



## LANDMARK UNIVERSITY, OMU-ARAN

### LECTURE NOTE

COLLEGE: COLLEGE OF SCIENCE AND ENGINEERING

DEPARTMENT: MECHANICAL ENGINEERING

Course code: MCE521

Course title: ADVANCED COMPUTATIONAL DYNAMICS.

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### **CFD CLASS WORK EXAMPLES.**

#### Major symbols

$AE, AW, AN,$   
 $AS, AP, Sp, Ak$

Coefficients in Discretised Equations

$B$

Body Force (N/kg) or Spalding Number

$B_i$   
an

represent a buoyancy force, a centrifugal and/or Coriolis force,

electromagnetic force, etc. Sometimes,  $B_i$  may also  
represent resistance forces.

CC

Convergence criterion

$FC_i$

Fractional change

FCMX

Maximum fractional change

GS

Gauss–Seidel method

$h$

Enthalpy (J/kg) or Heat Transfer Coefficient (W/m<sup>2</sup>-K)

$k$

Thermal Conductivity (W/m-K)

$P$

Peclet Number

$p$

Pressure (N/m<sup>2</sup>)

$q$

Heat Flux (W/m<sup>2</sup>)

$q'''$ ,  $Q'''$

Internal Heat Generation Rates (W/m<sup>3</sup>)

$S$ ,  $Su$

Source Term

$Su_i$

represent viscous terms

$T$

Temperature (°C or K)

$t$	Time (s)
$u, v, w$	$x$ -, $y$ -, $z$ -Direction Velocities (m/s)
$u_i$	Velocity in $x_i$ , $i = 1, 2, 3$ Direction
$V$	Volume ( $m^3$ )
$\Delta V$	<i>Control volume</i>
$\alpha$	Under relaxation Factor or Thermal Diffusivity ( $m^2/s$ )
$\beta$	Under relaxation Factor for Pressure or Coefficient of Volume Expansion ( $K^{-1}$ )
$\Psi$	Stream Function or Weighting Factor
$\Phi$	General Variable or Dimensionless Enthalpy
$\Gamma$	General Exchange Coefficient = $\mu$ , $\rho D$ , or $k/C_p$
P, N, S, E, W	Refers to Grid Nodes
n, s, e, w	Refers to Cell Faces
eff	Refers to Effective Value
f	Refers to Cell Face
$l$	Iteration Counter
o	Old Time
$u, v$	Refers to Momentum Equations
IOCV	Integration over a Control Volume Method
TDMA	Tridiagonal Matrix Algorithm
TSE	Taylor Series Expansion Method

The potential of fundamental laws (in association with some further empirical laws) for generating widely applicable and scale-neutral information has been known almost ever since they were invented nearly 200 years ago. The realization of this potential (meaning the ability to solve the relevant differential equations), however, has been made possible only with the availability of computers. The past five decades have witnessed almost exponential growth in the speed with which arithmetic operations can be performed on a computer.

By way of reminder, we note that the three laws governing transport are the following:

1. The law of conservation of mass (transport of mass),
2. Newton's second law of motion (transport of momentum), and

3. The first law of thermodynamics. (transport of energy).

### Transport Equations

The aforementioned laws are applied to an infinitesimally small *control volume* located in a moving fluid. Here, it will suffice to mention that the law of conservation of mass is written for a single-component fluid or for a mixture of several species. When applied to a single species of the mixture, the law yields the equation of mass transfer when an empirical law, namely, Fick's law of mass diffusion

( $m_i'' = -\rho D \partial \omega / \partial x_i$ ), is invoked. Newton's second law of motion, combined with Stokes's stress laws, yields three momentum equations for velocity in directions  $x_j$  ( $j = 1, 2, 3$ ). Similarly, the first law of thermodynamics in conjunction with Fourier's law of heat conduction ( $q_{i,\text{cond}} = -K \partial T / \partial x_i$ ) yields the so-called energy equation for the transport of temperature  $T$  or enthalpy  $h$ . Using tensor notation, we can state these laws as follows:

