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A HYBRID FIVE-POINT FINITE DIFFERENCE SCHEME FOR CONVECTION-DIFFUSION EQUATIONS

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Abstract. *In this paper, some five-point finite difference schemes for steady convection-diffusion problems are presented. To begin with, we use the finite volume method (FVM) to discretize the convection-diffusion equation. After that, we present two five-point difference schemes for the approximation of the first order derivatives on faces, one of which is central difference type scheme, the other is upwind difference type scheme. In both of the schemes, one node is always connected with its four neighbor nodes. As the central scheme is of fourth order accuracy, it is very accurate to employ for small Peclet numbers. But when Peclet number is large, the scheme can be unstable. In this case, the upwind scheme of third order accuracy is stable. As the upwind scheme can reflect the flow transportation, it can give stable numerical solution.*

Taking use the advantages of the above two schemes, we construct a hybrid scheme, which can be utilized not only for small Peclet numbers, but for large Peclet numbers. The new higher order difference scheme and the hybrid strategy might be extended to solve 2D and 3D fluid dynamics equations including Navier-Stokes equation. Some numerical examples are also presented to illustrate the discussion.

1 INTRODUCTION

In this paper, we consider the numerical solution for convection-diffusion problems. These problems play important roles in computational fluid dynamics.It can be described by following general partial equation(see[1, 2, 3]).

$$\frac{\partial(\rho\phi)}{\partial t} + div(\rho\mathbf{u}\phi) = div(\Gamma \cdot grad\phi) + S_\phi \tag{1}$$

where $\mathbf{u}, \rho, \Gamma$ and S_ϕ represent velocity vector, density, diffusion coefficient and source term respectively. In this equation, property ϕ can be internal energy i, or temperature T, or components of velocity vector $\mathbf{u}$ in x, y, z direction. In one dimensional steady flow field without source term S_ϕ, we present following problem.

Problem I. Property ϕ of a flow satisfy the following equation and boundary conditions.

$$\frac{d(\rho u\phi)}{dx} = \frac{d}{dx}(\Gamma\frac{d\phi}{dx}), 0 < x < L \tag{2}$$

$$\phi(0) = \phi_A, \phi(L) = \phi_B \tag{3}$$

where Γ is the diffusion coefficient, velocity u and density ρ of the flow are given in advance, ϕ_A and ϕ_B are given values.

The analytic solution of Problem I is (see[1])

$$\phi = \phi_A + \frac{\phi_B - \phi_A}{e^{\rho uL/\Gamma} - 1}(e^{\rho ux/\Gamma} - 1) \tag{4}$$

A lot of finite difference schemes have already been produced to compute the numerical solution of the convective-diffusion problems(see[1]) and similar problems(see[4]-[8]). The central difference scheme of second order accuracy may result in unstable solution because of its inability to identify flow direction. The upwind scheme takes into account flow direction, but its accuracy is only first order. The hybrid difference scheme of Spalding(1972) exploits the favorable properties of upwind and central difference schemes, but it is only first order accuracy. The QUICK scheme of Leonard(1979) is of second order accuracy, but it can be unstable. In this paper, we first present two five-point difference schemes for Problem I, one of which is central difference scheme, the other is upwind difference scheme. In both of these schemes, one inner node is always connected with its four neighbor nodes. As the central scheme is of fourth order accuracy, it is often employed for small Peclet numbers ($|P_e| < 2$). But when Peclet number is large ($|P_e| \geq 2$), the scheme is probably unstable. Under such condition, the upwind scheme is employed. Though the scheme is of third order accuracy, it can give stable numerical solution because it can identify the flow direction. Taking use the advantages of the above two schemes, we also construct a new hybrid scheme of third order accuracy, which can be utilized not only for small Peclet numbers, but for large Peclet numbers.

