Gas dynamics and Heat and Mass Transfer

Numerical Solution of the Convection–Diffusion Equations

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Contents

1 Convection–diffusion equations

In this section we derive the continuity equation and the general convection–diffusion equation. To begin, we present and prove Reynolds Transport Theorem, which is a generalization of Leibniz integral rule. Next we deduce the aforementioned equations using this theorem.

1.1 Notation and assumption

First of all, we shall introduce some notation that will be exhaustively used in the project.

- Let Ω be a subset of $\mathbb{R}^n$. The subsets $\partial\Omega$ and $\overline{\Omega}$ of $\mathbb{R}^n$ will denote the boundary and the closure of Ω, respectively.
- Let $x \in \mathbb{R}^n$ and $R > 0$. We will denote by $B(x,R) = \{y \in \mathbb{R}^n \mid \|x-y\| < R\}$ the open ball centered at x of radius R. The set $\overline{B(x,R)} = \{y \in \mathbb{R}^n \mid \|x-y\| \leq R\}$ is the closure $B(x,R)$.
- Let $U \subset \mathbb{R}^n$ be an open set. We will denote by $\mathcal{C}^k(U,\mathbb{R}^m)$ the set of k times continously differentiable functions $f\colon U \to \mathbb{R}^m$. If the codomain is clear from the context, we will use $\mathcal{C}^k(U)$. The set of continuous functions $f\colon U \to \mathbb{R}^m$ will be denoted $\mathcal{C}(U,\mathbb{R}^m)$ or $\mathcal{C}(U)$ when the codomain is clear.
- The velocity of a fluid will be the vector field $\mathbf{v} = \mathbf{v}(x,t)$. When working in $\mathbb{R}^2$ it will be written as $\mathbf{v} = u\mathbf{i} + v\mathbf{j}$.

Hereinafter, if $\mathcal{V} \subset \mathbb{R}^n$ is a control volume, we will assume it satisfies the following:

(i) $\mathcal{V}$ is an open set of $\mathbb{R}^n$, i.e. for all $x \in \mathcal{V}$ there exists $R > 0$ such that $B(x,R) \subset \mathcal{V}$.

(ii) $\mathcal{V}$ is bounded, that is to say, there exist $x_0 \in \mathbb{R}^n$ and $R > 0$ such that $\mathcal{V} \subset B(x_0,R)$.

(iii) $\mathcal{V}$ is a $\mathcal{C}^1$–domain. This implies that for every point $x \in \partial\mathcal{V}$ there exists a system of coordinates $(y_1,\ldots,y_{n-1},y_n) \equiv (\mathbf{y}',y_n)$ with origin at x, a ball $B(x,R)$ and a function φ defined in an open subset $\mathcal{N} \subset \mathbb{R}^{n-1}$ containing $\mathbf{y}' = \mathbf{0}'$, such that [1]:
   (a) $\varphi(\mathbf{0}') = 0$ and $\varphi \in \mathcal{C}^1(\mathcal{N},\mathbb{R})$ (φ is a $\mathcal{C}^1$ function from $\mathcal{N}$ to $\mathbb{R}$),
   (b) $\partial\mathcal{V} \cap B(x,R) = \{(\mathbf{y}',y_n) \mid y_n = \varphi(\mathbf{y}'),\ \mathbf{y}' \in \mathcal{N}\}$,
   (c) $\mathcal{V} \cap B(x,R) = \{(\mathbf{y}',y_n) \mid y_n > \varphi(\mathbf{y}'),\ \mathbf{y}' \in \mathcal{N}\}$.

Condition (i) will be useful to cast an integral equation into a differential equation. Condition (ii) prevents the integral of a continuous function defined on $\overline{\mathcal{V}}$ from becoming infinite. Moreover, an unbounded control volume, that is to say, a subset of $\mathbb{R}^n$ that extends indefinitely, makes no physical sense. Condition (iii), which is more technical, will allow us to apply vector calculus theorems.

Finally, we shall assume that all physical magnitudes, such as the velocity field $\mathbf{v}$, the density ρ or the temperature T are differentiable functions on their domains of definition as many times as necessary.

1.2 Reynolds Transport Theorem

Before stating and proving Reynolds Transport Theorem, we tackle the simpler Leibniz integral rule. To gain some physical intuition on it, suppose we have a very thin tube along the x–axis containing a fluid in motion. In this context we may assume that the fluid only moves along the tube direction. Let $f = f(x,t)$ be a magnitude of the fluid, for instance, the velocity u, the temperature T or the

concentration of some chemical species Y. So as to study how this magnitude variates on a portion of fluid, we consider a control volume $U(t) = [a(t), b(t)]$ that depends upon time. This situation is picture in figure 1.1. The total ammount of magnitude f in the control volume at time t, which we will denote by $\mathcal{F}(t)$, is given by

$$\mathcal{F}(t) = \int_{a(t)}^{b(t)} f(x,t)\,\mathrm{d}x \tag{1.1}$$

and its rate of variation

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}(t) = \frac{\mathrm{d}}{\mathrm{d}t}\int_{a(t)}^{b(t)} f(x,t)\,\mathrm{d}x \tag{1.2}$$

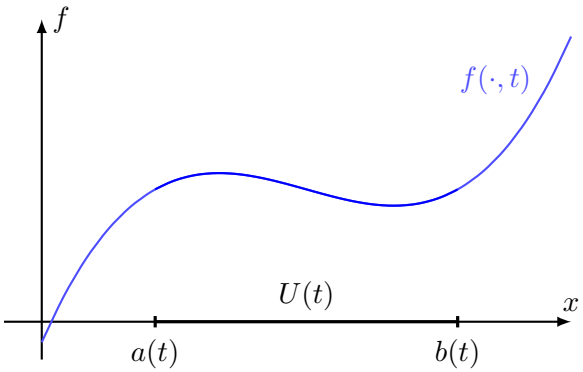


Figure 1.1. Control volume and magnitude f at time t.

Computing the derivative in equation (1.2) can be difficult depending on the case. Here is where Leibniz integral rule comes into play:

Theorem 1.1 (Leibniz integral rule)**.** Let $U \subset \mathbb{R}$ be a closed bounded interval and let $I = [t_1, t_2]$ be the time interval. Let $a, b\colon I \to U$ be differentiable functions with continuous derivative. Let $f\colon U \times I \to \mathbb{R}$, $(x,t) \mapsto f(x,t)$ be a differentiable function such that $\frac{\partial f}{\partial t}$ is also continuous. Then for all $t \in (t_1, t_2)$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{a(t)}^{b(t)} f(x,t)\,\mathrm{d}x = \int_{a(t)}^{b(t)} \frac{\partial f}{\partial t}\,\mathrm{d}x + f(b(t),t)b'(t) - f(a(t),t)a'(t) \tag{1.3}$$

Proof. See [2]. □

Consider the more general case where we have a fluid in n–dimensional space $\mathbb{R}^n$ and magnitude $f = f(x,t)$ defined on a control volume $\mathcal{V}(t) \subset \mathbb{R}^n$. The total ammount of f on $\mathcal{V}$ at time t and its variation are given by similar formulas,

$$\mathcal{F}(t) = \int_{\mathcal{V}(t)} f(x,t)\,\mathrm{d}x\,, \quad \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}(t) = \frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{V}(t)} f(x,t)\,\mathrm{d}x \tag{1.4}$$

however now computing the derivative might be impracticable. In this case we have Reynolds Transport Theorem:

Theorem 1.2 (Reynolds Transport Theorem [3])**.** Let $U \subset \mathbb{R}^n$ be a compact set (i.e. U is closed and bounded) and let $\mathcal{V}(t)$ be a control volume depending on time such that $\mathcal{V} \subset U$ for all $t \in I = [0, T]$ with $T > 0$. Let $\mathcal{S}(t) = \partial\mathcal{V}(t)$ be the boundary of $\mathcal{V}(t)$ and let $F \in \mathcal{C}^1(U \times I, \mathbb{R})$ be a scalar field.

Then for all $t \in I$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{V}(t)} F(x,t)\,\mathrm{d}x = \int_{\mathcal{V}(t)} \frac{\partial F}{\partial t}(x,t)\,\mathrm{d}x + \int_{\mathcal{S}(t)} F(x,t)\mathbf{b}\cdot\mathbf{n}\,\mathrm{d}S \tag{1.5}$$

where $\mathbf{b}\colon \mathcal{S}(t) \to \mathbb{R}^n$ is the local velocity of the control surface.

Proof. The moving control volume $\mathcal{V}(t)$ can be seen as the image of an initial region $\mathcal{V}(0)$ by a family of $\mathcal{C}^1$ maps $\xi\colon U \times I \subset \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$, that is to say, $\mathcal{V}(t) = \xi(\mathcal{V}(0), t)$ for all $t \in I$. Furthermore, by fixing one time t, the mapping $\xi(\cdot, t)\colon \mathcal{V}(0) \to \mathcal{V}(t)$ can be assumed to be a diffeomorphism. Since F is continuous, we can apply the Change of Variables Theorem taking $x = \xi(x_0, t)$,

$$\int_{\mathcal{V}(t)} F(x,t)\,\mathrm{d}x = \int_{\mathcal{V}(0)} F(\xi(x_0,t),t)\left|\det\left(\frac{\partial \xi}{\partial x_0}(x_0,t)\right)\right|\mathrm{d}x_0$$

where the determinant of the jacobian matrix $\det\left(\frac{\partial \xi}{\partial x_0}(x_0,t)\right)$ can be assumed to be positive for small enough T, hence the absolute value is dropped. Applying differentiation under the integral sign (Theorem A.1) with respect to t yields

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{V}(t)} F(x,t)\,\mathrm{d}x &= \int_{\mathcal{V}(0)} \frac{\partial}{\partial t}\left\{F(\xi(x_0,t),t)\ \det\left(\frac{\partial \xi}{\partial x_0}(x_0,t)\right)\right\}\mathrm{d}x_0 \\ &= \int_{\mathcal{V}(0)} \frac{\partial}{\partial t}\left\{F(\xi(x_0,t),t)\right\}\det\left(\frac{\partial \xi}{\partial x_0}(x_0,t)\right)\mathrm{d}x_0 + \int_{\mathcal{V}(0)} F(\xi(x_0,t),t)\,\frac{\partial}{\partial t}\left\{\det\left(\frac{\partial \xi}{\partial x_0}(x_0,t)\right)\right\}\mathrm{d}x_0\end{aligned}$$

On the one hand,

$$\frac{\partial}{\partial t}\left\{F(\xi(x_0,t),t)\right\}\det\left(\frac{\partial \xi}{\partial x_0}(x_0,t)\right) = \left\{\frac{\partial F}{\partial t}(\xi(x_0,t),t) + \boldsymbol{\nabla} F(\xi(x_0,t),t)\cdot\xi_t(x_0,t)\right\}\det\left(\frac{\partial \xi}{\partial x_0}(x_0,t)\right)$$

where $\xi_t = \frac{\partial \xi}{\partial t}$. On the other hand, using matrix calculus,

$$F(\xi(x_0,t),t)\,\frac{\partial}{\partial t}\left\{\det\left(\frac{\partial \xi}{\partial x_0}(x_0,t)\right)\right\} = F(\xi(x_0,t),t)\det\left(\frac{\partial \xi}{\partial x_0}(x_0,t)\right)\boldsymbol{\nabla}\cdot\xi_t(x_0,t)$$

Thereby the integral is written as

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{V}(t)} F(x,t)\,\mathrm{d}x &= \int_{\mathcal{V}(0)}\left\{\frac{\partial F}{\partial t} + \boldsymbol{\nabla}F\cdot\xi_t + F\boldsymbol{\nabla}\cdot\xi_t\right\}\det\left(\frac{\partial \xi}{\partial x_0}\right)\mathrm{d}x_0 \\ &= \int_{\mathcal{V}(0)}\left\{\frac{\partial F}{\partial t} + \boldsymbol{\nabla}\cdot(F\xi_t)\right\}\det\left(\frac{\partial \xi}{\partial x_0}\right)\mathrm{d}x_0\end{aligned}$$

So as to obtain an integral over $\mathcal{V}(t)$, the previous change of variables is reverted, that is, $x_0 = \xi^{-1}(x,t)$. In order not to complicate notation, let $\mathbf{b}(x,t) = \xi_t(\xi^{-1}(x,t),t)$, then

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{V}(t)} F(x,t)\,\mathrm{d}x = \int_{\mathcal{V}(t)}\left\{\frac{\partial F}{\partial t} + \boldsymbol{\nabla}\cdot(F\mathbf{b})\right\}(x,t)\,\mathrm{d}x$$

For a fixed $x_0 \in \mathcal{V}(0)$, $\xi(x_0,\cdot)$ is a function of time giving how x_0 moves, hence $\xi_t(x_0,t)$ is the instantaneous velocity of x_0. To end, an application of divergence theorem yields the final formula:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{V}(t)} F(x,t)\,\mathrm{d}x = \int_{\mathcal{V}(t)} \frac{\partial F}{\partial t}(x,t)\,\mathrm{d}x + \int_{\mathcal{S}(t)} F(x,t)\mathbf{b}\cdot\mathbf{n}\,\mathrm{d}S$$

□

1.3 Continuity equation

For the purposes of this project, where no nuclear nor relativistic effects are considered, mass is a property preserved over time. Let $\mathcal{V} \subset \mathbb{R}^n$ be a control volume, which may depend on time, and let $\rho = \rho(x,t)$ be the mass density defined over $\mathcal{V}$ for each time $t \in I$. The mass enclosed by $\mathcal{V}$ at time t is

$$m(t) = \int_{\mathcal{V}(t)} \rho(x,t)\,\mathrm{d}x = \int_{\mathcal{V}(t)} \rho\,\mathrm{d}x \tag{1.6}$$

and as a result of the mass conservation principle

$$\frac{\mathrm{d}}{\mathrm{d}t} m(t) = \frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathcal{V}(t)} \rho(x,t)\,\mathrm{d}x = 0 \tag{1.7}$$