### Conservation of Mass for the Mixture

$$\frac{\partial \rho_m}{\partial t} + \frac{\partial (\rho_m u_j)}{\partial x_j} = 0 \dots\dots\dots 1$$

### 1D Heat Conduction.

A wide variety of practical and interesting phenomena are governed by the 1D heat conduction equation. Heat transfer through a composite slab, radial heat transfer through a cylinder, and heat loss from a long and thin fin are typical examples. By 1D, we mean that the temperature is a function of only one space coordinate (say  $x$  or  $r$ ). This indeed is the case in steady-state problems. However, in unsteady state, the temperature is also a function of time. Thus, although there are two relevant independent variables (or dimensions), by convention, we refer to such problems as 1D *unsteady*-state problems. The extension *dimensional* thus always refers to the number of relevant space coordinates. The 1D heat conduction equation derived in the next section is equally applicable to some of the problems arising in *convective* heat transfer, in diffusion mass transfer, and in fluid mechanics, if the dependent and independent variables of the equation are appropriately interpreted. Our overall objective in this chapter is to develop a single computer program that is applicable to a wide variety of 1D problems.

### 1. 1D Conduction Equation.

Consider the 1D domain shown in Figure 1, in which the temperature varies only in the  $x$  direction although cross-sectional area  $A$  may vary with  $x$ . The temperature over the cross section is thus assumed to be uniform. We shall now invoke the first law of thermodynamics and apply it to a typical control volume of length  $\Delta x$ . The law states that (Rate of energy in) – (Rate of energy out) + (Rate of generation of energy) = (Rate of change of Internal energy), or

$$Q_x = Q_{x+\Delta x} + q''' A \Delta x = \frac{\partial}{\partial t} [\rho A \Delta x C T] \quad W, \dots\dots\dots 1$$

where  $q'''$  (W/m<sup>3</sup>) is the *volumetric* heat generation rate,  $C$  denotes specific heat (J/kg-K), and  $Q$  (W) represents the rate at which energy is conducted. Further, it is assumed that the control volume  $\Delta V = A(x) \times \Delta x$  does not change with time. Similarly, the density  $\rho$  is also assumed constant with respect to time but may vary with  $x$ . Therefore, dividing Equation 1 by  $\Delta V$ , we get