2 DISCRETIZATION FOR PROBLEM I

2.1 Grid generation

Now we use the finite volume method to discretize equation (2). We divide the domain [0,L] into some control volumes, as shown in Figure 1. The total number of the control volumes is denoted by n. Let us place n nodes inside the domain, one node in each of the control volumes and they are denoted by $1, 2, \cdots, n$ respectively. The boundary faces are A and B. A general nodal point is denoted by P. Its nearest pair of neighbor nodes in one-dimensional geometry, the nodes to the west and east of node P, are identified by W and E respectively. Similarly, its next two pairs of neighbor nodes are identified by W_1, E_2 and W_2, E_2. The west and east side faces of the control volume are denoted by w and e. The distances between the nodes W and P, and between P and E are denoted by δx_{WP} and δx_{PE}.

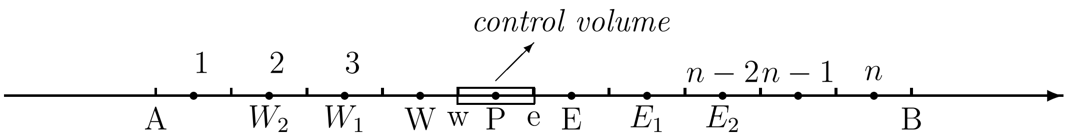

Figure 1: Discretization of the given domain [0,L]. The control volume at inner node P and its neighbor nodes.

2.2 discretization

Integration of equation (2) over a control volume containing node P yield a discretized equation

$$(\rho u A\phi)_e - (\rho u A\phi)_w = (\Gamma A\frac{d\phi}{dx})_e - (\Gamma A\frac{d\phi}{dx})_w \tag{5}$$

Here A is the cross-sectional area of the control volume. The flow must also satisfy continuity so that

$$\frac{d(\rho u)}{dx} = 0 \tag{6}$$

The integration of continuity equation (6) yields

$$(\rho u A)_e - (\rho u A)_w = 0 \tag{7}$$

To obtain difference equations for convective-diffusion problem we must approximate the derivative terms in equation(5). Now we define two variables F and D to represent the convective mass flux and diffusion conductance at cell faces:

$$F = \rho u A, \qquad D = \frac{\Gamma A}{\delta x} \tag{8}$$

Then (7) can be written as

$$F_e - F_w = 0 \tag{9}$$

We also define the non-dimensional cell Peclet number as a measure of the the relative strengths of convection and diffusion:

$$P_e = \frac{F}{D} = \frac{\rho u}{\Gamma/\delta x} \tag{10}$$

When the Peclet number is small($|P_e| < 2$), we say that the flow field is diffusive dominative. Otherwise, we say that the flow is convective dominative.

3 CENTRAL DIFFERENCE SCHEME

Now we use central difference scheme to calculate the numerical solution for Problem I. As Figure 1 shows, we have already discretized the domain in section 2. Here we presume that the widths of all the control volumes are the same, so are the distances between each of two neighbor nodes, and we denote them by δx.

Then we apply a cubic polynomial interpolation for cell face values in (5). We use a cubic function fit through four nodes, two of which on the upstream side, the other two on the downstream side, to evaluate the face values of ϕ and $\frac{d\phi}{dx}$ in (5). In other words, a cubic function fit through W_1, W, P and E is used to evaluate ϕ_w and $(\frac{d\phi}{dx})_w$, and a further cubic function fit through W, P, E and E_1 to evaluate ϕ_e and $(\frac{d\phi}{dx})_e$. For a uniform grid with step of δx, the values of ϕ and $\frac{d\phi}{dx}$ at the cell faces can be obtained by using cubic polynomial interpolation:

$$\phi_w = \frac{1}{16}(9\phi_W + 9\phi_P - \phi_{W_1} - \phi_E) + O(\delta x^4) \tag{11}$$

$$\phi_e = \frac{1}{16}(9\phi_P + 9\phi_E - \phi_W - \phi_{E_1}) + O(\delta x^4) \tag{12}$$

$$(\frac{d\phi}{dx})|_w = \frac{1}{24\delta x}(27\phi_P - 27\phi_W - \phi_E + \phi_{W_1}) + O(\delta x^4) \tag{13}$$

$$(\frac{d\phi}{dx})|_e = \frac{1}{24\delta x}(27\phi_E - 27\phi_P - \phi_{E_1} + \phi_W) + O(\delta x^4) \tag{14}$$

