

## Chapter 2

# Modelization of CFD problems

### 2.1 Description of the governing equations

The fluid flow and heat transfer phenomena assumed throughout this work can be summarized in the following hypotheses and restrictions:

- Two or three dimensional flow structure
- Steady or unsteady flow
- Laminar flow
- Newtonian and incompressible fluid
- Constant physical properties
- Buoyancy effect modeled by the Boussinesq's hypothesis
- Neglected viscous dissipation
- Neglected radiation
- Single phase fluid
- Single component

A detailed explanation of these hypothesis can be found in any book of fundamentals of CFD [31, 32, 33]. Under these hypotheses it is possible to cover a wide range of engineering applications.

The governing equations, i.e. the conservation of mass, momentum and energy equations give us the tools necessary to deal mathematically with these applications. These equations are written in differential form as:

- Conservation of mass (continuity equation)

$$\nabla \circ \vec{V} = 0$$

- Conservation of momentum (Navier-Stokes equations)

$$\frac{\partial \vec{V}}{\partial \tau} + \vec{V} (\nabla \circ \vec{V}) = -\frac{1}{\rho} \nabla P + \nu \nabla^2 \vec{V} + \vec{g} \beta (T - T_0)$$

- Conservation of energy

$$\frac{\partial T}{\partial \tau} + \vec{V} (\nabla \circ T) = \frac{\kappa}{\rho c_p} \nabla^2 T + \frac{S_T}{\rho c_p}$$

The solution of these equations reports a detailed information of the fluid-flow variables involved in the phenomena of study: the velocity  $\vec{V} = \{u, v, w\}$ , the pressure  $P$  and the temperature  $T$ .

Since the geometry of the domain of study has a strong influence in the pattern flow, it is suitable to choose the coordinate system which represent this pattern better. By doing so, generality is gained for the development of successive sections.

### 2.1.1 Cartesian and cylindrical coordinate systems

The governing equations are represented in two orthogonal coordinate systems: the cartesian  $\{x, y, z\}$  and the cylindrical  $\{r, \theta, z\}$  (see Fig. 2.1).

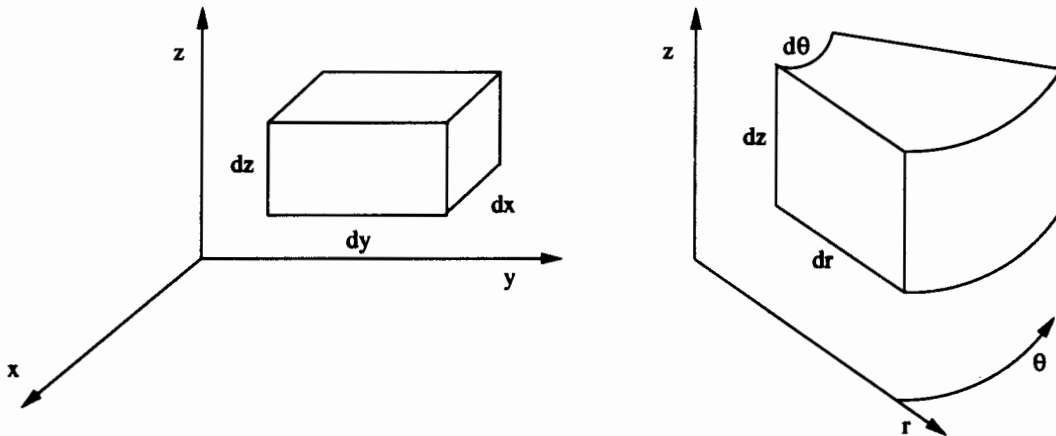


Figure 2.1: Coordinate systems: cartesian (left) and cylindrical (right).

Hence, the representation of the governing equations in the cartesian coordinate system leads to:

- Conservation of mass or continuity equation

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0$$

- Conservation of momentum in  $x$  direction

$$\frac{\partial u}{\partial \tau} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} = -\frac{1}{\rho} \frac{\partial P}{\partial x} + \nu \left[ \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right] + g_x \beta (T - T_0)$$

- Conservation of momentum in  $y$  direction

$$\frac{\partial v}{\partial \tau} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} = -\frac{1}{\rho} \frac{\partial P}{\partial y} + \nu \left[ \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} \right] + g_y \beta (T - T_0)$$

- Conservation of momentum in  $z$  direction

$$\frac{\partial w}{\partial \tau} + u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} = -\frac{1}{\rho} \frac{\partial P}{\partial z} + \nu \left[ \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right] + g_z \beta (T - T_0)$$

- Conservation of energy

$$\frac{\partial T}{\partial \tau} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} + w \frac{\partial T}{\partial z} = \frac{\kappa}{\rho c_p} \left[ \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right] + S_T$$

They are all summarized in the so called convection and diffusion equation [32] for the cartesian coordinate system as:

$$\frac{\partial \phi}{\partial \tau} + \frac{\partial u \phi}{\partial x} + \frac{\partial v \phi}{\partial y} + \frac{\partial w \phi}{\partial z} = \Gamma_\phi \left[ \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} \right] + S_\phi$$

Where the values of  $\phi$ ,  $\Gamma_\phi$  and  $S_\phi$  are summarized in table 2.1.