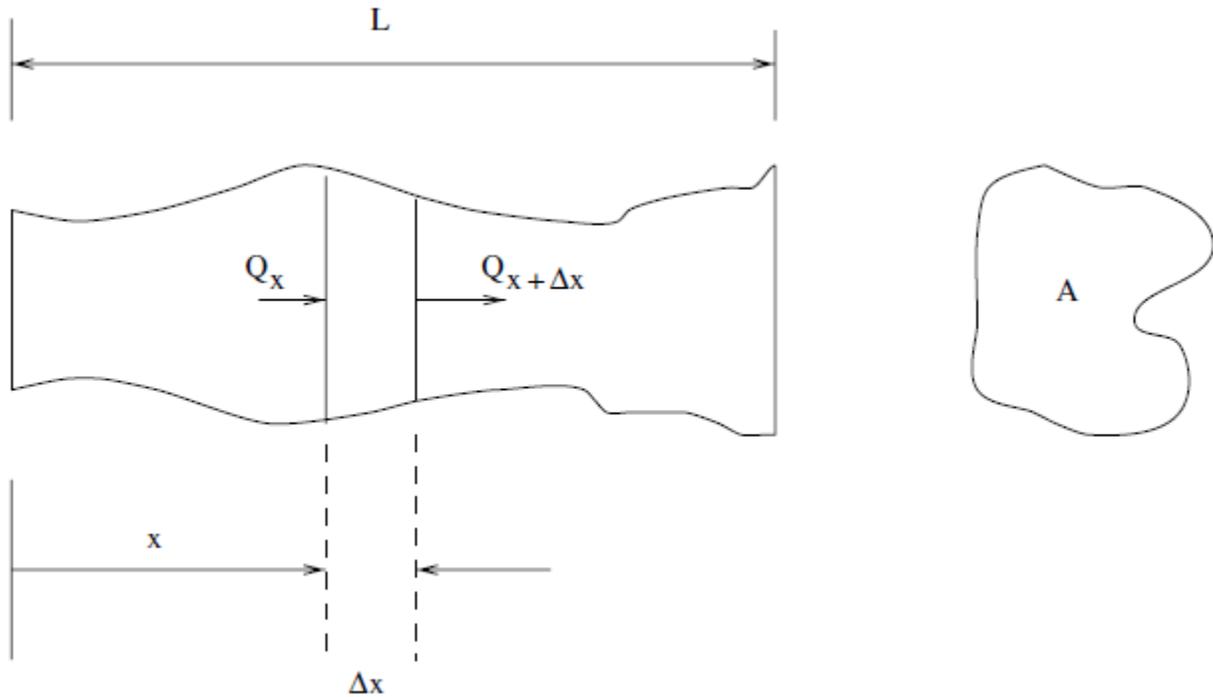


Figure 1. Typical 1D domain.

$$\frac{Q_x - Q_{x+\Delta x}}{A \Delta x} + q''' = \rho \frac{\partial(C T)}{\partial t}. \dots\dots\dots 2$$

Now, letting  $\Delta x \rightarrow 0$ , we obtain

$$-\frac{1}{A} \frac{\partial Q}{\partial x} + q''' = \rho \frac{\partial(C T)}{\partial t}. \dots\dots\dots 3$$

This partial differential equation contains two dependent variables,  $Q$  and  $T$ . The equation is rendered solvable by invoking Fourier's law of heat conduction. Thus,

$$Q = -kA \frac{\partial T}{\partial x}, \quad \dots\dots\dots 4$$

Where  $k$  is the thermal conductivity of the domain medium. Substituting Equation 4 in Equation 3 therefore yields

$$\frac{\partial}{\partial x} \left[ kA \frac{\partial T}{\partial x} \right] + q''' A = \rho A \frac{\partial (CT)}{\partial t}. \quad \dots\dots\dots 5$$

It will be instructive to make the following comments about Equation 5.

1. The equation is most general. It permits variation of medium properties  $\rho$ ,  $k$ , and  $C$  with respect to  $x$  and/or  $t$ .
2. The equation permits variation of cross-sectional area  $A$  with  $x$ . Thus, the equation is applicable to the case of a conical fin, for example. Similarly, the equation is also applicable to the case of cylindrical radial conduction if it is recognized that  $A = 2 \times \pi \times r$ , and if  $x$  is replaced by  $r$ .
3. The equation also permits variation of  $q'''$  with  $T$  or  $x$ . Thus, if an electric current is passed through the medium,  $q'''$  will be a function of electrical resistance and the latter will be a function of  $T$ . Similarly, in case of a fin losing heat to the surroundings due to convection,  $q'''$  will be negative and it will be a function of the heat transfer coefficient  $h$  and perimeter  $P$ .
4. Equation 5 is to be solved for boundary conditions at  $x = 0$  and  $x = L$  (say). Thus,  $0 \leq x \leq L$  specifies the domain of interest.

