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## ME-704 –CMTFE-KNI-15

### Introduction to Control Volume Formulation

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## TRANSPORT EQUATIONS

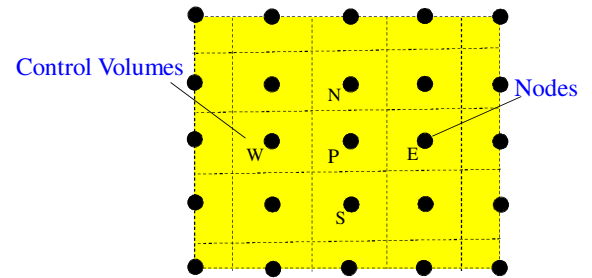
Generalised Transport Equation

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

Conservation Equation	Transported variable	Diffusion Coefficient	Source Term
Mass	1	0	0
X-momentum	u	$\mu$	$-\frac{\partial p}{\partial x} + \rho g_x$
Y-momentum	v	$\mu$	$-\frac{\partial p}{\partial y} + \rho g_y$

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## DOMAIN DISCRETISATION



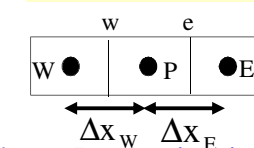
- The domain is divided into nodes and control faces are kept at the middle of these nodes
- The problem is to solve for the unknowns at the nodes

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## DISCRETISATION PRINCIPLES-1

Consider 1-D Convection-Diffusion Equation

$$\frac{d}{dx} \left( \rho u \phi - \Gamma \frac{\partial \phi}{\partial x} \right) = 0$$



Control Volume Integration implies

$$\int_w^e \frac{d}{dx} \left( \rho u \phi - \Gamma \frac{d\phi}{dx} \right) dx = 0$$

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## DISCRETISATION PRINCIPLES-II

$$\left(\rho u \phi - \Gamma \frac{\partial \phi}{\partial x}\right)_e - \left(\rho u \phi - \Gamma \frac{\partial \phi}{\partial x}\right)_w = 0 \quad \text{1}$$

For linear variation of the variable, we can write

$$\phi_c = \frac{\phi_E + \phi_P}{2}, \quad \phi_w = \frac{\phi_W + \phi_P}{2}, \quad \frac{\partial \phi}{\partial x}\bigg|_e = \frac{\phi_E - \phi_P}{\Delta x_E}, \quad \frac{\partial \phi}{\partial x}\bigg|_w = \frac{\phi_P - \phi_W}{\Delta x_W}$$

Substitution results in

$$\phi_E \left( \frac{\rho u|_e}{2} - \frac{\Gamma_c}{\Delta x_E} \right) - \phi_W \left( -\frac{\rho u|_w}{2} - \frac{\Gamma_w}{\Delta x_W} \right) + \phi_P \left( \frac{\rho u|_e}{2} + \frac{\Gamma_c}{\Delta x_E} - \frac{\rho u|_w}{2} + \frac{\Gamma_w}{\Delta x_W} \right) = 0$$

Central Difference Scheme

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## DISCRETISATION PRINCIPLES-III

### Difficulties of Central Difference

The previous equation can be written as

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

$$\text{where, } a_E = \left( \frac{\Gamma_e}{\Delta x_E} - \frac{\rho u|_e}{2} \right),$$

$$a_W = \left( \frac{\Gamma_w}{\Delta x_W} + \frac{\rho u|_w}{2} \right)$$

$$a_P = (a_E + a_W + \rho u|_e - \rho u|_w)$$

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## DISCRETISATION PRINCIPLES-IV

- For every node, a similar equation can be written
- If boundaries are known, we can write N equations for N interior nodes and the problem can be solved
- But the solution is found to be oscillatory for cases with large convection
- This was the overshoot problem

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## REASONS FOR THE DIFFICULTY

The coefficient for  $a_E$  can be written as

$$a_E = \frac{\Gamma_e}{\Delta x_E} \left( 1 - \frac{\rho u|_e \Delta x_E}{2\Gamma_e} \right) = \frac{\Gamma_e}{\Delta x_E} \left( 1 - \frac{P_e}{2} \right)$$

where  $p_e$  is defined as the cell Peclet number

The second term in the bracket can become negative at large velocities.

