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APPENDIX A

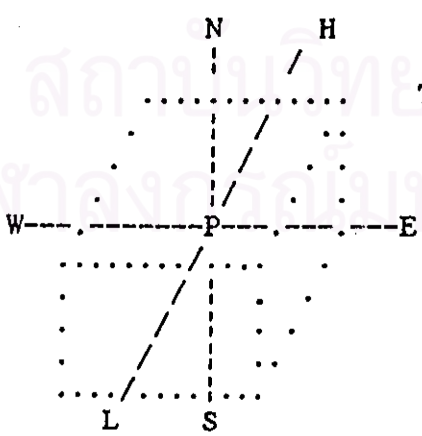
COMPUTATIONAL FLUID DYNAMICS TECHNIQUE

Computational fluid dynamics (CFD) is the art of replacing the governing equations of fluid dynamics with discretized algebraic forms , which in turn are solved to obtain numbers for the flow field values at discrete points in time and/or space.

The end product of CFD is indeed a collection of numbers , in contrast to a closed-form analytical solution. (Anderson , 1995)

In this study , integration of differential equations over the finite volume of a computational cell is applied with fully-implicit approach. Within each cell , a *grid point* is supposed to be located ; and each cell communicates with its neighbors across the intervening cell faces.

Figure A.1 illustrates the six links between grid point *P* and its six neighbors *N* , *S* , *E* , *W* , *H* and *L*.



The grid points shown are:-

P, the central point
N, the north neighbour
S, the south neighbour
E, the east neighbour
W, the west neighbour
H, the high neighbour
L, the low neighbour

Figure A.1 A control volume.

A.1 THE STRUCTURE OF THE DISCRETIZATION EQUATION

The general conservation equation contains four basic terms : the unsteady term , the convection term , the diffusion term and the source term respectively as below

$$\frac{\partial(\rho\phi)}{\partial t} + \frac{\partial(\rho u_j \phi)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\Gamma \frac{\partial \phi}{\partial x_j}\right) + S \qquad (A.1)$$

where ϕ is the general dependent variable.

and Γ is the diffusion coefficient of ϕ .

A discretization equation is an algebraic relation connecting the values of ϕ for a group of grid points. Such an equation is derived from the differential equation governing ϕ and thus express the same physical information as the differential equation.

That only a few grid points participate in a given discretization equation is a consequence of the piecewise nature of the profiles chosen. The value of ϕ at a grid point thereby influences the distribution of ϕ only in its immediate neighborhood.

As the number of grid points becomes very large , the solution of the discretization equations is expected to approach the exact solution of the corresponding differential equation. This follows from the consideration that , as the grid points get closer together , the change in ϕ between neighboring grid points becomes small , and then the actual details of the profile assumption become unimportant.

A.1.1 SCHEME

In case of a steady one-dimensional flow in which only the convection and diffusion terms are present , the governing differential equation is

$$\frac{d(\rho u \phi)}{dx} = \frac{d}{dx}\left(\Gamma \frac{d\phi}{dx}\right) \qquad (A.2)$$

where u represents the velocity in the x direction.

Also , the continuity equation (4.1) becomes

$$\frac{d(\rho u)}{dx} = 0 \quad \text{or} \quad \rho u = \text{constant} \qquad (A.3)$$

Using the three-grid-point cluster shown in figure A.2 to derive the discretization equation.

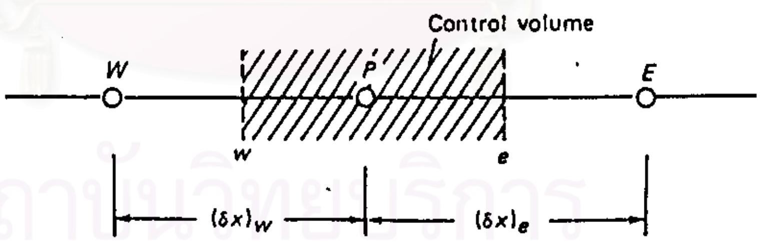


Figure A.2 Typical grid-point cluster for the one-dimensional problem.

Although the actual location of the control-volume face *e* and *w* would not influence the final formulation , it is convenient to assume that *e* is located midway between *P* and *E* , and *w* midway between *W* and *P*.

Integration of equation (A.2) over the control volume shown in figure A.2 gives

$$(\rho u\phi)_e - (\rho u\phi)_w = \left(\Gamma \frac{d\phi}{dx}\right)_e - \left(\Gamma \frac{d\phi}{dx}\right)_w \qquad (A.4)$$

The diffusion term $(\Gamma\, d\phi/dx)$ can be interpolated by piecewise-linear profile assumption between the grid points. For the convection term $(\rho u\phi)$, the same choice of profile would at first seem natural. The result is

$$\frac{1}{2}(\rho u)_e(\phi_E + \phi_P) - \frac{1}{2}(\rho u)_w(\phi_P + \phi_W) = \frac{\Gamma_e(\phi_E - \phi_P)}{(\delta x)_e} - \frac{\Gamma_w(\phi_P - \phi_W)}{(\delta x)_w} \qquad (A.5)$$

The factor $\frac{1}{2}$ arises from the assumption of the interfaces being midway , where

$$\phi_e = \frac{1}{2}(\phi_E + \phi_P) \quad \text{and} \quad \phi_w = \frac{1}{2}(\phi_P + \phi_W) \qquad (A.6)$$

The values of $(\rho u)_e$, $(\rho u)_w$, Γ_e and Γ_w can be obtained by appropriate interpolation as described later in subsection A.2.1.

