CHAPTER 4

MATHEMATICAL MODELING AND SIMULATION OF RAPID EXPANSION OF SUPERCRITICAL CARBON DIOXIDE

4.1 CFD modeling

The physical aspects of transport phenomena in the macro-scale are governed by Newton's laws of motion and the fundamental principles of mass, energy and species of conservation. Depending on the nature of the problem and the quantities of interest, these fundamental principles can be expressed in terms of algebraic equations, ordinary/partial differential equations or integral representations. Numerical simulation is by and large the technique of replacing the governing transport equations with algebraic equations and obtaining a final numerical description of the phenomenon in space and/or time domain. Irrespective of the nature of the problem, numerical simulation involves the manipulation and solution of numbers, leaving behind an end product, which is also a collection of numbers. This is in contrast to the symbolic expression of closed form analytical solution. The objective of investigations is to obtain a quantitative description of the problem, in terms of numbers. In this regard, numerical simulation techniques provide readily acceptable and often the most descriptive form of solutions to a variety of transport problems. Numerical simulation of practical problems generally involves the repetitive manipulation of thousands, or even millions, of calculation which is feasible only with the aid of a computer.

The Numerical simulation, Computational Fluid Dynamics or CFD, is the analysis of systems with fluid flow, heat transfer and associated phenomena such as chemical reactions by means of computer-based simulation. The technique is very powerful and covers a wide range of industrial and non-industrial applications. For examples,

- Aerodynamics of aircraft and vehicles : lift and drag
- Hydrodynamics of ships
- Power plant : combustion in IC engines and gas turbines
- Chemical process : mixing and separation
- Environmental engineering : distribution of pollutant and effluents

Moreover, it is possible to study existing system more quickly, economically and thoroughly than in the real system. Furthermore, with a suitable mathematical representation, it is possible to test extreme ranges of operating conditions, some of which might be impractical or unsafe to test in a real process.

4.2 Governing Equation

The governing two-dimensional equations for the rapid expansion of supercritical carbon dioxide are:

a) Equation of continuity

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho v)}{\partial y} + \frac{\partial (\rho w)}{\partial z} = 0 \qquad (4.1)$$

b) Momentum equation: Euler equations

y-component (horizontal direction)

$$\frac{\partial (\rho v)}{\partial t} + \frac{\partial}{\partial y}\left(\rho v^2 + p\right) + \frac{\partial}{\partial z}(\rho v w) = 0 \qquad (4.2)$$

z-component (vertical direction)

$$\frac{\partial (\rho w)}{\partial t} + \frac{\partial}{\partial y}(\rho v w) + \frac{\partial}{\partial z}\left(\rho w^2 + p\right) = 0 \qquad (4.3)$$

c) Equation of Energy

$$\frac{\partial E_t}{\partial t} + \frac{\partial}{\partial y}\left[(E_t + p)v + q_y\right] + \frac{\partial}{\partial z}\left[(E_t + p)w + q_z\right] = 0 \qquad (4.4)$$

Where

$$E_t = \rho\left(e + \frac{X^2}{2}\right) \tag{4.5}$$

$$\mathrm{Pr} = \frac{\mu Cp}{k} \tag{4.6}$$

$$q_y = -k\frac{\partial T}{\partial y} \tag{4.7}$$

$$q_z = -k\frac{\partial T}{\partial z} \tag{4.8}$$

$$e = CvT \tag{4.9}$$

$$X = \sqrt{v^2 + w^2} \tag{4.10}$$

$$k = \frac{\mu Cp}{\mathrm{Pr}} \tag{4.11}$$

$$p = \rho RT \tag{4.12}$$

$$\mu = \mu_{ref}\left(\frac{T}{T_{ref}}\right)^{\frac{3}{2}}\frac{T_{ref} + 110}{T + 110} \tag{4.13}$$

4.3 Numerical Approach

In this study an advanced explicit finite difference technique and implicit finite difference technique are used for comparing the result of each technique. An advanced explicit finite difference technique, namely the MacCormack's method, which is accurate up to second order of both space and time are used. For implicit technique, the current numerical method in computational fluid dynamics uses predictor–corrector types of algorithm because it allows a higher degree of accuracy with large time step.

4.3.1 Explicit and Implicit Approaches: Definitions and Contrasts

To solve the problem of flow field of a fluid in a specific domain, the technique that is used will fall into one or other of two different general approaches namely, an explicit approach or implicit approach.

Explicit

- Definition: each different equation contains only one unknown and therefore can be solved explicitly for this unknown in a straightforward manner.
- Advantage: relatively simple to set up and program.
- Disadvantage: the given Δx, Δt must be less than some limit imposed by stability constraints. In some cases Δt must be very small to maintain stability; this can result in long computer running times to make calculations over a given interval of t.

Implicit

- Definition: the unknown must be obtained by means of a simultaneous solution of the difference equations applied at all the grid points arrayed at the given time level.
- Advantage: stability can be maintain over much larger values of Δt, hence using considerable fewer time step to make calculations over a given interval of t. This results in less computer time.
- Disadvantage: more complicated to set up and program.
- Disadvantage: since massive matrix manipulations are usually required at each time step, the computer time per time step is much larger than in the explicit approach.

4.3.2 Explicit Finite Difference Method

In a slightly different form, all equations are rearranged into the following vector equations:

$$\frac{\partial U}{\partial t} + \frac{\partial E}{\partial y} + \frac{\partial F}{\partial z} = 0 \qquad (4.14)$$

Where U, E, and F are column vectors given by

d. At the Initial stage, atmospheric stability bed is stable.

e. The fluid flow is assumed to be non-isothermal and compressible.

f. The effects of inlet temperature, inlet-pressure and inlet-velocity on rapid expansion of supercritical carbon dioxide, especially near the nozzle area are simulated.

g. The two-dimensional rectangular coordinate is used.

h. A calorically-perfect fluid is assumed.

4.3.2.3 Algorithm of the explicit model

The basic idea behind the dynamic simulation is simply to model the given system by means of the mathematical equations, and then to determine its time-dependent behavior. The simplicity of the approach when combined with the computational power of a high-speed computer makes the simulation a powerful tool.

In this section the simulation algorithm for determination of the velocity profile, the temperature and pressure profile of rapid expansion of supercritical carbon dioxide, especially near the nozzle area, are presented and their simplified flow charts are illustrated in Figures 4.2 through 4.6. The simulation is carried out according to the following steps:

1. The grid size, maximum time step and basic properties of the flow as well as the required iteration number are specified.
2. Input all essential constant values for this algorithm, such as specific gas constant for CO_2 and C_p/C_v.
3. Calculate the density of fluid with the Equation of State (EOS), namely Soave Redlich-Kwong. This is done inside a subroutine called EOS where the initial pressure and temperature, which are, at the start, identical at all locations inside the system, are used to calculate the volume and, then, the gas density.

4. The initial temperature, y- and z-axis velocity, density and pressure inside the system are input as the fluid data at time 't'.
5. In the first iteration, parameters, i.e. temperature, y- and z-axis velocity, density and pressure in each individual point of the system, are read. At the boundary of the system, the velocities are set at zero. Regardless of the position, temperature, pressure, and density are equal to the initial T0, P0, and density are calculated through EOS, respectively.
6. With the Sutherland's law, the loop named the DYNVIS begins as follows:
   6.1 The number of cells inside the system both in the y- and z-axis are read.
   6.2 The reference temperature and viscosity are read and applied as constant values.
   6.3 For each individual location inside the system, the temperature is used to evaluate the viscosity according to the Sutherland's law.
   6.4 The temperature and viscosity at time 't' are recorded for use in the THERMC subroutine.
7. In the THERMC subroutine, conductivity of the fluid is calculated using the Prandtl number. The steps are as follows:
   7.1 The number of cells inside the system both in the y- and z-axis and the required iteration number are read.
   7.2 The C_p/C_v and Prandtl numbers are referred to as constants.
   7.3 The temperature and viscosity are recalled for each individual point inside the system.
   7.4 For each individual location inside the system, the heat capacity of the fuid is computed and recorded.
   7.5 Then, the thermal conductivity of the fluid in every single location at time 't' is computed through the Prandtl number.
8. The MacCormack's technique is applied for calculation of the fluid movement. The subroutine named "Mac" uses the balance of mass,

momentum and energy to calculate various properties of the fluid such as fluid velocity.

8.1 The number of cells inside the system both in the y- and z-axis and the required iteration number are read.

8.2 Various constants, composed of the time step, y- and z-axis grid size, Prandtl number, gas constant, initial velocity, reference viscosity, C_p/C_v, inlet temperature and pressure, are read.