Equation	$\phi$	$\Gamma_\phi$	$S_\phi$
Continuity	1	0	0
Momentum in $x$ direction	$u$	$\nu$	$-\frac{1}{\rho} \frac{\partial P}{\partial x} + g_x \beta (T - T_0)$
Momentum in $y$ direction	$v$	$\nu$	$-\frac{1}{\rho} \frac{\partial P}{\partial y} + g_y \beta (T - T_0)$
Momentum in $z$ direction	$w$	$\nu$	$-\frac{1}{\rho} \frac{\partial P}{\partial z} + g_z \beta (T - T_0)$
energy	$T$	$\frac{\kappa}{\rho c_p}$	$\frac{S_T}{\rho c_p}$

Table 2.1: Values of  $\phi$ ,  $\Gamma_\phi$  and  $S_\phi$  for the convection and diffusion equation in a cartesian coordinate system

The representation of the governing equations for the cylindrical coordinate system leads to:

- Conservation of mass or continuity equation

$$\frac{1}{r} \frac{\partial ru}{\partial r} + \frac{1}{r} \frac{\partial v}{\partial \theta} + \frac{\partial w}{\partial z} = 0$$

- Conservation of momentum in  $r$  direction

$$\begin{aligned} & \frac{\partial u}{\partial \tau} + u \frac{\partial u}{\partial r} + \frac{v}{r} \frac{\partial u}{\partial \theta} - \frac{v^2}{r} + w \frac{\partial u}{\partial z} = \\ & -\frac{1}{\rho} \frac{\partial P}{\partial r} + \nu \left[ \frac{\partial}{\partial r} \left( \frac{1}{r} \frac{\partial ru}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 v}{\partial \theta^2} - \frac{2}{r^2} \frac{\partial v}{\partial \theta} + \frac{\partial^2 u}{\partial z^2} \right] + g_r \beta (T - T_0) \end{aligned}$$

- Conservation momentum in  $\theta$  direction

$$\begin{aligned} & \frac{\partial v}{\partial \tau} + u \frac{\partial v}{\partial r} + \frac{v}{r} \frac{\partial v}{\partial \theta} + \frac{uv}{r} + w \frac{\partial v}{\partial z} = \\ & -\frac{1}{\rho r} \frac{\partial P}{\partial \theta} + \nu \left[ \frac{\partial}{\partial r} \left( \frac{1}{r} \frac{\partial rv}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 v}{\partial \theta^2} + \frac{2}{r^2} \frac{\partial u}{\partial \theta} + \frac{\partial^2 v}{\partial z^2} \right] + g_\theta \beta (T - T_0) \end{aligned}$$

- Conservation of momentum in  $z$  direction

$$\begin{aligned} & \frac{\partial w}{\partial \tau} + u \frac{\partial w}{\partial r} + \frac{v}{r} \frac{\partial w}{\partial \theta} + \frac{uw}{r} + w \frac{\partial w}{\partial z} = \\ & -\frac{1}{\rho r} \frac{\partial P}{\partial z} + \nu \left[ \frac{\partial}{\partial r} \left( \frac{1}{r} \frac{\partial rw}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 w}{\partial \theta^2} + \frac{2}{r^2} \frac{\partial u}{\partial \theta} + \frac{\partial^2 w}{\partial z^2} \right] + g_z \beta (T - T_0) \end{aligned}$$

- Conservation of energy

$$\frac{\partial T}{\partial \tau} + u \frac{\partial T}{\partial r} + \frac{v}{r} \frac{\partial T}{\partial \theta} + w \frac{\partial T}{\partial z} = \frac{\kappa}{\rho c_p} \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 T}{\partial \theta^2} + \frac{\partial^2 T}{\partial z^2} \right] + S_T$$

Analogously as in the cartesian coordinate system, they are written in the convection and diffusion equation for the cylindrical coordinate system.

$$\frac{\partial \phi}{\partial \tau} + \frac{1}{r} \frac{\partial ru\phi}{\partial r} + \frac{\partial v\phi}{\partial \theta} + \frac{\partial w\phi}{\partial z} = \Gamma_\phi \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \phi}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 \phi}{\partial \theta^2} + \frac{\partial^2 \phi}{\partial z^2} \right] + S_\phi$$

with  $\phi$ ,  $\Gamma_\phi$  and  $S_\phi$  values summarized in table 2.2

Equation	$\phi$	$\Gamma_\phi$	$S_\phi$
Continuity	1	0	0
Momentum in $r$ direction	$u$	$\nu$	$-\frac{1}{\rho} \frac{\partial P}{\partial r} + g_r \beta(T - T_0) + \frac{v^2}{r} - \nu \frac{2}{r^2} \frac{\partial v}{\partial \theta} - \nu \frac{u}{r^2}$
Momentum in $\theta$ direction	$v$	$\nu$	$-\frac{1}{\rho} \frac{\partial P}{\partial y} + g_r \beta(T - T_0) - \frac{uv}{r} + \nu \frac{2}{r^2} \frac{\partial v}{\partial \theta} - \nu \frac{v}{r^2}$
Momentum in $z$ direction	$w$	$\nu$	$-\frac{1}{\rho} \frac{\partial P}{\partial z} + g_z \beta(T - T_0)$
Energy	$T$	$\frac{\kappa}{\rho c_p}$	$\frac{S_T}{\rho c_p}$

Table 2.2: Values of  $\phi$ ,  $\Gamma_\phi$  and  $S_\phi$  for the convection and diffusion equation in a cylindrical coordinate system

These equations are written in differential form and all together, they represent a system of partial differential equations with non linear terms and coupling between variables. It is clear that no analytical solution is feasible in a general case. Conversely, numerical methods such as finite differences, finite elements or finite volumes can handle this problem.

## 2.2 Discretization by finite volume method

The finite volume method is used here because it is easy to understand from the physical point of view. In this sense, the work done by Patankar [32] for the discretization of the governing equations and the linking procedure between systems of equations was adopted and followed.

Firstly, the domain is discretized into a finite number of volumes covering all domain. The grid defined by this discretization is called the centered grid. At the center of these volumes, the scalar variables  $P$  and  $T$  are evaluated. In addition three staggered grids in each direction of the coordinate system, i.e. the  $\{x, y, z\}$  directions for the cartesian and the  $\{r, \theta, z\}$  directions for the cylindrical, are also used for the evaluation of each component of the velocity vector  $\vec{V} = \{u, v, w\}$ .

The integration of these partial differential equations in the respective grid can be briefly described by means of the integration of the convection and diffusion equation for a general grid whether it is centered or staggered.