To arrange the equation in a more compact form , two new symbols F and D are defined as follows

$$F \equiv \rho u \quad , \quad D \equiv \frac{\Gamma}{\delta x} \tag{A.7}$$

Both have the same dimensions ; F indicates the strength of the convection (or flow) , while D is the diffusion conductance. Note that , whereas D always remains positive , F can take either positive or negative values depending on the direction of the flow field.

With the new defenitions , the discretization equation becomes

$$a_P \phi_P = a_E \phi_E + a_W \phi_W \tag{A.8}$$

where

$$a_E = D_e - \frac{F_e}{2} \tag{A.9a}$$

$$a_W = D_w + \frac{F_w}{2} \tag{A.9b}$$

$$a_P = a_E + a_W + \left(F_e - F_w \right) \tag{A.9c}$$

The discretization equation (A.8) represents the implications of the piecewise-linear profile for ϕ. This form is also known as the *central-difference scheme* and is the natural outcome of a Taylor-series expansion.

However , the central-difference scheme was limited to low Reynolds number flow (i.e., to low values of $|F / D|$) because if out of this range , the unrealistic result will occur due to equations (A.9) indicate that the coefficients could , at times , become negative when $|F|$ exceeds 2 D. This violates the *four basic rules* which state that any discretization equations should be obeyed

, to ensure physical realism and overall balance. The details of these rules will be presented in the next subsection.

Since the foregoing preliminary formulation has resulted in an unacceptable discretization equation , the better formulations was required. A well-known remedy for the difficulties encountered is the *upwind-difference scheme*. This scheme recognizes that the weak point in the preliminary formulation is the assumption of the convected property ϕ_e at the interface is the average of ϕ_E and ϕ_P . Therefore , a better prescription is proposed. The formulation of the diffusion term is left unchanged , but the convection term is calculated from the following assumption.

The value of ϕ at an interface is equal to the value of ϕ at the grid point on the upwind side of the face.

Thus , $\phi_e = \phi_P$ if $F_e > 0$ (A.10a)

and $\phi_e = \phi_E$ if $F_e < 0$ (A.10b)

The value of ϕ_w can be definded similarly.

The conditional statements (A.10) can be written in a more compact form if a new operator $\| A , B \|$ is defined. This is equivalent to AMAX1 (A , B) in the computer language FORTRAN , to denote the greater of A and B. Then , the upwind-difference scheme implies

$$F_e\phi_e = \phi_P \| F_e , 0 \| - \phi_E \| -F_e , 0 \| \quad \text{(A.11)}$$

when equation (A.6) is replaced by this concept , the discretization equation becomes

$$a_P\phi_P = a_E\phi_E + a_W\phi_W \tag{A.12}$$

where

$$a_E = D_e + \| -F_e , 0 \| \tag{A.13a}$$

$$a_W = D_w + \| F_w , 0 \| \tag{A.13b}$$

$$a_P = a_E + a_W + \left(F_e - F_w \right) \tag{A.13c}$$

However , for a high Reynolds number flow (i.e., high values of $|F / D|$) , the diffusion is almost absent or the term $d\phi/dx$ is nearly zero but the upwind-difference scheme always calculates the diffusion term from the piecewise-linear profile and thus overestimates diffusion at large values of $|F / D|$.

In this study , the adopted scheme is the *hybrid-difference scheme*. The name hybrid is indicative of a combination of the central-difference and upwind-difference schemes. This scheme was developed to give a reasonable approximation to the exact solution according to conditions

$$\text{for} \quad F_e < -2D_e \quad \text{then} \quad a_E = -F_e \tag{A.14a}$$

$$\text{for} \quad -2D_e \le F_e \le 2D_e \quad \text{then} \quad a_E = D_e - \frac{F_e}{2} \tag{A.14b}$$

$$\text{for} \quad F_e > 2D_e \quad \text{then} \quad a_E = 0 \tag{A.14c}$$

The significance of the hybrid-difference scheme can be appreciated by recognizing that it is identical to the central-difference scheme for $\left| F_e \right| \leq 2 D_e$ and outside this range it reduces to the upwind-difference scheme in which the diffusion is set to zero.

The convection-diffusion discretization equation for the hybrid-difference scheme can be written as

$$a_P \phi_P = a_E \phi_E + a_W \phi_W \tag{A.15}$$

where

$$a_E = \left\| -F_e \ , \ D_e - \frac{F_e}{2} \ , \ 0 \right\| \tag{A.16a}$$

$$a_W = \left\| F_w \ , \ D_w + \frac{F_w}{2} \ , \ 0 \right\| \tag{A.16b}$$

$$a_P = a_E + a_W + \left(F_e - F_w \right) \tag{A.16c}$$

This formulation is valid for any arbitrary location of the interfaces between the grid points and is not limited to midway interfaces.

A.1.2 THE FOUR BASIC RULES

Rule 1 : Consistency at control-volume faces.

When a face is common to two adjacent control volumes , the flux across it must be represented by same expression in the discretization equations for the two control volumes.

Rule 2 : Positive coefficients.

All coefficients (the center-point coefficient a_P and the neighbor coefficients a_{nb}) must always be positive.

Rule 3 : Negative-slope linearization of the source term.

The source term S is linearized as $\overline{S} = S_C + S_P\phi_P$, where S_C stands for the constant part of the average value $\overline{S}$, while S_P is the coefficient of ϕ_P and must be less than or equal to zero.

