Convection – Diffusion

The 1D convection-diffusion equation reads (see Eq. 5.3 V & M)

$$\frac{d}{dx}(\rho U T) = \frac{d}{dx}\left(\Gamma\frac{dT}{dx}\right) + S,\ \Gamma = \frac{k}{c_p}$$

We discretize this equation in the same way as the diffusion equation. We start by integrating over the control volume (see figure below).

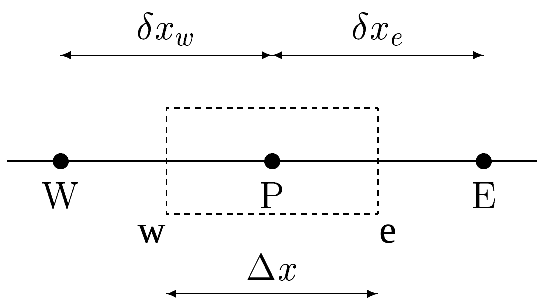


Figure. 1D control volume. Node P located in the middle of the control volume.

$$\int_w^e \frac{d}{dx}(\rho U T)\,dx = \int_w^e \left[\frac{d}{dx}\left(\Gamma\frac{dT}{dx}\right) + S\right] dx. \tag{17}$$

We start by the convective term (the left-hand side)

$$\int_w^e \frac{d}{dx}(\rho U T)\,dx = (\rho U T)_e - (\rho U T)_w\,.$$

We assume the velocity U to be known, or, rather, obtained from the solution of the Navier-Stokes equation. How to estimate T_e and T_w? The most natural way is to use linear interpolation (central differencing); for the east face this gives

$$(\rho UT)_e = (\rho U)_e T_e$$

where the convecting part, ρU, is taken by central differencing, and the convected part, T, is estimated with different differencing schemes. We start by using central differencing for T so that

$$(\rho UT)_e = (\rho U)_e T_e, \text{ where } T_e = f_x T_E + (1 - f_x) T_P$$

where f_x is the interpolation function (see Eq. 5, p. 9), and for constant mesh spacing $f_x = 0.5$. Assuming constant equidistant mesh (i.e. $\delta x_w = \delta x_e = \Delta x$) so that $f_x = 0.5$, inserting the discretized diffusion and the convection terms into Eq. 17 we obtain

$$\begin{aligned}
&(\rho U)_e \frac{T_E + T_P}{2} - (\rho U)_w \frac{T_P + T_W}{2} = \\
&= \frac{\Gamma_e (T_E - T_P)}{\delta x_e} - \frac{\Gamma_w (T_P - T_W)}{\delta x_w} + \bar{S}\Delta x
\end{aligned}$$

which can be rearranged as

$$\begin{aligned}
a_P T_P &= a_E T_E + a_W T_W + S_U \\
a_E &= \frac{\Gamma_e}{\delta x_e} - \frac{1}{2}(\rho U)_e, \; a_W = \frac{\Gamma_w}{\delta x_w} + \frac{1}{2}(\rho U)_w \\
S_U &= \bar{S}\Delta x, \; a_P = \frac{\Gamma_e}{\delta x_e} + \frac{1}{2}(\rho U)_e + \frac{\Gamma_w}{\delta x_w} - \frac{1}{2}(\rho U)_w
\end{aligned}$$

We want to compute a_P as the sum of its neighbour coefficients to ensure that $a_P \geq a_E + a_W$ which is the requirement to make sure that the iterative solver converges. We can add

$$(\rho U)_w - (\rho U)_e = 0$$

(the continuity equation) to a_P so that

$$a_P = a_E + a_W.$$

In general we have three requirements for a differencing scheme. It should be (see Section 5.4 in V & M):

1) conservative, 2) bounded and 3) transportive

• 1. Conservative. The flux *out* of a cell should be the same as that *into* the neighbour cell (e.g. the flux out of cell i through its face e should be the same as that into cell $i+1$ through its face w). This is automatically satisfied for finite volume methods.

• 2. Bounded. For the east face, for example, this means that T_e must not be smaller (or larger) than cell values used to compute T_e (see the figure on p. 27). If all coefficients are positive, this is satisfied.

• 3. Transportive. The scheme should reflect the way information is transported. The way information is transported through face e, for example, is dependent on the ratio between convection and diffusion [the Peclet number $Pe_e = (\rho U \delta x/\Gamma)_e$]. If Pe_e is small, the transport is dominated by diffusion, which transports information equally in all directions. If, on the other hand, $|Pe_e|$ is large, information is transported in the direction of U.

Above we have used the central differencing scheme. What about the three requirements?