The convection and diffusion equation composed by four terms, i.e. the convection, the diffusion, the source term and the unsteady term, is integrated in a generic volume  $\mathcal{V}$ . Fig. 2.2 shows the geometry of the volume, as well as the faces and distances between centers of the neighbour volumes.

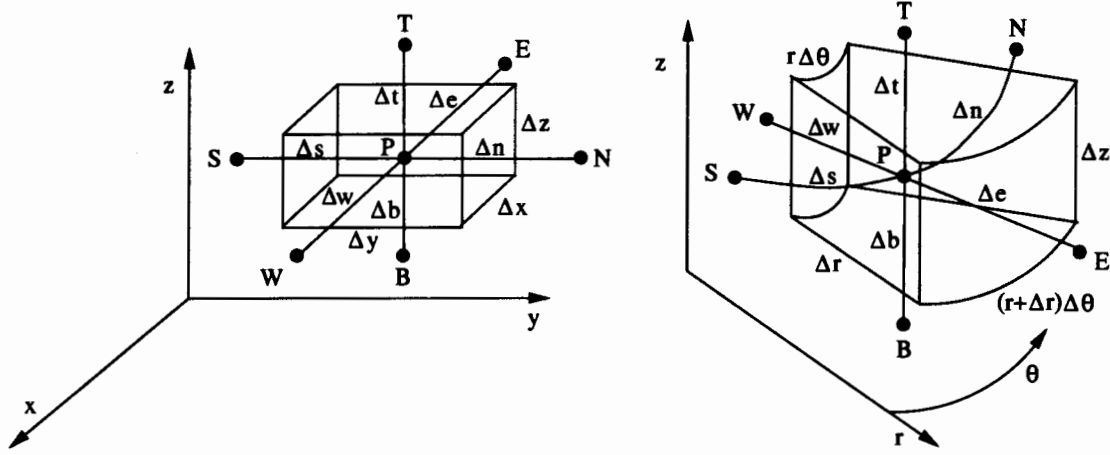


Figure 2.2: Coordinate systems: left, cartesian  $\{x, y, z\}$  and right, cylindrical  $\{r, \theta, z\}$ .

In both pictures, it is followed the same notation. The uppercase letters  $\{P, W, E, S, N, B, T\}$  represent the values of the variable  $\phi$  at the center of volumes whilst the lowercase letters represent the values at faces  $f = \{w, e, s, n, b, t\}$ .

Therefore, the resulting integrated convection and diffusion equation is expressed in algebraic form as

$$\begin{aligned}
 & \frac{\rho V}{\Delta \tau} (\phi_P - \phi_P^0) + \\
 & F_e \phi_e - F_w \phi_w + \\
 & F_n \phi_n - F_s \phi_s + \\
 & F_t \phi_t - F_b \phi_b = \\
 & D_e (\phi_E - \phi_P) - D_w (\phi_P - \phi_W) + \\
 & D_n (\phi_N - \phi_P) - D_s (\phi_P - \phi_S) + \\
 & D_t (\phi_T - \phi_P) - D_b (\phi_P - \phi_B) + S_\phi V
 \end{aligned}$$

where  $F_f$  and  $D_f$  are the convective and diffusive transport coefficients respectively of the variable  $\phi$  at face  $f$  with surface  $S_f$

$$F_f = (\rho u S)_f, \quad D_f = \left( \Gamma \frac{S}{\Delta} \right)_f$$

The algebraic equation for a given volume  $P$  can be solved to find the variable  $\phi$  at its center  $\phi_P$ .

It is worth noting that this equation contains also the variables of its neighbour volumes  $\phi_{NGB}$ . Values of variables at faces  $\phi_f$  are evaluated by interpolations of second order of accuracy or using higher order schemes that consider the closest values at centered points and the Peclet number at face  $f$ .

$$Pe_f = \frac{F_f}{D_f}$$

The deferred correction [34] is one of these approaches.

The set of coefficients of the resulting algebraic equation has the following structure

$$a_{P,\phi}\phi_P + \sum_{NGB} a_{NGB,\phi}\phi_{NGB} = b_{P,\phi}$$

where

$$\begin{aligned} a_{W,\phi} &= D_w A(Pe_w) + F_w \max(F_w, 0) \\ a_{E,\phi} &= D_e A(Pe_e) + F_e \max(-F_e, 0) \\ a_{S,\phi} &= D_s A(Pe_s) + F_s \max(F_s, 0) \\ a_{N,\phi} &= D_n A(Pe_n) + F_n \max(-F_n, 0) \\ a_{B,\phi} &= D_b A(Pe_b) + F_b \max(F_b, 0) \\ a_{T,\phi} &= D_t A(Pe_t) + F_t \max(-F_t, 0) \\ a_{P0} &= \frac{\rho(V)}{\Delta\tau} \\ a_{P,\phi} &= -(a_{W,\phi} + a_{E,\phi} + a_{S,\phi} + a_{N,\phi} + a_{B,\phi} + a_{T,\phi}) + \rho \frac{\mathcal{V}}{\Delta\tau} \\ b_{P,\phi} &= \rho \frac{\mathcal{V}}{\Delta\tau} \phi_P^0 + S_\phi \mathcal{V} \end{aligned}$$

where  $A(Pe_f)$  is a scheme function whose argument is the Peclet number. Further details of these implementations may be found in Patankar [32] and others [33].

The integration of the convection and diffusion equation for all volumes at all domain leads to an algebraic system of equations for a single variable  $\phi$ .

By doing so for the momentum equations at each direction and in the respective staggered grid and the energy equation in the centered grid, an amount of four algebraic systems of equations is obtained.

$$\begin{aligned} a_{P,u}u_P + \sum_{NGB} a_{NGB,u}u_{NGB} &= b_{P,u} \\ a_{P,v}v_P + \sum_{NGB} a_{NGB,v}v_{NGB} &= b_{P,v} \\ a_{P,w}w_P + \sum_{NGB} a_{NGB,w}w_{NGB} &= b_{P,w} \\ a_{P,T}T_P + \sum_{NGB} a_{NGB,T}T_{NGB} &= b_{P,T} \end{aligned}$$

Where the subscript  $P$  represent a generic point of the domain but into their respective grids.