Rule 4 : Sum of the neighbor coefficients.

The center-point coefficient a_P must equal to the sum of the neighbor coefficients a_{nb}. Thus , $a_P = \Sigma\, a_{nb}$. However , when the source term depends on ϕ , this case will be inapplicability of Rule 4. But if S_P is set to zero , this rule becomes applicable and is indeed obeyed.

A.1.3 DISCRETIZATION EQUATION FOR THREE DIMENSIONS

The three-dimensional form of equation (A.1) can be written as

$$\frac{\partial(\rho\phi)}{\partial t} + \frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} + \frac{\partial J_z}{\partial z} = S \qquad \text{(A.17)}$$

where J_x , J_y and J_z are the total of convection and diffusion fluxes defined by

$$J_x \equiv \rho u\phi - \Gamma\frac{\partial\phi}{\partial x} \qquad \text{(A.18a)}$$

$$J_y \equiv \rho v\phi - \Gamma\frac{\partial\phi}{\partial y} \qquad \text{(A.18b)}$$

$$J_z \equiv \rho w \phi - \Gamma \frac{\partial \phi}{\partial z} \qquad \text{(A.18c)}$$

and

where u , v and w denote the velocity components in the x , y and z directions respectively. The integration of equation (A.17) over the control volume give

$$\frac{\left(\rho_P \phi_P - \rho_P^o \phi_P^o \right) \Delta x \Delta y \Delta z}{\Delta t} + J_e - J_w + J_n - J_s + J_l - J_h = \left(S_C + S_P \phi_P \right) \Delta x \Delta y \Delta z \qquad \text{(A.19)}$$

For the unsteady term , ρ_P and ϕ_P are assumed to prevail over the whole control volume. The *old* values (i.e., the values at the beginning of the time step) are denoted by ρ_P^o and ϕ_P^o. In confirmity with the fully-implicit approach , all other values (i.e., those without a superscript) are to be regarded as the *new* values.

The quantities J_e , J_w , J_n , J_s , J_l and J_h are the integrated total fluxes over the control-volume faces ; that is , J_e stands for $\iint J_x \, dy \, dz$ over the interface *e* , and so on.

In a similar manner , the continuity equation (4.1) can be integrated over the control volume to give

$$\frac{\left(\rho_P - \rho_P^o \right) \Delta x \Delta y \Delta z}{\Delta t} + F_e - F_w + F_n - F_s + F_l - F_h = 0 \qquad \text{(A.20)}$$

Where F_e , F_w , F_n , F_s , F_l and F_h are the mass flow rates through the faces of the control volume. If ρu at point e is taken to prevail over the whole interface e ,

thus $$F_e = (\rho u)_e \, \Delta y \Delta z \quad \text{(A.21a)}$$

similarly $$F_w = (\rho u)_w \, \Delta y \Delta z \quad \text{(A.21b)}$$

$$F_n = (\rho v)_n \, \Delta x \Delta z \quad \text{(A.21c)}$$

$$F_s = (\rho v)_s \, \Delta x \Delta z \quad \text{(A.21d)}$$

$$F_l = (\rho w)_l \, \Delta x \Delta y \quad \text{(A.21e)}$$

$$F_h = (\rho w)_h \, \Delta x \Delta y \quad \text{(A.21f)}$$

By multiplying equation (A.20) by ϕ_P and subtracting it from equation (A.19) :

$$(\phi_P - \phi_P^{\circ}) \frac{\rho_P^{\circ} \Delta x \Delta y \Delta z}{\Delta t} + (J_e - F_e\phi_P) - (J_w - F_w\phi_P) + (J_n - F_n\phi_P)$$

$$-(J_s - F_s\phi_P) + (J_l - F_l\phi_P) - (J_h - F_h\phi_P) = (S_C + S_P\phi_P)\,\Delta x \Delta y \Delta z \quad \text{(A.22)}$$

The term such as $J_e - F_e\phi_P$ can be expressed and rearranged to be $a_E(\phi_P - \phi_E)$.

Similarly $$J_w - F_w\phi_P = a_W(\phi_W - \phi_P) \quad \text{(A.23a)}$$

$$J_n - F_n\phi_P = a_N(\phi_P - \phi_N) \qquad \text{(A.23b)}$$

$$J_s - F_s\phi_P = a_S(\phi_S - \phi_P) \qquad \text{(A.23c)}$$

$$J_l - F_l\phi_P = a_L(\phi_P - \phi_L) \qquad \text{(A.23d)}$$

and

$$J_h - F_h\phi_P = a_H(\phi_H - \phi_P) \qquad \text{(A.23e)}$$

Finally , the discretization equation based on the general differential equation (A.1) with the hybrid-difference scheme can be written as

$$a_P\phi_P = a_E\phi_E + a_W\phi_W + a_N\phi_N + a_S\phi_S + a_L\phi_L + a_H\phi_H + b \qquad \text{(A.24)}$$

where

$$a_E = \left\| -F_e \;,\; D_e - \frac{F_e}{2} \;,\; 0 \right\| \qquad \text{(A.25a)}$$

$$a_W = \left\| F_w \;,\; D_w + \frac{F_w}{2} \;,\; 0 \right\| \qquad \text{(A.25b)}$$

$$a_N = \left\| -F_n \;,\; D_n - \frac{F_n}{2} \;,\; 0 \right\| \qquad \text{(A.25c)}$$