A negative weight can give unphysical solutions

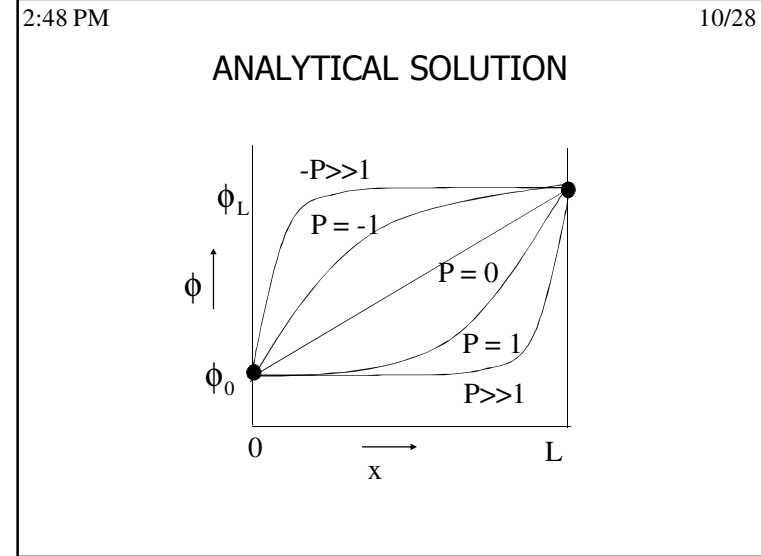
e.g.  $(50 \times 2 + 100 \times (-4))/(2-4) = -150$

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### THE REMEDY

➤ Better schemes can be derived from the analytical solution of the convection-diffusion equation

The analytical solution subject to boundary conditions,  
 $\phi(x=0) = \phi_0, \phi(x=L) = \phi_L$   
 is given by

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


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### EXPONENTIAL SCHEME-I

The values of the function and its derivative at the control surface 'e' can be obtained as

$$\phi_e = \phi_P + (\phi_E - \phi_P) \left( \frac{e^{\frac{\rho u|_e \delta x_e}{\Gamma_e} - 1}}{e^{\frac{\rho u|_e \Delta x_E}{\Gamma_e} - 1}} \right)$$

$$\frac{\partial \phi}{\partial x}|_e = (\phi_E - \phi_P) \left( \frac{e^{\frac{\rho u|_e \delta x_e}{\Gamma_e}}}{e^{\frac{\rho u|_e \Delta x_E}{\Gamma_e} - 1}} \right) \frac{\rho u|_e}{\Gamma_e}$$

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### EXPONENTIAL SCHEME-II

- Similarly the values at w can be computed and these can be substituted in Eq. (1) of slide 5 to get

$$a_p \phi_P = a_E \phi_E + a_w \phi_W,$$

where,  $a_E = \left( \frac{\rho u|_e}{e^{P_e} - 1} \right)$ ,  $a_w = \left( \frac{\rho u|_w e^{P_w}}{e^{P_w} - 1} \right)$  and  $a_p = (a_E + a_w + \rho u|_e - \rho u|_w)$


$a_E$  can be rewritten as

$$a_E = \frac{\Gamma_e}{\Delta x_E} \left( \frac{P_e}{e^{P_e} - 1} \right)$$

Note:  $a_E \rightarrow 0$  as  $P_e \gg 1$

The graph shows the relationship between the coefficient  $a_E/D_e$  and the Peclet number  $P_e$ . The curve starts at 1 for  $P_e = 0$  and asymptotically approaches 0 as  $P_e$  increases. The equation  $D_e = \frac{\Gamma_e}{\Delta x_E}$  is also shown.

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When convection dominates

$\phi_e = \phi_P$  and  $\phi_w = \phi_w$   
for  $u \gg 0$

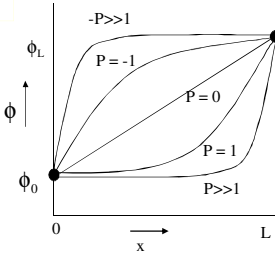
$\phi_e = \phi_E$  and  $\phi_w = \phi_P$   
for  $u \ll 0$

- Evaluating gradient by linear variation, we can write,

$$a_p \phi_P = a_E \phi_E + a_w \phi_w,$$

where,  $a_E = D_e + \langle -\rho u|_e, 0 \rangle$ ,  $a_w = D_w + \langle \rho u|_w, 0 \rangle$

and  $a_p = (a_E + a_w + \rho u|_e - \rho u|_w)$

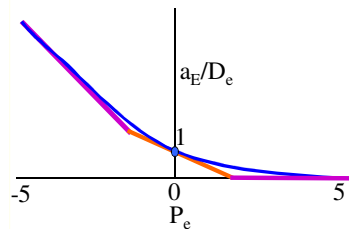


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### HYBRID SCHEME

➤ Properties of analytical solution of  $a_E/D_e$  are:

- $a_E/D_e = 1$  at  $P_e = 0$
- $a_E/D_e \rightarrow 0$  as  $P_e \gg 1$
- $a_E/D_e \rightarrow -P_e$  as  $-P_e \gg 1$
- $\frac{d(a_E/D_e)}{dP_e} = -0.5$  at  $P_e = 0$



$$a_p \phi_P = a_E \phi_E + a_w \phi_w,$$

where,  $a_E = \left\langle -\rho u|_e, D_e - \frac{\rho u|_e}{2}, 0 \right\rangle$ ,  $a_w = \left\langle \rho u|_w, D_w + \frac{\rho u|_w}{2}, 0 \right\rangle$

and  $a_p = (a_E + a_w + \rho u|_e - \rho u|_w)$

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### GENERALISATION OF ALL SCHEMES

All the schemes can be generalised using a function  $A(|P|)$

$$a_p \phi_P = a_E \phi_E + a_w \phi_w,$$

where,  $a_E = D_e A(|P_e|) + \langle -F_e, 0 \rangle$ ,

$$a_w = D_w A(|P_w|) + \langle F_w, 0 \rangle$$
 and
$$a_p = (a_E + a_w + F_e - F_w),$$

Scheme	$A( P )$
Central	$1 - 0.5  P $
Upwind	1
Hybrid	$\langle 0, 1 - 0.5 P  \rangle$
Exponential	$\frac{ P }{e^{ P } - 1}$

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### PRESSURE LINKED EQUATIONS

$$\frac{\partial p}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} = 0$$

$$\frac{\partial \rho u}{\partial t} + \frac{\partial}{\partial x} \left( \rho u u - \mu \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left( \rho u v - \mu \frac{\partial u}{\partial y} \right) = -\frac{\partial p}{\partial x} + \rho g_x$$

$$\frac{\partial \rho v}{\partial t} + \frac{\partial}{\partial x} \left( \rho u v - \mu \frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial y} \left( \rho v v - \mu \frac{\partial v}{\partial y} \right) = -\frac{\partial p}{\partial y} + \rho g_y$$

**There is no transport equation for p**

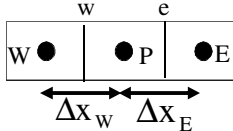
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### CHECKERBOARDING PROBLEM

- Early attempts at the solution led to oscillatory pressure fields
- A possible interpretation is given below


Control volume integration of pressure term leads to

$$\int_w^e -\frac{\partial p}{\partial x} dx = p|_w - p|_e$$

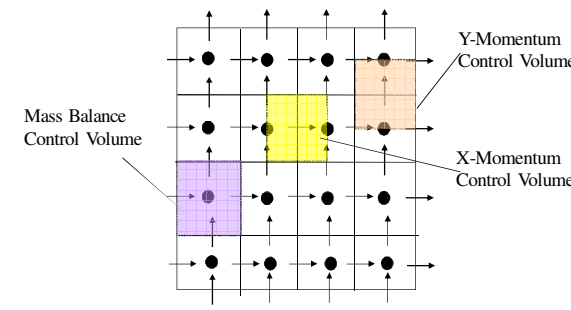
$$p_e = 0.5(p_p + p_E) \text{ and } p_w = 0.5(p_w + p_p)$$


$$\int_w^e -\frac{\partial p}{\partial x} dx = 0.5(p_w - p_E)$$

Equal increase of pressure in alternate nodes will not affect velocity

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### REMEDY – THE STAGGERED GRID



No interpolation of pressure required

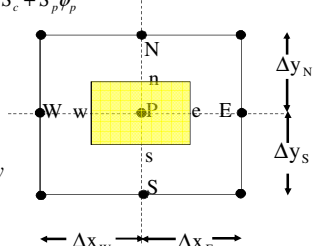
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### DRAWBACKS OF STAGGERED GRID

- Indices have to be carefully kept track
- Large number of coefficients have to be carried along
- Non-staggered Methods have been developed
- The principle is to manipulate the pressure gradient terms