Now applying Reynolds Transport Theorem to (1.7) setting $\mathbf{b} = \mathbf{v}$,

$$\int_{\mathcal{V}(t)} \frac{\partial \rho}{\partial t}\,\mathrm{d}x + \int_{\mathcal{S}(t)} \rho\mathbf{v}\cdot\mathbf{n}\,\mathrm{d}S = 0 \tag{1.8}$$

We apply the divergence theorem on the surface integral to transform it into a volume integral,

$$\int_{\mathcal{V}(t)} \frac{\partial \rho}{\partial t}\,\mathrm{d}x + \int_{\mathcal{V}(t)} \boldsymbol{\nabla}\cdot(\rho\mathbf{v})\,\mathrm{d}x = \int_{\mathcal{V}(t)} \left\{\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\mathbf{v})\right\}\mathrm{d}x = 0 \tag{1.9}$$

We claim that the integrand in equation (1.9) vanishes at every point in space and time. Indeed, assume there exists a time t_0 and a point $x_0 \in \mathcal{V}(t_0)$ such that

$$\left\{\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\mathbf{v})\right\}\Big|_{(x_0,t_0)} > 0 \tag{1.10}$$

Recall that we assumed the physical magnitudes are differentiable functions as many times as necessary. In particular, by fixing $t = t_0$, $(\partial_t\rho + \boldsymbol{\nabla}\cdot(\rho\mathbf{v}))(\cdot,t_0)$ is a continuous function of x. Since $\mathcal{V}(t_0)$ is open, there exists $\tilde{\delta} > 0$ such that $B(x_0,\tilde{\delta}) \subset \mathcal{V}(t_0)$. By continuity we can take $\delta > 0$, with $\delta < \tilde{\delta}$ such that for all $y \in B(x_0,\delta) \subset \mathcal{V}(t_0)$,

$$\left\{\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\mathbf{v})\right\}\Big|_{(y,t_0)} > 0 \tag{1.11}$$

Hence integrating on $B(x_0,\delta)$ yields

$$\int_{B(x_0,\delta)} \left\{\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\mathbf{v})\right\}\mathrm{d}x > 0 \tag{1.12}$$

a contradiction as it should be zero according to equation (1.9). The same contradiction is reached if we assume the existence of a point x_0 and a time t_0 where

$$\left\{\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\mathbf{v})\right\}\Big|_{(x_0,t_0)} < 0 \tag{1.13}$$

thereby proving our claim. Because this is true for each $x_0 \in \mathcal{V}(t_0)$ and $t_0 \in I$ is arbitrary, we obtain the continuity equation

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\mathbf{v}) = 0 \tag{1.14}$$

1.4 General convection–diffusion equation

Let $\mathcal{V} \subset \mathbb{R}^n$ be a control volume which may depend on time $t \in I \subset \mathbb{R}$ and let $\phi\colon \mathbb{R}^n \times I \to \mathbb{R}$, $(x,t) \mapsto \phi(x,t)$ be a magnitude of the fluid (such as the concentration of some chemical substance) per unit of mass. Then the total ammount of ϕ in $\mathcal{V}(t)$ is

$$\Phi(t) = \int_{\mathcal{V}(t)} \rho(x,t)\phi(x,t)\,\mathrm{d}x \tag{1.15}$$

and its variation over time is

$$\dot{\Phi}(t) = \frac{\mathrm{d}}{\mathrm{d}t}\Phi(t) = \frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{V}(t)} \rho(x,t)\phi(x,t)\,\mathrm{d}x \tag{1.16}$$

The variation of Φ is a consequence of two contributions: the flux of ϕ through the control surface $\mathcal{S}(t)$ and the generation/elimination of ϕ in $\mathcal{V}(t)$ due to source terms. Let $\mathbf{f}\colon \mathbb{R} \times \mathcal{S} \times I \to \mathbb{R}^n$, $(\phi,x,t) \mapsto \mathbf{f}(\phi,x,t)$ be the vector field which gives the flux of ϕ through $\mathcal{S}$. Then the total ammount of ϕ flowing through $\mathcal{S}(t)$ is given by

$$\mathscr{F}(t) = \int_{\mathcal{S}(t)} \mathbf{f}(\phi,x,t)\cdot\mathbf{n}\,\mathrm{d}S \tag{1.17}$$

In order to find out which sign has $\mathscr{F}(t)$, we may assume for a moment that there are no source terms. If $\mathscr{F}(t) > 0$, then ϕ is exiting $\mathcal{V}(t)$ and, as a result, $\dot{\Phi}(t) < 0$. Conversely, if $\mathscr{F}(t) < 0$, then $\dot{\Phi}(t) > 0$, therefore $\dot{\Phi}(t)$ and $F(t)$ have opposite signs. Now, let $\dot{s}_\phi\colon \to \mathbb{R}$ be te source term, which provides the ammount of ϕ generated/eliminated in $\mathcal{V}(t)$ per unit of time. Then the total ammount of ϕ generated/eliminated in $\mathcal{V}(t)$ is

$$\mathscr{S}(t) = \int_{\mathcal{V}(t)} \dot{s}_\phi(\phi,x,t)\,\mathrm{d}x \tag{1.18}$$

Assume that there is no flux of ϕ through $\mathcal{S}(t)$, that is to say, $\mathscr{F}(t) = 0$. If ϕ is generated in $\mathcal{V}(t)$, then $\mathscr{S}(t) > 0$, which implies $\dot{\phi}(t) > 0$; whereas if $\mathscr{S}(t) < 0$ then $\dot{\phi}(t) > 0$, thus $\dot{\phi}(t)$ and $\mathscr{S}(t)$ have the same sign. Introducing these terms in (1.16) leads to

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{V}(t)} \rho(x,t)\phi(x,t)\,\mathrm{d}x = -\int_{\mathcal{S}(t)} \mathbf{f}(\phi,x,t)\cdot\mathbf{n}\,\mathrm{d}S + \int_{\mathcal{V}(t)} \dot{s}_\phi(\phi,x,t)\,\mathrm{d}x \tag{1.19}$$

Hereinafter we shall become less formal by omitting on which variables depends each function. In order to relate the flux $\mathbf{f}$ and ϕ, we need to apply some constitutive law. Fourier's law for heat conduction and Fick's law for concentration state that $\mathbf{f}$ depends linearly on the gradient of ϕ with respect to the spatial variables [4], that is,

$$\mathbf{f} = -\Gamma_\phi \boldsymbol{\nabla}_x \phi = -\Gamma_\phi \begin{pmatrix} \dfrac{\partial\phi}{\partial x_1} & \cdots & \dfrac{\partial\phi}{\partial x_n} \end{pmatrix}^T \tag{1.20}$$

where Γ_ϕ is known as the diffusion coefficient. So as not to complicate the notation, we will write $\boldsymbol{\nabla}\phi$ in place of $\boldsymbol{\nabla}_x\phi$. Recall that $\boldsymbol{\nabla}\phi \in \mathbb{R}^n$ gives the direction of maximum growth of $\phi(\cdot,t)$ (the time is fixed because the gradient is computed with respect to x). The minus sign in (1.20) is the consequence of heat (concentration of a chemical) flowing from regions of higher to lower temperature (concentration) regions. With this in mind, equation (1.19) is rewritten as

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{V}(t)} \rho\phi\,\mathrm{d}x = \int_{\mathcal{S}(t)} \Gamma_\phi \boldsymbol{\nabla}\phi\cdot\mathbf{n}\,\mathrm{d}S + \int_{\mathcal{V}(t)} \dot{s}_\phi\,\mathrm{d}x \tag{1.21}$$

and applying Reynolds Transport Theorem on the left–hand side of (1.21) with $\mathbf{b} = \mathbf{v}$,

$$\int_{\mathcal{V}(t)} \frac{\partial(\rho\phi)}{\partial t}\,\mathrm{d}x + \int_{\mathcal{S}(t)} \rho\phi\mathbf{v}\cdot\mathbf{n}\,\mathrm{d}S = \int_{\mathcal{S}(t)} \Gamma_\phi \boldsymbol{\nabla}\phi\cdot\mathbf{n}\,\mathrm{d}S + \int_{\mathcal{V}(t)} \dot{s}_\phi\,\mathrm{d}x \tag{1.22}$$

To turn surface integrals into volume integrals we apply divergence theorem,

$$\int_{\mathcal{V}(t)} \frac{\partial(\rho\phi)}{\partial t}\,\mathrm{d}x + \int_{\mathcal{V}(t)} \boldsymbol{\nabla}\cdot(\rho\phi\mathbf{v})\,\mathrm{d}x = \int_{\mathcal{V}(t)} \boldsymbol{\nabla}\cdot(\Gamma_\phi\boldsymbol{\nabla}\phi)\,\mathrm{d}x + \int_{\mathcal{V}(t)} \dot{s}_\phi\,\mathrm{d}x \tag{1.23}$$

Proceeding in a similar way to the continuity equation, we assume the existence of a time t_0 and a point x_0 where

$$\left\{\frac{\partial(\rho\phi)}{\partial t}\,\mathrm{d}x + \boldsymbol{\nabla}\cdot(\rho\phi\mathbf{v})\,\mathrm{d}x - \boldsymbol{\nabla}\cdot(\Gamma_\phi\boldsymbol{\nabla}\phi)\,\mathrm{d}x - \dot{s}_\phi\,\mathrm{d}x\right\}\Big|_{(x_0,t_0)} \neq 0 \tag{1.24}$$

and we reach a contradiction, thereby obtaining the general convection diffusion equation:

$$\frac{\partial(\rho\phi)}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\phi\mathbf{v}) = \boldsymbol{\nabla}\cdot(\Gamma_\phi\boldsymbol{\nabla}\phi) + \dot{s}_\phi \tag{1.25}$$

The left–hand side of (1.25) can be expanded to find

$$\phi\left\{\frac{\partial\rho}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\mathbf{v})\right\} + \rho\frac{\partial\phi}{\partial t} + \rho\mathbf{v}\cdot\boldsymbol{\nabla}\phi = \boldsymbol{\nabla}\cdot(\Gamma_\phi\boldsymbol{\nabla}\phi) + \dot{s}_\phi \tag{1.26}$$

Since the term between keys is the continuity equation, (1.26) is simplified to

$$\rho\frac{\partial\phi}{\partial t} + \rho\mathbf{v}\cdot\boldsymbol{\nabla}\phi = \boldsymbol{\nabla}\cdot(\Gamma_\phi\boldsymbol{\nabla}\phi) + \dot{s}_\phi \tag{1.27}$$

Equations (1.25) and (1.27) are two equivalent forms of the same equation, each having its applications and benefits.

By taking ϕ to be the temperature T of the fluid or the concentration of the k–th chemical substance Y_k in the fluid, one obtains the energy conservation equation (1.28) and the k–species equation (1.29) [5]:

$$\frac{\partial(\rho T)}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\mathbf{v}T) = \boldsymbol{\nabla}\cdot\left(\frac{\lambda}{c_v}\boldsymbol{\nabla}T\right) + \left\{\frac{\tau\circ\boldsymbol{\nabla}\mathbf{v} - \boldsymbol{\nabla}\cdot\dot{\mathbf{q}}^R - p\boldsymbol{\nabla}\cdot\mathbf{v}}{c_v}\right\} \tag{1.28}$$

$$\frac{\partial(\rho Y_k)}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\mathbf{v}Y_k) = \boldsymbol{\nabla}\cdot(\rho D_{km}\boldsymbol{\nabla}Y_k) + \{\dot{\omega}_k\} \tag{1.29}$$

If ϕ is not a scalar magnitude but a vector magnitude, i.e. $\phi \equiv (\phi_1,\ldots,\phi_n)\colon \mathbb{R}^n\times I \to \mathbb{R}^n$, $(x,t)\mapsto\phi(x,t)$, the same process applied on each component function ϕ_i leads to n equations similar to (1.25) that can be gathered in the following vector equation

$$\frac{\partial(\rho\phi)}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\mathbf{v}\otimes\phi) = \boldsymbol{\nabla}\cdot(\mu\boldsymbol{\nabla}\phi) + \dot{s}_\phi \tag{1.30}$$

where $\mathbf{v}\otimes\phi$ is the exterior product:

$$\mathbf{v}\otimes\phi = \begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix}\begin{pmatrix} \phi_1 & \cdots & \phi_n \end{pmatrix} = \begin{pmatrix} v_1\phi_1 & \cdots & v_1\phi_n \\ \vdots & \ddots & \vdots \\ v_n\phi_1 & \cdots & v_n\phi_n \end{pmatrix} \tag{1.31}$$

The previous product can also be regarded as the tensor product of two 1–covariant tensors which yields a 2–covariant tensor. Notice that, in general, this product is not commutative, that is to say, $\mathbf{v}\otimes\phi \neq \phi\otimes\mathbf{v}$.

By taking ϕ to be the velocity $\mathbf{v}$ of the fluid, the momentum conservation equation is obtained [5]:

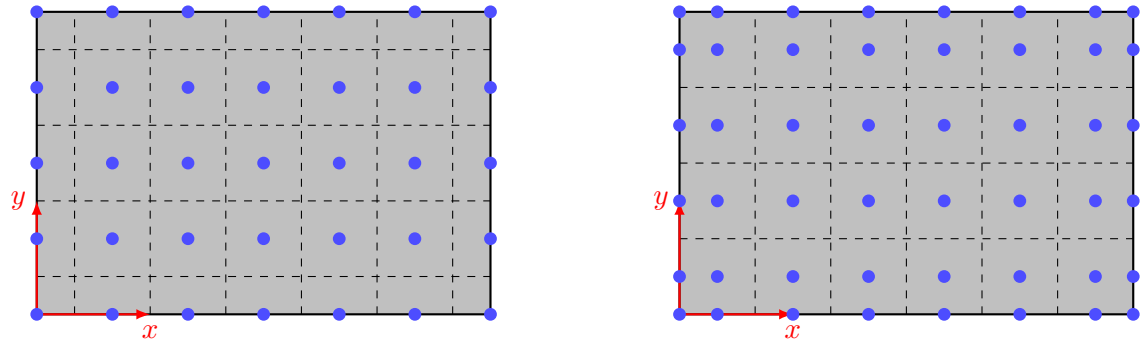
$$\frac{\partial(\rho\mathbf{v})}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\mathbf{v}\otimes\mathbf{v}) = \boldsymbol{\nabla}\cdot(\mu\boldsymbol{\nabla}\mathbf{v}) + \{\boldsymbol{\nabla}\cdot(\tau - \mu\boldsymbol{\nabla}\mathbf{v}) - \boldsymbol{\nabla}p + \rho\mathbf{g}\} \tag{1.32}$$

2 Numerical study of the convection–diffusion equations

2.1 Spatial and time discretization

The type of problems we will addressed in this project occur in a bounded rectangular domain $\Omega \subset \mathbb{R}^2$, that is to say, there exist non–degenerate intervals $[0, L]$ and $[0, W]$ such that $\Omega = [0, L] \times [0, W]$. In order to solve the problem numerically we shall follow a control–volume formulation. This methodology discretizes the domain into nonoverlapping control volumes along with a grid of points named discretization nodes. The resulting discretized domain is named mesh or numerical grid [6].