$$a_S = \left\| F_s \;,\; D_s + \frac{F_s}{2} \;,\; 0 \right\| \qquad \text{(A.25d)}$$

$$a_L = \left\| -F_l \;,\; D_l - \frac{F_l}{2} \;,\; 0 \right\| \qquad \text{(A.25e)}$$

$$a_H = \left\| \; F_h \;,\; D_h + \frac{F_h}{2} \;,\; 0 \; \right\| \qquad \text{(A.25f)}$$

$$a_P = a_E + a_W + a_N + a_S + a_L + a_H + a_P^\circ - S_P\, \Delta x \Delta y \Delta z \qquad \text{(A.25g)}$$

$$a_P^\circ = \frac{\rho_P^\circ\; \Delta x \Delta y \Delta z}{\Delta t} \qquad \text{(A.25h)}$$

$$b = S_C\, \Delta x \Delta y \Delta z + a_P^\circ \phi_P^\circ . \qquad \text{(A.25i)}$$

The diffusion conductances are defined as

$$D_e = \frac{\Gamma_e\, \Delta y \Delta z}{(\delta x)_e} \qquad \text{(A.26a)}$$

$$D_w = \frac{\Gamma_w\, \Delta y \Delta z}{(\delta x)_w} \qquad \text{(A.26b)}$$

$$D_n = \frac{\Gamma_n\, \Delta x \Delta z}{(\delta y)_n} \qquad \text{(A.26c)}$$

$$D_s = \frac{\Gamma_s\, \Delta x \Delta z}{(\delta y)_s} \qquad \text{(A.26d)}$$

$$D_l = \frac{\Gamma_l\, \Delta x \Delta y}{(\delta z)_l} \qquad \text{(A.26e)}$$

$$D_h = \frac{\Gamma_h\, \Delta x \Delta y}{(\delta z)_h} \qquad \text{(A.26f)}$$

As $\Delta t \rightarrow \infty$, equation (A.24) reduces to the steady-state discretization equation.

A.2 CALCULATION OF THE FLOW FIELD

The procedure for solving the general differential equation for ϕ in the presence of a given flow field has been formulated. The velocity components are governed by the momentum equations , which are special cases of the general differential equation for ϕ (with ϕ = u or $\overline{u}$, $\Gamma = \mu$ or μ_{eff} , and so on).

The pressure gradient forms a part of the source term for a momentum equation and also the velocity field lies in this unknown pressure field. There are some difficulties when using the control volume as shown in figure A.2 , the pressure field is calculated from the momentum equations then give zero pressure gradients or a uniform pressure field. A similar kind arises when the velocity components satisfied the continuity equation then also give the unrealistic solutions. (Patankar , 1980)

However , there is a remedy by stagger of the grid. The key feature is that pressures and velocities are calculated at different grid points. In the case of the velocity components , there is a significant benefit to be obtained by arranging them on grids that are different from the grid used for all other variables.

A.2.1 THE MOMENTUM EQUATIONS

A staggered control volume for the x-momentum equation is shown in figure A.3. If focus attention on the locations for u only by short arrows , there is nothing unusual about this control volume. Its faces lie between the point *e* and the corresponding locations for the neighbor u's.

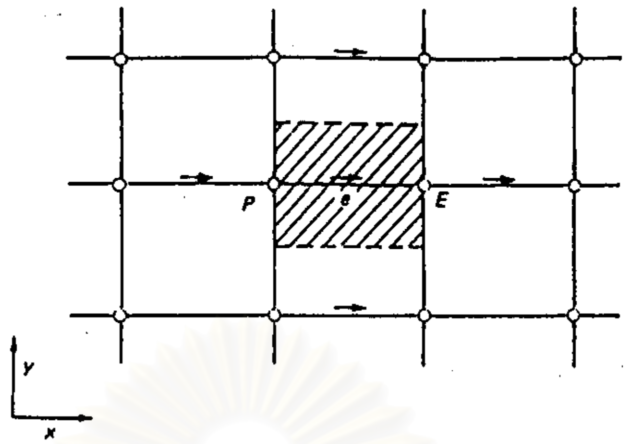


Figure A.3 Control volume for u.

The control volume is , however , staggered in relation to the normal control volume around the main grid point *P*. The staggering is in the x direction only , such that the faces normal to that direction pass through the main grid points *P* and *E*. This layout realizes one of the main advantages of the staggered grid : the pressure difference $P_P - P_E$ (or $\overline{P}_P - \overline{P}_E$) can be used to calculate the pressure force acting on the control volume for the velocity u.

The calculation of the diffusion coefficient and the mass flow rate at the faces of the u-control-volume shown in figure A.3 requires an appropriate interpolation. In this study , the *upwind side interpolation* is adopted.

The same formulation as described in subsection A.1.3 is applicable. The resulting discretization equation can be written as

$$a_e u_e \quad = \quad \sum a_{nb} u_{nb} \; + \; b \; + \; \left(P_P - P_E \right) A_e \qquad \text{(A.27)}$$

Here the number of neighbor terms depends on the dimensionality of the problem. The pressure gradient is not included in the source-term S_C and S_P but rise to the last term in equation (A.27). Since the pressure field is also to be ultimately calculated , it is inconvenient to absorb the pressures in the momentum source term.

A_e is the area on which the pressure difference acts and equals to $\Delta y \Delta z$ in the three-dimensional case. Then the momentum equations for the other directions are handled in a similar manner.