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### Discretisation of 2-D Transport Equation

$$\frac{\partial \rho \phi}{\partial t} + \frac{\partial}{\partial x} \left( \rho u \phi - \Gamma \frac{\partial \phi}{\partial x} \right) + \frac{\partial}{\partial y} \left( \rho v \phi - \Gamma \frac{\partial \phi}{\partial y} \right) = S_c + S_p \phi_p$$


$$\iint \frac{\partial \rho \phi}{\partial t} dx dy = \frac{\rho \phi|_p^{\Delta t} - \rho \phi|_p^0}{\Delta t} \Delta x \Delta y$$

$$\iint (S_c + S_p \phi_p) dx dy = [S_c + S_p \phi_p] \Delta x \Delta y$$

$$\iint \frac{\partial}{\partial y} \left( \rho u \phi - \Gamma \frac{\partial \phi}{\partial y} \right) dx dy = \left[ \left( \rho u \phi - \Gamma \frac{\partial \phi}{\partial y} \right)_n - \left( \rho u \phi - \Gamma \frac{\partial \phi}{\partial y} \right)_s \right] \Delta x$$

$$\iint \frac{\partial}{\partial x} \left( \rho u \phi - \Gamma \frac{\partial \phi}{\partial x} \right) dx dy = \left[ \left( \rho u \phi - \Gamma \frac{\partial \phi}{\partial x} \right)_e - \left( \rho u \phi - \Gamma \frac{\partial \phi}{\partial x} \right)_w \right] \Delta y$$

➤ Similar discretisation of mass balance will yield

$$\frac{\rho|_P^{\Delta t} - \rho|_P^0}{\Delta t} \Delta x \Delta y + (\rho u|_e - \rho u|_w) \Delta y + (\rho u|_n - \rho u|_s) \Delta x = 0$$

➤ Multiplying the above with  $\phi|_P^{\Delta t}$  and subtracting from the discretised momentum equation, we get

$$\frac{\phi|_P^{\Delta t} - \phi|_P^0}{\Delta t} \rho_p^0 \Delta x \Delta y + \left[ \left( \rho u \phi - \Gamma \frac{\partial \phi}{\partial x} \right)_e - \left( \rho u \phi - \Gamma \frac{\partial \phi}{\partial x} \right)_w - (\rho u|_e - \rho u|_w) \phi_p \right] \Delta y + \left[ \left( \rho u \phi - \Gamma \frac{\partial \phi}{\partial y} \right)_n - \left( \rho u \phi - \Gamma \frac{\partial \phi}{\partial y} \right)_s - (\rho u|_n - \rho u|_s) \phi_p \right] \Delta x = (S_c + S_p \phi_p) \Delta x \Delta y$$

➤ Plugging the profiles as done earlier, we get

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### Discretised of 2-D Transport Equation (Cont'd)

$$a_p \phi_P = a_E \phi_E + a_W \phi_W + a_N \phi_N + a_S \phi_S + b$$

where,  $a_E = D_e A(|P_e|) + \langle -F_e, 0 \rangle$ ,  $a_W = D_w A(|P_w|) + \langle F_w, 0 \rangle$ ,  
 $a_N = D_n A(|P_n|) + \langle -F_n, 0 \rangle$ ,  $a_S = D_s A(|P_s|) + \langle F_s, 0 \rangle$ ,  
 $b = S_c \Delta x \Delta y + \frac{\rho_p^0 \phi_p \Delta x \Delta y}{\Delta t}$

and  $a_p = \left( a_E + a_W + a_N + a_S + \frac{\rho_p^0 \Delta x \Delta y}{\Delta t} - S_p \Delta x \Delta y \right)$ ,  
 $D_e = \frac{\Gamma_e \Delta y}{\Delta x_E}$ ,  $D_w = \frac{\Gamma_w \Delta y}{\Delta x_W}$ ,  $D_n = \frac{\Gamma_n \Delta x}{\Delta y_N}$ ,  $D_s = \frac{\Gamma_s \Delta x}{\Delta y_S}$ ,  
 $F_e = \rho u|_e \Delta y$ ,  $F_w = \rho u|_w \Delta y$ ,  $F_n = \rho u|_n \Delta x$ ,  $F_s = \rho u|_s \Delta x$ ,  
 $P_e = \frac{F_e}{D_e}$ ,  $P_w = \frac{F_w}{D_w}$ ,  $P_n = \frac{F_n}{D_n}$ ,  $P_s = \frac{F_s}{D_s}$ .

