Development of the Numerical Schemes and Iteration Procedures

Nielsen, Peter Vilhelm

Published in:
Euroacademy on Ventilation and Indoor Climate

Publication date:
2008

Document Version
Publisher's PDF, also known as Version of record

Link to publication from Aalborg University

Citation for published version (APA):
Development of the numerical schemes and iteration procedures

Peter V. Nielsen, Aalborg University

Introduction

This lecture presents the basic theory behind the numerical method as well as the historical development. Some of the problems behind quality control are also illustrated. Main items in this chapter are:
- One-dimensional case
- False diffusion
- Iteration procedure

One-dimensional case

It is not possible to make a direct analytic solution of the differential equation system which can be established for room air distribution. Therefore, it is necessary to reformulate the differential equations into difference equations for which solutions can be found by a numerical method.

Most of this section is based on a simple one-dimensional case. This assumption should facilitate the understanding. Although the case is one-dimensional it can also be considered as a small part of a complicated flow which is one-dimensional in certain areas, parallel with grid lines and steady, see figure 1.

As a further simplification only the transport equation for mass fraction per unit of mass mixture (e.g. contaminant distribution) will be addressed in this chapter. This equation can be solved independently of the other flow equations assuming that the velocity and distribution of turbulence are known. The discretization of the Navier Stokes equations and the energy equation are further discussed in Awbi (2003) and in Versteeg and Malalasekera (1995).

Figure 1. Four grid points, with neighbouring points, in a flow domain where the flow is one-dimensional, parallel with the grid lines and steady.
The three-dimensional steady state version of this equation is given as

\[ \rho u \frac{\partial c}{\partial x} + \rho v \frac{\partial c}{\partial y} + \rho w \frac{\partial c}{\partial z} = \frac{\partial}{\partial x} \left( \Gamma_e \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial y} \left( \Gamma_e \frac{\partial c}{\partial y} \right) + \frac{\partial}{\partial z} \left( \Gamma_e \frac{\partial c}{\partial z} \right) + S_e \]  

(1)

And the one-dimensional equation is given as

\[ \rho u \frac{dc}{dx} = \Gamma_e \frac{d^2c}{dx^2} + S_e \]  

(2)

where \( x, t \) and \( \rho \) are position, time and density respectively. \( \Gamma_e \) is the turbulent diffusion coefficient and \( S_e \) is the specific source term.

**Finite volume expression**

The flow domain is divided into cells of the size \( \Delta x \cdot \Delta y \cdot \Delta z \), see Figure 2.

![Figure 2. Five grid points, WW, W, P, E and EE, and a cell around P with two surfaces, w and e.](image)

The finite volume equation for a grid point, \( P \), can either be developed from the transport equation, (Eq. 2), or it can be established direct from the cell shown in Figure 2, see Patankar (1980).

The convective mass transport to the volume is the difference between the convective mass transport through the two surfaces, \( e \) and \( w \).

\[ \rho(u_c - u_e)\Delta y \Delta z \]

The total diffusion over the two surfaces is equal to

\[ \Gamma_e \left[ \frac{dc}{dx} - \frac{dc}{dx} \right] \Delta y \Delta z \]

The source term is equal to

\[ S_e \Delta x \Delta y \Delta z \]

The steady state one-dimensional transport equation for contaminant distribution (mass fraction per unit of mass mixture) is therefore given by
\[ \rho(u_c c_e - u_e c_u) = \Gamma_e \left[ \frac{dc}{dx} \right]_e - \left[ \frac{dc}{dx} \right]_u + S \Delta x \]  

Equation (3) is called a control volume formulation because it can be considered to be an integration of the transport equation (differential equation (2)) over the length \( \Delta x \).

An important feature is the integral conservation of quantities such as mass, momentum and energy. This feature is valid not only for each control volume but also for the total flow domain, and it is independent of the grid distribution. Even a coarse-grid solution exhibits exact integral balances, Patankar (1980).

It is necessary to replace values at the cell surfaces, \( e \) and \( w \), with values at the grid points, \( WW, W, P, E \) and \( EE \), to obtain the final version of the discretization equation. Differing assumptions are made over the years. The examples in “solution of the transport equation” show the consequences of different schemes and the development of new schemes used in CFD software today. An original strategy was to let values on cell surfaces and the gradient \( dc/dx \) be replaced by the values obtained from a piecewise linear profile between grid points, as for example

\[ c_e = (c_P + c_F)/2 \]

and

\[ \left( \frac{dc}{dx} \right)_e = \frac{c_F - c_P}{\Delta x} \]

The two assumptions for convection and diffusion are both of second order accuracy.