Regarding these systems, the right hand side of the first three systems of equations contains the pressure gradient, the temperature effects over the density, i.e. the Boussinesq's hypothesis, and the source term derived from the cylindrical coordinate system on their respective directions.

$$b_{P,u} = -\frac{P_E - P_P}{\Delta_e} \mathcal{V}_u + S_u \mathcal{V}_u = -c_u (P_E - P_P) + S_u \mathcal{V}_u$$

$$b_{P,v} = -\frac{P_N - P_P}{\Delta_n} \mathcal{V}_v + S_u \mathcal{V}_v = -c_v (P_N - P_P) + S_v \mathcal{V}_v$$

$$b_{P,w} = -\frac{P_T - P_P}{\Delta_t} \mathcal{V}_w + S_u \mathcal{V}_w = -c_w (P_T - P_P) + S_w \mathcal{V}_w$$

Where  $\mathcal{V}_u$ ,  $\mathcal{V}_v$  and  $\mathcal{V}_w$  are the volumes for each staggered direction.

For the resulting four systems of equations, it is said to have a coupling between the fluid-flow variables  $\vec{V} = \{u, v, w\}$ ,  $T$  and  $P$ . The first three systems give the velocity components under the assumption of a pressure field, whilst the last one gives the temperature field. Therefore, the complete solution of the problem, i.e. the solution of the pressure  $P$ , would require an additional system of equations.

### 2.2.1 The SIMPLE-like algorithms

For the above three systems of equations that represent the momentum equations in each direction, a field of pressures  $P^*$  has to be guessed in order to solve the velocities say  $\vec{V}^*$ . This is written as:

$$a_{P,u} u_P^* + \sum_{NGB} a_{NGB,u} u_{NGB}^* = -c_u (P_E^* - P_P^*) + S_u \mathcal{V}_u$$

$$a_{P,v} v_P^* + \sum_{NGB} a_{NGB,v} v_{NGB}^* = -c_v (P_N^* - P_P^*) + S_v \mathcal{V}_v$$

$$a_{P,w} w_P^* + \sum_{NGB} a_{NGB,w} w_{NGB}^* = -c_w (P_T^* - P_P^*) + S_w \mathcal{V}_w$$

Since the velocities evaluated with momentum equations satisfy only the momentum, there is no guaranty about continuity. In this sense, the continuity equation serves to introduce the correction values of velocities  $\vec{V}'$ .

$$\vec{V} = \vec{V}^* + \vec{V}'$$

Moreover, it is necessary to evaluate the right value of the pressure  $P$ . This is carried out by the addition of a pressure correction  $P'$ .

$$P = P^* + P'$$

If the correction of the velocities  $\vec{V}'$  is set in function of a pressure correction rate  $\Delta P'$  such that

$$u_P = u_P^* + u_P' = u_P^* - d_u (P_E' - P_P')$$

$$u_P = u_P^* + u_P' = v_P^* - d_v (P_N' - P_P')$$

$$w_P = w_P^* + w_P' = w_P^* - d_w (P_T' - P_P')$$

The substitution of these expressions in the respective algebraic systems of equations under the assumption that the  $\vec{V}^*$  values satisfy each equation, the following systems of equations in  $\vec{V}'$  and  $P'$  are obtained.

$$a_{P,u} u_P' + \sum_{NGB} a_{NGB,u} u_{NGB}' = -d_u (P_E' - P_P')$$



$$a_{P,v}v'_P + \sum_{NGB} a_{NGB,v}v'_{NGB} = -d_v (P'_N - P'_P)$$

$$a_{P,w}w'_P + \sum_{NGB} a_{NGB,w}w'_{NGB} = -d_w (P'_T - P'_P)$$

For a first approach of  $d_u$ ,  $d_v$  and  $d_w$  the neighbour summation of each system can be neglected yielding to

$$d_u = -\frac{c_u}{a_{P,u}}, \quad d_v = -\frac{c_v}{a_{P,v}}, \quad d_w = -\frac{c_w}{a_{P,w}}$$

This approach has been named SIMPLE [32]. A much better improvement is SIMPLEC [35] which considers the neighbour summation.

$$d_u = -\frac{c_u}{a_{P,u} - \sum_{NGB} a_{NGB,u}}, \quad d_v = -\frac{c_v}{a_{P,v} - \sum_{NGB} a_{NGB,v}}, \quad d_w = -\frac{c_w}{a_{P,w} - \sum_{NGB} a_{NGB,w}}$$

Finally, the values of pressure corrections  $P'$  are obtained from the continuity equation by substitution of the velocities  $\vec{V}$  by the guessed velocities  $\vec{V}^*$  plus the corrections  $\vec{V}'$  expressed in terms of the pressure corrections.