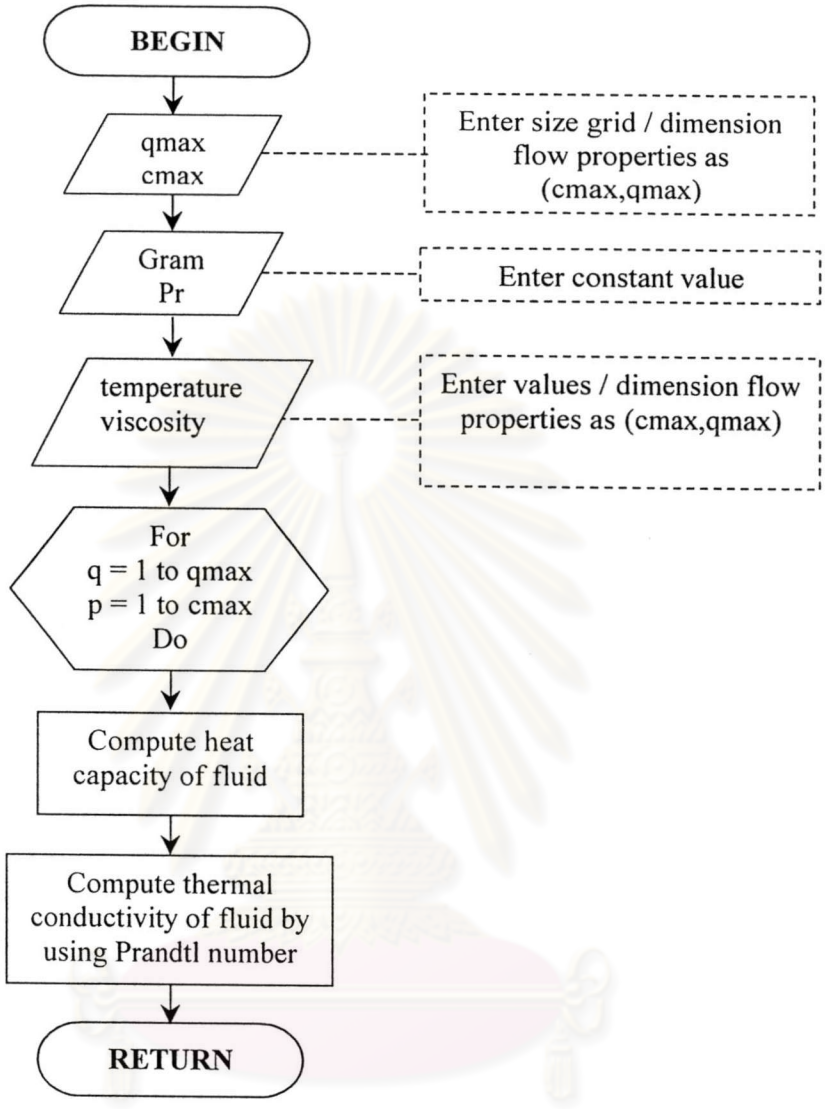
8.3 For each individual point inside the system at time 't', the characteristics of the fluid, including temperature, y- and z-axis velocity, thermal conductivity, density, pressure and heat capacity, are recalled.

8.4 The balance of mass, momentum and energy is then calculated through a set of matrixes to determine the temperature, y- and z-axis velocity, fluid density and pressure of all locations inside the system at time '$t + \Delta t$'.

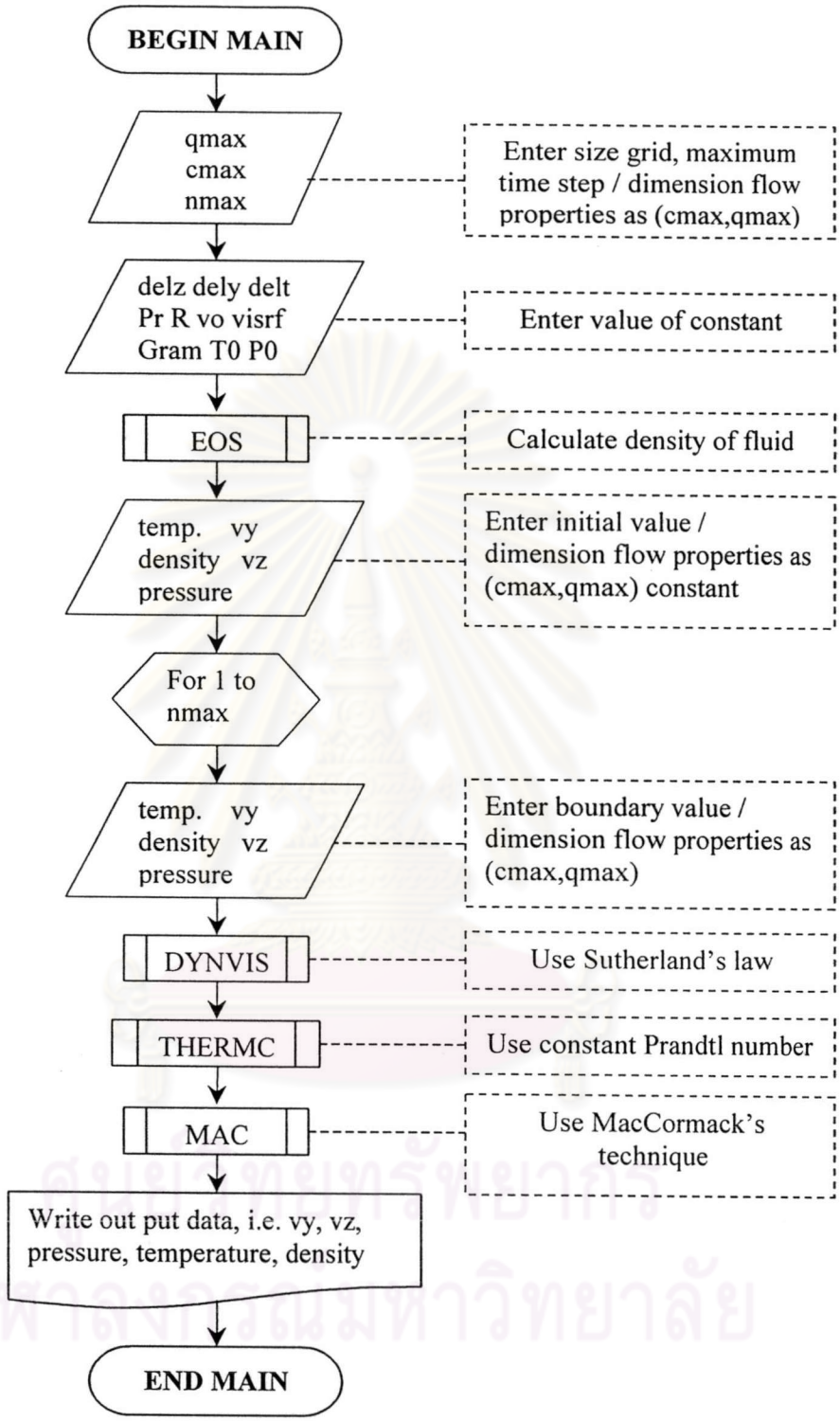
9. Show the results at time '$t + \Delta t$'.

10. Then, go back to (6) and do the next iteration, using the updated values of temperature, y- and z-axis velocity, fluid density and pressure for calculation. Repeat until the iteration number is equal to the required iteration number specified in (1).