So (5) can be written as

$$\begin{aligned} &\frac{1}{16}F_e(9\phi_P + 9\phi_E - \phi_W - \phi_{E_1}) - \frac{1}{16}F_w(9\phi_W + 9\phi_P - \phi_{W_1} - \phi_E) \\ =&\frac{1}{24}D_e(27\phi_E - 27\phi_P - \phi_{E_1} + \phi_W) - \frac{1}{24}D_w(27\phi_P - 27\phi_W - \phi_E + \phi_{W_1}) + O(\delta x^4) \end{aligned} \tag{15}$$

This can be re-arranged by deleting the truncation error term $O(\delta x^4)$ and utilizing (9) to give

$$a_P\phi_P = a_{W_1}\phi_{W_1} + a_W\phi_W + a_E\phi_E + a_{E_1}\phi_{E_1} + S_u \tag{16}$$

where $a_{W_1} = -D_w/24 - F_w/16, a_W = 9D_w/8 + 9F_w/16 + D_e/24 + F_e/16, a_E = 9D_w/8 - F_w/16 + D_e/24 - 9F_e/16, a_{E_1} = -D_e/24 + F_e/16, a_P = a_{W_1} + a_W + a_E + a_{E_1} - S_P$ with $S_P = 0, S_u = 0$.

At node 1, as shown by Figure 2, it is obvious that $\phi_w = \phi_A$. In order to use (5) evaluate ϕ_e, we make linear extrapolating at mirror node W, that is

$$\phi_W = 2\phi_A - \phi_P \tag{17}$$

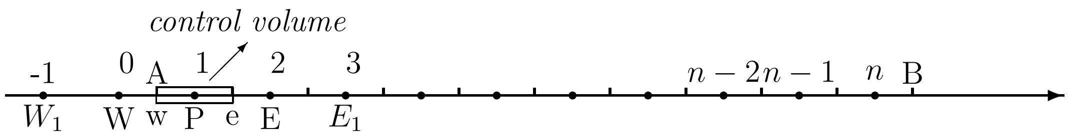

Figure 2: Discretization of the given domain [0,L]. The control volume at boundary node P and its neighbor nodes

Replacing ϕ_W in (12) with (17), and (12) becomes

$$\phi_e = \frac{1}{16}(10\phi_P + 9\phi_E - \phi_{E_1} - 2\phi_A) \tag{18}$$

A cubic function fit through four nodes P, E, E_1 and boundary node A is used to evaluate $(\frac{d\phi}{dx})_e$ and $(\frac{d\phi}{dx})_A$.

$$(\frac{d\phi}{dx})_e = \frac{1}{60\delta x}(8\phi_A - 75\phi_P + 70\phi_E - 3\phi_{E_1}) + O(\delta x^3) \tag{19}$$

$$(\frac{d\phi}{dx})_A = \frac{1}{60\delta x}(-184\phi_A + 225\phi_P - 50\phi_E + 9\phi_{E_1}) + O(\delta x^3) \tag{20}$$

According to (17)-(19) and (5), the discretization equation at node 1 can be written as

$$a_P\phi_P = a_E\phi_E + a_{E_1}\phi_{E_1} + S_u \tag{21}$$

where $a_E = \frac{5}{6}D_A + \frac{7}{6}D_e - \frac{9}{16}F_e; a_{E_1} = -\frac{3}{20}D_A - \frac{1}{20}D_e + \frac{1}{16}F_e; a_P = a_E + a_{E_1} - S_P; S_P = -(\frac{46}{15}D_A + F_A + \frac{2}{15}D_e + \frac{1}{8}F_e); S_u = (\frac{46}{15}D_A + F_A + \frac{2}{15}D_e + \frac{1}{8}F_e)\phi_A$.