Requirement 1: Yes;

Requirement 2: No, the coefficients can be negative (for example, $a_E < 0$ if $(\rho U)_e/2 > \Gamma_e/\delta x_e$); this occurs if the Peclet number is larger than two ($|Pe| > 2$);

Requirement 3: No, even if U becomes very large T_e is taken as the average of T_P and T_E.

We see that central differencing is second-order accurate (easily verified by Taylor expansion), i.e. the error is proportional to $(\Delta x)^2$. This is very important. If the number of cells in one direction is doubled, the error is reduced by a factor of four. By doubling the number of cells, we can verify that the discretization error is small, i.e. the difference between our algebraic, numerical solution and the exact solution of the differential equation.

Central differencing gives negative coefficients when $|Pe| > 2$; this condition is unfortunately satisfied in most of the computational domain in practice. The result is that mostly no convergent solution can be obtained at all, or, if a solution is obtained, the computed results contain oscillations. It's easy to understand why we get oscillations by looking how the derivative in the convective term is estimated in central differencing

$$\int_w^e \frac{dT}{dx}dx = T_e - T_w = \frac{T_E - T_W}{2}.$$

We see that T_P is not used when computing the derivative at node P. The right-hand side does not "feel" the value at P, and thus, as far as the right-hand side is concerned, T_P can take any value, i.e. oscillations are allowed. In order to avoid this we should use *upwind* biased discretization schemes.

First-Order Upwind Scheme

In this scheme the face value is estimated as

$$T_e = \begin{cases} T_P & \text{if } U_e \geq 0 \\ T_E & \text{otherwise} \end{cases}$$

- first-order accurate
- bounded

The large drawback with this scheme is that it is inaccurate.

For a derivation of the coefficients, see Section 5.6 in V & M.

Hybrid Scheme

This scheme is a blend of the central differencing scheme and the first-order upwind scheme. We learned that the central scheme is accurate and stable for $|Pe| \leq 2$. In the Hybrid scheme, the central scheme is used for $|Pe| \leq 2$; otherwise the first-order upwind scheme is used. This scheme is only marginally better than the first-order upwind scheme, as normally $|Pe| > 2$. It should be considered as a first-order scheme. For a derivation of the coefficients, see Section 5.7 in V & M.

Second-Order Upwind Scheme

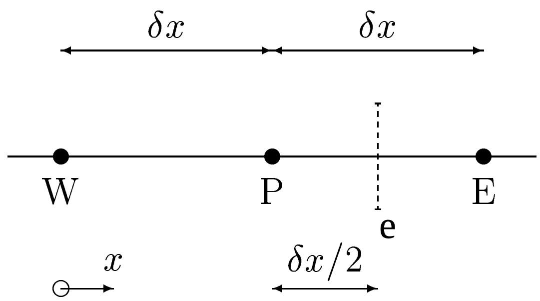


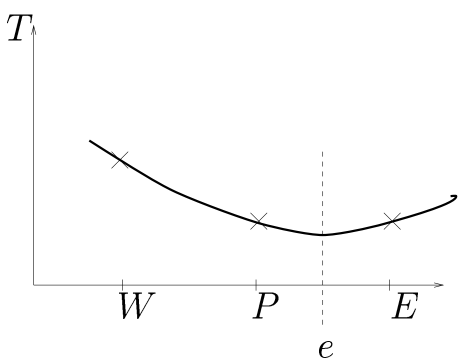
Figure. Constant mesh spacing. $U > 0$.

We use two nodes upstream and assume that the derivative between W and P is equal to that between P and e, i.e.

$$\frac{T_P - T_W}{\delta x} = \frac{T_e - T_P}{\frac{1}{2}\delta x} \Rightarrow T_e \simeq \frac{3}{2}T_P - \frac{1}{2}T_W \tag{18}$$

- second-order accurate

- unbounded (negative coefficients), i.e. $T_e < T_W$, $T_e < T_P$ or $T_e < T_E$ (see figure below), or vice versa.