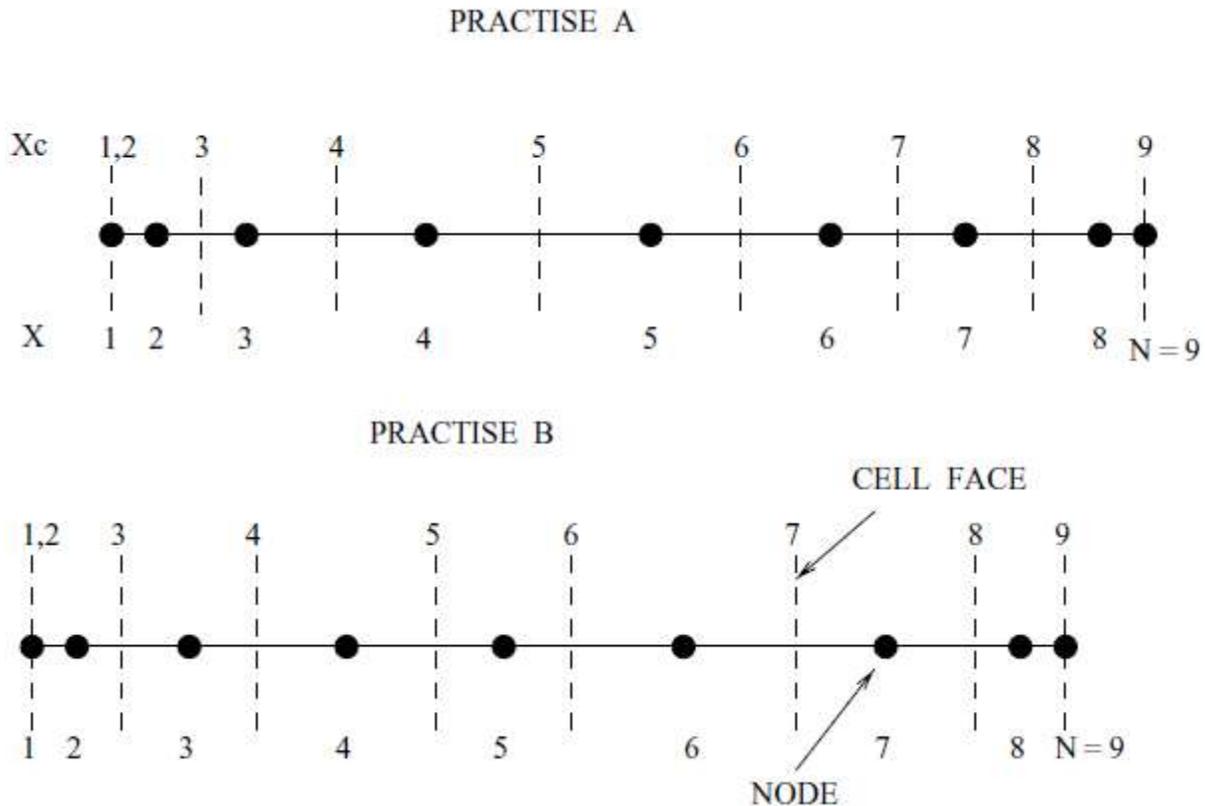
## 2. Grid Layout

Unlike analytical solutions, numerical solutions are obtained at a few *chosen points* within the domain. They are therefore called *discrete* solutions. Numerical solutions are obtained by employing numerical methods. The latter are really an intermediary between the physics embodied in the transport equations and the computers that can unravel them by generating numerical solutions. The process of arriving at numerical solutions is thus quite different from the process by which analytical solutions are developed. Before describing the essence of numerical methods, it is important to note that these methods, in principle, can overcome all three aforementioned impediments to obtaining analytical solutions. In fact, the history of CFD shows that numerical methods have been evolved precisely to overcome the impediments in the order of their mention. Selection of coordinates of such points (also called nodes) is called grid layout. Two practises are possible (see Figure 2).

### Practise A

In this practise, the locations of nodes (shown by filled circles) are first chosen and then numbered from 1 to  $N$ . Note that the chosen locations need not be equispaced. Now the control

volume faces (also called the cell faces) are placed *midway* between the nodes. When this is done, a difficulty arises at the near boundary nodes 2 and  $N - 1$ . For these nodes, the cell face to the west of node 2 is assumed to *coincide* with node 1 and, similarly, the cell face to the east of node  $N - 1$  is assumed to coincide with node  $N$ . As such, there is no cell face between nodes 1 and 2, nor between nodes  $N - 1$  and  $N$ . The space between the adjacent cell faces defines the *control volume*. In this practise therefore the nodes, in general, will not be at the *centre* of their respective control volumes. Also note that if  $N$  nodes are chosen, then there are  $N - 2$  control volumes.