Similarly, at node 2, the discretization equation becomes

$$a_P\phi_P = a_W\phi_W + a_E\phi_E + a_{E_1}\phi_{E_1} + S_u \tag{22}$$

where $a_W = \frac{5}{4}D_w + \frac{5}{8}F_w + \frac{1}{24}D_e + \frac{1}{16}F_e; a_E = \frac{1}{20}D_w - \frac{1}{16}F_w + \frac{9}{8}D_e - \frac{9}{16}F_e; a_{E_1} = -\frac{1}{24}D_e + \frac{1}{16}F_e; a_P = a_W + a_E + a_{E_1} - S_P; S_P = \frac{2}{15}D_w + \frac{1}{8}F_w; S_u = -(\frac{2}{15}D_w + \frac{1}{8}F_w)\phi_A$.

At node $n-1$, the discretization equation is

$$a_P\phi_P = a_W\phi_W + a_E\phi_E + a_{E_1}\phi_{E_1} + S_u \tag{23}$$

where $a_{W_1} = -\frac{1}{24}D_e - \frac{1}{16}F_e; a_W = \frac{9}{8}D_w + \frac{9}{16}F_w + \frac{1}{20}D_e + \frac{1}{16}F_e; a_E = \frac{1}{24}D_w - \frac{1}{16}F_w + \frac{5}{4}D_e - \frac{5}{8}F_e; a_P = a_{W_1} + a_W + a_E - S_P; S_P = \frac{2}{15}D_e + \frac{1}{8}F_e; S_u = -(\frac{2}{15}D_e + \frac{1}{8}F_e)\phi_A$.

At node n, we have

$$a_P\phi_P = a_{W_1}\phi_{W_1} + a_W\phi_W + S_u \tag{24}$$

where $a_{W_1} = -\frac{1}{20}D_w - \frac{1}{16}F_w - \frac{3}{20}D_B; a_W = \frac{7}{6}D_w + \frac{9}{16}F_w + \frac{5}{6}D_B; a_P = a_{W_1} + a_W - S_P; S_P = -\frac{2}{15}D_w + \frac{1}{8}F_w - \frac{46}{15}D_B + F_B; S_u = -(-\frac{2}{15}D_w + \frac{1}{8}F_w - \frac{46}{15}D_B + F_B)\phi_A$.

Now we discuss the property of the above central difference scheme.It is easy to prove that the scheme is of fourth order accuracy at inner nodes $i(2 < i < n-1)$, and is of third order accuracy at node 2 and $n-1$,and is first order at node 1 and n. So it is more accurate than the central difference scheme of second order accuracy.When $(-2 < P_e < 2)$, by using above scheme we can obtain highly accurate numerical solution, which is shown by Example 1. But when $P \geq 2$ or $P \leq -2$, the scheme might be unstable, which is shown by Example 2. For this reason, we introduce another scheme, third order upwind difference scheme in following section.

4 UPWIND DIFFERENCE SCHEME

When the flow is convective dominative, we also use four-points cubic interpolation to evaluate cell face values.The face values of ϕ and $\frac{d\phi}{dx}$ in (5) is obtained from a cubic function passing through four nodes too, but three of them on the upstream side, the other one on the downstream side. When $u_w > 0$ and $u_e > 0$, a cubic fit through W_2, W_1, W and P is used to evaluate ϕ_w and $(\frac{d\phi}{dx})_w$, and a further cubic fit through W_1, W, P and E to evaluate ϕ_e and $(\frac{d\phi}{dx})_e$. When $u_w < 0$ and $u_e < 0$, a cubic fit through W, P, E and E_1 is used to evaluate ϕ_w and $(\frac{d\phi}{dx})_w$, and a further cubic fit through P, E, E_1 and E_2 to evaluate ϕ_e and $(\frac{d\phi}{dx})_e$. Here we only discuss the the condtions when $u_e > 0$, $u_w > 0$. The condition when $u_w < 0$ and $u_e < 0$ can be dealt with similarly.