Now we'll use Taylor expansion to prove that the scheme is second-order accurate. We want to show that the convective term term $\partial T/\partial x$ is second-order accurate, i.e.

$$\frac{1}{\Delta x}\int \frac{dT}{dx}dx = \frac{T_e - T_w}{\Delta x}. \tag{19}$$

From Eq. 18 we have

$$T_e \simeq \frac{3}{2}T_P - \frac{1}{2}T_W,\; T_w \simeq \frac{3}{2}T_W - \frac{1}{2}T_{WW}.$$

Insertion into Eq. 19 gives

$$\frac{1}{\Delta x}\int \frac{dT}{dx}dx \simeq \frac{1}{\Delta x}\left(\frac{3}{2}T_P - \frac{1}{2}T_W - \frac{3}{2}T_W + \frac{1}{2}T_{WW}\right) = \frac{1}{2\Delta x}\left(T_{WW} - 4T_W + 3T_P\right). \tag{20}$$

Taylor expansion gives

$$\begin{aligned} T_W &= T_P - \Delta x\left(\frac{dT}{dx}\right)_P + \frac{(\Delta x)^2}{2}\left(\frac{d^2T}{dx^2}\right)_P - \frac{(\Delta x)^3}{6}\left(\frac{d^3T}{dx^3}\right)_P + \ldots \\ T_{WW} &= T_P - 2\Delta x\left(\frac{dT}{dx}\right)_P + \frac{(2\Delta x)^2}{2}\left(\frac{d^2T}{dx^2}\right)_P - \frac{(2\Delta x)^3}{6}\left(\frac{d^3T}{dx^3}\right)_P + \ldots \end{aligned} \tag{21}$$

Eqs. 20 and 21 now give

$$\begin{aligned} \frac{1}{\Delta x}\int \frac{dT}{dx}dx &= \frac{1}{2\Delta x}\left(T_{WW} - 4T_W + 3T_P\right) + \mathcal{O}((\Delta x^2)) \\ &= \frac{1}{2\Delta x}\left[2\Delta x\left(\frac{dT}{dx}\right)_P + \left(-\frac{8}{3} + \frac{4}{6}\right)\left(\frac{d^3T}{dx^3}\right)_P \Delta x^3\right] + \ldots \\ &= \left(\frac{dT}{dx}\right)_P - \left(\frac{d^3T}{dx^3}\right)_P \Delta x^2 + \ldots, \end{aligned}$$

which is what we wanted to show.

QUICK

Quadratic Upwind Interpolation for Convective Kinematics. Two nodes upstream and one node downstream are used. A second-order polynomial is fitted through W, P and E (see figure on p. 27)

$$T(x) = ax^2 + bx + c.$$

The conditions

$$T(x=0) = T_W,\ T(x=\delta x) = T_P,\ T(x=2\delta x) = T_E$$

are used to determine the coefficients a, b and c, so that

$$T(x=1.5\delta x) \equiv T_e = \frac{3}{4}T_P + \frac{3}{8}T_E - \frac{1}{8}T_W$$

For a derivation of the coefficients, see Section 5.9 in V & M.

QUICK is

- third-order accurate
- unbounded

Bounded Second-Order Upwind Scheme

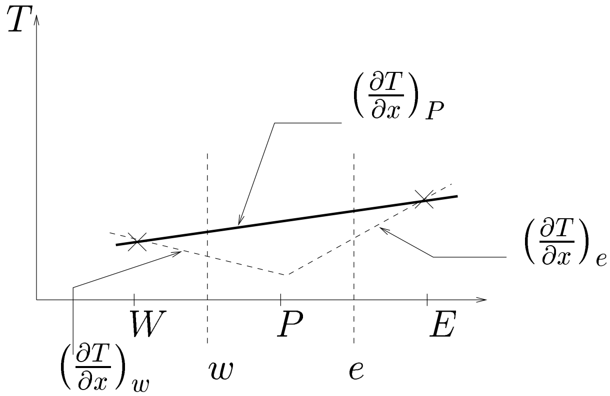
Above a second-order upwind scheme was presented. However, this scheme was unbounded, and therefore numerical problems are often encountered for this scheme. Mostly, bounded second-order upwind schemes are used. One example is the Van Leer scheme. This scheme reads as follows ($U_e > 0$ assumed):

$$T_e = \begin{cases} T_P + \frac{T_E - T_P}{T_E - T_W}(T_P - T_W) & \text{if } |T_E - 2T_P + T_W| \leq |T_E - T_W| \\ T_P & \text{otherwise} \end{cases}$$

If the variation of T is smooth then

$$\frac{T_E - T_P}{T_E - T_W} \simeq \frac{1}{2},$$

and we find that van Leer scheme gives $T_e = 1.5T_P - 0.5T_W$, i.e. it returns to the second-order upwind scheme (see p. 27).



If T has, for example, a minimum at node P (see figure above), then the second derivative $[T_E - 2T_P + T_W = T_E - T_W + 2(T_W - T_P)]$ is larger than than the derivative evaluated between P and E (i.e. $T_E - T_W$). When so, the first-order upwind scheme is used.

The van Leer scheme

- is second-order accurate, except at local minima and maxima where is only first-order accurate. It can be regarded as a second-order scheme.

- is bounded