**Figure 2: Grid layout practices.**

### Practise B

In this practise, the location of cell faces is first chosen and then the grid nodes are placed *at the centre* of the control volumes thus formed. Note again that the chosen locations of the cell faces need not be equi-spaced. Both practises have their advantages and disadvantages that become apparent only as one encounters multidimensional situations. Yet, a choice must be made. In this lecture, much of the discussion is carried out using practise A, but it will be shown that a generalized code can be written to accommodate either practise.

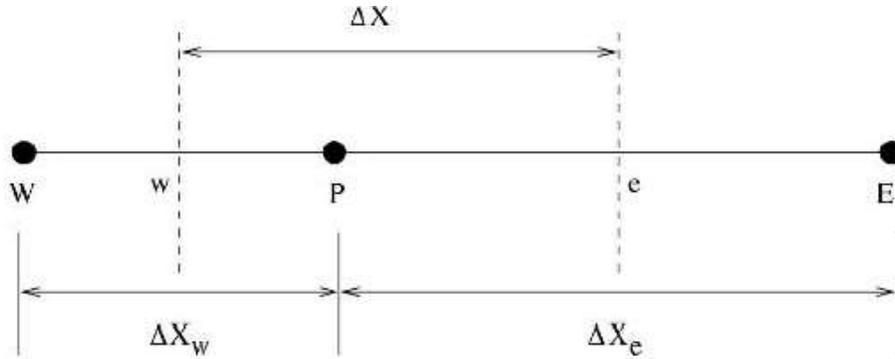


Figure 3. Typical node P – Practise A.

### 3. Discretisation

Having chosen the grid layout, our next step is to convert the PDE (5) to an algebraic one. This process of conversion is called discretisation. Here again, there are two possible approaches:

1. a Taylor series expansion (TSE) method or
2. an integration over a control volume (IOCV) method.

In both methods, a typical node P is chosen along with nodes E and W to east and west of P, respectively (see Figure 3). The cell face at *e* is midway between P and E, likewise, the cell face at *w* is midway between P and W. Before describing these methods, it is important to note an important aspect of discretisation. Equation 5 is a partial differential equation. The time derivative on the right-hand side (RHS), therefore, must be evaluated at a fixed *x*. We choose this fixed location to be node P. The left-hand side (LHS) of Equation 5, however, contains a partial second derivative with respect to *x* and, therefore, this derivative must be evaluated at a fixed time. The choice of this fixed time, however, is not so straightforward because over a time step  $\Delta t$ , one may evaluate the LHS at time *t*, or *t* +  $\Delta t$ , or at an intermediate time between *t* and *t* +  $\Delta t$ . In general, therefore, we may write Equation 5 as

$$\psi (LHS)_P^n + (1 - \psi)(LHS)_P^o = RHS|_P \dots\dots\dots 6$$

where  $\psi$  is a weighting factor, superscript n refers to the new time *t* +  $\Delta t$ , and superscript o refers to the old time *t*. If we choose  $\psi = 1$  then the discretisation is called *implicit*, if  $\psi = 0$  then it is called *explicit*, and if  $0 < \psi < 1$ , it is called *semiimplicit* or *semi-explicit*. Each choice has a bearing on economy and convenience with which a numerical solution is obtained. The choice of  $\psi$  is therefore made by the numerical analyst depending on the problem at hand. The main issues involved will become apparent following further developments.