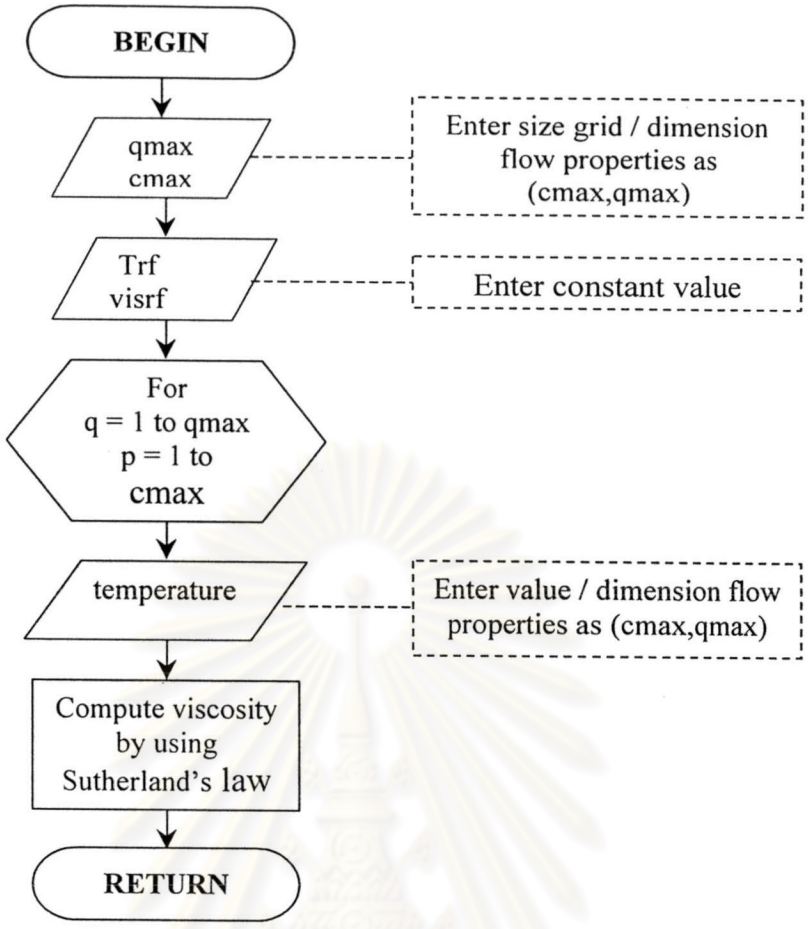
11. The final results are shown at the end of program.



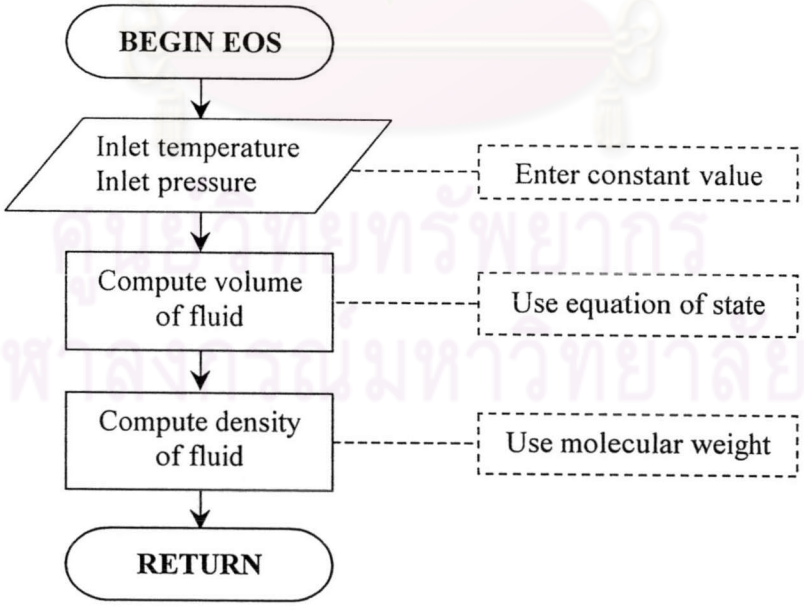
Figures 4.2 Block diagram of computation viscosity by using Prandtl number



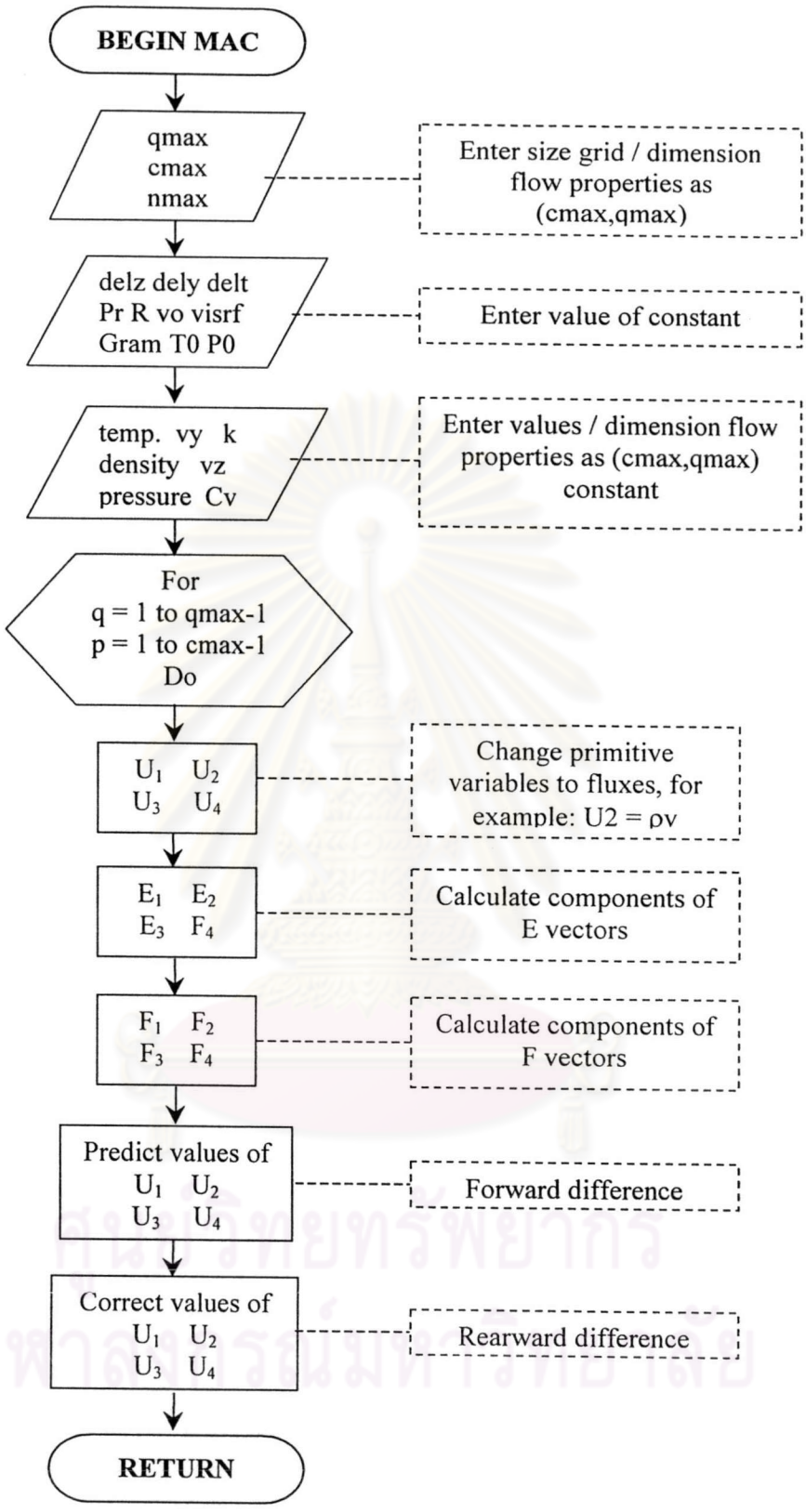
Figures 4.3 Block diagram simulation of rapid expansion of supercritical carbon dioxid by explicit finite difference technique



Figures 4.4 Block diagram of computation viscosity by using Sutherland's law



Figures 4.5 Block diagram of Equation of State



Figures 4.6 Block diagram of MacCormack's technique

4.3.3 Implicit Finite Difference Method

4.3.3.1 The numerical Method

The implicit finite-difference method is widely used to solve fluid flow problems because it allows a higher degree of accuracy with large time step. Two momentum equations, one continuity equation, a two-dimensional energy equation and equation of state are solved. The conventional staggered-grid formalism is used, which means that momentum fluxes are defined at node interfaces, whereas scalar variables, such as temperature, density, and pressure are defined at node center.