For a uniform grid with step of δx, the value of ϕ and $\frac{d\phi}{dx}$ at the cell faces can be obtained by using cubic interpolation:

$$\phi_w = \frac{1}{16}(\phi_{W_2} - 5\phi_{W_1} + 15\phi_W + 5\phi_P) + O(\delta x^3) \tag{25}$$

$$\phi_e = \frac{1}{16}(\phi_{W_1} - 5\phi_W + 15\phi_P + 5\phi_E) + O(\delta x^3) \tag{26}$$

$$(\frac{d\phi}{dx})_w = \frac{1}{24\delta x}(\phi_{W_2} - 3\phi_{W_1} - 21\phi_W + 23\phi_P) + O(\delta x^3) \tag{27}$$

$$(\frac{d\phi}{dx})_e = \frac{1}{24\delta x}(\phi_{W_1} - 3\phi_W - 21\phi_P + 23\phi_E) + O(\delta x^3) \tag{28}$$

Replacing the terms ϕ_w, ϕ_e, $(\frac{d\phi}{dx})_w$ and $(\frac{d\phi}{dx})_e$ with (25)-(28), we can obtain the discretized equation at the general node $i(3 < i < n)$ as following.

$$a_P\phi_P = a_{W_2}\phi_{W_2} + a_{W_1}\phi_{W_1} + a_W\phi_W + a_E\phi_E + S_u \tag{29}$$

where $a_{W_2} = -\frac{1}{24}D_w + \frac{1}{16}F_w, a_{W_1} = \frac{1}{8}D_w - \frac{5}{16}F_w + \frac{1}{24}D_e - \frac{1}{16}F_e, a_W = \frac{7}{8}D_w + \frac{5}{16}F_w - \frac{1}{8}D_e + \frac{5}{16}F_e, a_E = \frac{23}{24}D_e - \frac{5}{16}F_e, a_P = a_{W_2} + a_{W_1} + a_W + a_E - S_P, S_P = 0, S_u = 0.$

As same as the method showed in section 3, the discretization equations at nodes near the boundary can also be obtained.

At node 1, we use the first order upwind difference scheme to discretize the (2) and give

$$a_P\phi_P = a_E\phi_E + S_u \tag{30}$$

where $a_E = D_e, a_P = a_E - S_P, S_P = -(2D_A + F_A), S_u = (2D_A + F_A)\phi_A$.

At node 2, the discretization equation is

$$a_P\phi_P = a_W\phi_W + a_E\phi_E + a_{E_1}\phi_{E_1} + S_u \tag{31}$$

where $a_W = \frac{5}{4}D_w + \frac{5}{4}F_w - \frac{1}{4}D_e + \frac{3}{8}F_e, a_E = \frac{1}{20}D_w + \frac{19}{20}D_e - \frac{5}{16}F_e, a_P = a_W + a_E + F_e - F_w - S_P, S_P = \frac{2}{15}D_w - \frac{1}{2}F_w - \frac{2}{15}D_e + \frac{1}{8}F_e, S_u = -(\frac{2}{15}D_w - \frac{1}{2}F_w - \frac{2}{15}D_e + \frac{1}{8}F_e)\phi_A$.

At node 3, the discretization equation becomes

$$a_P\phi_P = a_{W_1}\phi_{W_1} + a_W + a_E\phi_E + S_u \tag{32}$$

where $a_{W_1} = \frac{1}{4}D_w - \frac{3}{8}F_w + \frac{1}{24}D_e - \frac{1}{16}F_e, a_W = \frac{5}{6}D_w + \frac{15}{16}F_w - \frac{1}{8}D_e + \frac{5}{16}F_e, a_E = \frac{23}{24}D_e - \frac{5}{16}F_e, a_P = a_{W_1} + a_W + a_E + F_e - F_w - S_P, S_P = \frac{2}{15}D_w - \frac{1}{8}F_w, S_u = -(\frac{2}{15}D_w + \frac{1}{8}F_w)\phi_A$.

At node n, we use the first order upwind difference scheme to discretize the (2) and the discretization equation takes the form

$$a_P\phi_P = a_W\phi_W + S_u \tag{33}$$

where $a_W = D_w + F_w, a_P = a_W - S_P, S_P = -2D_B, S_u = 2D_B\phi_B$.