In the following section the velocity, \( u \), is considered to be constant and the source term is equal to zero in the flow regime. The finite volume equation will therefore have the form

\[ 4\Gamma e c_P = (2\Gamma e + \rho\Delta xu)c_F + (2\Gamma e - \rho\Delta xu)c_e \]

The equation shows the connection between the concentration, \( c_P \), in the grid point, \( P \), and the concentration in the neighbouring points, \( c_W \) and \( c_E \).

**Finite difference equation**

The discretization equation can also be developed as a finite difference equation. The first and the second derivatives in equation (2) are replaced with the expressions developed from Taylor Series

\[ \frac{dc}{dx} = \frac{c_F - c_W}{\Delta x} \]

\[ \frac{d^2 c}{dx^2} = \frac{c_W - 2c_P + c_E}{\Delta x^2} \]

The obtained equation will express a direct connection between the neighbouring grid points.

**Solution of the transport equation**
The finite volume transport equation (4) is often expressed in the general form

\[ a_P c_P = a_W c_W + a_E c_E + b \]  

(5)

As an example, the flow is studied in a case for which the length, \( x \), is equal to 4, see Figure 3. The velocity, \( u \), is equal to 0.1, and \( \Gamma_c \) and \( \rho \) are both 1.0. The boundary values, \( c_0 \) and \( c_3 \), are equal to 1.0 and 0.0, respectively.

Figure 3. Grid point distribution with four internal grid points. Points 0 and 3 are temporary boundaries for the one-dimensional predictions.

Figure 4 shows the predictions of the one-dimensional concentration distribution at a low velocity of \( u = 0.1 \). The predictions are close to the straight line between the two boundary values 1.0 and 0.0. The straight line is the solution when the velocity is zero and transport occurs only as diffusion.

Experience shows that unstable (oscillatory or wiggly) solutions are obtained for high velocity, \( u \), or for an increased grid point distance, \( \Delta x \). It is shown that the Peclet number

\[ Pe = \frac{\rho \Delta x u}{\Gamma_c} \]  

(6)
must be smaller than 2 to ensure convergence and stable solutions. This is a very disadvantageous situation because most engineering applications have a high Reynolds number or a high convective flux and a small diffusion.

Figure 5 shows the solution of Equation (4) for a velocity of \( u = 3.0 \). The numerically unstable solution is typical of a control volume formulation with a central difference in the convection term and a large Peclet number (\( Pe = 4 \) in this case). The increase in concentration, \( c \), between the co-ordinations 1 and 2 cannot be a physical effect because the transport equation is without any source term, but it is a numerical error which is obtained by the central difference scheme and a high Peclet number.

This was a typical situation in the 1950s and in the 1960s. Solutions with increasing Reynolds numbers were therefore obtained by reducing the distance between the grid points to get a small Peclet number. On the other hand, this remedy often led to a number of grid points far too high for computers of that time.

It is recognized that convection is an asymmetric phenomenon, i.e. the upstream conditions have a greater influence than the downstream conditions. Therefore, it is essential that the discretization scheme reflects this in one way or another, otherwise physically unrealistic solutions might occur.

![Figure 5](image)

**Figure 5.** Numerical solution of the concentration distribution in a one-dimensional flow at high velocity \( (u = 3.0) \). Convection term with central difference.

A large step forward was therefore taken when Courant et al. (1952) suggested the upwind scheme which has almost unconditional stability. The upwind scheme defines the values, for example on the control-volume surface, \( w \), in the convection term by

\[
\begin{align*}
    c_w &= c_w & u & \geq 0 \\
    c_w &= c_p & u & < 0
\end{align*}
\]

The upwind scheme is of first order of accuracy. Instead of the mean value given in equation (4) the following discretization equation will be obtained when the upwind scheme is introduced in equation (3)

\[
(2\Gamma_c + \rho\Delta x u)c_p = (\Gamma_c + \rho\Delta x u)c_w = \Gamma_c c_E
\]
A solution of a transport equation with an upwind scheme in the convection term and high Peclet number ($Pe = 4$) is shown in Figure 5.6 for both $\rho$ and $\Gamma_c$ equal to 1.0. The solution is physically correct with a continuously decreasing $c$ value as a function of the distance, $x$.