#### 3.1 TSE Method

To employ this method, Equation 5 is first written in a *non-conservative* form. Thus,

$$\text{LHS}|_P = kA \frac{\partial^2 T}{\partial x^2} + \frac{\partial(kA)}{\partial x} \frac{\partial T}{\partial x} + q''' A, \quad \dots\dots\dots 7$$

$$\text{RHS}|_P = \rho A \frac{\partial(C T)}{\partial t}. \quad \dots\dots\dots 8$$

Equation 7 contains first and second derivatives of  $T$  with respect to  $x$ . To represent these derivatives we employ a Taylor series expansion:

$$T_E = T_P + \Delta x_e \left. \frac{\partial T}{\partial x} \right|_P + \frac{\Delta x_e^2}{2} \left. \frac{\partial^2 T}{\partial x^2} \right|_P + \dots, \quad \dots\dots\dots 9$$

$$T_W = T_P - \Delta x_w \left. \frac{\partial T}{\partial x} \right|_P + \frac{\Delta x_w^2}{2} \left. \frac{\partial^2 T}{\partial x^2} \right|_P + \dots. \quad \dots\dots\dots 10$$

From these two expressions, it is easy to show that

$$\left. \frac{\partial T}{\partial x} \right|_P = \frac{\Delta x_w^2 T_E - \Delta x_e^2 T_W + (\Delta x_e^2 - \Delta x_w^2) T_P}{\Delta x_e \Delta x_w (\Delta x_e + \Delta x_w)}, \quad \dots\dots\dots 11$$

$$\left. \frac{\partial^2 T}{\partial x^2} \right|_P = \frac{\Delta x_w T_E + \Delta x_e T_W - (\Delta x_e + \Delta x_w) T_P}{\Delta x_e \Delta x_w (\Delta x_e + \Delta x_w)/2}. \quad \dots\dots\dots 12$$

Note that, in Equations 9 and 10, terms involving derivative orders greater than 2 are ignored. Therefore, Equations 11 and 12 are called second-order accurate representations of first- and second-order derivatives with respect to  $x$ .

Now to evaluate the time derivative, we write,

$$(C T)_P^n = (C T)_P^o + \Delta t \left. \frac{\partial(C T)}{\partial t} \right|_P + \dots, \quad \dots\dots\dots 13$$

or

$$\left. \frac{\partial(C T)}{\partial t} \right|_P = \frac{(C T)_P^n - (C T)_P^o}{\Delta t}. \quad \dots\dots\dots 14$$

In Equation 13, derivatives of order higher than 1 are ignored; therefore, Equation 14 is only a first-order-accurate representation of the time derivative. Inserting Equations 11 and 12 in Equation 7 and Equation 14 in Equation 8 and employing Equation 6, we can show that

$$\left[ \frac{\rho \Delta V C^n}{\Delta t} \Big|_P + \psi (AE + AW) \right] T_P^n = \psi [AE T_E^n + AW T_W^n] + S, \quad ..15$$

with

$$AE = \frac{2}{\Delta x_e} \left[ (kA)_P + \frac{\Delta x_w}{2} \frac{d(kA)}{dx} \Big|_P \right] \frac{\Delta x}{(\Delta x_e + \Delta x_w)}, \quad \dots\dots\dots 16$$

$$AW = \frac{2}{\Delta x_w} \left[ (kA)_P - \frac{\Delta x_e}{2} \frac{d(kA)}{dx} \Big|_P \right] \frac{\Delta x}{(\Delta x_e + \Delta x_w)}, \quad \dots\dots\dots 17$$

$$S = [\psi q_P'''^n + (1 - \psi) q_P'''^o] \Delta V + (1 - \psi) [AE T_E^o + AW T_W^o] + \left[ \frac{\rho \Delta V C^o}{\Delta t} \Big|_P - (1 - \psi)(AE + AW) \right] T_P^o, \quad \dots\dots\dots 18$$

Where  $\Delta V = A \Delta x$ . Note that if the cell faces were midway between adjacent nodes,  $2 \Delta x = \Delta x_e + \Delta x_w$ . Before leaving the discussion of the TSE method, we make the following observations:

1. Calculation of coefficients  $AE$  and  $AW$  requires evaluation of the derivative  $d(kA)/dx|_P$ . This derivative can be evaluated using expressions such as (11) in which  $T$  is replaced by  $kA$ .
2. For certain variations of  $(kA)$  and choices of  $\Delta x_e$  and  $\Delta x_w$ ,  $AE$  and/or  $AW$  can become negative.
3. For certain choices of  $\Delta t$ , the multiplier of  $T_P^o$  in Equation 18 can become negative.
4. In steady-state problems,  $\Delta t = \infty$  and  $T^o$  has no meaning. Therefore, in such problems,  $\psi$  always equals 1.