The momentum equations can be solved only when the pressure field is given or is somehow estimated. Unless the correct pressure field is employed , the resulting velocity field will not satisfy the continuity equation. Such an imperfect velocity field based on a guessed pressure field P^* will be denoted by u^* , v^* , w^*. This *starred* velocity field can be calculated from the following discretization equations.

$$a_e u_e^* = \sum a_{nb} u_{nb}^* + b + \left(P_P^* - P_E^* \right) A_e \qquad (A.28)$$

$$a_n v_n^* = \sum a_{nb} v_{nb}^* + b + \left(P_P^* - P_N^* \right) A_n \qquad (A.29)$$

$$a_l w_l^* = \sum a_{nb} w_{nb}^* + b + \left(P_P^* - P_L^* \right) A_l \qquad (A.30)$$

A.2.2 THE PRESSURE AND VELOCITY CORRECTIONS

The next aim is to find a way of improving the guessed pressure P^* such that the resulting starred velocity field will progressively get closer to satisfying the continuity equation. The proposal of the correct pressure P is obtained from

$$P = P^{*} + P' \qquad (A.31)$$

where P' will be called the *pressure correction*.

The corresponding velocity corrections u' , v' , w' can be introduced in a similar manner :

$$u = u^{*} + u' \qquad (A.32a)$$

$$v = v^{*} + v' \qquad (A.32b)$$

$$w = w^{*} + w' \qquad (A.32c)$$

If subtract equation (A.28) from equation (A.27) , then obtain

$$a_e u'_e = \sum a_{nb} u'_{nb} + \left(P'_P - P'_E \right) A_e \qquad (A.33)$$

Following Patankar (1980) , set the term $\sum a_{nb} u'_{nb}$ equal to zero and the result is

$$a_e u'_e = \left(P'_P - P'_E \right) A_e \qquad (A.34)$$

or

$$u'_e = d_e \left(P'_P - P'_E \right) \qquad (A.35)$$

where

$$d_e \equiv \frac{A_e}{a_e} \qquad (A.36)$$

Equation (A.35) is called the *velocity-correction formula* , which can also be written as

$$u_e \quad = \quad u_e^* \quad + \quad d_e \left(P_P' - P_E' \right) \qquad \text{(A.37)}$$

This shows how the starred velocity u_e^* is to be corrected in response to the pressure corrections to produce u_e.

The correction formulae for the velocity components in other directions can be written similarly

$$v_n \quad = \quad v_n^* \quad + \quad d_n \left(P_P' - P_N' \right) \qquad \text{(A.38)}$$

$$w_l \quad = \quad w_l^* \quad + \quad d_l \left(P_P' - P_L' \right) \qquad \text{(A.39)}$$

Returning to the continuity equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z} = 0 \qquad \text{(A.40)}$$

Integrate this over the same control volume which was used for deriving the discretization equation for the general variable ϕ as described in subsection A.1.3 , then the integrated form of equation (A.40) becomes same as equation (A.20).

If substitute for all the velocity components the expressions given by the velocity-correction formulae such as equations (A.37) - (A.39) into equation (A.20) , after rearrangement , obtain the following discretization equation for P'

$$a_P P_P' = a_E P_E' + a_W P_W' + a_N P_N' + a_S P_S' + a_L P_L' + a_H P_H' + b \qquad \text{(A.41)}$$

where $a_E \quad = \quad \rho_e d_e \, \Delta y \Delta z$ (A.42a)

$$a_W = \rho_w d_w \, \Delta y \Delta z \tag{A.42b}$$

$$a_N = \rho_n d_n \, \Delta x \Delta z \tag{A.42c}$$

$$a_S = \rho_s d_s \, \Delta x \Delta z \tag{A.42d}$$

$$a_L = \rho_l d_l \, \Delta x \Delta y \tag{A.42e}$$

$$a_H = \rho_h d_h \, \Delta x \Delta y \tag{A.42f}$$

$$a_P = a_E + a_W + a_N + a_S + a_L + a_H \tag{A.42g}$$

$$b = \frac{\left(\rho_P^o - \rho_P \right) \Delta x \Delta y \Delta z}{\Delta t} + \left[\left(\rho u^* \right)_w - \left(\rho u^* \right)_e \right] \Delta y \Delta z$$

$$+ \left[\left(\rho v^* \right)_s - \left(\rho v^* \right)_n \right] \Delta x \Delta z + \left[\left(\rho w^* \right)_h - \left(\rho w^* \right)_l \right] \Delta x \Delta y \tag{A.42h}$$

From equation (A.42h) , if the term b is zero , it means that the starred velocities , in conjunction with the available value of $\left(\rho_P^o - \rho_P \right)$, do satisfy the continuity equation , and no pressure correction is needed. The term b thus represents a *mass source* which the pressure corrections (through their associated velocity corrections) must annihilate.

A.2.3 THE NUMERICAL PROCEDURE

The procedure that was developed for the calculation of the flow field called SIMPLE , which stands for *S*emi-*I*mplicit *M*ethod for *P*ressure-*L*inked

Equations. The words *semi-implicit* have been used to acknowledge the omission of the term $\sum a_{nb}u'_{nb}$ in equation (A.33). This term represents an indirect or implicit influence of the pressure correction on velocity ; pressure corrections at nearby locations can alter the neighboring velocities and thus cause a velocity correction at the point under consideration. When this influence is not included , thus work with a scheme that is only partially , and not totally , implicit.