In equation (7) the convection term is of first order of accuracy and the diffusion term is of second order of accuracy. This means that the whole equation is a first order equation (the lowest order will count).

**False diffusion**

In the early 1970s, it seemed that the use of an upwind scheme had opened the way to make numerical simulations of flow phenomena at indefinitely high Reynolds numbers. However, before the end of the decade it had become clear that there were errors in the predictions, although high stability was obtained. The error is connected with a flow which has an angle to the grid lines, and the error has a maximum at 45°. A “false” or “numerical” diffusion is the result and it is proportional to the velocity and to the distance between the grid points. Huang et al. (1985) conclude that many studies at the end of the 1970s had a false diffusion which could be larger than the actual physical diffusion.

An improvement was obtained by introducing an upwind scheme with a second order of accuracy. The value on the cell surface, $c_w$, is in this case based on values in two upstream notes instead of one upstream note

\[
c_w = \begin{cases} 
\frac{3}{2} c_w - \frac{1}{2} c_{yw} & u \geq 0 \\
\frac{3}{2} c_p - \frac{1}{2} c_e & u \leq 0
\end{cases}
\]

The second order upwind scheme introduced in equation (3) gives the following discretization equation

\[
(4\Gamma_c + 3\rho \Delta xu)c_p = -\rho u \Delta x c_{yw} + (2\Gamma_c + 4\rho \Delta xu)c_{yw} + 2\Gamma_c c_e
\]  

(8)

A solution of this transport equation for $\rho = 1.0$ and $\Gamma_c = 1.0$ is also shown in Figure 6.
The QUICK scheme by Leonard (1979) is another improved scheme for the convection term, which has a small false diffusion and a high accuracy. The scheme is addressed here, because it has some of the qualities which are typical for new schemes in commercial programs. The scheme can be interpreted as a central difference scheme with a stabilizing upstream weighted curvature correction arising from the second order polynomial fit. The value, $c_w$, on the control volume surface of equation (3) has the following formulation

$$\begin{align*}
c_w &= \frac{3}{4} c_w + \frac{3}{8} c_p - \frac{1}{8} c_{ww} & u \geq 0 \\
c_w &= \frac{3}{4} c_p + \frac{3}{8} c_w - \frac{1}{8} c_e & u < 0
\end{align*}$$

The van Leer scheme is a scheme which also takes into account the fact that the upstream conditions have a greater influence on the variable in point, $P$, than the downstream conditions.

The treatment of the convection in the different schemes is illustrated in Figures 7 and 8. The black curve shows the analytical solution $c = f(x)$ of mass fraction distribution per unit of mass mixture.

The second order central difference is shown in blue for the cell surface, $w$, in Figure 7. It indicates that, $c_w$, is the mean value of $c_w$ and $c_p$, or in other terms, that a piecewise linear profile is used for the description of the convection term.

![Figure 7. Central difference description of the cell surface value $c_w$.](image)

Figure 8 shows that in a first order upwind scheme the cell surface value is simply given as the upstream value, $c_w$. In the second order upwind scheme the cell surface obtains the value extrapolated from the assumption of a straight line through $c_{ww}$ and $c_w$. In the QUICK scheme three points are used for the formulation of the cell surface value and it is given from a polynomial fit of the grid points.

An increasing accuracy is indicated in the Figures 8 A, B and C. It is also obvious that the cell surface value, $c_w$, is unbounded in figures B and C, which means that, $c_w$, might have a value above or below $c_{ww}$, $c_w$ and $c_p$ if the curve $c = f(x)$ has a large variation between the grid points. This is a source of non-physical wiggles in the prediction.
The second order upwind scheme and the QUICK scheme were introduced to minimize the false diffusion and Figure 9 illustrates the effect. Figure 9A shows the prediction of flow from a wall-mounted opening of the size 6.8 cm x 52 cm located in a wall 0.5 m below the ceiling in a room. The flow is directed upward from the opening \((u, v = 3.1, 2.6 \text{ m/s})\) and the predictions are using a grid with 30000 cells. The grid is rectangular and the flow close to the opening has therefore an angle to the grid lines. Figure 9B shows the predicted profile below the ceiling 1 m from the wall. The two profiles show the large change which is obtained by the use of a second order upwind scheme instead of a first order scheme. Predictions made by a second order upwind scheme indicate non-physical wiggles which in this case are the result of an insufficient number of grid points. This is also an indication of the fact that convergence problems may arise when the second order upwind scheme is used.