There exist several types of grids according to the shape of control volumes and the ammount of subdivisions the domain has been partitioned into, namely, a structured (regular) grid, a block–structured grid and an unstructured grid [7]. However, henceforth we will only consider structured regular grids. This formulation allows for two manners to discretize the domain, namely, cell–centered and node–centered discretizations. The former places discretization nodes over the domain and generates a control–volume centered on each node. The latter first generates the control–volumes, next places a node at the center of each one and finally sets nodes at the border if necessary.



(a) Cell–centered uniform discretization. **(b)** Node–centered uniform discretization.

Figure 2.1. Comparison of the cell–centered and the node–centered uniform discretizations.

As it can be noticed when uniform discretizations are used, the node–centered discretization approach offers higher resolution near the boundary of the domain. Notwithstanding, it also generates singular nodes located at the corners which need a special treatment, whilst the cell–centered does not. Furthermore, we can distinguish between uniform discretizations, where distances between adjacent internal nodes are constant along the domain, and non–uniform discretizations, meaning the opposite.

Later we will deal with the discretization of the convection–diffusion equations in a cell–centered discretized domain. In order to enumerate the nodes, we will start from the lower left corner of Ω, where node $(0, 0)$ is located. We will use the notation (i, j) to refer the i–th node in x–coordinate and j–th node in y–coordinate. Given an arbitrary node (i, j) that we denote by P, its neighbour nodes are the west node $(i - 1, j)$, the east node $(i + 1, j)$, the south node $(i, j - 1)$ and the north node $(i, j + 1)$. This scheme is pictured in figure 2.2. The calligraphic letter $\mathcal{V}$ will be used to denote a control volume. For instance, $\mathcal{V}_P$ is the control volume associated to node P. The volume of $\mathcal{V}_P$ is V_P. The notation $\mathcal{S}_{Pi}$ will denote the interface between the control volumes $\mathcal{V}_P$ and $\mathcal{V}_I$. As an example, $\mathcal{S}_{Pw}$ is the surface between the control volumes $\mathcal{V}_P$ and $\mathcal{V}_W$. The distance between the control volumes associated to nodes A and B is $d_{AB} = \|(x_A - x_B, y_A - y_B)\|$. The distance between the node P and one of its control surfaces i is given by d_{Pi}, for example, d_{Pw}.

In regards to time, the problems we consider last for finite time. Therefore the time interval is $I = [0, T] \subset \mathbb{R}$ with $T > 0$ finite. The discretization of I is simply a partition of it, that is to say, a

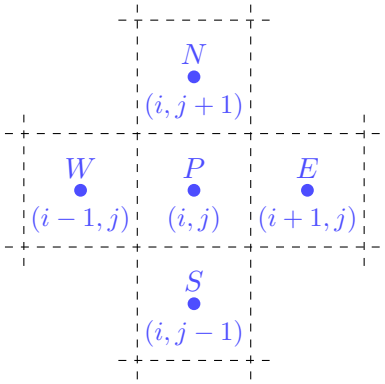


Figure 2.2. Central node P and neighbour nodes.

finite set of points $P(I) = \{t_0 = 0, t_1, \ldots, t_{m-1}, t_m = T\}$ with $t_{i+1} > t_i$ for all $0 \leq i < m$. The time discretization is said to uniform whenever there exists $\Delta t > 0$ such that $t_{i+1} - t_i = \Delta t$ for all i, and non–uniform otherwise. In the case of a uniform time discretization, the number Δt is know as time step. We shall only consider uniform time discretizations, nevertheless non–uniform discretizations might be convenient in problems combining fast and low transient processes.

2.2 Discretization of the continuity equation

As we have previously seen, the continuity equation in differential form is

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \mathbf{v}) = 0 \quad (x, t) \in \Omega \times I \tag{2.1}$$

Since the above relation is true in $\Omega \times I$, fixing one time $t \in I$ and integrating over a control volume $\mathcal{V}_P \subset \Omega$ gives

$$\int_{\mathcal{V}_P} \frac{\partial \rho}{\partial t} \, \mathrm{d}x + \int_{\mathcal{V}_P} \boldsymbol{\nabla} \cdot (\rho \mathbf{v}) \, \mathrm{d}x = 0 \tag{2.2}$$

Let $\mathcal{S}_P = \partial \mathcal{V}_P$ be the control surface, i.e. the boundary of the control volume. Then applying the divergence theorem on the second term of equation (2.2),

$$\int_{\mathcal{V}_P} \frac{\partial \rho}{\partial t} \, \mathrm{d}x + \int_{\mathcal{S}_P} \rho \mathbf{v} \cdot \mathbf{n} \, \mathrm{d}S = 0 \tag{2.3}$$

So as to simplify the first term of (2.3), we define the average density of the control volume as

$$\overline{\rho}_P = \frac{1}{V_P} \int_{\mathcal{V}_P} \rho \, \mathrm{d}x \tag{2.4}$$

Introducing this relation in equation (2.3),

$$\frac{\mathrm{d}\overline{\rho}_P}{\mathrm{d}t} V_P + \int_{\mathcal{S}_P} \rho \mathbf{v} \cdot \mathbf{n} \, \mathrm{d}S = 0 \tag{2.5}$$

The mass flow term can be further simplified because we know the geometry of the boundary of $\mathcal{V}_P$. Since the control surface is $\mathcal{S}_P = \mathcal{S}_{Pe} \cup \mathcal{S}_{Pw} \cup \mathcal{S}_{Pn} \cup \mathcal{S}_{Ps}$, we can rewrite the mass flow term as

$$\begin{aligned} \int_{\mathcal{S}_P} \rho \mathbf{v} \cdot \mathbf{n} \, \mathrm{d}S &= \underbrace{\int_{\mathcal{S}_{Pe}} \rho \mathbf{v} \cdot \mathbf{n} \, \mathrm{d}S}_{\dot{m}_e} + \underbrace{\int_{\mathcal{S}_{Pw}} \rho \mathbf{v} \cdot \mathbf{n} \, \mathrm{d}S}_{-\dot{m}_w} + \underbrace{\int_{\mathcal{S}_{Pn}} \rho \mathbf{v} \cdot \mathbf{n} \, \mathrm{d}S}_{\dot{m}_n} + \underbrace{\int_{\mathcal{S}_{Ps}} \rho \mathbf{v} \cdot \mathbf{n} \, \mathrm{d}S}_{-\dot{m}_s} \\ &= \dot{m}_e - \dot{m}_w + \dot{m}_n - \dot{m}_s \end{aligned} \tag{2.6}$$

Since evaluating each integral may be computationally expensive or impossible, the following approach is followed. Given a face f, the normal outer vector is constant on $\mathcal{S}_{Pf}$. Indeed, if $\mathbf{n}_f$ denotes the normal outer vector to face f, then $\mathbf{n}_e = \mathbf{i}$, $\mathbf{n}_w = -\mathbf{i}$, $\mathbf{n}_n = \mathbf{j}$ and $\mathbf{n}_s = -\mathbf{j}$. Since $\mathbf{v} = u\mathbf{i} + v\mathbf{j}$, the dot products are $\mathbf{v}\cdot\mathbf{n}_e = u$, $\mathbf{v}\cdot\mathbf{n}_w = -u$ and so on. Moreover, the integrand $(\rho\mathbf{v}\cdot\mathbf{n})_f$ can be approximated by the value each term takes at the face center, i.e.

$$(\rho\mathbf{v}\cdot\mathbf{n})_f \approx \rho_f(\mathbf{v}\cdot\mathbf{n})_f \tag{2.7}$$

Therefore the integral over $\mathcal{S}_{Pe}$ on equation (2.6) is simplified as follows:

$$\int_{\mathcal{S}_{Pe}} \rho\mathbf{v}\cdot\mathbf{n}\,\mathrm{d}S \approx \int_{\mathcal{S}_{Pe}} (\rho\mathbf{v}\cdot\mathbf{n})_e\,\mathrm{d}S \approx \int_{\mathcal{S}_{Pe}} \rho_e(\mathbf{v}\cdot\mathbf{n})_e)\,\mathrm{d}S = \int_{\mathcal{S}_{Pe}} \rho_e u_e\,\mathrm{d}S = \rho_e u_e S_{Pe} =: \dot{m}_e \tag{2.8}$$

The same simplifications are applied to the other integrals. Defining $\dot{m}_w$ and $\dot{m}_s$ as the negative integral makes the mass flow terms be positive in the positive coordinate direction. Introducing these in (2.5) yields

$$\frac{\mathrm{d}\overline{\rho}_P}{\mathrm{d}t}V_P + \dot{m}_e - \dot{m}_w + \dot{m}_n - \dot{m}_s = 0 \tag{2.9}$$

The average density of the control volume is roughly the density at the discretization node, i.e. $\overline{\rho}_P \approx \rho_P$. Integrating (2.9) over the time interval $[t^n, t^{n+1}]$ gives

$$V_P \int_{t^n}^{t^{n+1}} \frac{\mathrm{d}\rho_P}{\mathrm{d}t}\,\mathrm{d}t + \int_{t^n}^{t^{n+1}} (\dot{m}_e - \dot{m}_w + \dot{m}_n - \dot{m}_s)\,\mathrm{d}t = 0 \tag{2.10}$$

The first term of (2.10) has a straightforward simplification applying a corollary of the fundamental theorem of calculus. Regarding the second term, numerical integration is used,

$$\begin{aligned}(\rho_P^{n+1} - \rho_P^n)V_P + \beta(\dot{m}_e^{n+1} - \dot{m}_w^{n+1} + \dot{m}_n^{n+1} - \dot{m}_s^{n+1})(t^{n+1} - t^n) \\ + (1-\beta)(\dot{m}_e^n - \dot{m}_w^n + \dot{m}_n^n - \dot{m}_s^n)(t^{n+1} - t^n) = 0\end{aligned} \tag{2.11}$$

where $\beta \in \{0, \frac{1}{2}, 1\}$ depends on the chosen integration scheme. For the sake of simplicity, superindex $n+1$ shall be dropped and the time instant n will be denoted by the superindex 0. Since we assume a uniform time discretization with time step Δt, the resulting discretized continuity equation is

$$\frac{\rho_P - \rho_P^0}{\Delta t}V_P + \beta(\dot{m}_e - \dot{m}_w + \dot{m}_n - \dot{m}_s) + (1-\beta)(\dot{m}_e^0 - \dot{m}_w^0 + \dot{m}_n^0 - \dot{m}_s^0) = 0 \tag{2.12}$$

Finally, when an implicit scheme is selected for the time integration,

$$\frac{\rho_P - \rho_P^0}{\Delta t}V_P + \dot{m}_e - \dot{m}_w + \dot{m}_n - \dot{m}_s = 0 \tag{2.13}$$

If a 3D–mesh is being used, the contributions of top (T) and bottom (B) nodes must be considered. In this case, the control surface is the union $\mathcal{S}_P = \mathcal{S}_{Pe} \cup \mathcal{S}_{Pw} \cup \mathcal{S}_{Pn} \cup \mathcal{S}_{Ps} \cup \mathcal{S}_{Pt} \cup \mathcal{S}_{Pb}$, hence equation (2.13) incorporates two new terms

$$\frac{\rho_P - \rho_P^0}{\Delta t}V_P + \dot{m}_e - \dot{m}_w + \dot{m}_n - \dot{m}_s + \dot{m}_t - \dot{m}_b = 0 \tag{2.14}$$

2.3 Discretization of the general convection–diffusion equation

The generalized convection–diffusion for a real valued function $\phi\colon \Omega \times I \subset \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}$ is

$$\frac{\partial(\rho\phi)}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\mathbf{v}\phi) = \boldsymbol{\nabla}\cdot(\Gamma_\phi\boldsymbol{\nabla}\phi) + \dot{s}_\phi, \quad (x,t) \in \Omega \times I \tag{2.15}$$

whereas for a vector valued function $\phi = (\phi_1, \ldots, \phi_n)\colon \Omega \times I \subset \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$ it is written as

$$\frac{\partial(\rho\phi)}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \mathbf{v} \otimes \phi) = \boldsymbol{\nabla} \cdot (\Gamma_\phi \boldsymbol{\nabla}\phi) + \dot{s}_\phi, \quad (x,t) \in \Omega \times I \tag{2.16}$$

where $\otimes$ denotes the outer product of $\mathbf{v}\colon \Omega \times I \subset \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$ and ϕ, which is a $n \times n$ matrix. Since the generalized convection–diffusion equation for a vector valued function actually comprises n equations, one for each component function, we will only study the discretization for a real valued function.