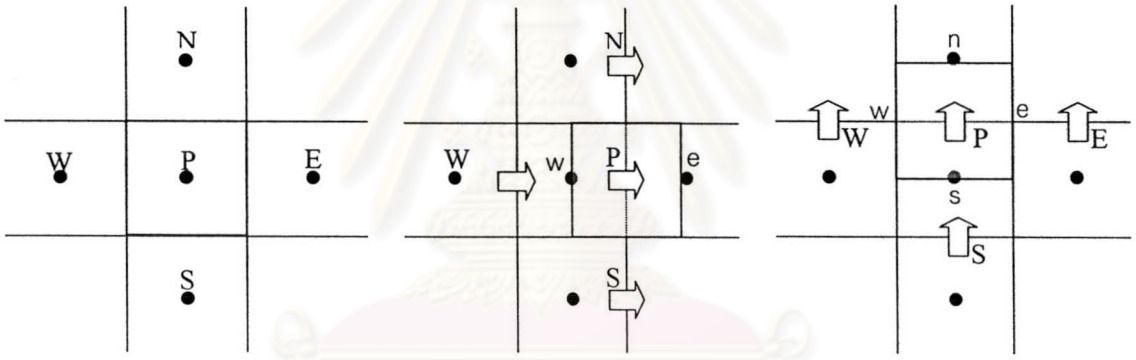


Figure 4.7 Control volume for scalar variables (left),
y-direction velocity (middle)
z-direction velocity (right)

Continuity equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho v)}{\partial y} + \frac{\partial (\rho w)}{\partial z} = 0$$

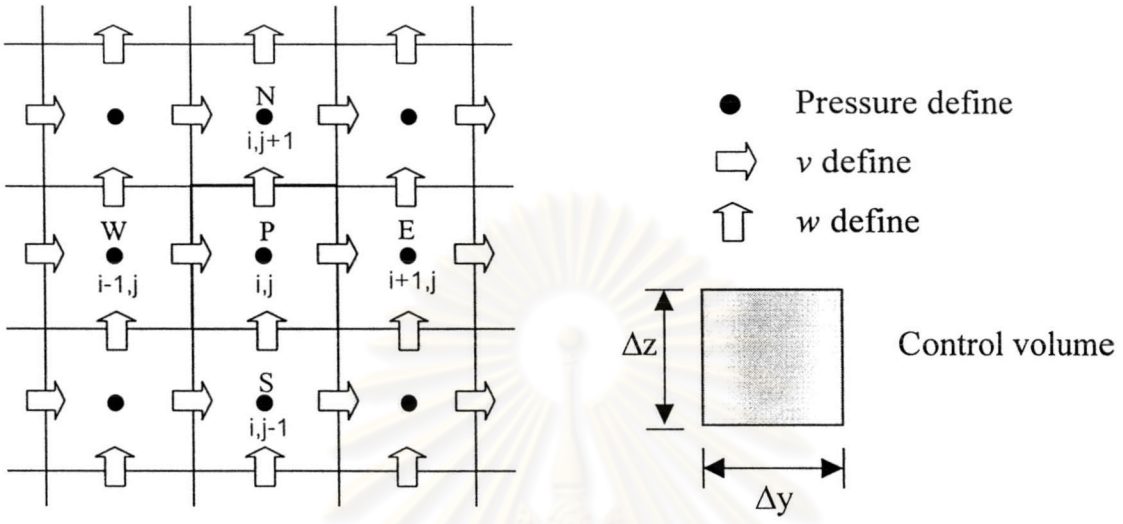


Figure 4.8 Control volume for continuity equation

Integrate the continuity equation in the control volume with provide

$$\int_{t}^{t+\Delta t} \frac{\partial \rho}{\partial t} dt + \int_{t}^{t+\Delta t} \int_{s}^{n} \int_{w}^{e} \frac{\partial (\rho v)}{\partial y} dydzdt + \int_{t}^{t+\Delta t} \int_{w}^{e} \int_{s}^{n} \frac{\partial (\rho w)}{\partial z} dzdydt = 0 \qquad (4.23)$$

$$\frac{\Delta y \Delta z}{\Delta t}(\rho_{i,j} - \rho_{i,j}^{0}) + \frac{(\rho_{i,j} + \rho_{i+1,j})}{2} v_{i,j} \Delta z - \frac{(\rho_{i,j} + \rho_{i-1,j})}{2} v_{i-1,j} \Delta z$$
$$+ \frac{(\rho_{i,j} + \rho_{i,j+1})}{2} w_{i,j} \Delta y - \frac{(\rho_{i,j} + \rho_{i,j-1})}{2} w_{i,j-1} \Delta y = 0$$

$$\frac{(\rho_{i,j} + \rho_{i+1,j})}{2} v_{i,j} \Delta z = F_e$$

$$\frac{(\rho_{i,j} + \rho_{i-1,j})}{2} v_{i-1,j} \Delta z = F_w$$

$$\frac{(\rho_{i,j} + \rho_{i,j+1})}{2} w_{i,j} \Delta y = F_n$$

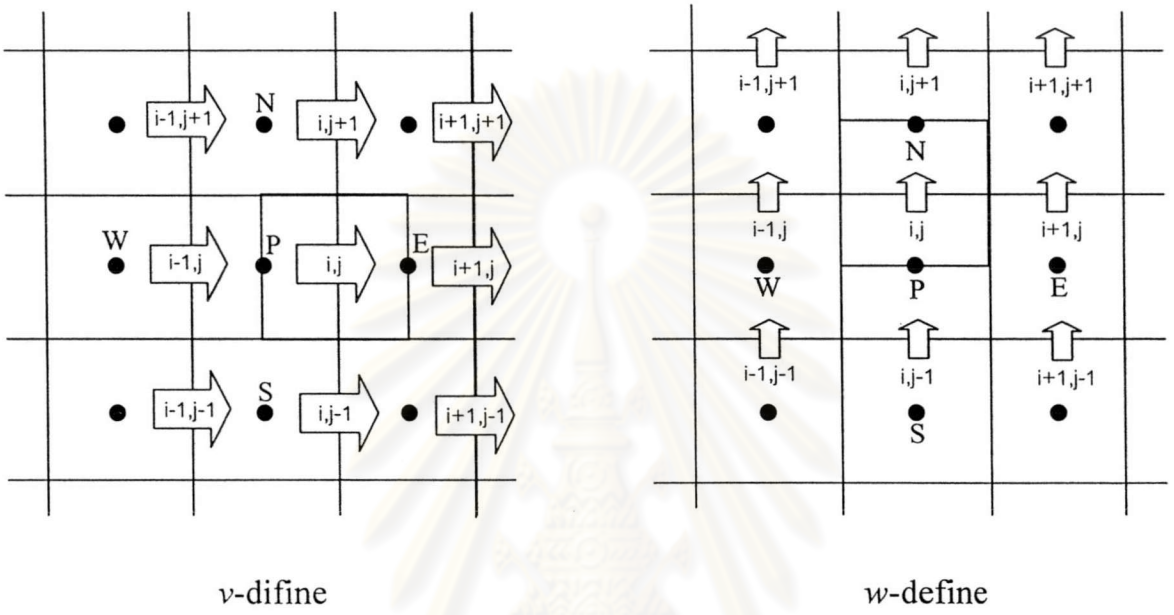
$$\frac{(\rho_{i,j} + \rho_{i,j-1})}{2} w_{i,j-1} \Delta y = F_z$$

Then $$\frac{(\rho_p - \rho_p^0)}{\Delta t} \Delta z \Delta y + F_e - F_w + F_n - F_z = 0 \qquad (4.24)$$

Momentum equation:

$$\text{y-direction:} \quad \frac{\partial(\rho v)}{\partial t}+\frac{\partial}{\partial y}\left(\rho v^2+p\right)+\frac{\partial}{\partial z}(\rho v w)=0$$

$$\text{z-direction:} \quad \frac{\partial(\rho w)}{\partial t}+\frac{\partial}{\partial y}(\rho v w)+\frac{\partial}{\partial z}\left(\rho w^2+p\right)=0$$



v-difine *w*-define

Figure 4.9 Control volume for momentum equations

Similarly, integrate the equation of momentum in the control volume with provide

y-direction:

$$\int_w^e\int_s^n\int_t^{t+\Delta t}\frac{\partial \rho v}{\partial t}dtdzdy+\int_t^{t+\Delta t}\int_s^n\int_w^e\frac{\partial(\rho v^2+p)}{\partial y}dydzdt+\int_t^{t+\Delta t}\int_w^e\int_s^n\frac{\partial(\rho v w)}{\partial z}dzdydt=0 \tag{4.25}$$

z-direction:

$$\int_w^e\int_s^n\int_t^{t+\Delta t}\frac{\partial \rho w}{\partial t}dtdzdy+\int_t^{t+\Delta t}\int_s^n\int_w^e\frac{\partial(\rho v w)}{\partial y}dydzdt+\int_t^{t+\Delta t}\int_w^e\int_s^n\frac{\partial(\rho w^2+p)}{\partial z}dzdydt=0 \tag{4.26}$$