Figure 9B illustrates two different types of error. The first order upwind solution shows a diffusive error and the second order upwind solution shows a dispersive error.
The selection of a numerical scheme with a high order of accuracy improves the results if it is difficult to obtain a grid-independent solution. Sørensen and Nielsen (2003) have shown the influence of false diffusion in a case called the Smith and Hutton problem (1982). Figure 10A shows the case. The air is defined as a two-dimensional flow in a “death end channel” and the velocities are given by an analytical description. The situation is typical of room air movement (in certain areas) with mixing ventilation as indicated on the right side of Figure 10B.

A transport equation, e.g. the contaminant transport equation, is solved in the flow field in Figure 10A. This transport equation is without physical diffusion terms. The concentration will therefore be transported along with the flow, preserving the inlet values all the way to the outlet. Consequently, at the outlet any deviations between the exact and the computed concentration fields are due to inaccuracies in the numerical solution of the transport equation (false diffusion).

Figure 10. The Smith and Hutton problem at the top (A), and typical flow in a room with mixing ventilation and slot inlet at the bottom (B).

Figure 11. Concentration distributions predicted by three different discretization schemes. (A): first order upwind scheme, (B): second order scheme, (C): third order QUICK scheme. Grid size is 80 × 40 cells. Contours are shown for concentration levels of 0.01, 0.05, 0.5, 1.0, 1.5, 1.95 and 1.99.

The computational grids are made with 80 × 40 cells in the x and y directions, respectively. Steady calculations are made with three different discretization schemes. Figure 11 shows the concentration distributions for a first order upwind scheme (Figure 11 (A)), a second order scheme (B) and a third order QUICK scheme (C). Recalling that the distribution at the outlet should equal the distribution at the inlet,
the false diffusion is evidenced by the large smearing of the distribution. The second order scheme transports the concentration with less smearing. Finally, the third order scheme transports the concentration almost without change. Thus, the example shows that higher order schemes perform significantly better than lower order schemes for a given grid size. The predictions in Figure 11 are made by 3200 grid points which are a small number. An equivalent grid density in the whole room in Figure 10 (with three-dimensional flow) demands about one million grid points which in practice is typical of many predictions. Other predictions with a lower and a higher number of grid points are also given by Sørensen and Nielsen (2003). It is shown that an increased number of grid points improve the first and second order schemes.

The selection of the numerical scheme has some influence on the results when it is difficult to obtain grid independent solutions. It is always recommended to use a scheme of second order accuracy if it is available and if convergence can be obtained, see Casey and Wintergerste (2000) and Sørensen and Nielsen (2003).

**Iteration procedure**

The one-dimensional case is finalized by the following discussion of the iteration procedure. Older methods are mentioned because they exhibit, in an illustrative way, the typical problems in numerical methods.

A Gauss-Seidel procedure was used earlier in the 1960s, while a Tri-Diagonal-Matrix has been used together with a line-by-line up to now.

The Gauss-Seidel iteration is a very simple method in which the values of the variable are calculated by visiting each grid point in a certain order. The discretization equation (Eq. 5) can be rearranged in the form

$$c_P = C_W c_W + C_E c_E + D$$

where $C_w = a_W/a_P$, $C_E = a_E/a_P$ and $D = b/a_P$

Figure 12. Temporary boundaries and grid distribution for the one-dimensional test case in section 5.2.

Figure 12 shows the grid distribution for the one-dimensional test case. $c_0$ and $c_{m+1}$ are temporary boundaries for the one-dimensional predictions. The figure shows how $c_P$ is calculated from the neighbour points. One of the points has been updated ($c_W$) and the other point has the value from the earlier iteration. All $m$ grid points are visited during iterations $n+1$ according to the discretization equation for the test case

$$c_P^{n+1} = C_W c_W^{n+1} + C_E c_E^{n}$$

The value of a point $P$ will converge towards the level which is the solution of all the algebraic equations during the iteration.
A grid distribution as shown in Figure 3 gives the following discretization equation in the grid points 1 and 2 in the case of a low velocity and a central difference assumption in the convective terms.

\[
\begin{align*}
x = 1.333 & \Rightarrow \quad c_1 = 0.4667 \ c_2 + 0.5333 \\
x = 2.667 & \Rightarrow \quad c_2 = 0.5333 \ c_1
\end{align*}
\]

Table 1 shows the converged Gauss-Seidel iteration of the equation with 0.0 as the internal starting values.

