1 Introduction

2 The convection–diffusion equations

2.1 Reynolds transport theorem

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{V(t)} F(\mathbf{x},t)\,\mathrm{d}\mathbf{x} = \int_{V(t)} \frac{\partial F}{\partial t}\,\mathrm{d}\mathbf{x} + \int_{A(t)} F(\mathbf{x},t)\mathbf{b}\cdot\mathbf{n}\,\mathrm{d}S \tag{2.1}$$

2.2 Continuity equation

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\mathbf{v}) = 0 \tag{2.2}$$

2.3 Momentum equation

$$\frac{\partial(\rho\mathbf{v})}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\mathbf{v}\otimes\mathbf{v}) = \boldsymbol{\nabla}\cdot(\mu\boldsymbol{\nabla}\mathbf{v}) + \{\boldsymbol{\nabla}\cdot(\tau - \mu\boldsymbol{\nabla}\mathbf{v}) - \boldsymbol{\nabla}p + \rho\mathbf{g}\} \tag{2.3}$$

2.4 Energy equation

$$\frac{\partial(\rho T)}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\mathbf{v}T) = \boldsymbol{\nabla}\cdot\left(\frac{\lambda}{c_v}\boldsymbol{\nabla}T\right) + \left\{\frac{\tau\circ\boldsymbol{\nabla}\mathbf{v} - \boldsymbol{\nabla}\cdot\dot{\mathbf{q}}^R - p\boldsymbol{\nabla}\cdot\mathbf{v}}{c_v}\right\} \tag{2.4}$$

2.5 Species equation

$$\frac{\partial(\rho Y_k)}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\mathbf{v}Y_k) = \boldsymbol{\nabla}\cdot(\rho D_{km}\boldsymbol{\nabla}Y_k) + \{\dot{\omega}_k\} \tag{2.5}$$

2.6 Convection–diffusion equations

3 Numerical study

3.1 Assumptions

In order to solve the convection–diffusion equations numerically, we must make some assumptions which will simplify our study.

1. The location where the problem takes place is a closed connected set K contained in a bounded open connected set $\Omega \subset \mathbb{R}^m$, where $m = 1, 2, 3$ depends on the dimension of the problem. Both K and Ω are $\mathcal{C}^1$ or Lipschitz domains, allowing us to use vector calculus theorems.

2. The problem lasts for finite time, starting at time $t = 0$ and ending at time $t = t_{\max}$. Therefore the time interval is $I = (0, t_{\max}) \subset \mathbb{R}$.

3. The closed connected set K can be expressed as the union of finitely many closed sets $\mathcal{V}_1, \dots, \mathcal{V}_r$, that is, $K = \mathcal{V}_1 \cup \dots \cup \mathcal{V}_r$. Moreover, these sets

The control volume centered at node P will be denoted by $\mathcal{V}_P$. Its boundary, known as the control surface, will be expressed as $\mathcal{S}_P = \partial\mathcal{V}_P$. The volume $\mathcal{V}_P$ occupies in $\mathbb{R}^m$

3.2 Spatial discretization

The type of problems we are studying occur in a bounded domain $\Omega \subset \mathbb{R}^m$ with $1 \leq m \leq 3$ depending on the case. In order to solve the problem numerically, the domain is discretized into nonoverlapping control volumes and a control node is placed at the center of each one [**patankar2018numerical**]. There exist two manners to discretize the domain, namely, the cell–centered and the 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 and then places a node at the center of each one.