If expressions such as $a_{nb}u'_{nb}$ were retained , they would have to be expressed in terms of the pressure corrections and the velocity corrections at the neighbors of u_{nb}. These neighbors would , in turn , bring their neighbors , and so on. Ultimately , the velocity-correction formula would involve the pressure correction at all grid points in the calculation domain , and the resulting pressure-correction equation would become unmanageable. The omission of the term $\sum a_{nb}u'_{nb}$ enables the same form as the general ϕ equation to be applied to cast the P' equation.

Moreover , it so happens that the converged solution given by SIMPLE does not contain any error resulting from the omission of the term $\sum a_{nb}u'_{nb}$. The details of the construction of the pressure-correction equation then become irrelevant to the correctness of the converged solution. (Patankar , 1980)

The step-by-step procedure for the SIMPLE algorithm is as follows :

1. Guess the pressure field P^*.
2. Solve the momentum equation , such as equations (A.28) - (A.30) , to obtain u^* , v^* , w^*.

3. Solve the pressure-correction equation (A.41) to obtain P'.
4. Calculate P from equation (A.31) by adding P' to P^*.
5. Calculate u , v , w from their starred values using the velocity-correction formulae (A.37) - (A.39).
6. Solve the discretization equation for other ϕ 's such as turbulence quantities.
7. Treat the corrected pressure P as a new guessed pressure P^* , return to step 2. , and repeat the whole procedure until a converged solution is obtained.

A.3 SOLUTION OF THE ALGEBRAIC EQUATIONS

The solution of the discretization equations for the one-dimensional situation can be obtained by the standard Gaussian-elimination method , because of the particularly simple form of the equations , this is sometimes called the *Thomas algorithm* or TDMA (*Tri**D*iagonal-*M*atrix *A*lgorithm).

For convenience in presenting the algorithm , it is necessary to use somewhat different nomenclature. Suppose the grid points were numbered 1 , 2 , 3 , ... , N , with points 1 and N denoting the boundary points. The discretization equations can be written as

$$L_i\phi_{i-1} + M_i\phi_i + U_i\phi_{i+1} = D_i \qquad \text{(A.43)}$$

for i = 1 , 2 , 3 , ... , N.

The designation TDMA refers to the fact that when the matrix of the coefficients of these equations is written , all the nonzero coefficients align themselves along three diagonals of the matrix. Consider a system of N linear , simultaneous algebraic equations with N unknowns , ϕ_1 , ϕ_2 , ϕ_3 , ... , ϕ_N , given in the form as belows.

$$M_1\phi_1 + U_1\phi_2 = D_1 \quad \text{(A.44a)}$$

$$L_2\phi_1 + M_2\phi_2 + U_2\phi_3 = D_2 \quad \text{(A.44b)}$$

$$L_3\phi_2 + M_3\phi_3 + U_3\phi_4 = D_3 \quad \text{(A.44c)}$$

$$\vdots$$

$$L_{N-1}\phi_{N-2} + M_{N-1}\phi_{N-1} + U_{N-1}\phi_N = D_{N-1} \quad \text{(A.44d)}$$

$$L_N\phi_{N-1} + M_N\phi_N = D_N \quad \text{(A.44e)}$$

This is a tridiagonal system , i.e., a system of equations with finite coefficients only on the main diagonal (the M_i's) , the lower diagonal (the L_i's) and the upper diagonal (the U_i's).

In summary of TDMA , this system will be changed at first into an upper bidiagonal form by dropping the first term in each equation (involving the L_i's) , replacing the coefficient of the main diagonal term by following equation.

$$M_i' = M_i - \frac{L_i U_{i-1}}{M_{i-1}'} \quad \text{(A.45)}$$

for i = 2 , 3 , ... , N.

And also replacing the right-hand side with following equation.

$$D'_i = D_i - \frac{L_i D'_{i-1}}{M'_{i-1}} \qquad (A.46)$$

for i = 2 , 3 , ... , N.

This results in the last equation in the system in having only one unknown , namely ϕ_N. Solve for ϕ_N from the equation below.

$$\phi_N = \frac{D'_N}{M'_N} \qquad (A.47)$$

Then , all other unknowns are found in sequence from the equation below.

$$\phi_i = \frac{D'_i - U_i \phi_{i+1}}{M'_i} \qquad (A.48)$$

Starting with $\phi_i = \phi_{N-1}$ and ending with $\phi_i = \phi_1$.

For solution of the multidimensional discretization equations , using *direct methods* such as TDMA for solving the algebraic equations in two- or three-dimensional problems are much more complicated and require rather large amounts of computer storage and time.

The alternative , then , is *iterative methods* for the solution of algebraic equations. These start from a guessed field of ϕ (the dependent variable) and use the algebraic equations in some manner to obtain an improved field. Successive repetitions of the algorithm finally lead to a solution that is sufficiently close to the correct solution of the algebraic equations. Iterative methods usually require very small additional storage in the computer.

The simplest of all iterative methods is the *Gauss-Seidel point-by-point method* in which the values of the variable are calculated by visiting each grid point in a certain order. Only one set of ϕ 's is held in computer storage. In the beginning , these represent the initial guess or values from the previous iteration.

As each grid point is visited , the corresponding value of ϕ in the computer storage is altered as follows : if the discretization equation is written as

$$a_P\phi_P = \sum a_{nb}\phi_{nb} + b \qquad \text{(A.49)}$$

then ϕ_P at the visited grid point is calculated from

$$\phi_P = \frac{\sum a_{nb}\phi^*_{nb} + b}{a_P} \qquad \text{(A.50)}$$

where ϕ^*_{nb} is the neighbor-point value in the computer storage.