Integrating (2.15) over $\mathcal{V}_P \times [t^n, t^{n+1}] \subset \Omega \times I$ and using Fubini's theorem (Fubini's theorem) to swap the order of integration

$$\int_{t^n}^{t^{n+1}} \int_{\mathcal{V}_P} \frac{\partial(\rho\phi)}{\partial t} \,\mathrm{d}x\,\mathrm{d}t + \int_{t^n}^{t^{n+1}} \int_{\mathcal{V}_P} \boldsymbol{\nabla} \cdot (\rho \mathbf{v} \phi) \,\mathrm{d}x\,\mathrm{d}t = \\ = \int_{t^n}^{t^{n+1}} \int_{\mathcal{V}_P} \boldsymbol{\nabla} \cdot (\Gamma_\phi \boldsymbol{\nabla}\phi) \,\mathrm{d}x\,\mathrm{d}t + \int_{t^n}^{t^{n+1}} \int_{\mathcal{V}_P} \dot{s}_\phi \,\mathrm{d}x\,\mathrm{d}t \tag{2.17}$$

The simplification of the first term is analogous to that of the continuity equation. The average value of $\rho\phi$ on $\mathcal{V}_P$ at time t is defined by

$$(\rho\phi)_P = \frac{1}{V_P} \int_{\mathcal{V}_P} \rho\phi \,\mathrm{d}x \tag{2.18}$$

although the following approximation is needed:

$$(\rho\phi)_P \approx \rho_P \phi_P \tag{2.19}$$

Then the transient term is:

$$\int_{t^n}^{t^{n+1}} \int_{\mathcal{V}_P} \frac{\partial(\rho\phi)}{\partial t} \,\mathrm{d}x\,\mathrm{d}t = \int_{t^n}^{t^{n+1}} \frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathcal{V}_P} \rho\phi \,\mathrm{d}x\,\mathrm{d}t = \int_{t^n}^{t^{n+1}} \frac{\mathrm{d}(\rho\phi)_P}{\mathrm{d}t} V_P \,\mathrm{d}t \approx \left\{\rho_P \phi_P - \rho_P^0 \phi_P^0\right\} V_P \tag{2.20}$$

Divergence theorem must be applied to simplify the convective term,

$$\int_{t^n}^{t^{n+1}} \int_{\mathcal{V}_P} \boldsymbol{\nabla} \cdot (\rho \mathbf{v} \phi) \,\mathrm{d}x\,\mathrm{d}t = \int_{t^n}^{t^{n+1}} \int_{\mathcal{S}_P} \rho\phi \mathbf{v} \cdot \mathbf{n} \,\mathrm{d}S\,\mathrm{d}t = \int_{t^n}^{t^{n+1}} \sum_i \int_{\mathcal{S}_{Pi}} \rho\phi \mathbf{v} \cdot \mathbf{n} \,\mathrm{d}S\,\mathrm{d}t \tag{2.21}$$

The value that ϕ takes on $\mathcal{S}_{Pi}$ can be approximated by its value at a representative point, for instance, the point at face center, that is to say, $\phi \approx \phi_i$. Therefore,

$$\int_{t^n}^{t^{n+1}} \sum_i \int_{\mathcal{S}_i} \rho\phi \mathbf{v} \cdot \mathbf{n} \,\mathrm{d}S\,\mathrm{d}t \approx \int_{t^n}^{t^{n+1}} \sum_i \int_{\mathcal{S}_i} \rho\phi_i \mathbf{v} \cdot \mathbf{n} \,\mathrm{d}S\,\mathrm{d}t = \int_{t^n}^{t^{n+1}} \sum_i \dot{m}_i \phi_i \,\mathrm{d}t = \\ = \left\{\beta \sum_i \dot{m}_i \phi_i + (1-\beta) \sum_i \dot{m}_i^0 \phi_i^0\right\} \Delta t \tag{2.22}$$

In regard to the diffusion term,

$$\int_{t^n}^{t^{n+1}} \int_{\mathcal{V}_P} \boldsymbol{\nabla} \cdot (\Gamma_\phi \boldsymbol{\nabla}\phi) \,\mathrm{d}x\,\mathrm{d}t = \int_{t^n}^{t^{n+1}} \int_{\mathcal{S}_P} \Gamma_\phi \boldsymbol{\nabla}\phi \cdot \mathbf{n} \,\mathrm{d}S\,\mathrm{d}t = \int_{t^n}^{t^{n+1}} \sum_i \int_{\mathcal{S}_{Pi}} \Gamma_\phi \boldsymbol{\nabla}\phi \cdot \mathbf{n} \,\mathrm{d}S\,\mathrm{d}t \tag{2.23}$$

The outer normal vector to the face $\mathcal{S}_{Pi}$ is constant and points in the direction of some coordinate axis, hence the dot product $\boldsymbol{\nabla}\phi \cdot \mathbf{n}$ in the face $\mathcal{S}_{Pi}$ equals the partial derivative with respect to x_i

times ± 1, depending on the direction of $\mathbf{n}$. For east, north and top faces the sign is positive, whilst for west, south and bottom faces the sign is negative. Again, Γ_ϕ will be approximated by the value at the face center, and partial derivatives will be approximated by a finite centered difference. In order to simplify the notation, we shall drop the subindex ϕ in the diffusion coefficient Γ_ϕ and define the coefficients

$$D_f = \frac{\Gamma_f S_f}{d_{PF}} \tag{2.24}$$

$$D_f^0 = \frac{\Gamma_f^0 S_f}{d_{PF}} \tag{2.25}$$

where f and F refer to the face and to the node, respectively. For a 2D–mesh, equation (2.23) results in

$$\begin{aligned}
&\int_{t^n}^{t^{n+1}} \sum_i \int_{\mathcal{S}_{Pi}} \Gamma_\phi \boldsymbol{\nabla}\phi \cdot \mathbf{n}\, \mathrm{d}S\, \mathrm{d}t \approx \\
&\approx \int_{t^n}^{t^{n+1}} \Big\{ D_e(\phi_E - \phi_P) - D_w(\phi_P - \phi_W) + D_n(\phi_N - \phi_P) - D_s(\phi_P - \phi_S) \Big\}\, \mathrm{d}t \approx \\
&\approx \beta \left\{ D_e(\phi_E - \phi_P) - D_w(\phi_P - \phi_W) + D_n(\phi_N - \phi_P) - D_s(\phi_P - \phi_S) \right\} \Delta t + \\
&+ (1-\beta) \Big\{ D_e^0(\phi_E - \phi_P) - D_w^0(\phi_P - \phi_W) + D_n^0(\phi_N - \phi_P) - D_s^0(\phi_P - \phi_S) \Big\} \Delta t
\end{aligned} \tag{2.26}$$

In the case of a 3D–mesh, the contributions of top and bottom faces must be accounted for.

So as to discretize the source term, the mean value of the source function in $\mathcal{V}_P$ at time t is given by

$$\overline{\dot{s}}_\phi = \frac{1}{V_P} \int_{\mathcal{V}_P} \dot{s}_\phi \, \mathrm{d}x \tag{2.27}$$

If the value of s_ϕ is known, the relation $\overline{\dot{s}}_\phi = \dot{\overline{s}}_\phi$ is true. Indeed, applying differentiation under the integral sign (Theorem A.1)

$$\dot{\overline{s}}_\phi = \frac{\mathrm{d}}{\mathrm{d}t}\overline{s}_\phi = \frac{1}{V_P}\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{V}_P} s_\phi \, \mathrm{d}x = \frac{1}{V_P}\int_{\mathcal{V}_P} \dot{s}_\phi \, \mathrm{d}x = \overline{\dot{s}}_\phi \tag{2.28}$$

In most cases, the dependence of $\dot{\overline{s}}_\phi$ on ϕ is complicated. Since the equations obtained until now are linear, the relation between the source term and the variable would ideally be linear. This linearity is imposed as follows

$$\dot{\overline{s}}_\phi = S_C^\phi + S_P^\phi \phi_P \tag{2.29}$$

where the values of S_C^ϕ and S_P^ϕ may vary with ϕ [6]. Making use of these relations, the source term integral is discretized as

$$\int_{t^n}^{t^{n+1}} \int_{\mathcal{V}_P} \dot{s}_\phi \, \mathrm{d}x \, \mathrm{d}t = \int_{t^n}^{t^{n+1}} \dot{\overline{s}}_{\phi P} V_P \Delta t = \left(S_C^\phi + S_P^\phi \phi_P \right) V_P \Delta t \tag{2.30}$$

As we shall discuss later, the term S_P^ϕ must be non–positive.

The discretization of the 2D generalized convection–diffusion equation is

$$\begin{aligned}
&\frac{\rho_P\phi_P - \rho_P^0\phi_P^0}{\Delta t}V_P + \\
&+ \beta\Big(\dot{m}_e\phi_e - \dot{m}_w\phi_w + \dot{m}_n\phi_n - \dot{m}_s\phi_s\Big) + (1-\beta)\left(\dot{m}_e^0\phi_e^0 - \dot{m}_w^0\phi_w^0 + \dot{m}_n^0\phi_n^0 - \dot{m}_s^0\phi_s^0\right) = \\
&= \beta\Big\{D_e(\phi_E - \phi_P) - D_w(\phi_P - \phi_W) + D_n(\phi_N - \phi_P) - D_s(\phi_P - \phi_S)\Big\} + \\
&+ (1-\beta)\Big\{D_e^0(\phi_E^0 - \phi_P^0) - D_w^0(\phi_P^0 - \phi_W^0) + D_n^0(\phi_N^0 - \phi_P^0) - D_s^0(\phi_P^0 - \phi_S^0)\Big\} + \\
&+ \left(S_C^\phi + S_P^\phi\phi_P\right)V_P
\end{aligned} \tag{2.31}$$

In the case of a implicit integration scheme, i.e. $\beta = 1$, equation (2.31) is simplified to:

$$\begin{aligned}
&\frac{\rho_P\phi_P - \rho_P^0\phi_P^0}{\Delta t}V_P + \dot{m}_e\phi_e - \dot{m}_w\phi_w + \dot{m}_n\phi_n - \dot{m}_s\phi_s = \\
&\quad = D_e(\phi_E - \phi_P) - D_w(\phi_P - \phi_W) + D_n(\phi_N - \phi_P) - D_s(\phi_P - \phi_S) + (S_C^\phi + S_P^\phi\phi_P)V_P
\end{aligned} \tag{2.32}$$

An equivalent and more useful form of the discretization equation can be found by multiplying (2.13) times ϕ_P and subtracting it from (2.32), which results in

$$\begin{aligned}
&\rho_P^0\frac{\phi_P - \phi_P^0}{\Delta t}V_P + \dot{m}_e(\phi_e - \phi_P) - \dot{m}_w(\phi_w - \phi_P) + \dot{m}_n(\phi_n - \phi_P) - \dot{m}_s(\phi_s - \phi_P) = \\
&\quad = D_e(\phi_E - \phi_P) - D_w(\phi_P - \phi_W) + D_n(\phi_N - \phi_P) - D_s(\phi_P - \phi_S) + (S_C^\phi + S_P^\phi\phi_P)V_P
\end{aligned} \tag{2.33}$$

The 3D analog of (2.33) includes the top and bottom faces contributions:

$$\begin{aligned}
\rho_P^0\frac{\phi_P - \phi_P^0}{\Delta t}V_P &+ \dot{m}_e(\phi_e - \phi_P) - \dot{m}_w(\phi_w - \phi_P) + \dot{m}_n(\phi_n - \phi_P) \\
&- \dot{m}_s(\phi_s - \phi_P) + \dot{m}_t(\phi_t - \phi_P) - \dot{m}_b(\phi_b - \phi_P) \\
&= D_e(\phi_E - \phi_P) - D_w(\phi_P - \phi_W) + D_n(\phi_N - \phi_P) \\
&- D_s(\phi_P - \phi_S) + D_t(\phi_T - \phi_P) - D_b(\phi_P - \phi_B) + (S_C^\phi + S_P^\phi\phi_P)V_P
\end{aligned} \tag{2.34}$$

2.4 Evaluation of the convective terms

The discretized version of the generalized convection–diffusion equation requires the values of ϕ at points different from the nodes. In this subsection we study several methods to compute the value of ϕ at faces. We will assume that ρ and Γ are known at the nodal points. For the sake of simplicity, we will evaluate the convective term at east face, although the generalization to the remaining faces is straightforward. The references for this subsection are [6] and [8].

2.4.1 Upwind–Difference Scheme (UDS)

Incompressible flows and gases at low Mach number are more influenced by upstream conditions than downstream conditions. Let $(\mathbf{v}\cdot\mathbf{n})_e$ denote the value of the dot product $\mathbf{v}\cdot\mathbf{n}$ at east face $\mathcal{S}_{Pe}$. If $(\mathbf{v}\cdot\mathbf{n})_e > 0$, fluid flows from node P to node E, hence P is the upstream node and E is the downstream node. Conversely, if $(\mathbf{v}\cdot\mathbf{n})_e < 0$, nodes interchange their roles as fluid flows from node E to node P. Whenever $(\mathbf{v}\cdot\mathbf{n})_e = 0$, it implies that $\mathbf{v}_e$ lies in the orthogonal subspace to the vector space generated by $\mathbf{n}$. As a result, given the approximations taken, there is no fluid flow through face $\mathcal{S}_{Pe}$.

The Upwind–Difference Scheme assigns ϕ_e the value of ϕ at the upstream node, that is,

$$\phi_e = \begin{cases} \phi_P & \text{if } (\mathbf{v}\cdot\mathbf{n})_e > 0 \\ \phi_E & \text{if } (\mathbf{v}\cdot\mathbf{n})_e < 0 \end{cases} \tag{2.35}$$

The scheme is summarized in figures 2.3 and 2.4.

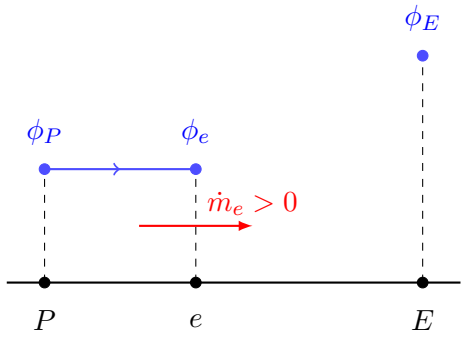


Figure 2.3. UDS when $(\mathbf{v}\cdot\mathbf{n})_e > 0$.