5 HYBRID DIFFERENCE SCHEME

For the fourth order central difference scheme is more accurate when $|P_e| < 2$, but the third order upwind difference scheme is more stable when $|P_e| \geq 2$, we now utilize their advantages to construct a hybrid scheme. That is, when $|P_e| < 2$, we use central difference scheme introduced in section 3 to discretize (2). Otherwise, we take use of upwind scheme introduced in section 4 to discretize (2). As have already been deduced in section 3 and section 4, the discretization equation for Problem I at inner node $i(3 < i < n-2)$ takes the form

$$a_P\phi_P = a_{W_2}\phi_{W_2} + a_{W_1}\phi_{W_1} + a_W\phi_W + a_E\phi_E + a_{E_1}\phi_{E_1} + a_{E_2}\phi_{E_2} + S_u \tag{34}$$

where

$$a_P = a_{W_2} + a_{W_1} + a_W + a_E + a_{E_1} + a_{E_2} - S_P \tag{35}$$

and $a_{W_2}, a_{W_1}, a_W, a_E, a_{E_1}, a_{E_2}, S_P, S_u$ are given in Table 1.

At the nodes near the boundary, the discretized equations also take the form of (34), and the coefficients of these equations can also be obtained from section 3 and section 4. For the restriction to the magnitude of this paper, we no longer present them here. At the inner nodes, as the central scheme is of fourth order accuracy, and the upwind scheme of third order accuracy, then the hybrid scheme is of third order accuracy at least. As in this scheme we take account into the flow direction, it is more stable too.

	$P_e > 2$	$-2 \le P_e \le 2$	$P_e < -2$
a_{W_2}	$-\frac{1}{24}D_w + \frac{1}{16}F_w$	0	0
a_{W_1}	$\frac{1}{8}D_w - \frac{5}{16}F_w + \frac{1}{24}D_e - \frac{1}{16}F_e$	$-\frac{1}{24}D_w - \frac{1}{16}F_w$	0
a_W	$\frac{7}{8}D_w + \frac{15}{16}F_w - \frac{1}{8}D_e + \frac{5}{16}F_e$	$\frac{1}{24}D_w + \frac{9}{16}F_w + \frac{9}{8}D_e + \frac{1}{16}F_e$	$\frac{23}{24}D_w + \frac{5}{16}F_w$
a_E	$\frac{23}{24}D_e - \frac{5}{16}F_e$	$\frac{9}{8}D_w - \frac{1}{16}F_w + \frac{1}{24}D_e - \frac{9}{16}F_e$	$-\frac{1}{8}D_w - \frac{5}{16}F_w + \frac{7}{8}D_e - \frac{15}{16}F_e$
a_{E_1}	0	$-\frac{1}{24}D_e + \frac{1}{16}F_e$	$\frac{1}{24}D_w - \frac{1}{16}F_w + \frac{1}{8}D_e - \frac{5}{16}F_e$
a_{E_2}	0	0	$-\frac{1}{24}D_e - \frac{1}{16}F_e$
S_P	0	0	0
S_u	0	0	0

Table 1: Coefficients of the difference equations obtained from the hybrid scheme.

6 NUMERICAL EXAMPLES

Example 1 In Problem I, presuming that all of the cross-sectional area of control volumes A are the same, $A = 1.0, \rho = 1.0, \Gamma = 0.05, u = 0.2, n = 10, L = 1.0$.

Here $\delta x = 0.1$, at all of the e and w faces,$F = \rho u A = 0.2, D = \Gamma A/\delta x = 0.5$, $P_e = \dfrac{F}{D} = 0.4$. By using above scheme we give its numerical solution. The numerical and analytic solutions are compared in Figure 3. The maximum percentage error is only 0.10%.