For neighbors that have already been visited during the current iteration , ϕ^*_{nb} is the current value ; for yet-to-be-visited neighbors , ϕ^*_{nb} is the value from the previous iteration. In any case , ϕ^*_{nb} is the latest available value for the neighbor-point dependent variable. When all grid points have been visited in this manner , one iteration of the Gauss-Seidel method is complete.

However , a major disadvantage of the otherwise attractive Gauss-Seidel method is that its convergence is too slow , especially when a large number of grid points are involved. This is because the method transmits the boundary-condition information at a rate of one grid interval per iteration.

The convergence of the line-by-line method is faster , because the boundary-condition information from the ends of the line is transmitted *at once* to the interior of the domain , no matter how many grid points lie along the line.

APPENDIX B

COMPUTER CODE

```
TALK=T;RUN( 1, 1);VDU=VGAMOUSE
IRUNN   =        1 ;LIBREF =       0
************************************************************
 Group 1. Run Title
TEXT(3-BLADE , 30 DEGREE ANGLE                    )
************************************************************
 Group 2. Transience
STEADY  =    T
************************************************************
 Groups 3, 4, 5  Grid Information
   * Overall number of cells, RSET(M,NX,NY,NZ,tolerance)
RSET(M,5,30,50)
   * Set overall domain extent:
   *        xulast  yvlast  zwlast    name
XSI= 1.524E-01;YSI= 1.524E-01;ZSI= 7.620E+00;RSET(D,DUCT    )
************************************************************
 Group 6. Body-Fitted coordinates
BFC=T
   * Copy/Transfer/Block grid planes
GSET(T,K1,F,K10,1,5,1,30,5.85)
GSET(C,J24,F,J28,1,5,10,50,+,0,0,0,INC,1)
GSET(C,J14,F,J18,1,5,10,50,+,0,0,0,INC,1)
GSET(C,J4,F,J8,1,5,10,50,+,0,0,0,INC,1)
GSET(T,J4,F,J1,1,5,10,50,1)
GSET(T,J14,F,J4,1,5,10,50,1)
GSET(T,J24,F,J14,1,5,10,50,1)
GSET(T,J31,F,J24,1,5,10,50,1)
GSET(T,K5,F,K10,1,5,1,30,1)
GSET(T,K1,F,K5,1,5,1,30,3.63)
GSET(T,K51,F,K10,1,5,1,30,2.35)
GSET(T,J31,F,J1,1,5,15,50,1)
GSET(T,K15,F,K10,1,5,1,30,1)
GSET(T,K51,F,K15,1,5,1,30,1.83)
   **********
NONORT  =    T
   * X-cyclic boundaries switched
************************************************************
```

```
 Group 7. Variables: STOREd,SOLVEd,NAMEd
ONEPHS  =     T
   * Non-default variable names
NAME(45) =NPOR ; NAME(46) =ENUT
NAME(47) =WCRT ; NAME(48) =VCRT
NAME(49) =DEN1 ; NAME(50) =UCRT
   * Solved variables list
SOLVE(P1  ,U1  ,V1  ,W1  ,KE  ,EP  )
   * Stored variables list
STORE(UCRT,DEN1,VCRT,WCRT,ENUT,NPOR)
   * Additional solver options
SOLUTN(P1  ,Y,Y,Y,N,N,N)
SOLUTN(U1  ,Y,Y,N,N,N,N)
SOLUTN(V1  ,Y,Y,N,N,N,N)
SOLUTN(W1  ,Y,Y,N,N,N,N)
SOLUTN(KE  ,Y,Y,N,N,N,N)
SOLUTN(EP  ,Y,Y,N,N,N,N)
************************************************************
 Group 8. Terms & Devices
TERMS (P1  ,Y,Y,Y,N,Y,N)
TERMS (U1  ,Y,Y,Y,N,Y,N)
TERMS (V1  ,Y,Y,Y,N,Y,N)
TERMS (W1  ,Y,Y,Y,N,Y,N)
TERMS (KE  ,N,Y,Y,N,Y,N)
TERMS (EP  ,N,Y,Y,N,Y,N)
NEWENT  =     T
************************************************************
 Group 9. Properties
RHO1     = 1.185E+00
PRESS0   = 1.013E+05
CP1      = 1.005E+03
EL1      = GRND4
ENUL     = 1.555E-05 ;ENUT    = GRND3
PRT    (EP  ) =  1.314E+00
************************************************************
 Group 10.Inter-Phase Transfer Processes
************************************************************
 Group 11.Initialise Var/Porosity Fields
RESTRT(ALL)

CONPOR(PLT1     ,  0.00,NORTH ,-#1,-#1,-#1,-#1,-#2,-#2)

CONPOR(PLT2     ,  0.00,NORTH ,-#1,-#1,-#3,-#3,-#2,-#2)

CONPOR(PLT3     ,  0.00,NORTH ,-#1,-#1,-#5,-#5,-#2,-#2)

RSTGRD  =     F

INIADD  =     F
************************************************************
 Group 12. Convection and diffusion adjustments
************************************************************
```

```
 Group 13. Boundary & Special Sources

 PATCH (KESOURCE,PHASEM,1,NX,1,NY,1,NZ,1,LSTEP)