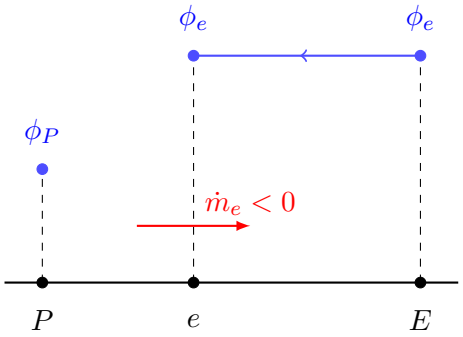


Figure 2.4. UDS when $(\mathbf{v}\cdot\mathbf{n})_e < 0$.

Equation (2.35) can be expressed in a more compact fashion as follows,

$$\dot{m}_e(\phi_e - \phi_P) = \frac{\dot{m}_e - |\dot{m}_e|}{2}(\phi_E - \phi_P) \tag{2.36}$$

since the approximation to compute $\dot{m}_e$ is related to $(\mathbf{v}\cdot\mathbf{n})_e$ through the relation $\dot{m}_e = (\mathbf{v}\cdot\mathbf{n})_e S_{Pe}$. The extension of (2.36) to the remaining faces is the following:

$$\dot{m}_w(\phi_w - \phi_P) = \frac{\dot{m}_w + |\dot{m}_w|}{2}(\phi_W - \phi_P) \tag{2.37}$$

$$\dot{m}_n(\phi_n - \phi_P) = \frac{\dot{m}_n - |\dot{m}_n|}{2}(\phi_N - \phi_P) \tag{2.38}$$

$$\dot{m}_s(\phi_s - \phi_P) = \frac{\dot{m}_s + |\dot{m}_s|}{2}(\phi_S - \phi_P) \tag{2.39}$$

UDS is a stable scheme, however it suffers from numerical diffusion. Indeed, assuming the upstream node is P, expanding ϕ about point x_P in its Taylor expansion up to 2^{nd} degree and using Lagrange's remainder,

$$\phi_e = \phi_P + \left(\frac{\partial\phi}{\partial x}\right)_P d_{Pe} + \left(\frac{\partial^2\phi}{\partial x^2}\right)_{\xi_1} \frac{d_{Pe}^2}{2} \tag{2.40}$$

it is apparent that UDS retains the first term on the left–hand side of (2.40). As a consequence, the error highest order is $(\partial_x\phi)_P d_{Pe}$, which is proportional to the distance between P and the face $\mathcal{S}_{Pe}$. This term resembles to a diffusion flux given, for instance, by Fourier's or Fick's laws of diffusion. The same result is obtained when E is the upstream node,

$$\phi_e = \phi_E - \left(\frac{\partial\phi}{\partial x}\right)_E d_{Ee} + \left(\frac{\partial^2\phi}{\partial x^2}\right)_{\xi_2} \frac{d_{Ee}^2}{2} \tag{2.41}$$

whence it can be deduced that the error is bounded by $\max\{|(\partial_x\phi)_E d_{Pe}|, |(\partial_x\phi)_E d_{Ee}|\}$. The numerical diffusion issue is magnified in multidimensional problems, where peaks of rapid variation can be obtained, hence very fine grids are required.

2.4.2 Central–Difference Scheme (CDS)

The Central–Difference Scheme assumes a linear distribution for ϕ as illustrated in figure 2.5.

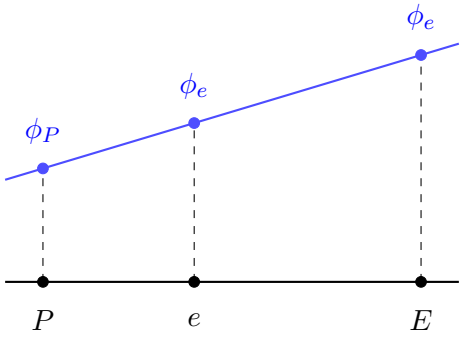


Figure 2.5. Central Difference Scheme (CDS).

Thereby ϕ_e can be obtained interpolating between ϕ_P and ϕ_E,

$$\phi_e - \phi_P = \frac{d_{Pe}}{d_{PE}}(\phi_E - \phi_P) \tag{2.42}$$

as well as the remaining faces values,

$$\phi_w - \phi_P = \frac{d_{Pw}}{d_{PW}}(\phi_W - \phi_P) \tag{2.43}$$

$$\phi_n - \phi_P = \frac{d_{Pn}}{d_{PN}}(\phi_N - \phi_P) \tag{2.44}$$

$$\phi_s - \phi_P = \frac{d_{Ps}}{d_{PS}}(\phi_S - \phi_P) \tag{2.45}$$

This yields a 2^{nd} order approximation for ϕ_e if $d_{Pe} = d_{Ee}$. In effect, applying Taylor's theorem about point x_e,

$$\phi_P = \phi_e - \left(\frac{\partial \phi}{\partial x}\right)_e d_{Pe} + \frac{1}{2}\left(\frac{\partial^2 \phi}{\partial x^2}\right)_e d_{Pe}^2 + \frac{1}{6}\left(\frac{\partial^3 \phi}{\partial x^3}\right)_{\xi_1} d_{Pe}^3 \tag{2.46}$$

The 2^{nd} order approximation of $(\partial_x \phi)_e$ is given by

$$\left(\frac{\partial \phi}{\partial x}\right)_e = \frac{\phi_E - \phi_P}{d_{PE}} - \left(\frac{\partial^3 \phi}{\partial x^3}\right)_{\xi_2} \frac{d_{PE}^2}{3!} = \frac{\phi_E - \phi_P}{d_{PE}} - \left(\frac{\partial^3 \phi}{\partial x^3}\right)_{\xi_2} \frac{(d_{Pe} + d_{Ee})^2}{3!} \tag{2.47}$$

Introducing (2.47) in (2.46) and imposing $d_{Pe} = d_{Ee}$,

$$\phi_e - \phi_P = \frac{d_{Pe}}{d_{PE}}(\phi_E - \phi_P) - \left(\frac{\partial^2 \phi}{\partial x^2}\right)_e \frac{d_{Pe}^2}{2} - \left\{\left(\frac{\partial^3 \phi}{\partial x^3}\right)_{\xi_1} + 4\left(\frac{\partial^3 \phi}{\partial x^3}\right)_{\xi_2}\right\} \frac{d_{Pe}^3}{6} \tag{2.48}$$

As CDS retains the first term on the left–hand side of (2.48), the highest order term of the error is $\frac{1}{2}(\partial_x^2 \phi)_e d_{Pe}^2$, proving that CDS provides a 2^{nd} order approximation of ϕ_e when $d_{Pe} = d_{Ee}$. Nonetheless, this scheme is prone to stability problems producing oscillatory outputs since the approximation is of order higher than 1.

2.4.3 Exponential–Difference Scheme (EDS)

The exponential difference scheme assumes a distribution for ϕ based on the steady 2–dimensional generalized convection–diffusion equation with no source term, that is to say,

$$\frac{\mathrm{d}}{\mathrm{d}x}(\rho u \phi) = \frac{\mathrm{d}}{\mathrm{d}x}\left(\Gamma \frac{\mathrm{d}\phi}{\mathrm{d}x}\right) \tag{2.49}$$

So as to ease the study, ρu and Γ are assumed to be constant. Thereby the initial value problem obtained is

$$\begin{cases} \dfrac{\mathrm{d}^2\phi}{\phi x^2} - \dfrac{\rho u}{\Gamma}\dfrac{\mathrm{d}\phi}{\mathrm{d}x} = 0 \quad \text{in } (x_P, x_E) \subset \mathbb{R} \\ \phi(x_P) = \phi_P \\ \phi(x_E) = \phi_E \end{cases} \tag{2.50}$$

Since the initial value problem (2.50) is a second order linear ODE with two boundary conditions, its solutions exists, is unique THEOREM, and is given by

$$\phi(x) = \phi_P + \frac{e^{\frac{\rho u}{\Gamma}(x - x_P)} - 1}{e^{\frac{\rho u}{\Gamma} d_{PE}} - 1}(\phi_E - \phi_P) \tag{2.51}$$

Péclet's number is defined as the ratio between of strengths of convection and diffusion [6],

$$\mathrm{Pe} = \frac{\text{convection transport rate}}{\text{diffusion transport rate}} = \frac{\rho u L}{\Gamma} \tag{2.52}$$

where L is a characteristic length of the problem. Taking d_{PE} as characteristic length and evaluating (2.51) at $x = x_e$, the approximation of ϕ_e given by EDS in terms of Péclet's number is written as

$$\phi_e - \phi_P = \frac{e^{\mathrm{Pe}_e \frac{d_{Pe}}{d_{PE}}} - 1}{e^{\mathrm{Pe}_e} - 1}(\phi_E - \phi_P) \tag{2.53}$$

The extension of (2.53) to the face f is done by taking d_{PF} as characteristic length, that is, if $f = w$, then the characteristic length is d_{PW}. Thereby EDS gives the following face values:

$$\phi_w = \left(1 - \frac{e^{\mathrm{Pe}_w \frac{d_{Ww}}{d_{PW}}} - 1}{e^{\mathrm{Pe}_w} - 1}\right)\phi_W + \frac{e^{\mathrm{Pe}_w \frac{d_{Ww}}{d_{PW}}} - 1}{e^{\mathrm{Pe}_w} - 1}\phi_P \tag{2.54}$$

$$\phi_n - \phi_P = \frac{e^{\mathrm{Pe}_n \frac{d_{Pn}}{d_{PN}}} - 1}{e^{\mathrm{Pe}_n} - 1}(\phi_N - \phi_P) \tag{2.55}$$

$$\phi_s = \left(1 - \frac{e^{\mathrm{Pe}_s \frac{d_{Ss}}{d_{PS}}} - 1}{e^{\mathrm{Pe}_s} - 1}\right)\phi_S + \frac{e^{\mathrm{Pe}_s \frac{d_{Ss}}{d_{PS}}} - 1}{e^{\mathrm{Pe}_s} - 1}\phi_P \tag{2.56}$$

2.4.4 Second–order Upwind Linear Extrapolation (SUDS)

As previously mentioned, incompressible flows and fluids at low Mach number are more influenced by upstream condition than by downstream conditions. In order to account for this fact and to ease the study, we introduce a new notation. When located at the face separating two control volumes, f refers to the face, D is the downstream node, C is the first upstream node and U is the most upstream node. Some books may use U and UU instead of C and U, respectively.

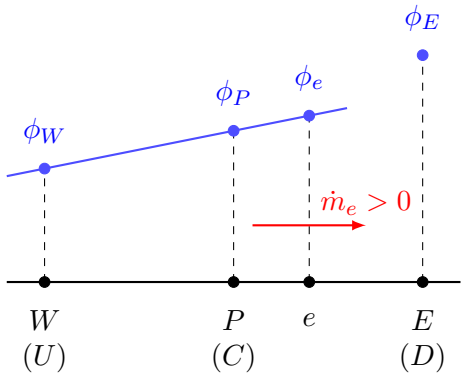


Figure 2.6. SUDS when $(\mathbf{v}\cdot\mathbf{n})_e > 0$.

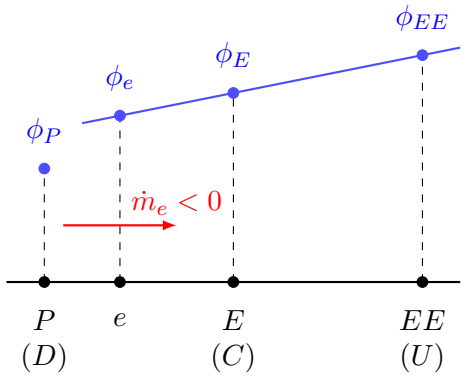


Figure 2.7. SUDS when $(\mathbf{v}\cdot\mathbf{n})_e < 0$.

The Second–order Upwind Linear Extrapolation scheme takes profit of this idea since it extrapolates ϕ_e using a straight line between the values of ϕ at nodes C and U. The two possible situations are pictured in figures 2.6 and 2.7.

On the one hand, when $(\mathbf{v}\cdot\mathbf{n})_e > 0$, the line between points (x_W, ϕ_W) and (x_P, ϕ_P) is given by

$$\phi(x) = \phi_W + \frac{\phi_P - \phi_W}{d_{PW}}(x - x_W) \tag{2.57}$$

and substituting at $x = x_e$, the formula for ϕ_e is obtained:

$$\phi_e = \phi_W + \frac{\phi_P - \phi_W}{d_{PW}}(x_e - x_W) = \phi_P + \frac{d_{Pe}}{d_{PW}}(\phi_P - \phi_W) \tag{2.58}$$

On the other hand, in the case of $(\mathbf{v}\cdot\mathbf{n})_e < 0$, the line between points (x_E, ϕ_E) and (x_{EE}, ϕ_{EE}) is

$$\phi(x) = \phi_E + \frac{\phi_{EE} - \phi_E}{d_{E,EE}}(x - x_E) \tag{2.59}$$

and the approximation of ϕ_e is

$$\phi_e = \phi_E + \frac{\phi_{EE} - \phi_E}{d_{E,EE}}(x_e - x_E) = \phi_E + \frac{d_{Ee}}{d_{E,EE}}(\phi_E - \phi_{EE}) \tag{2.60}$$

Using the DCU notation, (2.58) and (2.60) are both rewritten in the following manner:

$$\phi_f - \phi_C = \frac{d_{Cf}}{d_{CU}}(\phi_C - \phi_U) \tag{2.61}$$

In order to prove that SUDS is a second order scheme when a uniform mesh is used and $(\mathbf{v}\cdot\mathbf{n})_e > 0$, consider the Taylor expansion up to 2^{nd} degree of ϕ about point x_W,

$$\phi_e = \phi_W + \left(\frac{\partial\phi}{\partial x}\right)_W d_{We} + \left(\frac{\partial^2\phi}{\partial x^2}\right)_{\xi_1} \frac{d_{We}^2}{2} \tag{2.62}$$

The first derivative of ϕ with respect to x can be replaced by its first order approximation, namely,

$$\left(\frac{\partial\phi}{\partial x}\right)_W = \frac{\phi_P - \phi_W}{d_{PW}} - \left(\frac{\partial^2\phi}{\partial x^2}\right)_{\xi_2} \frac{d_{PW}}{2} \tag{2.63}$$

thereby,

$$\begin{aligned}\phi_e &= \phi_W + \frac{d_{We}}{d_{PW}}(\phi_P - \phi_W) + \left(\frac{\partial^2\phi}{\partial x^2}\right)_{\xi_1} \frac{d_{We}^2}{2} - \left(\frac{\partial^2\phi}{\partial x^2}\right)_{\xi_2} \frac{d_{We}d_{PW}}{2} \\ &= \phi_P + \frac{d_{Pe}}{d_{PW}}(\phi_P - \phi_W) + \left(\frac{\partial^2\phi}{\partial x^2}\right)_{\xi_1} \frac{(d_{PW}+d_{Pe})^2}{2} - \left(\frac{\partial^2\phi}{\partial x^2}\right)_{\xi_2} \frac{(d_{PW}+d_{Pe})d_{PW}}{2}\end{aligned} \tag{2.64}$$

The scheme retains the two first terms on the right–hand side of (2.64), therefore the error is composed by the last two terms. The uniform mesh hypothesis implies $d_{PW} = 2d_{Pe} = L$, therefore the error term is multiplied by L^2,

$$\phi_e = \phi_P + \frac{d_{Pe}}{d_{PW}}(\phi_P - \phi_W) + \frac{3L^2}{4}\left\{3\left(\frac{\partial^2\phi}{\partial x^2}\right)_{\xi_1} - \left(\frac{\partial^2\phi}{\partial x^2}\right)_{\xi_2}\right\} \tag{2.65}$$

whence the second order of SUDS is deduced. The proof in the case of $(\mathbf{v}\cdot\mathbf{n})_e < 0$ is analogous.