From equation (4.25)

$$\int_w^e\int_s^n\int_t^{t+\Delta t}\frac{\partial(\rho v)}{\partial t}dtdzdy=\left((\rho v)_p-(\rho v)_p^0\right)\Delta y\Delta z$$

$$\int_t^{t+\Delta t}\int_s^n\int_w^e \frac{\partial(\rho v^2)}{\partial y}dydzdt = \left(\rho v^2\right)_e \Delta z\Delta t - \left(\rho v^2\right)_w \Delta z\Delta t$$

$$\int_t^{t+\Delta t}\int_w^e\int_s^n \frac{\partial(\rho vw)}{\partial z}dzdydt = \left(\rho vw\right)_n \Delta y\Delta t - \left(\rho vw\right)_s \Delta y\Delta t$$

$$\int_t^{t+\Delta t}\int_s^n\int_w^e \frac{\partial(p)}{\partial y}dydzdt = \left(p_e - p_w\right)\Delta z\Delta t = \left(p_E - p_P\right)\Delta z\Delta t$$

$$\left(\rho v^2\right)_e \Delta z\Delta t = J_e\Delta t = F_e v_e \Delta t$$
$$\left(\rho v^2\right)_w \Delta z\Delta t = J_w\Delta t = F_w v_w \Delta t$$
$$\left(\rho vw\right)_n \Delta y\Delta t = J_n\Delta t = F_n v_n \Delta t$$
$$\left(\rho vw\right)_s \Delta y\Delta t = J_s\Delta t = F_s v_s \Delta t$$

Then
$$\frac{\left((\rho v)_p - (\rho v)_p^0\right)}{\Delta t}\Delta y\Delta z + J_e - J_w + J_n - J_s = -\left(p_E - p_P\right)\Delta z \quad (4.27)$$

Multiply equation (4.24) by v_p (y-direction velocity at i,j):

$$\frac{\left(v_p\rho_p - v_p\rho_p^0\right)}{\Delta t}\Delta z\Delta y + v_p F_e - v_p F_w + v_p F_n - v_p F_z = 0 \quad (4.28)$$

Subtract equation (4.27) by equation (4.28):

$$\frac{\left(v_p - v_p^0\right)\rho_p^0}{\Delta t}\Delta y\Delta z + (J_e - v_p F_e) - (J_w - v_p F_w) + (J_n - v_p F_n) - (J_s - v_p F_s) = -\left(p_E - p_P\right)\Delta z \quad (4.29)$$

For upwind scheme: the control volume and direction of velocity are shown in Fig. 4.10

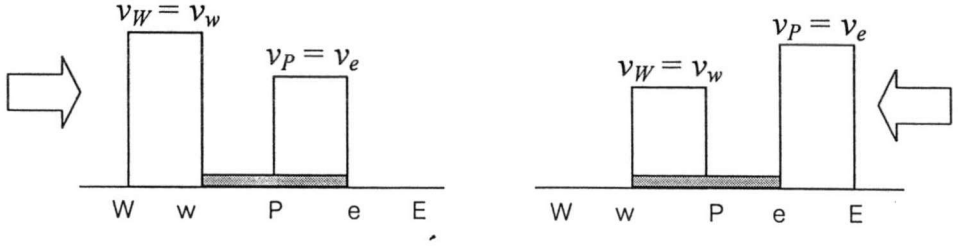


Fig. 4.10 velocity for Upwind scheme

When F_e is flow rate through e-surface

For $F_e > 0$, $v_e = v_{i,j}$

$F_e < 0$, $v_e = v_{i+1,j}$

Then $J_e = F_e v_e = v_{i,j} \max [F_e, 0] - v_{i+1,j} \max [-F_e, 0]$

$F_e v_p = v_{i,j} \max [F_e, 0] - v_{i,j} \max [-F_e, 0]$

So $J_e - F_e v_p = \max [-F_e, 0] (v_{i,j} - v_{i+1,j})$

In the same way

$$J_w - F_w v_p = \max [F_w, 0] (v_{i-1,j} - v_{i,j})$$

$$J_n - F_n v_p = \max [-F_n, 0] (v_{i,j} - v_{i,j+1})$$

$$J_s - F_s v_p = \max [F_s, 0] (v_{i,j-1} - v_{i,j})$$

Give $a_e = \max [-F_e, 0]$

$a_w = \max [F_w, 0]$

$a_n = \max [-F_n, 0]$

$a_s = \max [F_s, 0]$

Then
$$a_p v_p = a_e v_e + a_w v_w + a_n v_n + a_s v_s + by + (p_p - p_E)\Delta z \qquad (4.30)$$

Where
$$a_p = a_e + a_w + a_n + a_s + \frac{(\rho_p^0 + \rho_e^0)\Delta y \Delta z}{2\Delta t}$$

$$by = \frac{(\rho_p^0 + \rho_e^0) v_p^0 \Delta y \Delta z}{2\Delta t}$$

In the same way, from equation (4.26)

$$\int_w^e \int_s^n \int_t^{t+\Delta t} \frac{\partial(\rho w)}{\partial t} dt dz dy = \left((\rho w)_p - (\rho w)_p^0\right)\Delta y \Delta z$$

$$\int_t^{t+\Delta t} \int_s^n \int_w^e \frac{\partial(\rho v w)}{\partial y} dy dz dt = (\rho v w)_e \Delta z \Delta t - (\rho v w)_w \Delta z \Delta t$$

$$\int_t^{t+\Delta t} \int_w^e \int_s^n \frac{\partial(\rho w^2)}{\partial z} dz dy dt = (\rho w^2)_n \Delta y \Delta t - (\rho w^2)_s \Delta y \Delta t$$

$$\int_t^{t+\Delta t} \int_w^e \int_s^n \frac{\partial(p)}{\partial z} dz dy dt = (p_n - p_s)\Delta y \Delta t = (p_N - p_P)\Delta y \Delta t$$

Give

$$(\rho vw)_e \Delta z \Delta t = J_e \Delta t = F_e v_e \Delta t$$
$$(\rho vw)_w \Delta z \Delta t = J_w \Delta t = F_w v_w \Delta t$$
$$(\rho ww)_n \Delta y \Delta t = J_n \Delta t = F_n v_n \Delta t$$
$$(\rho ww)_s \Delta y \Delta t = J_s \Delta t = F_s v_s \Delta t$$

Then
$$\frac{\left((\rho w)_p - (\rho w)_p^0\right)}{\Delta t} \Delta y \Delta z + J_e - J_w + J_n - J_s = -(p_N - p_P)\Delta y \quad (4.31)$$

Multiply equation (4.24) by w_p (y-direction velocity at i,j):

$$\frac{\left(w_p \rho_p - w_p \rho_p^0\right)}{\Delta t} \Delta z \Delta y + w_p F_e - w_p F_w + w_p F_n - w_p F_z = 0 \quad (4.32)$$

Subtract equation (4.31) by equation (4.32)

$$\frac{\left(w_p - w_p^0\right)\rho_p^0}{\Delta t} \Delta y \Delta z + (J_e - w_p F_e) - (J_w - w_p F_w) + (J_n - w_p F_n)$$
$$- (J_s - w_p F_s) = -(p_N - p_P)\Delta y \quad (4.33)$$

Give
$$J_e - F_e w_p = \max [-F_e, 0] (w_{i,j} - w_{i+1,j})$$
$$J_w - F_w w_p = \max [F_w, 0] (w_{i-1,j} - w_{i,j})$$
$$J_n - F_n w_p = \max [-F_n, 0] (w_{i,j} - w_{i,j+1})$$
$$J_s - F_s w_p = \max [F_s, 0] (w_{i,j-1} - w_{i,j})$$
$$a_e = \max [-F_e, 0]$$
$$a_w = \max [F_w, 0]$$
$$a_n = \max [-F_n, 0]$$
$$a_s = \max [F_s, 0]$$

Then
$$a_{pz} v_p = a_e v_e + a_w v_w + a_n v_n + a_s v_s + bz + (p_P - p_N)\Delta y \quad (4.34)$$

Where
$$a_{pz} = a_e + a_w + a_n + a_s + \frac{(\rho_p^0 + \rho_n^0)\Delta y \Delta z}{2\Delta t}$$

$$bz = \frac{(\rho_p^0 + \rho_n^0) v_p^0 \Delta y \Delta z}{2\Delta t}$$

Energy Equation :

$$\frac{\partial E_t}{\partial t}+\frac{\partial}{\partial y}\left[(E_t+p)v+q_y\right]+\frac{\partial}{\partial z}\left[(E_t+p)w+q_z\right]=0$$

