gives the mean value within the domain.

7. Discretization of 1-D diffusion and convection eq.

$$\frac{d(\rho u\phi)}{dx} = \frac{d}{dx}(\Gamma \frac{d\phi}{dx}), \quad x = 0, \ \phi = \phi_0; \ x = L, \ \phi = \phi_L$$

$$x = 0, \ \phi = \phi_0; \ x = L, \ \phi = \phi_L$$

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

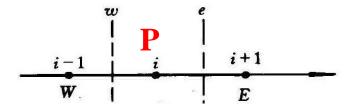
$$a_P \phi_P = a_E \phi_E + a_W \phi_W$$
 $a_P = a_E + a_W + (F_e - F_W)$

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

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 CV—interpolation of interface always takes upstream grid value

$$\phi_{e} = \begin{cases} \phi_{P}, u_{e} > 0 \\ \phi_{E}, u_{e} < 0 \end{cases} O(\Delta x) \phi_{w} = \begin{cases} \phi_{W}, u_{w} > 0 \\ \phi_{P}, u_{w} < 0 \end{cases}$$





2. Compact form (紧凑形式)

For the convenience of discussion, combining interface value 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:

$$(\rho u\phi)_{e} = \phi_{P} \llbracket F_{e}, 0 \rrbracket - \phi_{E} \llbracket -F_{e}, 0 \rrbracket$$

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 $a_E \ge 0$, $a_W \ge 0$ 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.



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





4.3 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



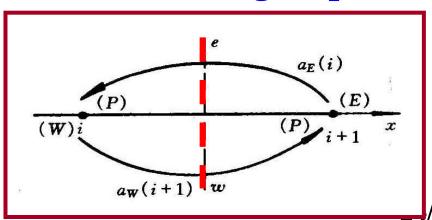


4.3 Hybrid and Power-Law Schemes

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

For CD:

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

convection effect on grid (i+1).

$$(W)_{i} \qquad (E)$$

$$a_{w}(i+1) \qquad w \qquad (E)$$

$$(W)_{i} \qquad (E)$$

$$a_{w}(i+1) \qquad w \qquad (I+1)$$

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

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

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 convection effect on i; $a_E(i)$ has no convection effect on grid i, while $a_W(i+1)$ has some





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

$$\frac{a_{W}(i+1)}{D} - \frac{a_{E}(i)}{D} = 1 + ||P_{\Delta}, 0|| - (1 + ||-P_{\Delta}, 0||) = ||P_{\Delta}, 0|| - ||-P_{\Delta}, 0|| = P_{\Delta}$$

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

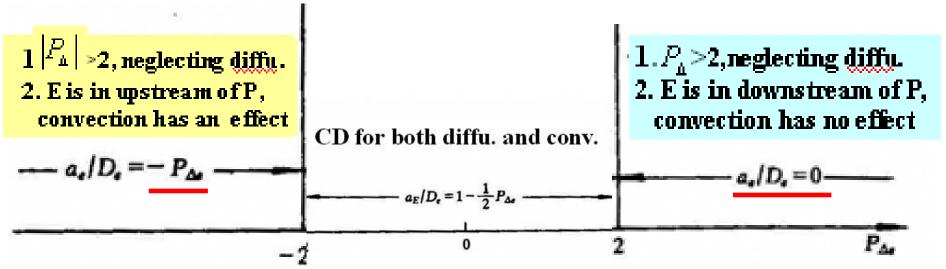
Thus defining a scheme can be conducted just by defining one coefficient. We will define the E-coeff.