2.4.5 Quadratic Upwind Interpolation for Convective Kinematics (QUICK)

A logical improvement of CDS is using a parabola to interpolate between nodal points rather than a straight line. To construct a parabola three points are needed. As aforementioned, upstream conditions have a greater influence on flow properties than downstream conditions for incompressible flows and low Mach number gases. QUICK scheme takes profit of this fact.

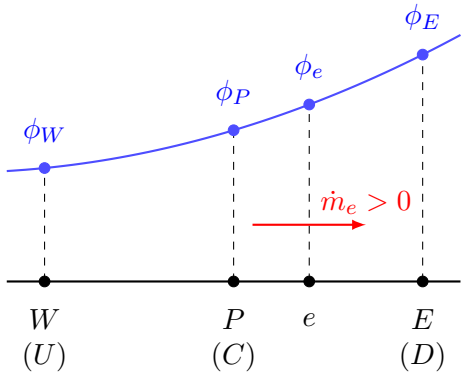


Figure 2.8. QUICK when $(\mathbf{v}\cdot\mathbf{n})_e > 0$.

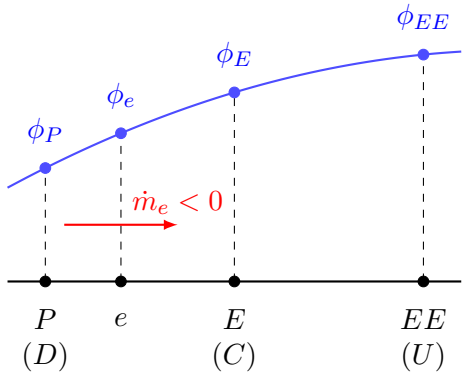


Figure 2.9. QUICK when $(\mathbf{v}\cdot\mathbf{n})_e < 0$.

Let (x_0,ϕ_0), (x_1,ϕ_1), (x_2,ϕ_2) be the points which the polynomial $p(x)$ must interpolate, that is, $p(x_0) = \phi_0$, $p(x_1) = \phi_1$ and $p(x_2) = \phi_2$, satisfying $x_0 < x_1 < x_2$. If $(\mathbf{v}\cdot\mathbf{n})_e > 0$ then $x_0 = x_W$, $x_1 = x_P$ and $x_2 = x_E$, whereas $x_0 = x_P$, $x_1 = x_E$ and $x_2 = x_{EE}$ in the case of $(\mathbf{v}\cdot\mathbf{n})_e < 0$. Let $p(x)$ be the following polynomial

$$p(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)(x - x_1), \quad a_0, a_1, a_2 \in \mathbb{R} \tag{2.66}$$

Since the interpolating polynomial exists and is unique (see [9], Theorem 8.1), by imposing the interpolating condition, $p(x)$ will be the desired polynomial. The interpolating condition is,

$$\left.\begin{aligned} p(x_0) &= a_0 = \phi_0 \\ p(x_1) &= a_0 + a_1(x_1 - x_0) = \phi_1 \\ p(x_2) &= a_0 + a_1(x_2 - x_0) + a_2(x_2 - x_0)(x_2 - x_1) = \phi_2 \end{aligned}\right\} \tag{2.67}$$

which yields the following linear system:

$$\begin{pmatrix} 1 & 0 & 0 \\ 1 & x_1 - x_0 & 0 \\ 1 & x_2 - x_0 & (x_2 - x_1)(x_2 - x_0) \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \end{pmatrix} \tag{2.68}$$

The determinant of the system matrix is non-zero because the abscissae are distinct, therefore the solution is given by

$$\left.\begin{aligned} a_0 &= \phi_0 \\ a_1 &= \frac{\phi_1 - \phi_0}{x_1 - x_0} \\ a_2 &= \frac{\phi_2 - \phi_0}{(x_2 - x_1)(x_2 - x_0)} - \frac{\phi_1 - \phi_0}{(x_2 - x_1)(x_1 - x_0)} \end{aligned}\right\} \tag{2.69}$$

and the polynomial is

$$p(x) = \phi_0 - \frac{(x - x_2)(x - x_0)}{(x_2 - x_1)(x_1 - x_0)}(\phi_1 - \phi_0) + \frac{(x - x_1)(x - x_0)}{(x_2 - x_1)(x_2 - x_0)}(\phi_2 - \phi_0) \tag{2.70}$$

In terms of the *DCU* notation, we have the following:

$$p(x) = \begin{cases} \phi_U - \dfrac{(x - x_D)(x - x_U)}{(x_D - x_C)(x_C - x_U)}(\phi_C - \phi_U) + \dfrac{(x - x_C)(x - x_U)}{(x_D - x_C)(x_D - x_U)}(\phi_D - \phi_U) & \text{if } (\mathbf{v} \cdot \mathbf{n})_e > 0 \\ \phi_D - \dfrac{(x - x_U)(x - x_D)}{(x_U - x_C)(x_C - x_D)}(\phi_C - \phi_D) + \dfrac{(x - x_C)(x - x_D)}{(x_U - x_C)(x_U - x_D)}(\phi_U - \phi_D) & \text{if } (\mathbf{v} \cdot \mathbf{n})_e < 0 \end{cases} \tag{2.71}$$

Assuming a uniform grid, i.e. $x_1 - x_0 = x_2 - x_1 = L$ and the face f located at the midpoint between nodal points, the approximation of ϕ_e given by QUICK scheme is

$$\phi_e = -\frac{1}{8}\phi_0 + \frac{6}{8}\phi_1 + \frac{3}{8}\phi_2 \tag{2.72}$$

and depending on the sign of $(\mathbf{v} \cdot \mathbf{n})_e$,

$$\phi_e = \begin{cases} -\dfrac{1}{8}\phi_U + \dfrac{6}{8}\phi_C + \dfrac{3}{8}\phi_D & \text{if } (\mathbf{v} \cdot \mathbf{n})_e > 0 \\ -\dfrac{1}{8}\phi_D + \dfrac{6}{8}\phi_C + \dfrac{3}{8}\phi_U & \text{if } (\mathbf{v} \cdot \mathbf{n})_e < 0 \end{cases} \tag{2.73}$$

The output (2.73) provided by QUICK scheme is second–order accurate.

2.4.6 Normalization of variables

Owing to numerical reasons, it is convenient to normalize spatial and convective variables, that is to say, define new variables which take a rather small range of values. This is accomplished using the *DCU* notation and defining

$$\hat{x} = \frac{x - x_U}{x_D - x_U} \tag{2.74}$$

$$\hat{\phi} = \frac{\phi - \phi_U}{\phi_D - \phi_U} \tag{2.75}$$

Of course, $(\hat{x}_U, \hat{\phi}_U) = (0, 0)$, $(\hat{x}_D, \hat{\phi}_D) = (1, 1)$ and $\hat{x}_C, \hat{x}_f \in [0, 1]$. However, $\hat{\phi}$ is not necessarily in $[0, 1]$ for all $x \in [0, 1]$, nor does it have to be an increasing function. These situations are represented in figures 2.10 and 2.11.

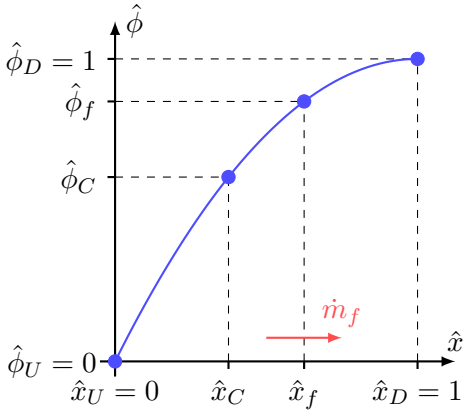


Figure 2.10. Scheme of normalized variables when $\hat{\phi}(x)$ is a strictly increasing function.

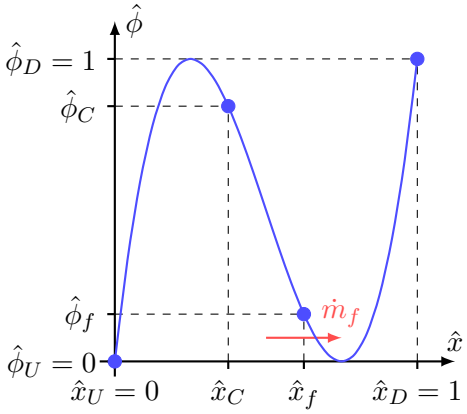


Figure 2.11. Scheme of normalized variables when $\hat{\phi}(x)$ is not a strictly increasing function.

Some schemes, such as SMART, give the value of the normalized variable at face $\hat{\phi}_f$ directly as equation (2.77) shows. Based on $\hat{\phi}_f$, the variable at face is calculated by

$$\phi_f = \phi_U + \hat{\phi}_f(\phi_D - \phi_U) \tag{2.76}$$

2.4.7 Sharp and Monotonic Algorithm for Realistic Transport (SMART)

As aforementioned, schemes whose order is higher than one might be unstable, producing oscillatory outputs for the convective variables. For instance, CDS, SUDS and QUICK are not bounded schemes. The conditions for stability and accuracy are formulated in [10]:

(i) $\hat{\phi}_f$ must be a continuous function of $\hat{\phi}_C$.

(ii) If $\hat{\phi}_C = 0$, then $\hat{\phi}_f = 0$.

(iii) If $\hat{\phi}_C = 1$, then $\hat{\phi}_f = 1$.

(iv) If $0 < \hat{\phi}_f < 1$, then $\hat{\phi}_C < \hat{\phi}_f < 1$.

Conditions (i) through (iv) are represented in figure 2.12. A bounded convective scheme must output results lying within the shadowed region.

The SMART scheme (Sharp and Monotonic Algorithm for Realistic Transport) is a bounded convective scheme [10], given by:

$$\hat{\phi}_f = \begin{cases} -\dfrac{\hat{x}_f(1 - 3\hat{x}_C + 2\hat{x}_f)}{\hat{x}_C(\hat{x}_C - 1)}\hat{\phi}_C & \text{if} \quad 0 < \hat{\phi}_C < \dfrac{\hat{x}_C}{3} \\ \dfrac{\hat{x}_f(\hat{x}_f - \hat{x}_C)}{1 - \hat{x}_C} + \dfrac{\hat{x}_f(\hat{x}_f - 1)}{\hat{x}_C(\hat{x}_C - 1)}\hat{\phi}_C & \text{if} \quad \dfrac{\hat{x}_C}{3} < \hat{\phi}_C < \dfrac{\hat{x}_C(1 + \hat{x}_f - \hat{x}_C)}{\hat{x}_f} \\ 1 & \text{if} \quad \dfrac{\hat{x}_C(1 + \hat{x}_f - \hat{x}_C)}{\hat{x}_f} < \hat{\phi_C} < 1 \\ \hat{\phi}_C & \text{otherwise} \end{cases} \tag{2.77}$$

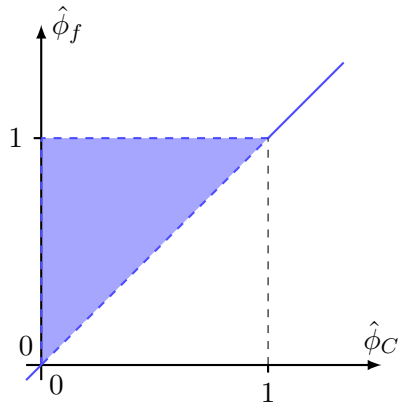


Figure 2.12. High–order bounded convection schemes conditions for stability.

2.5 Final form of the generalized convection–diffusion equation

The purpose of this subsection is to obtain a discretization equation of the form

$$\mathcal{A}_P\phi_P + \sum_F \mathcal{A}_F\phi_F = \mathcal{Q}_P \tag{2.78}$$

so that it can be easily implemented to be solved numerically, starting from equation (2.32) and the studied schemes to evaluate convective properties. Among the revised schemes, some use only the surrounding nodes, whilst others involve a larger amount of nodes. As a consequence of the different treatment needed, separate subsections are devoted to each type of scheme.

2.5.1 Small molecule schemes

Small molecule schemes are those which only involve adjacent nodes to the volume faces. That is, index I in (2.78) refers to nodes E, W, N and S. As a result, these schemes can be introduced in a compact form as Patankar suggests [6]. However a different approach will be followed here.