Integrating the convection and diffusion equation for  $\phi = 0$  there is the continuity equation:

$$\rho u_e S_e - \rho u_w S_w + \rho v_n S_n - \rho v_s S_s + \rho w_t S_t - \rho w_b S_b = 0$$

where the velocities at faces are

$$u_e = u_P^*|_e - d_u|_e (P'_E - P'_P) = u_e^* - d_u|_e (P'_E - P'_P)$$

$$v_n = v_P^*|_n - d_v|_n (P'_N - P'_P) = v_n^* - d_v|_n (P'_N - P'_P)$$

$$w_t = w_P^*|_t - d_w|_t (P'_T - P'_P) = w_t^* - d_w|_t (P'_T - P'_P)$$

Substituting these velocities in the continuity equation leads to

$$\rho (u_e^* - d_u|_e (P'_E - P'_P)) S_e - \rho (u_w^* - d_u|_w (P'_P - P'_W)) S_w +$$

$$\rho (v_n^* - d_v|_n (P'_N - P'_P)) S_n - \rho (v_s^* - d_v|_s (P'_P - P'_S)) S_s +$$

$$\rho (w_t^* - d_w|_t (P'_T - P'_P)) S_t - \rho (w_b^* - d_w|_b (P'_P - P'_B)) S_b = 0$$

The arrangement of terms of  $\vec{V}^*$  to the right hand side gives the so called pressure correction equation.

$$a_{P,P'} P'_P + \sum_{NGB} a_{NGB,P'} P'_{NGB} = b_{P'}$$

Where

$$a_{W,P'} = D_w A(Pe_w) + \max(F_w, 0)$$

$$a_{E,P'} = D_e A(Pe_e) + \max(-F_e, 0)$$

$$a_{S,P'} = D_s A(Pe_s) + \max(F_s, 0)$$

$$a_{N,P'} = D_n A(Pe_n) + \max(-F_n, 0)$$

$$a_{B,P'} = D_b A(Pe_b) + \max(F_b, 0)$$

$$a_{T,P'} = D_t A(Pe_t) + \max(-F_t, 0)$$

$$a_{P,P'} = -(a_{W,P'} + a_{E,P'} + a_{S,P'} + a_{N,P'} + a_{B,P'} + a_{T,P'})$$

$$b_{P'} = \rho u_w^* S_w - \rho u_e^* S_e + \rho v_s^* S_s - \rho v_n^* S_n + \rho w_b^* S_b - \rho w_t^* S_t$$

Solving this system of algebraic equations the desired map of pressure corrections  $P'$  is obtained. With it, the pressure and velocities are corrected satisfying both criteria momentum and continuity.

Finally, the system of equations for the temperature is solved with the corrected velocities. By doing so iteratively, the coupling between all variables  $\vec{V}$ ,  $P$  and  $T$  is achieved. The coupling of the segregated systems is summarized in the so called SIMPLE-like algorithm (see Alg. 1).

---

**Algorithm 1** SIMPLE-like
 

---

**start with**  $k = 0$   
 $\vec{V}^{(k)}, P^{(k)}, T^{(k)}$   
**do**  
   **new iteration**  $k = k + 1$   
   **guess fluid flow variables**  
      $\vec{V}^* = \vec{V}^{(k-1)}, P^* = P^{(k-1)}, T^* = T^{(k-1)}$   
   **evaluate coefficients of Navier-Stokes equation using:**  $\vec{V}^*, P^*, T^*$   
   **solve**  $a_{P,u} u_P^{(k)} + \sum_{NGB} a_{NGB,u} u_{NGB}^{(k)} = b_{P,u}$   
   **solve**  $a_{P,v} v_P^{(k)} + \sum_{NGB} a_{NGB,v} v_{NGB}^{(k)} = b_{P,v}$   
   **solve**  $a_{P,w} w_P^{(k)} + \sum_{NGB} a_{NGB,w} w_{NGB}^{(k)} = b_{P,w}$   
   **evaluate coefficients of continuity equation using:**  $\vec{V}^{(k)}$   
   **solve**  $a_{P,P'} P_P'^{(k)} + \sum_{NGB} a_{NGB,P'} P_{NGB}'^{(k)} = b_{P,P'}$   
   **correct the velocity and the pressure**  
      $\vec{V}^{(k)} = \vec{V}^{(k)} + \alpha_V \vec{V}'^{(k)}$   
      $P^{(k)} = P^{(k)} + \alpha_P P'^{(k)}$   
   **evaluate coefficients of energy equation using:**  $\vec{V}^{(k)}, T^*$   
   **solve**  $a_{P,T} T_P^{(k)} + \sum_{NGB} a_{NGB,T} T_{NGB}^{(k)} = b_{P,T}$   
**until** (mass, momentum and energy conservation)

---

Notice that the velocities and pressures are underrelaxed with  $\alpha_V, \alpha_P$  for convergence at time of the correction step. Typical values of these parameters are  $\alpha_V = 0.5$  and  $\alpha_P = 0.8$ .

### 2.2.2 Time marching algorithm

The algorithm outlined below enable us to evaluate all variables for a given instant of time  $\tau$ , say  $\vec{V}^\tau, P^\tau$  and  $T^\tau$  under the initial conditions at previous time step  $\tau - \Delta\tau$ . This algorithm so called time marching [32] is carried out advancing in time until arriving at the steady state of all variables.

This algorithm completes the full simulation from an initial state which originates an unsteady state and the evolution to a final steady state. The full algorithm (see Alg. 2) including the time marching and coupling of systems is written down.

**Algorithm 2** SIMPLE-like plus time marching

---

```

start with  $\tau = 0$ 
 $\vec{V}^\tau, P^\tau, T^\tau$ 
do

  new time step  $\tau = \tau + \Delta\tau$ 
  start with  $k = 0$ 
 $\vec{V}^{(k)} = \vec{V}^{\tau-\Delta\tau}, P^{(k)} = P^{\tau-\Delta\tau}, T^{(k)} = T^{\tau-\Delta\tau}$ 
  do

    new iteration  $k = k + 1$ 
    guess fluid flow variables
 $\vec{V}^* = \vec{V}^{(k-1)}, P^* = P^{(k-1)}, T^* = T^{(k-1)}$ 

    evaluate coefficients of Navier-Stokes equations using:  $\vec{V}^*, P^*, T^*$ 
    solve  $a_{P,u} u_P^{(k)} + \sum_{NGB} a_{NGB,u} u_{NGB}^{(k)} = b_{P,u}$ 
    solve  $a_{P,v} v_P^{(k)} + \sum_{NGB} a_{NGB,v} v_{NGB}^{(k)} = b_{P,v}$ 
    solve  $a_{P,w} w_P^{(k)} + \sum_{NGB} a_{NGB,w} w_{NGB}^{(k)} = b_{P,w}$ 

    evaluate coefficients of continuity equation using:  $\vec{V}^{(k)}$ 
    solve  $a_{P,P'} P_P'^{(k)} + \sum_{NGB} a_{NGB,P'} P_{NGB}'^{(k)} = b_{P,P'}$ 

    correct the velocity and the pressure
 $\vec{V}^{(k)} = \vec{V}^{(k)} + \alpha_V \vec{V}'^{(k)}$ 
 $P^{(k)} = P^{(k)} + \alpha_P P'^{(k)}$ 

    evaluate coefficients of energy equation using:  $\vec{V}^{(k)}, T^*$ 
    solve  $a_{P,T} T_P^{(k)} + \sum_{NGB} a_{NGB,T} T_{NGB}^{(k)} = b_{P,T}^{(k)}$ 

  until (mass, momentum and energy conservation)
 $\vec{V}^\tau = \vec{V}^{(k)}, P^\tau = P^{(k)}, T^\tau = T^{(k)}$ 

until (steady state of all variables)