### 3.2 IOCV Method

In this method, the RHS and LHS of Equation 5 are *integrated* over a control volume  $\Delta x$  and over a time step  $\Delta t$ . Thus,

$$\text{Int(LHS)} = \int_t^{t'} \int_w^e \frac{\partial}{\partial x} \left[ kA \frac{\partial T}{\partial x} \right] dx dt + \int_t^{t'} \int_w^e q''' A dx dt, \quad .. 19$$

Where  $t' = t + \Delta t$ . It is now *assumed* that the integrands are constant over the time interval  $\Delta t$ . Further,  $q'''$  is assumed constant over the control volume and since the second-order derivative is evaluated at a fixed time, we may write

$$\text{Int(LHS)} = \left[ kA \frac{\partial T}{\partial x} \Big|_e - kA \frac{\partial T}{\partial x} \Big|_w \right] \Delta t + q_P''' A \Delta x \Delta t. \dots\dots\dots 20$$

It is further assumed that  $T$  varies *linearly* with  $x$  between adjacent nodes. Then

$$\frac{\partial T}{\partial x} \Big|_e = \frac{T_E - T_P}{\Delta x_e}, \quad \frac{\partial T}{\partial x} \Big|_w = \frac{T_P - T_W}{\Delta x_w}. \dots\dots\dots 21$$

Note that when the cell faces are midway between the nodes, these representations of the derivatives are second-order accurate (see Equation 11). Using Equation 21 therefore gives

$$\begin{aligned} \text{Int(LHS)} = & \left[ \frac{kA}{\Delta x} \Big|_e (T_E - T_P) + \frac{kA}{\Delta x} \Big|_w (T_W - T_P) \right] \Delta t \\ & + q_P''' A \Delta x \Delta t. \dots\dots\dots 22 \end{aligned}$$

Similarly,

$$\begin{aligned} \text{Int(RHS)} = & \rho A \int_t^{t'} \int_w^e \frac{\partial(C T)}{\partial t} dx dt \\ = & (\rho A \Delta x)_P [(C T)^n - (C T)^o]_P. \dots\dots\dots 23 \end{aligned}$$

Substituting Equations 22 and 23 into the integrated version of Equation 6, therefore, we can show that

$$\left[ \frac{\rho \Delta V C^n}{\Delta t} \Big|_P + \psi (AE + AW) \right] T_P^n = \psi [AE T_E^n + AW T_W^n] + S, \dots\dots\dots 24$$

Where

$$AE = \frac{kA}{\Delta x} \Big|_e \dots\dots\dots 25$$

$$AW = \frac{kA}{\Delta x} \Big|_w \dots\dots\dots 26$$

$$S = [\psi q_P'''^{,n} + (1 - \psi) q_P'''^{,o}] \Delta V + (1 - \psi) [AE T_E^o + AW T_W^o] + \left[ \frac{\rho \Delta V C^o}{\Delta t} \Big|_P - (1 - \psi)(AE + AW) \right] T_P^o. \dots\dots\dots 27$$

Note that Equation 24 has the same form as Equation 15, but there are important differences:

1. Coefficients  $AE$  and  $AW$  can never be negative since  $kA/\Delta x$  can only assume positive values.
2.  $AE$  and  $AW$  are also amenable to physical interpretation; they represent conductances.
3. Again, in steady-state problems,  $\psi = 1$  because  $t = \infty$ . In unsteady problems, for certain choices of  $\Delta t$ , however, the multiplier of  $T_P^o$  can still be negative. This observation is in common with the TSE method.