As it can be noted from the expressions for schemes UDS (equations (2.36) to (2.39)), CDS (equations (2.42) to (2.45)) and EDS (equations (2.53) to (2.56)), once a face f is chosen, the formula for ϕ_f has the following form

$$\phi_f - \phi_P = A_f(\phi_F - \phi_P) \tag{2.79}$$

where A_f is a coefficient which depends on the face and the scheme. Particularizing for each face,

$$\phi_e - \phi_P = A_e(\phi_E - \phi_P) \tag{2.80}$$
$$\phi_w - \phi_P = A_w(\phi_W - \phi_P) \tag{2.81}$$
$$\phi_n - \phi_P = A_n(\phi_N - \phi_P) \tag{2.82}$$
$$\phi_s - \phi_P = A_s(\phi_S - \phi_P) \tag{2.83}$$

The values of A_f and B_f for each face and scheme are collected in table 2.1.

Introducing equations (2.80) through (2.83) in (2.33), a general discretization equation comprising

Face	UDS	CDS	EDS
East	$\frac{\dot{m}_e - \lvert\dot{m}_e\rvert}{2\dot{m}_e}$	$\frac{d_{Pe}}{d_{PE}}$	$\frac{e^{\mathrm{Pe}_e \frac{d_{Pe}}{d_{PE}}} - 1}{e^{\mathrm{Pe}_e} - 1}$, $\mathrm{Pe}_e = \frac{\rho_e u_e d_{PE}}{\Gamma_e}$
West	$\frac{\dot{m}_w + \lvert\dot{m}_w\rvert}{2\dot{m}_w}$	$\frac{d_{Pw}}{d_{PW}}$	$\mathrm{Pe}_w = \frac{\rho_w u_w d_{PW}}{\Gamma_w}$
North	$\frac{\dot{m}_n - \lvert\dot{m}_n\rvert}{2\dot{m}_n}$	$\frac{d_{Pn}}{d_{PN}}$	$\frac{e^{\mathrm{Pe}_n \frac{d_{Pn}}{d_{PN}}} - 1}{e^{\mathrm{Pe}_n} - 1}$, $\mathrm{Pe}_n = \frac{\rho_n v_n d_{PN}}{\Gamma_n}$
South	$\frac{\dot{m}_s + \lvert\dot{m}_s\rvert}{2\dot{m}_s}$	$\frac{d_{Ps}}{d_{PS}}$	$\mathrm{Pe}_s = \frac{\rho_s v_s d_{PS}}{\Gamma_s}$

Table 2.1. Coefficient A_f of equation $\phi_f - \phi_P = A_f(\phi_F - \phi_P)$ for east, west, north and south faces, and for schemes UDS, CDS and EDS.

UDS, CDS and EDS can be obtained:

$$\begin{aligned}
&\left\{D_e - \dot{m}_e A_e + D_w + \dot{m}_w A_w + D_n - \dot{m}_n A_n + D_s + \dot{m}_s A_s + \frac{\rho_P^0 V_P}{\Delta t} - S_P^\phi V_P\right\}\phi_P \\
&= \Big\{D_e - \dot{m}_e A_e\Big\}\phi_E + \Big\{D_w + \dot{m}_w A_w\Big\}\phi_W + \Big\{D_n - \dot{m}_n A_n\Big\}\phi_N + \Big\{D_s + \dot{m}_s A_s\Big\}\phi_S \\
&+ \left\{S_C^\phi + \frac{\rho_P^0 \phi_P^0}{\Delta t}\right\} V_P
\end{aligned} \tag{2.84}$$

In order to make (2.84) more tractable, the following discretization coefficients are defined:

$$a_E = D_e - \dot{m}_e A_e \tag{2.85}$$
$$a_W = D_w + \dot{m}_w A_w \tag{2.86}$$
$$a_N = D_n - \dot{m}_n A_n \tag{2.87}$$
$$a_S = D_s + \dot{m}_s A_s \tag{2.88}$$
$$a_P = a_W + a_E + a_S + a_N + \frac{\rho_P^0 V_P}{\Delta t} - S_P^\phi V_P \tag{2.89}$$
$$b_P = S_C^\phi V_P + \frac{\rho_P^0 \phi_P^0}{\Delta t} V_P \tag{2.90}$$

Thereby the discretization equation is:

$$a_P \phi_P = a_W \phi_W + a_E \phi_E + a_S \phi_S + a_N \phi_N + b_P \tag{2.91}$$

2.5.2 Large molecule schemes

High–resolution schemes (HRS) such as SUDS, QUICK and SMART, not only use adjacent nodes to the faces but also the most upstream nodes, that is to say, involve a larger molecule. Since a larger molecule increases the memory usage and the computational effort, it is desirable to keep it as low as possible. Therefore, the aim is to obtain a discretization equation such as (2.91), where only the surrounding nodes participate, while upstream nodes are computed by different means and collected in b_P.

The first logical solution would be to use small molecule schemes, although it must be kept in mind the lower order of the approximations. The second solution would be to compute the upstream node

value using the data of the previous iteration and introduce this term in the equation as a contribution to b_P. Nevertheless, this may lead to the divergence of the iterations since the terms treated explicitly may be substantial [11].

The solution is to compute the approximated terms with a higher order approximation explicitly and put them on the right–hand side of equation (2.78). Then a simpler approximation to these terms, for instance one that provides a smaller molecule, is put on the left–hand side and on the right–hand side, computing it using explicit values. Then the right–hand side is the difference between two approximations of the same value, hence is likely to be small. This technique is known as deferred correction, and is used with higher–order approximations, as well as grid non–orthogonality and correction to prevent undesirable effects in solutions [11].

Given a face f, the idea is approximate ϕ_f as

$$\phi_f^{\text{HRS}} - \phi_P = (\phi_f^{\text{UDS}} - \phi_P) + (\phi_f^{\text{HRS},*} - \phi_f^{\text{UDS},*}) \tag{2.92}$$

ϕ_f^{HRS} and ϕ_f^{UDS} are the current calculated values of ϕ using the chosen HRS and UDS, whereas $\phi_f^{\text{HRS},*}$ and $\phi_f^{\text{UDS},*}$ are the computed values in the previous iteration. As stated above, when convergence is achieved, $\phi_f^{\text{HRS}} = \phi_f^{\text{HRS},*}$ and $\phi_f^{\text{UDS}} = \phi_f^{\text{UDS},*}$ [5]. Substituting $\phi_f - \phi_P$ by $\phi_f^{\text{HRS}} - \phi_P$ in (2.31)

$$\begin{aligned}\rho_P^0 \frac{\phi_P - \phi_P^0}{\Delta t} V_P + \dot{m}_e(\phi_e^{\text{HRS}} - \phi_P) - \dot{m}_w(\phi_w^{\text{HRS}} - \phi_P) + \dot{m}_n(\phi_n^{\text{HRS}} - \phi_P) - \dot{m}_s(\phi_s^{\text{HRS}} - \phi_P) = \\ = D_e(\phi_E - \phi_P) - D_w(\phi_P - \phi_W) + D_n(\phi_N - \phi_P) - D_s(\phi_P - \phi_S) + (S_C^\phi + S_P^\phi \phi_P)V_P\end{aligned} \tag{2.93}$$

and using relation (2.92)

$$\begin{aligned}\rho_P^0 \frac{\phi_P - \phi_P^0}{\Delta t} V_P + \dot{m}_e(\phi_e^{\text{UDS}} - \phi_P) - \dot{m}_w(\phi_w^{\text{UDS}} - \phi_P) + \dot{m}_n(\phi_n^{\text{UDS}} - \phi_P) - \dot{m}_s(\phi_s^{\text{UDS}} - \phi_P) = \\ = D_e(\phi_E - \phi_P) - D_w(\phi_P - \phi_W) + D_n(\phi_N - \phi_P) - D_s(\phi_P - \phi_S) + (S_C^\phi + S_P^\phi \phi_P)V_P + \\ - \dot{m}_e(\phi_e^{\text{HRS},*} - \phi_e^{\text{UDS},*}) + \dot{m}_w(\phi_w^{\text{HRS},*} - \phi_w^{\text{UDS},*}) - \dot{m}_n(\phi_n^{\text{HRS},*} - \phi_n^{\text{UDS},*}) + \dot{m}_s(\phi_s^{\text{HRS},*} - \phi_s^{\text{UDS},*})\end{aligned} \tag{2.94}$$

Replacing the corresponding terms with expressions (2.36) through (2.39) and rearranging terms, the desired expression is found

$$a_P \phi_P = a_W \phi_W + a_E \phi_E + a_S \phi_S + a_N \phi_N + b_P \tag{2.95}$$

with the following coefficients:

$$a_E = D_e - \frac{\dot{m}_e - |\dot{m}_e|}{2} = \frac{\Gamma_e S_e}{d_{PE}} - \frac{\dot{m}_e - |\dot{m}_e|}{2} \tag{2.96}$$

$$a_W = D_w + \frac{\dot{m}_w + |\dot{m}_w|}{2} = \frac{\Gamma_w S_w}{d_{PW}} + \frac{\dot{m}_w + |\dot{m}_w|}{2} \tag{2.97}$$

$$a_N = D_n - \frac{\dot{m}_n - |\dot{m}_n|}{2} = \frac{\Gamma_n S_n}{d_{PN}} - \frac{\dot{m}_n - |\dot{m}_n|}{2} \tag{2.98}$$

$$a_S = D_s + \frac{\dot{m}_s + |\dot{m}_s|}{2} = \frac{\Gamma_s S_s}{d_{PS}} + \frac{\dot{m}_s + |\dot{m}_s|}{2} \tag{2.99}$$

$$a_P = a_W + a_E + a_S + a_N + \frac{\rho_P^0 V_P}{\Delta t} - S_P^\phi V_P \tag{2.100}$$

$$\begin{aligned}b_P = \frac{\rho_P^0 \phi_P^0}{\Delta t} V_P + S_C^\phi V_P - \dot{m}_e(\phi_e^{\text{HRS},*} - \phi_e^{\text{UDS},*}) + \dot{m}_w(\phi_w^{\text{HRS},*} - \phi_w^{\text{UDS},*}) \\ - \dot{m}_n(\phi_n^{\text{HRS},*} - \phi_n^{\text{UDS},*}) + \dot{m}_s(\phi_s^{\text{HRS},*} - \phi_s^{\text{UDS},*})\end{aligned} \tag{2.101}$$

2.6 Treatment of boundary conditions

In Cauchy problems involving Partial Differential Equations (PDEs), there exist several kinds of boundary conditions which must be prescribed in order to guarantee the existence and uniqueness of solution, although in this project we will only consider two types. So as to illustrate how these conditions are set, let $U \subset \mathbb{R}^n$ be a bounded open subset of $\mathbb{R}^n$. The heat or diffusion equation is the PDE

$$u_t - \Delta u = f(x,t) \quad (x,t) \in U \times (0,\infty) \tag{2.102}$$

where $\Delta = \sum_{i=1}^{m} \frac{\partial^2}{\partial x_i^2}$ is Laplace's operator and f models the internal sources for magnitude u [4]. This equation models the evolution in time of the density u of some quantity such as heat, chemical concentration, etc. Let $g\colon U \to \mathbb{R}$ be the initial value for u. The typical Cauchy problem for diffusion equation is

$$\begin{cases} u_t - \Delta u = f(x,t) & \text{in } U \times (0,\infty) \\ u = g & \text{on } U \times \{t=0\} \\ \text{Boundary conditions} \end{cases} \tag{2.103}$$

The boundary conditions considered are:

- Dirichlet boundary condition: the value of u is prescribed on $\partial U \times (0,\infty)$, that is to say, if $d\colon \partial U \times (0,\infty) \to \mathbb{R}$, $(x,t) \mapsto d(x,t)$ describes the boundary condition, then (2.103) is written as

$$\begin{cases} u_t - \Delta u = f(x,t) & \text{in } U \times (0,\infty) \\ u = g & \text{on } U \times \{t=0\} \\ u = d & \text{on } \partial U \times (0,\infty) \end{cases} \tag{2.104}$$

  When (2.102) is thought of as describing the propagation of heat, then d fixes the temperature at the boundary of U for each time.

- Neumann boundary condition: the normal derivative of u to the boundary of U is prescribed on $\partial U \times (0,\infty)$, i.e. if $n\colon \partial U \times (0,\infty) \to \mathbb{R}$ describes the boundary condition, then (2.103) is written as

$$\begin{cases} u_t - \Delta u = f(x,t) & \text{in } U \times (0,\infty) \\ u = g & \text{on } U \times \{t=0\} \\ \partial_\nu u = n & \text{on } \partial U \times (0,\infty) \end{cases} \tag{2.105}$$

  where ν is the outer normal vector to ∂U. In terms of heat, this boundary condition sets the conduction heat transfer through U for each time.

The numerical treatment of boundary conditions is straightforward, specially is our case as we are using a cartesian mesh on a rectangular domain. In the case of a Dirichlet boundary condition, such as the one shown in figure 2.13, the value at face must be equal to the prescribed value at boundary, that is,

$$\phi_e = \phi_E \tag{2.106}$$

and flux per unit of surface can be easily computed as

$$j_e = -\Gamma_P \frac{\phi_e - \phi_P}{d_{Pe}} \tag{2.107}$$

In contrast, when a Neumann boundary condition with flux j_e is imposed, the value at face is

$$\phi_e = \phi_P - \frac{j_e d_{Pe}}{\Gamma_P} \tag{2.108}$$

This second situation is pictured in figure 2.14.

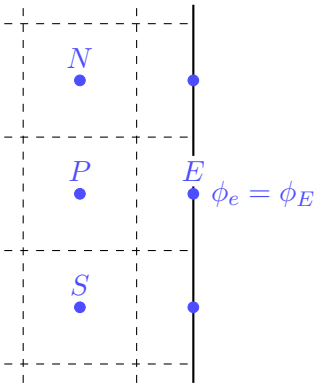


Figure 2.13. Dirichlet boundary condition.