```

---

**2.2.3 Calculation of the time step**

In previous sections a spatial  $\Delta x, \Delta y, \Delta z$  and temporal  $\Delta\tau$  discretizations of the CFD problem were supposed. Since the formulation is fully implicit, there is no stability criterion that needs to be met in determining the time step  $\Delta\tau$ . However, in order to model the transient phenomena properly, it is necessary to set  $\Delta\tau$  at least one order of magnitude smaller than the smallest time constant in the system being modeled. A good way to judge the choice of  $\Delta\tau$  is to observe the number of iterations SIMPLE-like algorithm needs to converge at each time step. The ideal number of iterations per time step is 10-20. If SIMPLE-like algorithm needs substantially more, the time step is too large. If SIMPLE-like algorithm needs only a few iterations per time step,  $\Delta\tau$  may be increased. Frequently a time-dependent problem has a very fast startup transient that decays rapidly. It is thus often wise to choose a conservatively small  $\Delta\tau$  for the first 5-10 time steps.  $\Delta\tau$  may then

be gradually increased as the calculation proceeds.

At glance, a conservative approach [36] to  $\Delta\tau$  for implicit methods is obtained from an explicit criteria based on the Courant-Friedrichs-Levy condition (CFL) and applied to all  $ijk$  point of the domain:

$$\Delta t \leq \min_{ijk} \left( \left[ \frac{|u|}{\Delta x} + \frac{|v|}{\Delta y} + \frac{|w|}{\Delta z} + 2\mu \left( \frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2} \right) \right]^{-1} \right)$$

The physical meaning underlying this expression is that, the time step  $\Delta\tau$  has to be small enough to take account of variations of fluid flow due to the convection and diffusion effects produced in small regions of dimension  $\mathcal{V} = \Delta x \times \Delta y \times \Delta z$ .

## 2.3 Boundary conditions

In previous section, the time marching algorithm and the set of initial conditions were described and they closed the problem in the temporal direction. With respect to the spatial directions, the problem is constrained by the boundary conditions. Due to the importance of the discretization of the boundary conditions this section is reserved.

### 2.3.1 Dirichlet and Neumann conditions

The first kind of boundary conditions to be treated is the Dirichlet boundary condition. It sets a prescribed value  $\bar{\phi}$  to the variable  $\phi$  at fixed points  $P$  of the domain.

$$\phi|_P = \bar{\phi}$$

An example of this condition for viscous flows is the non-slip condition  $\vec{V}_{wall} = 0$  that appears in wall bounded viscous flows (see Fig. 2.3).

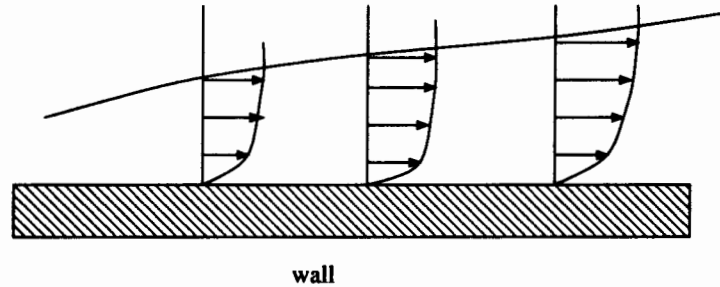


Figure 2.3: Velocity profiles and non-slip boundary condition at wall due to the viscous effects.

This condition is added to the rest of equations of momentum in their respective directions as

$$u|_{wall} = 0, \quad v|_{wall} = 0, \quad w|_{wall} = 0$$

If the problem has inlets the value of the velocity at these entrances is prescribed with either a fixed value or a velocity profile. For thermal problems, some regions of the domain can be fixed at a prescribed distribution of temperatures.

$$T|_{wall} = \bar{T}$$

In general, the Dirichlet condition is translated into an algebraic expression and included within the rest of the algebraic equations in order to close the system. The set of coefficients that represents this condition are

$$a_{P,\phi} = 1, \quad b_{P,\phi} = \bar{\phi}, \quad a_{NGB,\phi} = 0$$

The second kind of boundary condition is the Neumann boundary condition. It is associated to the numerical treatment of the phenomena where the derivative of the variable  $\phi$  is prescribed. Let  $P$  be a point of the boundary of the domain, the prescription with a value  $\bar{q}_\phi$  is written as

$$\left. \frac{\partial \phi}{\partial x} \right|_P = \bar{q}_\phi$$

For example, the free-slip condition or the null derivative of velocities should be fixed at outlets, where the structure of the flow remains constant downstream. For instance, a fully developed channel flow should consider this condition written as

$$\left. \frac{\partial \vec{V}}{\partial x} \right|_{outlet} = 0$$

For wall bounded domains and due to the non-slip condition, a zero pressure gradient at the pressure correction equation is set.

$$\left. \frac{\partial P}{\partial x} \right|_W = 0, \quad \left. \frac{\partial P}{\partial x} \right|_E = 0$$

$$\left. \frac{\partial P}{\partial y} \right|_S = 0, \quad \left. \frac{\partial P}{\partial y} \right|_N = 0$$

$$\left. \frac{\partial P}{\partial z} \right|_B = 0, \quad \left. \frac{\partial P}{\partial z} \right|_T = 0$$

For thermal problems, Neumann conditions describe heat fluxes (e.g. adiabatic walls).

$$\left. \frac{\partial T}{\partial x} \right|_W = \bar{q}_T$$

See Fig. 2.4 for a schematic representation of the points involved in the discretization of the adiabatic wall condition.