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### SIMPLE (Semi-IMplicit procedure for solving Pressure Linked Equations)

1. Assume a pressure field and velocity field
2. Compute coefficients for x and y momentum equations
3. Solve for u's and v's using x and y momentum equations
4. Check whether it satisfies mass balance
5. Obtain a new guess for pressure field systematically so that the resulting velocity would satisfy mass balance
6. Repeat steps 2-5 till convergence is obtained

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### The Pressure Correction Equation

Let  $p^*$  be the assumed pressure field

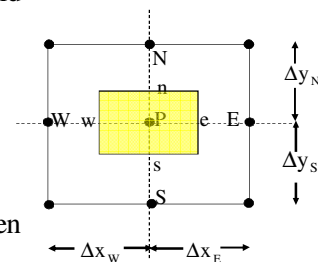
X-momentum  
 $a_c u_c^* = \sum a_{nb} u_{nb}^* + b_c + (p_P^* - p_E^*) \Delta y$

Y-momentum  
 $a_n v_n^* = \sum a_{nb} v_{nb}^* + b_n + (p_P^* - p_N^*) \Delta x$

If  $p$  is the correct pressure field then

$$a_c u_c = \sum a_{nb} u_{nb} + b_c + (p_P - p_E) \Delta y$$

$$a_n v_n = \sum a_{nb} v_{nb} + b_n + (p_P - p_N) \Delta x$$



Subtraction of the approximate fields from the correct fields lead to ➡

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### The Pressure Correction Equation (cont'd)


$$a_e u'_e = \sum a_{nb} u'_{nb} + (p'_p - p'_E) \Delta y \quad a_n v'_n = \sum a_{nb} v'_{nb} + (p'_p - p'_N) \Delta x$$

$$u'_e = (p'_p - p'_E) \frac{\Delta y}{a_e} \quad v'_n = (p'_p - p'_N) \frac{\Delta x}{a_n}$$

Control volume integration of mass balance leads to

$$\frac{\rho'_p - \rho'_E}{\Delta t} \Delta x \Delta y + (\rho'_e (u'_e + u'_e) - \rho'_w (u'_w + u'_w)) \Delta y +$$

$$(\rho'_e (v'_n + v'_n) - \rho'_s (v'_s + v'_s)) \Delta x = 0$$

Substitution of  $u'_e$ ,  $v'_n$  from above  
and rearranging leads to 

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### The Pressure Correction Equation (cont'd)

$$a_p p'_p = a_E p'_E + a_W p'_W + a_N p'_N + a_S p'_S + b$$

where,  $a_E = \rho'_e \frac{\Delta y}{a_e} \Delta y$ ,  $a_W = \rho'_w \frac{\Delta y}{a_w} \Delta y$ ,  $a_N = \rho'_n \frac{\Delta x}{a_n} \Delta x$ ,  $a_S = \rho'_s \frac{\Delta x}{a_s} \Delta x$ ,

and  $a_p = a_E + a_W + a_N + a_S$ ,

$$b = (\rho'_e u'_e - \rho'_w u'_w) \Delta y + (\rho'_n v'_n - \rho'_s v'_s) \Delta x + \frac{(\rho'_p - \rho'_E) \Delta x \Delta y}{\Delta t}$$

The source term for pressure correction is the mass imbalance. Thus the correction will cease when the mass balance is satisfied.

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### Details of the Procedure

1. Assume arbitrary  $u$ ,  $v$  and  $p$  fields
2. Compute the coefficients for  $x$  and  $y$  momentum equations on lines given in Eq. (33). Proper labelling of indices have to be taken care of
3. Solve for  $u^*$  and  $v^*$  using computed coefficients in step 2 and assume pressure field in step 1
4. Compute mass imbalance ( $b$ ) in Eq. (43).
5. If mass imbalance is low every where, then the obtained  $u^*$ ,  $v^*$  and the assumed  $p^*$  are the solutions.

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### Details of the Procedure (cont'd)

6. If step 5 is not satisfied, then obtain coefficients for pressure correction equation Eq. (43).
7. Solve for  $p'$ , Eq. (43)
8. Correct  $u$ ,  $v$  and  $p$  as,  $p = p^* + \alpha_p p'$ ,  
 $u = u^* + \alpha_u u'$  and  $v = v^* + \alpha_v v'$ , where  $\alpha$ 's are under relaxation coefficients to prevent the procedure from diverging. Typical values these are 0.5-0.7.
9. Repeat steps 2-8 as many times as is required to satisfy step 5.