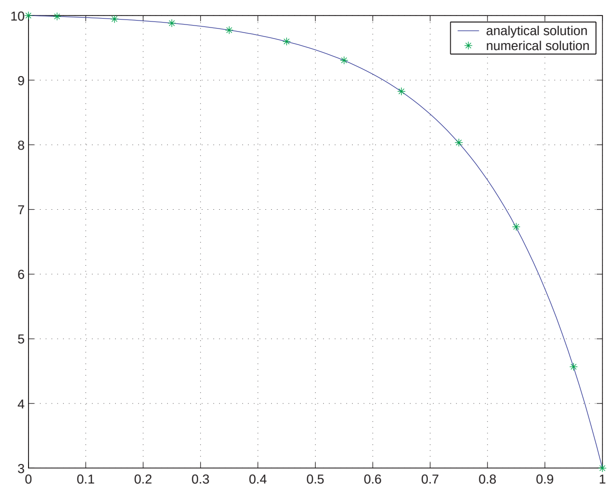

Figure 3: Numerical solution of the central difference scheme for problem I when $P_e = 0.4$.

Example 2 In Problem I, presuming that all of the cross-sectional area of control volumes A are the same, $A = 1.0, \rho = 1.0, \Gamma = 0.05, u = 2.5, n = 10, L = 1.0$.

Here $\delta x = 0.1$,at e and w faces of all control volumes, $D = 0.5, F = 2.5, P_e = \dfrac{F}{D} = 5$. The numerical and analytic solutions are compared in Figure 4. As the maximum percentage error arrives at 38.85%.

Example 3. Use the upwind scheme just introduced to solve the problem of Example 2 again, and compare the numerical solution of the upwind scheme with the QUICK

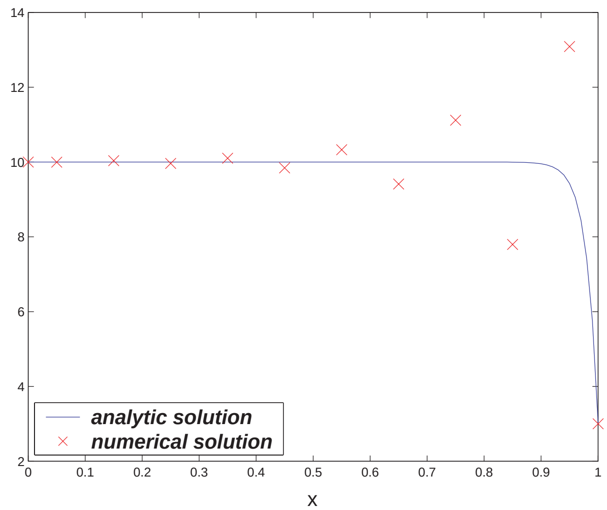

Figure 4: Numerical solution of the central difference scheme for problem I when $P_e = 5$

scheme.

We can obtain the numerical solution by using the upwind scheme, which is compared with its analytic solution and numerical solution by using the QUICK scheme in Figure 5. The maximum percentage error of the upwind scheme and the QUICK scheme are 11.11% and 62.73% respectively.

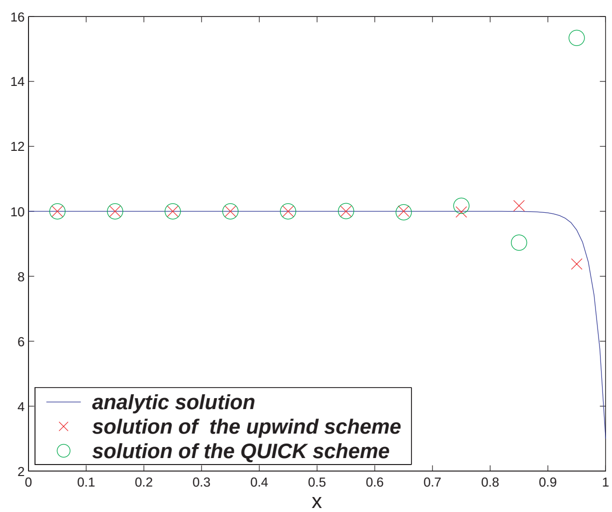

Figure 5: Solution of the upwind difference scheme and the QUICK scheme for problem I when $P_e = 5$.

7 CONCLUSIONS

- In this paper, five-point difference schemes and some hybrid strategy are presented and discussed. The schemes are of higher order accuracy in theory.
- One dimensional steady convection-diffusion problem tests indicate that the new scheme are suitable for convection dominant problems.
- The schemes might also be extended to solve 2D and 3D convection-diffusion problems.

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