 COVAL (KESOURCE,KE   , GRND4     , GRND4     )
 COVAL (KESOURCE,EP   , GRND4     , GRND4     )

 INLET (BFCIN    ,LOW   ,#1,#1,#1,#7,#1,#1,#1,#1)
 VALUE (BFCIN    ,P1  , GRND1     )
 VALUE (BFCIN    ,U1  , GRND1     )
 VALUE (BFCIN    ,V1  , GRND1     )
 VALUE (BFCIN    ,W1  , GRND1     )
 VALUE (BFCIN    ,KE  , 2.000E-02)
 VALUE (BFCIN    ,EP  , 2.315E-01)
 VALUE (BFCIN    ,WCRT, 4.000E+00)
 VALUE (BFCIN    ,DEN1, 1.185E+00)

 PATCH (OUT      ,HIGH  ,#1,#1,#1,#7,#4,#4,#1,#1)
 COVAL (OUT      ,P1  , FIXVAL    , 0.000E+00)
 COVAL (OUT      ,KE  , 0.000E+00, SAME      )
 COVAL (OUT      ,EP  , 0.000E+00, SAME      )

 PATCH (WALL1    ,SWALL ,#1,#1,#1,#1,#1,#4,#1,#1)
 COVAL (WALL1    ,U1  , GRND2     , 0.000E+00)
 COVAL (WALL1    ,W1  , GRND2     , 0.000E+00)
 COVAL (WALL1    ,KE  , GRND2     , GRND2     )
 COVAL (WALL1    ,EP  , GRND2     , GRND2     )

 PATCH (WALL2    ,NWALL ,#1,#1,#7,#7,#1,#4,#1,#1)
 COVAL (WALL2    ,U1  , GRND2     , 0.000E+00)
 COVAL (WALL2    ,W1  , GRND2     , 0.000E+00)
 COVAL (WALL2    ,KE  , GRND2     , GRND2     )
 COVAL (WALL2    ,EP  , GRND2     , GRND2     )

 PATCH (WALL3    ,WWALL ,#1,#1,#1,#7,#1,#4,#1,#1)
 COVAL (WALL3    ,V1  , GRND2     , 0.000E+00)
 COVAL (WALL3    ,W1  , GRND2     , 0.000E+00)
 COVAL (WALL3    ,KE  , GRND2     , GRND2     )
 COVAL (WALL3    ,EP  , GRND2     , GRND2     )

 PATCH (WALL4    ,EWALL ,#1,#1,#1,#7,#1,#4,#1,#1)
 COVAL (WALL4    ,V1  , GRND2     , 0.000E+00)
 COVAL (WALL4    ,W1  , GRND2     , 0.000E+00)
 COVAL (WALL4    ,KE  , GRND2     , GRND2     )
 COVAL (WALL4    ,EP  , GRND2     , GRND2     )

BFCA     = 1.185E+00
************************************************************
 Group 14. Downstream Pressure For PARAB
************************************************************
 Group 15. Terminate Sweeps
LSWEEP   =    10000
SELREF   =      T
RESFAC   = 1.000E-06
************************************************************
```

```
 Group 16. Terminate Iterations
************************************************************
 Group 17. Relaxation
RELAX(P1  ,LINRLX, 3.000E-01)
RELAX(U1  ,LINRLX, 3.000E-01)
RELAX(V1  ,LINRLX, 3.000E-01)
RELAX(W1  ,LINRLX, 3.000E-01)
RELAX(KE  ,LINRLX, 3.000E-01)
RELAX(EP  ,LINRLX, 3.000E-01)
KELIN    =       0
************************************************************
 Group 18. Limits
************************************************************
 Group 19. EARTH Calls To GROUND Station
GENK     =    T
************************************************************
 Group 20. Preliminary Printout
ECHO     =    F
************************************************************
 Group 21. Print-out of Variables
OUTPUT(P1  ,N,N,N,N,N,N)
OUTPUT(U1  ,N,N,N,N,N,N)
OUTPUT(V1  ,N,N,N,N,N,N)
OUTPUT(KE  ,N,N,N,N,N,N)
OUTPUT(EP  ,N,N,N,N,N,N)
OUTPUT(NPOR,N,N,N,N,N,N)
OUTPUT(ENUT,N,N,N,N,N,N)
OUTPUT(WCRT,N,N,N,N,N,N)
OUTPUT(VCRT,N,N,N,N,N,N)
OUTPUT(DEN1,N,N,N,N,N,N)
OUTPUT(UCRT,N,N,N,N,N,N)
************************************************************
 Group 22. Monitor Print-Out
IXMON    =       3 ;IYMON    =      15 ;IZMON    =      45
TSTSWP   =      -1
************************************************************
 Group 23.Field Print-Out & Plot Control
NXPRIN   =       1
IXPRF    =       1 ;IXPRL    =       5
NYPRIN   =       1
IYPRF    =       1 ;IYPRL    =      30
NZPRIN   =       1
IZPRF    =       1 ;IZPRL    =      10
ITABL    =       1
  No PATCHes used for this Group
************************************************************
 Group 24. Dumps For Restarts
************************************************************
MENSAV(S,RELX,DEF,5.0800E-03,3,3.0000E-01)
MENSAV(S,PHSPROP,DEF,200,298,1.1850E+00,1.5550E-05)
MENSAV(S,FLPRP,DEF,K-E,CONSTANT,AIR-CONSTANT)
STOP
```

BIOGRAPHY

Mr. Santi Wattananusorn was born in Bangkok , Thailand , on September 23 , 1969. He attended the Kasetsart University. In 1988 and 1989 , he received the gold medaled-student awards and graduating in 1991 with a Bachelor of Chemistry Science Degree.