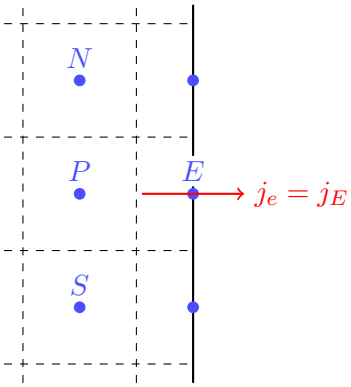


Figure 2.14. Neumann boundary condition.

2.7 Solving algorithm

The procedure to solve of a transient convection–diffusion problem with 2D–cartesian mesh is shown in Algorithm 1.

Hereinafter, the term iteration will be used to refer to the iterative procedure to solve the linear system on step **4.3**. It must not be confused with the next time instant term.

On step **4** the next time instant is computed. This is the most computationally expensive step in the algorithm, specially part **4.3** where the resolution of the linear system of discretized equations is carried out. As a result of the convection–diffusion equations nature, the system matrix A and the vector of independent terms b change each time the convergence condition is not fulfilled on step (**4.4**). Since A and b depend on the previous iteration value of ϕ, that is to say, $A = A(\phi^*)$ and $b = b(\phi^*)$, the linear system of equations is

$$A(\phi^*)\,\phi = b(\phi^*) \tag{2.109}$$

In the case both A and b were constant, the algorithm needed to solve the linear system (2.109) would be clear at first glance. Since each node is influenced only by the adjacent nodes, A is a pentadiagonal by blocks matrix, therefore A is sparse, i.e. most of the elements are zero, hence an iterative method for solving the linear system would be convenient. Let A_{ij} denote the element in the i-th row and j-th column of A. If A is, in addition, a strictly diagonally dominant (SDD) matrix, that is to say,

$$|A_{ii}| \geq \sum_{\substack{j=1 \\ j\neq i}}^{n} |A_{ij}| \tag{2.110}$$

then Gauss–Seidel algorithm is guaranteed to converge and eventually solve the system. In terms of the discretization coefficients, condition (2.110) is written as

$$|a_P[i][j]| \geq |a_W[i][j]| + |a_E[i][j]| + |a_S[i][j]| + |a_N[i][j]| \tag{2.111}$$

Nonetheless the SDD condition is not assured as a consequence of the discretization coefficients.

As the execution of an iterative procedure to solve the linear system may diverge, arguably the most convenient is a direct method.

Algorithm 1 Resolution of a transient convection–diffusion problem with 2D–cartesian mesh.

1 Input data:

1.1 Physical data: geometry, thermophysical properties, initial and boundary conditions.

1.2 Numerical data: mesh, Δt (time step), δ (convergence criterion).

2 Mesh generation: nodes position, faces position, distances, surfaces and volumes.

3 Initial map: $n \leftarrow 0$, $t^n \leftarrow 0$, $\phi^0[i][j] = \phi(x, y, t)|_{t=0}$.

4 Compute the new time step: $t^{n+1} = t^n + \Delta t$.

4.1 Initial estimated values: $\phi^*[i][j] \leftarrow \phi^0[i][j]$.

4.2 Evaluation of the discretization coefficients: $a_E[i][j]$, $a_W[i][j]$, $a_N[i][j]$, $a_S[i][j]$, $a_P[i][j]$, $b_P[i][j]$.

4.3 Resolution of the linear system

$$a_P[i][j]\,\phi[i][j] = a_E[i][j]\,\phi[i+1][j] + a_W[i][j]\,\phi[i-1][j] + a_N[i][j]\,\phi[i][j+1] + a_S[i][j]\,\phi[i][j-1] + b_P[i][j]$$

4.4 Is $\max_{i,j} |\phi^*[i][j] - \phi[i][j]| < \delta$?

- Yes: continue.
- No: $\phi^*[i][j] \leftarrow \phi[i][j]$, go to **4.2**.

5 New time step?

- Yes: $n \leftarrow n + 1$, go to **4**.
- No: continue.

6 Final computations, print results.

7 End.

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A Some results on Measure Theory

In this appendix we gather two important theorems needed to justify some steps in the derivation of conservation laws in section 1. Despite these results are basic, a previous study of real analysis is required in order to understand and prove them. A good reference for the interested reader is Real and Complex Analysis of Walter Rudin [12].

A.1 Differentiation under the integral sign

Differentiation under the integral sign allows us to compute the derivative of an integral of a function of two parameters in a simple way. It is needed, for instance, when the mass conservation law or the heat diffusion equation are derived.

Let $(X, \mathcal{A}, \mu)$ be a measure space and let $[a, b] \subset \mathbb{R}$. Hereinafter we deal with functions $f\colon X \times [a, b] \to \mathbb{R}$, where $t \in [a, b]$ is the parameter on which f depends. We assume that $f(\cdot, t)$ is a measurable function for each $t \in [a, b]$.

Theorem A.1 (Differentiation under the integral sign)**.** Let $F(t) = \int_X f(\mathbf{x}, t)\,\mathrm{d}\mu$. Assume that

(i) $f(\mathbf{x}, t_0)$ is an integrable function for some $t_0 \in [a, b]$.

(ii) $\dfrac{\partial f}{\partial t}(\mathbf{x}, t)$ is defined for all $(\mathbf{x}, t) \in X \times [a, b]$.

(iii) There exists an integral function $g\colon X \to \mathbb{R}$ such that $\left|\dfrac{\partial f}{\partial t}(\mathbf{x}, t)\right| \leq g(\mathbf{x})$ for all $(\mathbf{x}, t) \in X \times [a, b]$.

Then F is a differentiable function and

$$F'(t) = \frac{\mathrm{d}}{\mathrm{d}t}F(t) = \int_X \frac{\partial f}{\partial t}(\mathbf{x}, t)\,\mathrm{d}\mu$$

For the applications needed in this project, $X = \mathbb{R}^m$ with $1 \leq m \leq 3$, $\mathcal{A}$ is the Borel σ–algebra on $\mathbb{R}^m$ and μ is Lebesgue's measure on $\mathbb{R}^m$, which for most of the "natural" sets of $\mathcal{A}$ coincides with the usual notion of m–dimensional volume.

A.2 Lebesgue's differentiation lemma

A common way to derive a conservation law is to integrate some functions in a control volume, then apply Differentiation under the integral sign to obtain an integral equation and finally get to a differential equation using Lebesgue's differentiation lemma.

An intuitive way to understand and to motivate Lebesgue's differentiation lemma is the following. Let $f\colon \mathbb{R} \to \mathbb{R}$ be a continuous function, let $a \in \mathbb{R}$ be a fixed point and let $F(x) = \int_a^x f(y)\,\mathrm{d}y$, which is a differentiable function. Due to a corollary of the Fundamental Theorem of Calculus, we have $F'(x) = f(x)$. Using the definition of derivative,

$$F'(x) = \lim_{h\to 0} \frac{F(x+h) - F(x)}{h} = \lim_{h\to 0} \frac{1}{h}\left\{\int_a^{x+h} f(y)\,\mathrm{d}y - \int_a^x f(y)\,\mathrm{d}y\right\} = \lim_{h\to 0} \frac{1}{h}\int_x^{x+h} f(y)\,\mathrm{d}y = f(x)$$

Notice that the integral is divided by the length of the interval $[x, x + h]$, otherwise the limit would be zero. Lebesgue's lemma generalizes the previous equality by considering functions $f\colon \mathbb{R}^n \to \mathbb{R}$ and integrating them on open balls $B(\mathbf{x_0}, r) = \{x \in \mathbb{R}^n \mid \|\mathbf{x} - \mathbf{x_0}\| < r\}$. Furthermore, the integral is divided by the n–dimensional volume of $B(\mathbf{x_0}, r)$, which is denoted by $|B(\mathbf{x_0}, r)|$.

Theorem A.2 (Lebesgue's differentiation lemma [13])**.** Let $f\colon \mathbb{R}^n \to \mathbb{R}$ be a locally integrable function.

(1) Then for almost everywhere point $\mathbf{x_0} \in \mathbb{R}^n$,

$$\frac{1}{|B(\mathbf{x_0}, r)|} \int_{B(\mathbf{x_0}, r)} f(\mathbf{x})\, \mathrm{d}\mathbf{x} \to f(\mathbf{x_0}) \quad \text{as } r \to 0$$

(2) In fact, for almost everywhere point $\mathbf{x_0} \in \mathbb{R}^n$,

$$\frac{1}{|B(\mathbf{x_0}, r)|} \int_{B(\mathbf{x_0}, r)} |f(\mathbf{x}) - f(\mathbf{x_0})|\, \mathrm{d}\mathbf{x} \to 0 \quad \text{as } r \to 0$$

B Ordinary Differential Equations

In this section we present the Picard–Lindelöf theorem which aids on proving the existence and uniqueness of solution to initial value problems involving ordinary differential equations (ODEs) initial value problems. We begin with the definition of a Lipschitz function:

Definition B.1. A function $f\colon \Omega \subset \mathbb{R}^n \to \mathbb{R}^m$ is said to be Lipschitz or Lipschitz continuous if there exists a constant L such that

$$\|f(\mathbf{x}) - f(\mathbf{y})\| \leq L\|\mathbf{x} - \mathbf{y}\| \tag{B.1}$$

for every $\mathbf{x}, \mathbf{y} \in \Omega$. The constant L is called the Lipschitz constant of f [1].

It can be easily proven that every Lipschitz function on Ω is also a continuous function in the usual sense on Ω. The converse is not true in general, and depends on the properties of Ω. The Lipschitz continuity is actually a very restrictive condition, since it imposes that the function can grow at most as a linear function.

Definition B.2. Let $(E, \|\cdot\|_E)$ and $(F, \|\cdot\|_F)$ be two finite dimensional normed vector spaces and let $A\colon E \to F$ be a linear mapping between them. The norm of A is defined to be

$$\|A\| := \sup\{\|Ax\|_F \mid x \in E,\ \|x\|_E \leq 1\} \tag{B.2}$$

It is a well known fact that $\|A\|$ is finite. In some cases, proving that a function is Lipschitz continuous is a laborious task. In these situations we have the following theorems:

Theorem B.3 (Corollary of the mean value theorem [14])**.** Let $\Omega \subset \mathbb{R}^n$ an open set and let $f\colon \Omega \subset \mathbb{R}^n \to \mathbb{R}^m$ a differentiable function on Ω. Let $\mathbf{x}, \mathbf{y} \in \Omega$ such that the segment $\overline{\mathbf{xy}} = \{\lambda\mathbf{x} + (1-\lambda)\mathbf{y} \mid \lambda \in [0,1]\}$ is contained in Ω. Then the following inequality holds:

$$\|f(\mathbf{x}) - f(\mathbf{y})\| \leq \sup_{\mathbf{z} \in \overline{\mathbf{xy}}} \|Df(\mathbf{z})\|\|\mathbf{x} - \mathbf{y}\| \tag{B.3}$$

Proof. See [14], page 78. □

Theorem B.4. Let $\Omega \subset \mathbb{R}^n$ a compact convex set and let $f \equiv (f_1, \ldots, f_m)\colon \Omega \subset \mathbb{R}^n \to \mathbb{R}^m$ a $\mathcal{C}^1(\Omega)$ function. Then f is Lipschitz in Ω.

Proof. The differential of Df, given by

$$Df = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_n} \end{pmatrix} \tag{B.4}$$

is a linear mapping $Df\colon \mathbb{R}^n \to \mathbb{R}^m$. Since f is $\mathcal{C}^1(\Omega)$ function, the partial derivatives $\frac{\partial f_1}{\partial x_1}, \ldots, \frac{\partial f_m}{\partial x_n}$ are continuous functions on Ω. Moreover, the norm of the differential depends continuously on the partial derivatives $\frac{\partial f_1}{\partial x_1}, \ldots, \frac{\partial f_m}{\partial x_n}$ and on $\mathbf{z}$. As a consequence, $\|Df\|$ is a continuous function on Ω. By Weierstrass theorem, $\|Df\|$ reaches a maximum M on Ω. Applying theorem B.3 we have

$$\|f(\mathbf{x}) - f(\mathbf{y})\| \leq \sup_{\mathbf{z}\in\overline{\mathbf{xy}}} \|Df(\mathbf{z})\|\|\mathbf{x}-\mathbf{y}\| \leq M\|\mathbf{x}-\mathbf{y}\| \tag{B.5}$$

for all $\mathbf{x}, \mathbf{y} \in \Omega$, hence f is Lipschitz on $\overline{\Omega}$. □

Finally we can state the Picard–Lindelöf theorem. Let U be an open subset of $\mathbb{R}^{n+1}$ and let $f \in C(U, \mathbb{R})$, $(t_0, \mathbf{x_0}) \in U$. Consider the following IVP:

$$\begin{cases} \dot{\mathbf{x}}(t) = f(t, \mathbf{x}) \\ \mathbf{x}(t_0) = \mathbf{x_0} \end{cases} \tag{B.6}$$

The Picard–Lindelöf theorem gives us the existence and uniqueness of solution for (B.6).

Theorem B.5 (Picard–Lindelöf [15])**.** Suppose $f \in \mathcal{C}(U, \mathbb{R}^n)$, where U is an open subset of $\mathbb{R}^{n+1}$, and $(t_0, \mathbf{x_0}) \in U$. If f is locally Lipschitz continuous in the second argument, uniformly with respect to the first, then there exists a unique local solution $vbx(t) \in \mathcal{C}^1(I)$ of the initial value problem (B.6), where I is some interval around t_0.

More specifically, if $V = [t_0, t_0 + T] \times \overline{B(\mathbf{x_0}, \delta)} \subset U$ and M denotes the maximum of $|f|$ on V, then the solution exists at least for $t \in [t_0, t_0 + T_0]$ and remains in $\overline{B(\mathbf{x_0}, \delta)}$ where $T_0 = \min\left\{T, \frac{\delta}{M}\right\}$. The analogous result holds for the interval $[t_0 - T, t_0]$.

Proof. See [15], page 38. □

C Numerical resolution of linear systems

C.1 Gauss–Seidel algorithm

C.2 LU factorization