- 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)



$$\frac{a_E}{D_e} = \left\{ \begin{array}{c} 0, P_{\Delta} > 2\\ 1 - \frac{1}{2}P_{\Delta}, |P_{\Delta}| \le 2\\ -P_{\Delta}, P_{\Delta} < -2 \end{array} \right\}$$

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 $J=const$





$$J_e = J_w$$

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

Substituting the analytical solution of ϕ into J:

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

$$Pe = \frac{\rho uL}{\Gamma}$$

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

$$\rho u\phi$$

$$\Gamma d\phi / dx$$

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

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

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



2. Expressions of total flux for e,w interfaces

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

For w:
$$\phi_0 = \phi_W$$
, $\phi_L = \phi_P$, $L = (\delta x)_W$: $J_W = F_W [\phi_W + \frac{\phi_W - \phi_P}{\exp(P_{\Delta W}) - 1}]$

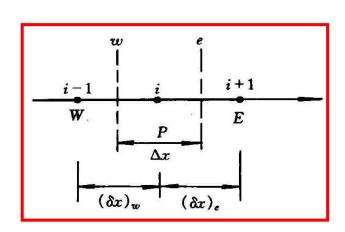
Substituting the two expressions into $J_e = J_w$ and

rewrite into algebraic equation among $\phi_{\!\scriptscriptstyle W},\phi_{\!\scriptscriptstyle P},\phi_{\!\scriptscriptstyle E}$

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

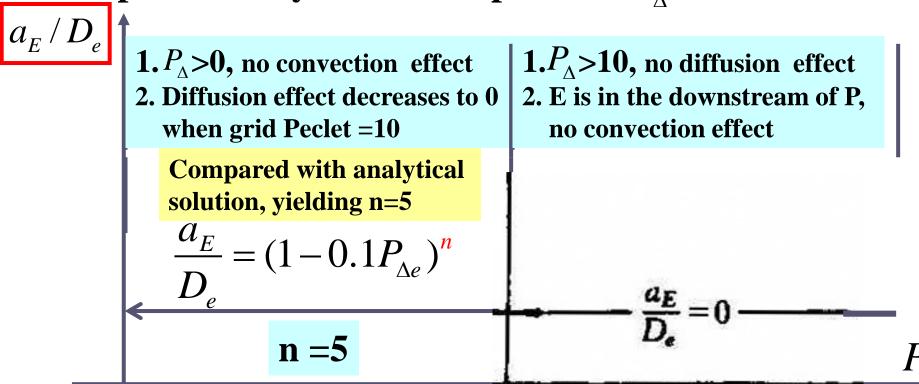
$$a_E = \frac{F_e}{\exp(P_{\Delta e}) - 1} a_W = \frac{F_w \exp(P_{\Delta w})}{\exp(P_{\Delta w}) - 1}$$

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



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 $P_{\lambda} > 0$:





For
$$P_{\Lambda} < 0$$

$$a_E/D_e$$

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

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

- 1. P_{\triangle} <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 $P_{\Lambda} > 0$