### 3.3 Stability and Convergence

Before discussing the issues of stability and convergence, we recognize that there will be one equation of the type (24) [or (15)] for each node  $P$ . To minimize writing, we designate each node by a running index  $i = 1, 2, 3, \dots, N$ , where  $i = 1$  and  $i = N$  are boundary nodes. Thus, Equations 24 are written as

$$AP_i T_i = \psi [AE_i T_{i+1} + AW_i T_{i-1}] + S_i, \quad i = 2, 3, \dots, N - 1, \dots 28$$

Where superscript  $n$  is now dropped for convenience. In these equations,  $AP_i$  represents multiplier of  $T_P$  in Equation 24. It will be shown later that this equation set can be written in a matrix form  $[A][T]=[S]$ , where  $[A]$  is the coefficient matrix and  $[T]$  and  $[S]$  are column vectors. This set can be solved by a variety of *direct* and *iterative* methods. The methods yield *converged* solutions only when the condition for convergence (also known as Scarborough's criterion is satisfied) is satisfied. To put it simply, the criterion states that,

#### Condition for Convergence

$$\frac{\psi [ |AE_i| + |AW_i| ]}{|AP_i|} \leq 1 \quad \text{for all nodes, } \dots\dots 29$$

$$\frac{\psi [ |AE_i| + |AW_i| ]}{|AP_i|} < 1 \quad \text{for at least one node. .... 30}$$

### 3.4 Explicit Procedure $\psi = 0$

In this case, Equation 28 will read as

$$\left[ \frac{\rho \Delta V_i C_i^n}{\Delta t} \right] T_i = AE_i T_{i+1}^o + AW_i T_{i-1}^o + q_i^{''' , o} A_i \Delta x + \left[ \frac{\rho \Delta V_i C_i^o}{\Delta t} - (AE_i + AW_i) \right] T_i^o. \quad \text{..... 31}$$

Equation 31 shows that the values of  $T_i$  at a new time step are now calculable explicitly in terms of values  $T_{i-1}^o$ ,  $T_i^o$ , and  $T_{i+1}^o$ . Terms containing  $T_{i+1}$  and  $T_{i-1}$  do not appear on the RHS. Therefore, the equation is explicit and no iterations are required. This situation is also depicted in Figure 4. Thus, starting with known initial temperature distribution at  $t = 0$ , one can evaluate temperatures at each new time step. Such a solution procedure is called a *marching* solution procedure. It is very easy to devise computer code for a marching procedure. In an explicit procedure, the issue of convergence is irrelevant but the stability of the calculation procedure requires that the coefficient of  $T_i^o$  always be positive. From Equation 31 it is clear that this requirement is satisfied when

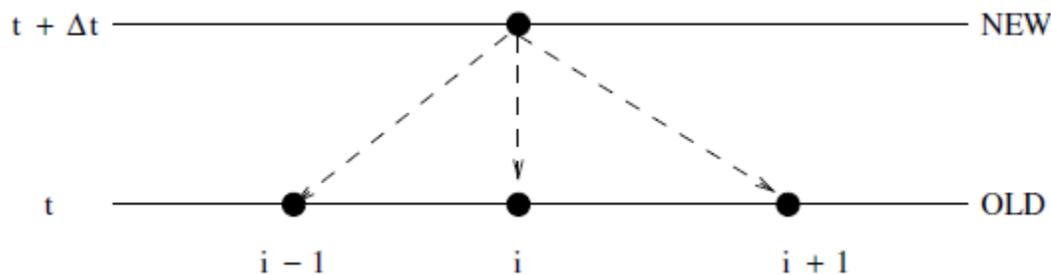


Figure 4. Explicit procedure.

$$\Delta t < \left[ \frac{\rho \Delta V_i C_i^o}{AE_i + AW_i} \right]_{\min} \quad \text{..... 32}$$

Note,

This condition of positiveness is strictly meant for the case of  $\psi = 0$ . For  $\psi = 1$ , the condition is automatically satisfied. For  $0 < \psi < 1$ , however, the condition again holds but can be violated without impairing stability of the solution procedure.