**Table 1. Gauss-Seidel iteration of the equation system based on the grid in Figure 3**

<table>
<thead>
<tr>
<th>n</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\Omega)</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
</tr>
<tr>
<td>(c_1)</td>
<td>0.000</td>
<td>0.5333</td>
<td>0.6660</td>
<td>0.6991</td>
<td>0.7073</td>
<td>0.7093</td>
<td>0.7098</td>
<td>0.7100</td>
</tr>
<tr>
<td>(c_2)</td>
<td>0.000</td>
<td>0.2844</td>
<td>0.3552</td>
<td>0.3728</td>
<td>0.3772</td>
<td>0.3783</td>
<td>0.3786</td>
<td>0.3786</td>
</tr>
<tr>
<td>(c_3)</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
</tbody>
</table>

The discretization equation can also be rearranged in the Tri-Diagonal-Matrix Algorithm (TDMA)

\[
\begin{align*}
x = 1.333 & \Rightarrow \quad BV + a_P c_1 + a_E c_2 = 0 \\
x = 2.667 & \Rightarrow \quad a_W c_1 + a_P c_2 + BV = 0
\end{align*}
\]

The TDMA method is a direct solution of the above equation system. \(c_1\) in the second equation is substituted by \(c_1 = \text{func} (c_2)\) from the first equation whereby \(c_2\) known. \(c_1\) is then found by back-substitution. The process can be made for any number of equations in the \(x\)-direction.

The solution of the discretization equations for the one-dimensional test case can thus be obtained direct by the TDMA method. This method is also called the Thomas algorithm or the Gaussian-elimination method. The designation TDMA refers to the three diagonals in the matrix formed by the coefficients of the discretization equation.
The line-by-line method is a convenient combination of the TDMA method for one-dimensional situations and the Gauss-Seidel method. Figure 13 shows how the line-by-line method can be used for the two-dimensional situation. The neighbour points to a line with unknown values are assumed to be known from the latest iteration. The TDMA method is used at the line with unknown values with the effect that the boundary conditions are transmitted into the inner field in an efficient way. The next line is now treated as a line with unknown values, while the neighbour points have the known values, and the TDMA method is repeated at this line. Figure 13 indicates how this process sweeps over all the grid points during one iteration. The sweep direction can be changed. It is always efficient to consider the sweep direction in connection with the flow field which has to be predicted. Sweeps in the flow direction should e.g. be used when convection occurs in the flow field.

The coupling between pressure and velocity is handled by a SIMPLE procedure. This procedure uses the staggered grid for the velocities in order to avoid non-physical oscillations in the pressure field. Furthermore, the continuity equation is rewritten as an equation for pressure correction. A detailed description is given by Patankar (1980) and Versteeg and Malalasekera (1995).

The procedures described here are the classical ones and serve as an easily understandable starting point for more sophisticated numerical solution techniques. Modern algorithms handle more complex cell forms too and usually apply multi-grid acceleration techniques.

The multi-grid method is based on the observation that numerical wiggling are especially damped for wiggling patterns which have a periodicity of the same length as the grid distance. Larger wavelength wiggling patterns are much less affected by successive iterations.

Therefore a coarser grid is constructed (typically a coarsening factor of 2 is used), and the values are interpolated from the original grid and some iterations are performed on this grid.

Sometimes an even coarser grid is formed and the same procedure is applied. After that the intermediate solution is transferred back to the less coarse grid, and iterations are done. This solution is then transferred to the original grid and further iterations are performed.

In total the procedure accelerates the convergence considerably. Figure 14 shows an example of an iteration procedure on grids of different coarsenesses. The exact procedure is adjusted to the properties of the specific code. All the steps described are performed automatically without need of a user interaction. The method is used in most modern codes.
Figure 14. Multi-grid method. Above: 2 coarser grids formed from original grid. Below: Schematic drawing of successive iterations on different grids.

Literature