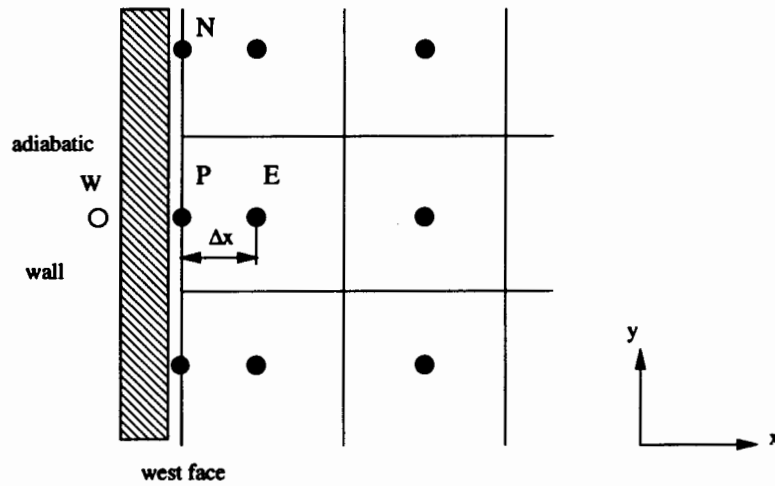


Figure 2.4: Adiabatic wall at west face of a domain.

Analogously to the Dirichlet condition, the Neumann condition is translated to an algebraic expression and included within the rest of algebraic equations and closing the system. For instance, let us to specify an adiabatic wall condition in the west face of a square box domain. The adiabatic wall condition is mathematically expressed as:

$$-\Gamma \frac{\partial T}{\partial x} \Big|_w = 0$$

Using the Taylor's series the derivative is expanded and truncated to the first term.

$$-\Gamma \frac{\partial T}{\partial x} \Big|_w = -\Gamma \frac{T_E - T_P}{\Delta x} = 0$$

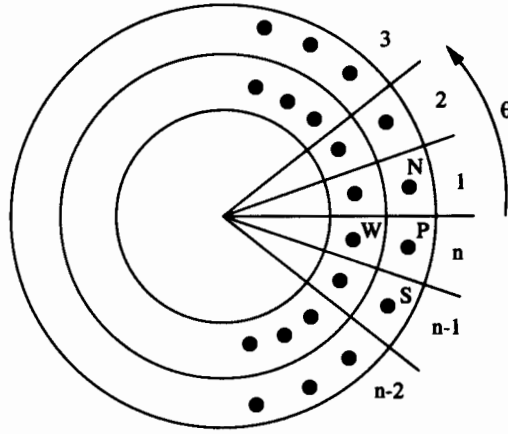
And rearranging terms it yields

$$a_{P,T} = 1, \quad a_{E,T} = -1, \quad b_{P,T} = 0, \quad a_{NGB,T} = 0$$

Discretization of these boundary conditions with higher accuracies [37] are out of scope of this work.

### 2.3.2 Periodic condition

For those problems where the discretization is done in the cylindrical coordinate system, there appears a spatial periodicity condition in the angular direction  $\theta$ . That implies a connection between the variables at the beginning and end of the angular coordinate. Fig. 2.5 shows graphically this connection.

Figure 2.5: Periodicity in the angular direction  $\theta$ .

Where

$$\phi_{N,n} = \phi_{P,n+1} = \phi_{P,1}$$

$$\phi_{S,1} = \phi_{P,0} = \phi_{P,n}$$

There are two ways to implement these conditions and to close the system of equations. The first one is simply adding explicitly the periodicity by including the two previous expressions in the system as follows:

$$\theta = n + 1, \quad a_{P,\phi} = 1, \quad b_{P,\phi} = \phi_{P,1}, \quad a_{NGB,\phi} = 0$$

$$\theta = 0, \quad a_{P,\phi} = 1, \quad b_{P,\phi} = \phi_{P,n}, \quad a_{NGB,\phi} = 0$$

A similar treatment [38] is also used in cartesian coordinate systems for periodic and antiperiodic boundary conditions where an inlet flow is given by the outlet flow.

The second one is considering implicitly the periodicity in the solver and then no additional algebraic equations are needed. This implicit treatment of the periodicity will be discussed in the next chapter.

## 2.4 Stopping criteria for a simulation

An important issue in a simulation is the stopping criteria. The stopping criteria have mainly to cover two issues: the coupling and the transition to the steady state.

The first one is the coupling between the velocity field  $\vec{V}$ , the pressure  $P$  and the temperature  $T$  at each time step. For this purpose, after the correction of velocities (mass balance satisfied), the balance of momentum of each component of the velocity field and the balance of energy must be guaranteed.

The measure of the conservation of the momentum and energy is summarized into a global value by joining all balances previously normalized and non dimensionalized. The normalization adopted in this work is based on the 2-norm  $\|\cdot\|_2$  of the residual  $r^{(k)}$  at a given iteration  $k$  of each algebraic system.