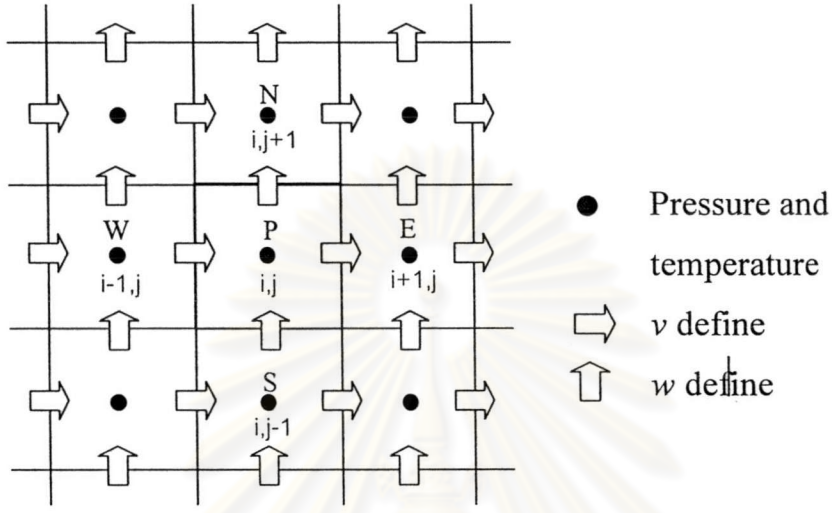


Figure 4.11 Control volume for energy equations

Integrate the equation of energy in the control volume

$$\int_w^e\int_s^n\int_t^{t+\Delta t}\frac{\partial E_t}{\partial t}dtdzdy+\int_t^{t+\Delta t}\int_s^n\int_w^e\frac{\partial\left[(E_t+p)v+q_y\right]}{\partial y}dydzdt+\int_t^{t+\Delta t}\int_w^e\int_s^n\frac{\partial\left[(E_t+p)w+q_z\right]}{\partial z}dzdydt=0 \tag{4.35}$$

From equation (4.35)

$$\int_w^e\int_s^n\int_t^{t+\Delta t}\frac{\partial E_t}{\partial t}dtdzdy=\left[\left(\rho C_vT+\frac{\rho v^2}{2}+\frac{\rho w^2}{2}\right)_p-\left(\rho C_vT+\frac{\rho v^2}{2}+\frac{\rho w^2}{2}\right)_p^0\right]\Delta z\Delta y$$

$$\int_t^{t+\Delta t}\int_s^n\int_w^e\frac{\partial\left[(E_t+p)v+q_y\right]}{\partial y}dydzdt=\left[\left(\rho C_vTv+\frac{\rho w^2v}{2}+\frac{\rho v^3}{2}+pv+q_y\right)_{e-w}\right]\Delta z\Delta t$$

$$\int_t^{t+\Delta t}\int_w^e\int_s^n\frac{\partial\left[(E_t+p)w+q_z\right]}{\partial z}dzdydt=\left[\left(\rho C_vTw+\frac{\rho v^2w}{2}+\frac{\rho w^3}{2}+pw+q_z\right)_{n-s}\right]\Delta y\Delta t$$

Give

$$ap = \rho_{i,j} C_{v i,j} \frac{\Delta y \Delta z}{\Delta t} + \frac{1}{2}\left(\frac{\rho_{i,j} + \rho_{i+1,j}}{2}\right)\left(\frac{C_{v i,j} + C_{v i+1,j}}{2}\right) v_{i,j} \Delta z$$
$$- \frac{1}{2}\left(\frac{\rho_{i,j} + \rho_{i-1,j}}{2}\right)\left(\frac{C_{v i,j} + C_{v\, i-1,j}}{2}\right) v_{i-1,j} \Delta z + \frac{(k_{i+1,j} - k_{i-1,j})}{2} \frac{\Delta z}{\Delta y}$$
$$+ \frac{1}{2}\left(\frac{\rho_{i,j} + \rho_{i,j+1}}{2}\right)\left(\frac{C_{v i,j} + C_{v i,j+1}}{2}\right) w_{i,j} \Delta y - \frac{1}{2}\left(\frac{\rho_{i,j} + \rho_{i,j-1}}{2}\right)\left(\frac{C_{v i,j} + C_{v i,j-1}}{2}\right) w_{i,j-1} \Delta y$$
$$+ \frac{\left(k_{i,j+1} - k_{i,j-1}\right)}{2} \frac{\Delta y}{\Delta z}$$

$$F_e = \left[\frac{1}{2}\left(\frac{\rho_{i,j} + \rho_{i+1,j}}{2}\right)\left(\frac{C_{v i,j} + C_{v i+1,j}}{2}\right) v_{i,j} - \left(\frac{k_{i,j} + k_{i+1,j}}{2\Delta y}\right)\right] T_{i+1,j} \Delta z$$

$$F_w = \left[\frac{1}{2}\left(\frac{\rho_{i,j} + \rho_{i-1,j}}{2}\right)\left(\frac{C_{v i,j} + C_{v i-1,j}}{2}\right) v_{i-1,j} - \left(\frac{k_{i,j} + k_{i-1,j}}{2\Delta y}\right)\right] T_{i-1,j} \Delta z$$

$$F_n = \left[\frac{1}{2}\left(\frac{\rho_{i,j} + \rho_{i,j+1}}{2}\right)\left(\frac{C_{v i,j} + C_{v i,j+1}}{2}\right) w_{i,j} - \left(\frac{k_{i,j} + k_{i,j+1}}{2\Delta z}\right)\right] T_{i,j+1} \Delta y$$

$$F_s = \left[\frac{1}{2}\left(\frac{\rho_{i,j} + \rho_{i,j-1}}{2}\right)\left(\frac{C_{v i,j} + C_{v,j-1}}{2}\right) w_{i,j-1} - \left(\frac{k_{i,j} + k_{i,j-1}}{2\Delta z}\right)\right] T_{i,j-1} \Delta y$$

$$ba = \left(\rho_{i,j} C_{v_{i,j}} T_{i,j} + \frac{\rho_{i,j} v_{i,j}^2}{2} + \frac{\rho_{i,j} w_{i,j}^2}{2}\right)^0 \frac{\Delta y \Delta z}{\Delta t}$$

$$bb = -\frac{1}{2}\left(\frac{\rho_{i,j} + \rho_{i+1}}{2}\right) v_{i,j}^2 w_{i,j} \Delta z + \frac{1}{2}\left(\frac{\rho_{i,j} + \rho_{i-1,j}}{2}\right) v_{i-1,j}^2 w_{i-1,j} \Delta z$$
$$- \frac{1}{2}\left(\frac{\rho_{i,j} + \rho_{i+1,j}}{2}\right) v_{i,j}^3 \Delta z + \frac{1}{2}\left(\frac{\rho_{i,j} + \rho_{i-1,j}}{2}\right) v_{i-1}^3 \Delta z$$
$$- \frac{1}{2}\left(\frac{\rho_{i,j} + \rho_{i,j+1}}{2}\right) v_{i,j} w_{i,j}^2 \Delta y + \frac{1}{2}\left(\frac{\rho_{i,j} + \rho_{i,j-1}}{2}\right) v_{i,j-1} w_{i,j-1}^2 \Delta y$$
$$- \frac{1}{2}\left(\frac{\rho_{i,j} + \rho_{i,j+1}}{2}\right) w_{i,j}^3 \Delta y + \frac{1}{2}\left(\frac{\rho_{i,j} + \rho_{i,j-1}}{2}\right) w_{i,j-1}^3 \Delta y$$
$$- \frac{\left(p_{i,j} + p_{i+1,j}\right)}{2} v_{i,j} \Delta z + \frac{\left(p_{i,j} + p_{i-1,j}\right)}{2} v_{i-1,j} \Delta z$$
$$- \frac{\left(p_{i,j} + p_{i,j+1}\right)}{2} w_{i,j} \Delta y + \frac{\left(p_{i,j} + p_{i,j-1}\right)}{2} w_{i,j-1} \Delta y$$

Give $a_e = \max [-F_e, 0]$

$a_w = \max [F_w, 0]$

$a_n = \max [-F_n, 0]$

$a_s = \max [F_s, 0]$

Then $apT_{i,j} = a_e + a_w + a_n + a_s + ba + bb$ (4.36)

For the system of equations for two-dimensional problems, the Thomas algorithm or the tri-diagonal matrix algorithm (TDMA) is a technique that is used. The TDMA is actually a direct method for one-dimensional situations, but it can be applied, in a line-by-line fashion, to solve multi-dimensional problems and is widely used in CFD program.