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

Λ

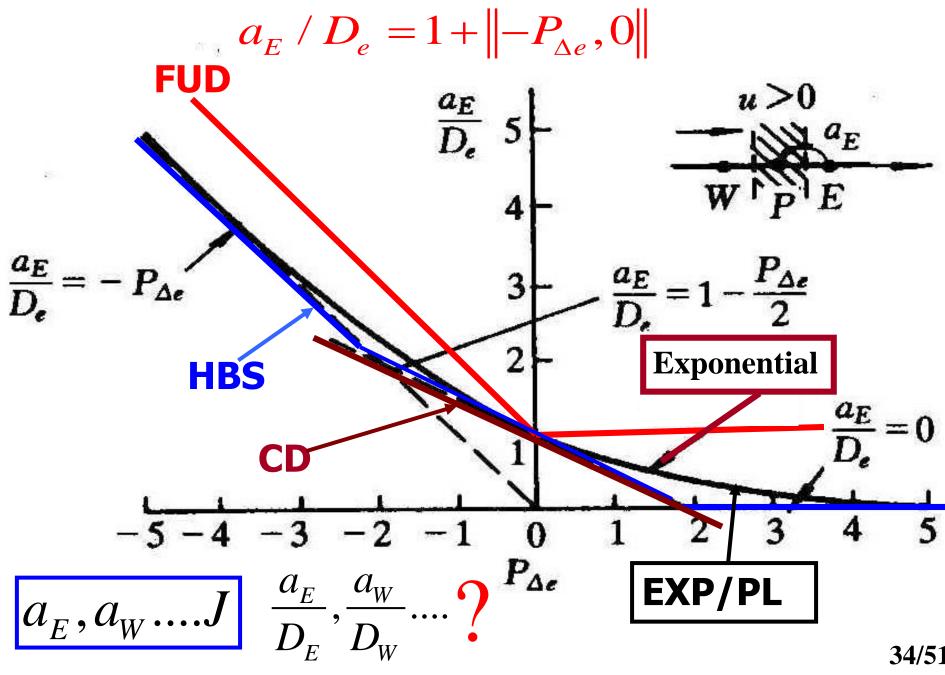


Compact form of the power-law scheme

$$\frac{a_E}{D_e} = \begin{vmatrix} 0, (1-0.1|P_{\Delta e}|)^5 \\ & + \|0, -P_{\Delta e}\| \end{vmatrix}$$
Diffusion effect
Convection effect

4.3.5. Coefficient expressions of five schemes and graph illustration (a_F / D_e)

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







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



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:

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

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



2. Discretized form of J^*

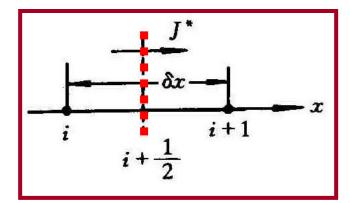
For the three-point scheme J^* at interface can be expressed by a combination of variables at nearby two grids.

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_A

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^* :

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

From the discretized expression of J^* :

Analytical= Discretized!

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



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

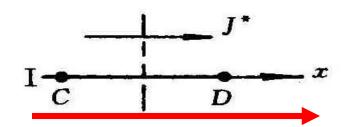
$$B-A=P_{\Delta}$$

 $B - A = P_{\Lambda}$ | Summation-subtraction (和差特性)

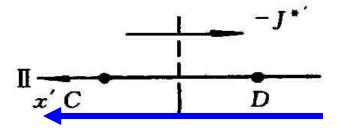
2. Symmetry character

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

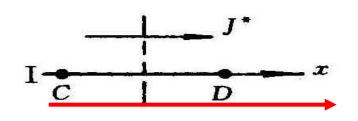




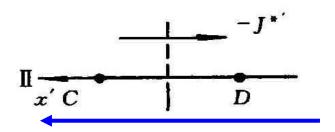
For the same flux, in coordinate I it is denoted by J^* , while in II denoted by J^* , then we have

For I C-behind/D-ahead

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



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.

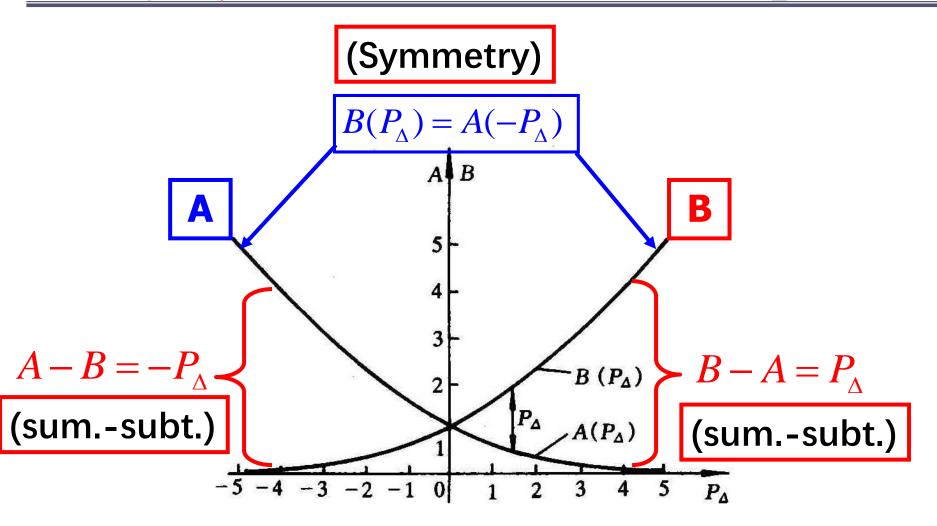
is valid for any ϕ_D, ϕ_C , it is required:

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

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

Symmetry character (对称特性)

Taking $P_{\Lambda} = 0$ 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.** 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

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

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

Either $P_{\Lambda} > 0$ or $P_{\Lambda} < 0$

$$A(P) = \begin{cases} A(P_{\Delta}), P \ge 0 \\ A(|P_{\Delta}|) + |P_{\Delta}|, P_{\Delta} < 0 \end{cases} A(|P_{\Delta}|) + ||-P_{\Delta}|, 0||$$

2. We show that for $B(P_{\wedge})$ above statement is also valid.

Sum.-subt. From
$$A$$
 (P) expression
$$A(|P_{\Delta}|) + ||-P_{\Delta}, 0|| + P_{\Delta} \longrightarrow A(|P_{\Delta}|) + ||P_{\Delta}, 0||$$
Thus $B(P_{\Delta}) = A(|P_{\Delta}|) + ||P_{\Delta}, 0||$
Finished!

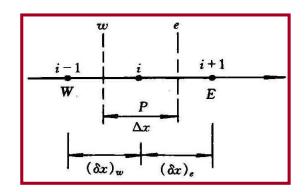


4.4.4 Derivation of general expression for a_E, a_W from coefficient characters

Basic idea

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

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



- (2) Expressing J^* via A, B and the related grid value;
- (3) Expressing A,B via $A(|P_{\wedge}|)$;
- (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:

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

$$a_{W} = D_{w}A(|P_{\Delta w}|) + ||F_{w},0||$$

$$a_{P} = a_{E} + a_{W} + (F_{e} - F_{w})$$

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	$\llbracket [0,1-0.5 \mid P_{\Delta} \mid 1 \rrbracket$
Exponential	$ P_{\Delta} /(\exp(P_{\Delta})-1)$
Power-law	$[0,(1-0.1 P_{\Delta})^{5}]$



aw(i+1) w

4.4.5 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

$$a_{W}(i+1) = \{D_{W}A(|P_{\Delta w}|) + ||F_{W},0||\}_{i+1} \qquad (D_{W})_{i+1} = (D_{e})_{i}$$

$$a_{E}(i) = \{D_{e}A(|P_{\Delta e}|) + ||-F_{e},0||\}_{i} \qquad (F_{W})_{i+1} = (F_{e})_{i}$$

$$a_{W}(i+1) - a_{E}(i) = ||F,0|| - ||-F,0|| = F \qquad (P_{\Delta w})_{i+1} = (P_{\Delta e})_{i}$$



Appendix 1 of Section 5-4

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

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

$$\phi_P[D_eB(P_{\Delta e}) + D_wA(P_{\Delta w})] = [D_eA(P_{\Delta e})]\phi_E + [D_wB(P_{\Delta W})]\phi_W$$

$$a_P$$

$$a_P$$

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

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

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

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

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

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

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

$$D_{e}A(|P_{\Delta e}|) + ||F_{e}, 0|| + D_{w}A(|P_{\Delta w}|) + ||-F_{w}, 0|| =$$

$$D_{e}A(|P_{\Delta e}|) + ||F_{e},0|| + F_{e} - F_{e} + D_{w}A(|P_{\Delta w}|) + ||-F_{w},0|| + F_{w} - F_{w} = 0$$

$$a_E$$
 $\left\|-F_e,0\right\|$

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

$$a_P = a_E + a_W + (F_W - F_W)$$





同舟共济 渡彼岸!

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