Rewriting each algebraic systems of equations for their respective variable  $\phi = \{u, v, w, T\}$  for a given  $k$  iteration, there are:

$$A_u^{(k)} u^{(k)} = b_u^{(k)} \longrightarrow r_u^{(k)} = b_u^{(k)} - A_u^{(k)} u^{(k)}$$

$$A_v^{(k)} v^{(k)} = b_v^{(k)} \longrightarrow r_v^{(k)} = b_v^{(k)} - A_v^{(k)} v^{(k)}$$

$$A_w^{(k)} w^{(k)} = b_w^{(k)} \longrightarrow r_w^{(k)} = b_w^{(k)} - A_w^{(k)} w^{(k)}$$

$$A_T^{(k)} T^{(k)} = b_T^{(k)} \longrightarrow r_T^{(k)} = b_T^{(k)} - A_T^{(k)} T^{(k)}$$

where  $A_\phi^{(k)}$  is the matrix of coefficients,  $\phi^{(k)}$  the variable expressed as a vector and the right hand side  $b_\phi^{(k)}$  another vector, all of them at iteration  $k$ .

The normalization and nondimensionalization, say  $coupling_\phi^{(k)}$ , is evaluated by

$$coupling_\phi^{(k)} = \frac{\|r_\phi^{(k)}\|_2}{\|b_\phi^{(k)}\|_2}$$

The addition of all of these quantities is the overall criterion of coupling of the systems for a given time step  $t$ .

$$coupling^{(k)} = coupling_u^{(k)} + coupling_v^{(k)} + coupling_w^{(k)} + coupling_T^{(k)}$$

Another coupling criterion based on the mass balance may be used rather than the described above. The reason is that the coupling among systems is strongly affected by the velocities and pressure. Hence the guarantee of the continuity (after the correction step) for each volume and in overall is an enough criterion to ensure the coupling among all variables.

The normalized mass balance based coupling criterion may be written as

$$coupling^{(k)} = \frac{\sqrt{\sum_{ijk} (\rho u_w^{(k)} S_w - \rho u_e^{(k)} S_e + \rho v_s^{(k)} S_s - \rho v_n^{(k)} S_n + \rho w_b^{(k)} S_b - \rho w_t^{(k)} S_t)^2}}{\frac{\sum_{ijk} \rho V}{\Delta \tau}}$$

The second issue is the transition of the fluid flow from the unsteady state to the steady state. After the steady state there is no need to continue evaluating the variables at new time steps. Therefore a simply comparison of each variable in two close time steps is enough to decide if the steady state is achieved. For a given variable  $\phi$  evaluated at time step  $\tau$  the steady state  $steady_\phi^t$  is measured as follows:

$$steady_\phi^\tau = \frac{\sum_{ijk} |\phi^\tau - \phi^{\tau-\Delta\tau}|}{\sum_{ijk} |\phi^\tau|}$$

where  $|\cdot|$  is the absolute value of the quantity between bars.

Since the steady state of the fluid flow is achieved when all variables have arrived at the steady state, all measures in a single value are joined:

$$steady^\tau = steady_u^\tau + steady_v^\tau + steady_w^\tau + steady_T^\tau$$



Once evaluate both measures  $coupling^{(k)}$  and  $steady^T$  the stopping criteria for numerical simulations is fixed in the following values:

$$coupling^{(k)} \leq 10^{-6}, \quad steady^T \leq 10^{-3}$$

These values have been chosen experimentally in order to guarantee the numerical coupling of variables at each time step and an estimated situation of the steady state. Higher values of the coupling criterion may not ensure convergence of the pressure correction system or produce inaccurate field solutions. And higher values of the steady criterion may stop a slow fluid flow transition, for example in natural convection phenomena. Conversely, smaller values of the steady criterion may never stop the algorithm. The numerical perturbations of the algorithm and solvers masquerade the steady fluid flow state, and hence, the sensibility of the criterion cannot detect that the simulation has already reached the steady state.

## 2.5 Nomenclature

$A$	discretization matrix
$a$	coeff. in $A$
$b$	discretization right hand side
$CV$	control volume
$c_p$	specific heat
$D$	diffusion coefficient
$d$	coeff. of the pressure diff. term
$F$	flow rate through the $CV$ face
$f$	general face
$\vec{g}$	gravitational force
$P$	pressure
$Pe$	Peclet number
$q$	net flux
$r$	residual, radial coordinate
$S$	general source term
$T$	temperature
$\vec{V}$	fluid flow velocity vector
$\{u, v, w\}$	fluid flow velocity components
$\{x, y, z\}$	cartesian coordinates
$\{r, \theta, z\}$	cylindrical coordinates

### Greek symbols

$\beta$	thermal volumetric expansion coeff.
$\Delta$	general width of a $CV$
$\Delta r$	$r$ -direction width of $CV$
$\Delta x$	$x$ -direction width of $CV$
$\Delta y$	similar to $\Delta x$
$\Delta z$	similar to $\Delta x$
$\Delta \tau$	time step
$\Delta \theta$	similar to $\Delta x$
$\Gamma$	general diffusion coeff.
$\kappa$	thermal conductivity
$\epsilon$	precision
$\mu$	dynamic viscosity
$\nu$	kinematic viscosity
$\rho$	density
$\phi$	general dependent variable
$\tau$	time
$\theta$	angular coordinate

### Other symbols

$S$	surface of $CV$
$\mathcal{V}$	volume of $CV$

### Subscripts

$B$	neighbour at the bottom
$b$	$CV$ face between $P$ and $B$
$E$	neighbour at the east side
$e$	$CV$ face between $P$ and $E$
$N$	neighbour on the north side
$NGB$	general neighbour grid point
$n$	$CV$ face between $P$ and $N$
$P$	central grid point
$S$	neighbour on the south side
$s$	$CV$ face between $P$ and $S$
$T$	neighbour at the top
$t$	$CV$ face between $P$ and $T$
$W$	neighbour at the west side
$w$	$CV$ face between $P$ and $W$

### Superscripts

$(k)$	$k$ -th iteration
$\tau$	time value
*	guessed value
'	correction value
-	prescribed value