The tri-diagonal matrix algorithm

Consider a system of equations that has a tri-diagonal from

$$\begin{aligned}
\phi_1 &= C_1 \\
-\beta_2\phi_1 + D_2\phi_2 - \alpha_2\phi_3 &= C_2 \\
-\beta_3\phi_2 + D_3\phi_3 - \alpha_3\phi_4 &= C_3 \\
-\beta_4\phi_3 + D_4\phi_4 - \alpha_3\phi_4 &= C_4 \\
\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots &= \ldots \\
-\beta_n\phi_{n-1} + D_n\phi_n - \alpha_n\phi_{n+1} &= C_n \\
\phi_{n+1} &= C_{n+1}
\end{aligned}$$

In the above set of equations ϕ_1 and ϕ_{n+1} are know boundary values. The general form of any single equation is

$$-\beta_j\phi_{j-1} + D_j\phi_j - \alpha_j\phi_{j+1} = C_j \quad (4.37)$$

The set of equations can be rewritten as

$$\phi_2 = \frac{\alpha_2}{D_2}\phi_3 + \frac{\beta_2}{D_2}\phi_1 + \frac{C_2}{D_2} \quad (4.38a)$$

$$\phi_3 = \frac{\alpha_3}{D_3}\phi_4 + \frac{\beta_3}{D_3}\phi_2 + \frac{C_3}{D_3} \quad (4.38b)$$

$$\phi_4 = \frac{\alpha_4}{D_4}\phi_5 + \frac{\beta_4}{D_4}\phi_3 + \frac{C_4}{D_4} \qquad (4.38c)$$

.....

$$\phi_n = \frac{\alpha_n}{D_n}\phi_{n+1} + \frac{\beta_n}{D_n}\phi_{n-1} + \frac{C_n}{D_n}$$

These equations can be solved by the forward elimination and back-substitution. The forward elimination process starts by moving ϕ_2 from equation (4.38b) substitution from the equation (4.38a) to give

$$\phi_3 = \left(\frac{\alpha_3}{D_3 - \beta_3\frac{\alpha_2}{D_2}}\right)\phi_4 + \left(\frac{\beta_3\left(\frac{\beta_2}{D_2}\phi_1 + \frac{C_2}{D_2}\right) + C_3}{D_3 - \beta_3\frac{\alpha_2}{D_2}}\right) \qquad (4.39a)$$

Give $A_2 = \frac{\alpha_2}{D_2}$ and $C_2' = \frac{\beta_2}{D_2}\phi_1 + \frac{C_2}{D_2}$ (4.39b)

Equation (4.39a) can be written as

$$\phi_3 = \left(\frac{\alpha_3}{D_3 - \beta_3 A_2}\right)\phi_4 + \left(\frac{\beta_3 C_2' + C_3}{D_3 - \beta_3 A_2}\right) \qquad (4.39c)$$

If $A_3 = \left(\frac{\alpha_3}{D_3 - \beta_3 A_2}\right)$ and $C_3' = \left(\frac{\beta_3 C_2' + C_3}{D_3 - \beta_3 A_2}\right)$

One will be able to re-cast equation (4.39c) as

$$\phi_3 = A_3\phi_4 + C_3' \qquad (4.40)$$

Formula (4.40) can now be used to eliminate ϕ_3 from (4.38c) and procedure can be repeated up to the last equation of the set. This constitutes the forward elimination process.

For back-substitution, from the general form (4.40)

$$\phi_j = A_j\phi_{j+1} + C_j' \qquad (4.41a)$$

Where $A_j = \left(\frac{\alpha_j}{D_j - \beta_j A_{j-1}} \right)$ and $C'_j = \left(\frac{\beta_j C'_{j-1} + C_j}{D_j - \beta_j A_{j-1}} \right)$

(4.41b,4.41c)

The formulae can be made to apply at the boundary points $j = 1$ and $j = n+1$ by setting the following values for A and C'

$$A_1 = 0 \quad \text{and} \quad C'_1 = \phi_1$$

$$A_{n+1} = 0 \quad \text{and} \quad C'_{n+1} = \phi_{n+1}$$

In order to solve a system of equations, it should be arranged in form of equation (4.37) and α_j, β_j,D_j and C'_1 are identified. The values of A_j and C'_1 are subsequently calculated starting at $j = 2$ and going up to $j = n$ using (4.41c). Since the value of ϕ_3 is known at boundary location (n+1) the values for ϕ_j can be obtained in reverse order (ϕ_n, ϕ_{n-1}, ϕ_{n-2},..., ϕ_2) by means of the recurrence formula (4.41a).

For solving a system of equations for two-dimension problems, a general two-dimensional discretised transport equation of the form

$$a_p\phi_p = a_e\phi_e + a_w\phi_w + a_n\phi_n + a_s\phi_s + b \qquad (4.42)$$

To solve the system TDMA is applied along chosen, for example north-south (*n-s*), lines. The discretised equation is rearranged in the form

$$-a_s\phi_s + a_p\phi_p - a_n\phi_n = a_w\phi_w + a_e\phi_e + b \qquad (4.43)$$

the right hand side of (4.43) is assumed to be temporarily known. Equation (4.43) is in the form of equation (4.37)

Where $\alpha_j \equiv a_n$, $\beta_j \equiv a_s$

$D_j \equiv a_p$, $C_j \equiv a_w\phi_w + a_e\phi_e + b$

Along *n-s* direction of the chosen line can be solved for the values $j = 2$, 3, 4,.., n. The calculation is moved to the next north-south line. The sequence in which lines are chosen is known as the sweep direction. Sweeping from west to east, the values of ϕ_w to the west point P are known from the calculations on the previous line. Values of ϕ_e to its east, however, are unknown so the solution

process must be iterative. At each iteration cycle ϕ_e is taken to have its value at the end of the previous iteration or a given initial value at the first iteration. The line-by-line calculation procedure is repeated several times until a converged solution is obtained.

4.3.3.2 Assumptions used in the implicit model

For simplicity, the present model is based on the following assumptions:

a. Investigated system consists of chemically non-reactive substances.
b. The high velocity inlet fluid is injected from nozzle at the central part of the bed.
c. Investigated bed is formed in cylindrical vessel.
d. At the Initial stage, atmospheric stability bed is stable.
e. The fluid flow is assumed to be non-isothermal and compressible.
f. The effects of inlet temperature, inlet-pressure and inlet-velocity on RESS process especially near the nozzle area are simulated.
g. The two-dimensional rectangular coordinate is used.
h. A calorically-perfect fluid is assumed.

4.3.3.3 Algorithm of the implicit model

The simulation algorithm of the implicit model for determination of the velocity profile, the temperature and pressure profile of rapid expansion of supercritical solution process, especially near the nozzle area are presented and their simplified flow charts are illustrated in Figures 4.12 and Figures 4.13. The simulation is carried out according to the following steps:

1. The grid size, maximum time step and basic properties of the flow as well as the required iteration and interval number are specified.
2. Input all essential constant values for this algorithm, such as specific gas constant for CO_2 and C_p/C_v.

3. Calculate the density of fluid with the Equation of State (EOS), namely Soave Redlich-Kwong. This is done inside a subroutine called EOS where the initial pressure and temperature, which are, at the start, identical at all locations inside the system, are used to calculate the volume and, then, the gas density.
4. The initial temperature, y- and z-axis velocity, density and pressure inside the system are input as the fluid data at time 't'.
5. Solve the set of equations to obtain the temperature, y- and z-axis velocity, thermal conductivity, density, pressure and heat capacity for each individual point inside the system at time 't+Δt' by the loop named FLUID.
   5.1 In the first iteration, parameters, i.e. temperature, y- and z-axis velocity, density and pressure in each individual point of the system, are read. At the boundary of the system, the velocities are set at zero. Regardless of the position, temperature, pressure, and density are equal to the initial T0, P0, and density are calculated through EOS, respectively.
   5.2 Heat capacity and thermal conductivity are calculated in the loop named the HEAT which begins as follows:
      - The number of cells inside the system both in the y- and z-axis are read.
      - The reference temperature and viscosity are read and applied as constant values.
      - For each individual location inside the system, the temperature is used to evaluate the viscosity.
      - The thermal conductivity of the fluid in every single location at time 't' is computed through the Prandtl number and viscosity at time 't'.
   5.3 Regardless of the position, temperature, pressure, heat capacity and density are saved for the first iteration in the loop named MEM.

5.4 Calculate the values of Coefficient on boundary.

5.5 Solve the momentum equations to obtain the momentum distribution by the loop named MOMENTUM.

5.6 Solve the continuity equation to obtain the density distribution by the loop named CON_DEN.

5.7 For new iteration, the heat capacity and thermal conductivity are calculated in the loop named the HEAT again.

5.8 Solve the energy equation to obtain the temperature distribution by the loop named ENERGY.

5.9 For new iteration, the pressure is saved in the loop named MEM_PRE to use for comparing with the new values that will obtain from the loop named PRESSURE.