(a) A subfigure **(b)** A subfigure

Figure 3.1. A figure with two subfigures

3.3 Time discretization

3.4 Discretization of the continuity equation

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

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \mathbf{v}) = 0 \quad (\mathbf{x}, t) \in \Omega \times I \tag{3.1}$$

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

$$\int_{\mathcal{V}} \frac{\partial \rho}{\partial t} \,\mathrm{d}\mathbf{x} + \int_{\mathcal{V}} \boldsymbol{\nabla} \cdot (\rho \mathbf{v}) \,\mathrm{d}\mathbf{x} = 0 \tag{3.2}$$

Let $\mathcal{S} = \partial\mathcal{V}$ be the control surface, i.e. the boundary of the control volume. Then applying the divergence theorem on the second term of equation (3.2) gives

$$\int_{\mathcal{V}} \frac{\partial \rho}{\partial t} \,\mathrm{d}\mathbf{x} + \int_{\mathcal{S}} \rho \mathbf{v} \cdot \mathbf{n} \,\mathrm{d}S = 0 \tag{3.3}$$

With the aim of simplifying the first term of (3.3), we define the average density of the control volume as

$$\overline{\rho} = \frac{1}{V} \int_{\mathcal{V}} \rho \,\mathrm{d}\mathbf{x} \tag{3.4}$$

Introducing this relation in equation (3.3) gives

$$\frac{\mathrm{d}\overline{\rho}}{\mathrm{d}t} V + \int_{\mathcal{S}} \rho \mathbf{v} \cdot \mathbf{n} \,\mathrm{d}S = 0 \tag{3.5}$$

The mass flow term can be further simplified if we are using a cartesian mesh. In case of a 2D–mesh, the control surface can be partitioned into four different faces, namely, the east, west, north and south faces. In this context the control surface is $\mathcal{S} = \mathcal{S}_e \cup \mathcal{S}_w \cup \mathcal{S}_n \cup \mathcal{S}_s$ and we may express the mass flow term as

$$\int_{\mathcal{S}} \rho \mathbf{v} \cdot \mathbf{n} \,\mathrm{d}S = \sum_i \int_{\mathcal{S}_i} \rho \mathbf{v} \cdot \mathbf{n} \,\mathrm{d}S = \dot{m}_e + \dot{m}_w + \dot{m}_n + \dot{m}_s \tag{3.6}$$

If we use a 3D–mesh, we must consider the contributions of top and bottom faces. The control surface is the union $\mathcal{S} = \mathcal{S}_e \cup \mathcal{S}_w \cup \mathcal{S}_n \cup \mathcal{S}_s \cup \mathcal{S}_t \cup \mathcal{S}_b$, and therefore the mass flow incorporates two new terms

$$\int_{\mathcal{S}} \rho \mathbf{v} \cdot \mathbf{n} \,\mathrm{d}S = \sum_i \int_{\mathcal{S}_i} \rho \mathbf{v} \cdot \mathbf{n} \,\mathrm{d}S = \dot{m}_e + \dot{m}_w + \dot{m}_n + \dot{m}_s + \dot{m}_n + \dot{m}_b \tag{3.7}$$

In both cases equation (3.5) is rewritten in the following way

$$\frac{\mathrm{d}\overline{\rho}}{\mathrm{d}t} V + \sum_i \dot{m}_i = 0 \tag{3.8}$$

The average density of the control volume is roughly the density at the discretization node, that is, $\overline{\rho} \approx \rho$. Integrating (3.8) over the time interval $[t^n, t^{n+1}]$ gives

$$V \int_{t^n}^{t^{n+1}} \frac{\mathrm{d}\overline{\rho}}{\mathrm{d}t} \,\mathrm{d}t + \int_{t^n}^{t^{n+1}} \sum_i \dot{m}_i \,\mathrm{d}t = 0 \tag{3.9}$$

The first term of (3.9) has a straightforward simplification applying a corollary of the fundamental theorem of calculus. Regarding the second term, we use numerical integration which, in general, gives a non–exact result,

$$V(\rho^{n+1} - \rho^n) + \left(\beta \sum_i \dot{m}_i^{n+1} + (1-\beta) \sum_i \dot{m}_i^n \right) (t^{n+1} - t^n) = 0 \tag{3.10}$$

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

$$\frac{\rho - \rho^0}{\Delta t} V + \beta \sum_i \dot{m}_i + (1-\beta) \sum_i \dot{m}_i^0 = 0 \tag{3.11}$$

3.5 Discretization of the general convection diffusion equation