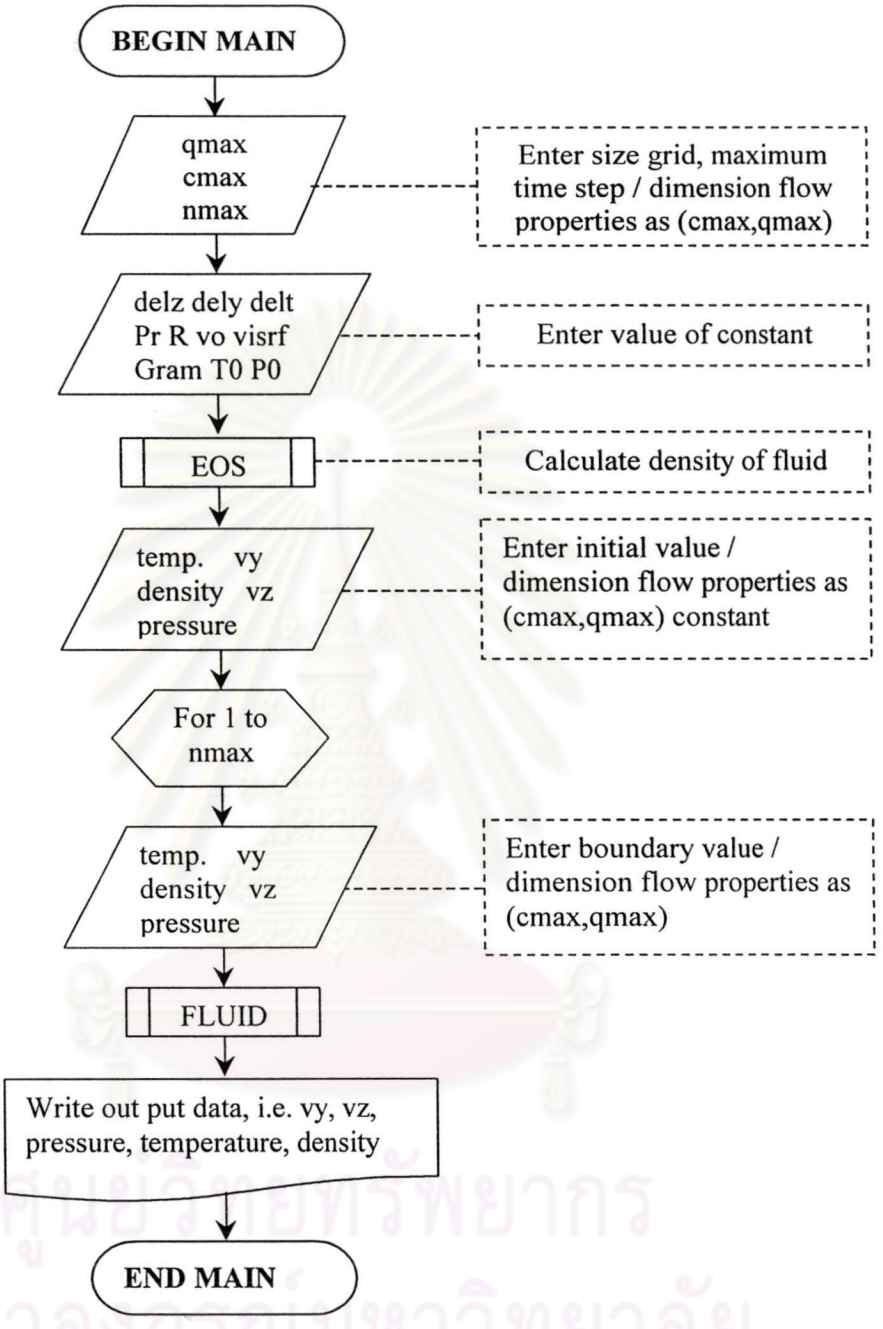
5.10 In the loop named PRESSURE, the equation of state, namely Soave Redlich-Kwong is solved to obtain the pressure distribution .

5.11 Comparison the previous pressure and the pressure that obtains from PRESSURE loop. If the remainder is not acceptable, go back to (5.1), using the updated values of temperature, y- and z-axis velocity, fluid density and pressure for calculation. The calculation procedure is repeated several times until a converged solution is obtained

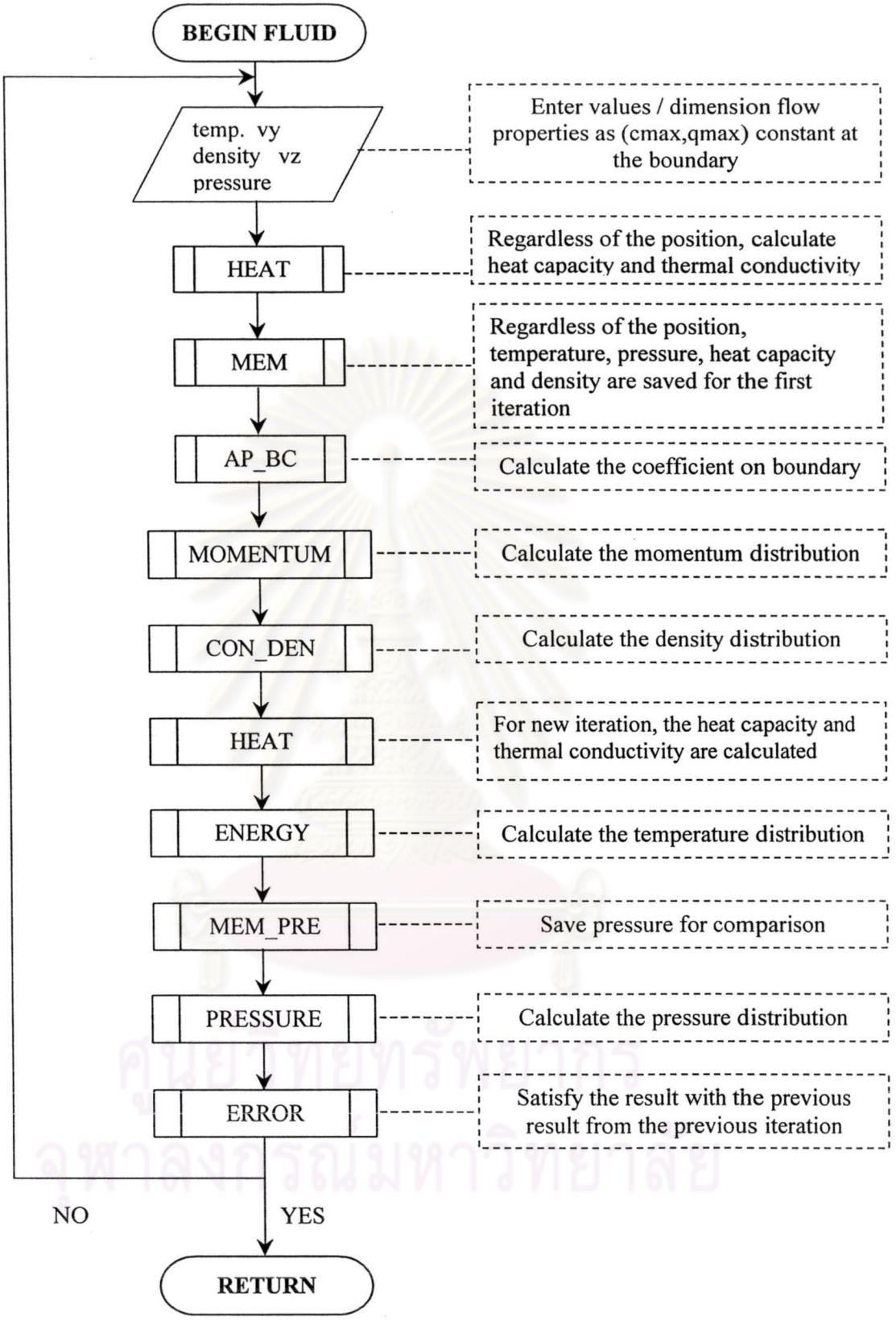
5.12 Show the results at time '$t + \Delta t$'.

6. Then, go back to (5) and do the next interval, Repeat until the interval number is equal to the required interval number specified in (1).

7. The final results are write at the end of program in the loop named SAVEDATA.



Figures 4.12 Block diagram simulation of rapid expansion of supercritical carbon dioxide by implicit finite difference technique



Figures 4.13 Block diagram of Fluid loop in implicit finite difference technique