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PERFORMANCE OF FINITE VOLUME DISCRETIZATION SCHEMES FOR THE CONVECTIVE-DIFFUSIVE LINEAR TRANSPORT EQUATION. PART I: LOW EIGENVALUE-PECLET RATIOS

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Abstract. *Various numerical aspects of several discretization schemes are evaluated by using the two-dimensional transport problem of a scalar property in uniform flow. This problem is modeled by the convective-diffuse transport equation, here discretized by the finite volume method. It is proposed a methodology that evaluates the Peclet number's influence and the dependence on the angle between flow and grid lines on the rms error of the numerical schemes: central differencing, upwind, simple exponential, second order upwind, QUICK, LOADS and UNIFAES. The discretization-generated algebraic system is solved by the ADI method for the five-node schemes. However, the source terms of UNIFAES and LOADS are computed explicitly. The boundary conditions are of the Dirichlet type. The scalar property's values at the domain boundary are provided by analytical solutions. Schemes that employ the generating equation's source term, i.e. UNIFAES and LOADS, present the best performance in nearly all functions, alongside the QUICK scheme. UNIFAES shows the lowest dependence with the flow direction. With the increase of the Peclet number, UNIFAES and QUICK outperform the others, being closely followed by LOADS. However, UNIFAES has the advantage of being unconditionally stable for all Peclet numbers, while QUICK may show wiggly behavior.*

Keywords: *Numerical Methods, Finite Volumes, Finite Differences, UNIFAES, CFD.*

1. INTRODUCTION

The classical methods of finite differences, finite volumes and finite elements, when applied in the discretization of convective-diffusive transport equations, present some shortcomings. The second order central difference schemes in finite volumes and in finite differences, and the Galerkin method in finite elements can be employed, with good accuracy, in problems with low to moderate Peclet, Reynolds or Rayleigh numbers. Yet, for high values they show either spatially oscillating solutions or numerical instability, depending on the solution method of equations. On the other hand, unconditionally stable schemes, such as upwind for finite differences and finite volumes, and Petrov-Galerkin method in finite elements, produce inaccurate slowly convergent first order solutions.

The insufficiency of the classical discretizations has generated intensive research in development of schemes, in order to better numerically express the behavior of the function in the discrete interval. Thus, several other schemes have been developed. The selection of discretization schemes has a strong influence on the numerical solution of problems involving transport phenomena and fluid mechanics. Among the most used, within the finite volume approach, are the QUICK scheme, originally developed by Leonard (1979), and the second order upwind (SOU) presented by Shyy (1985).

Among these alternatives, one can consider the family of exponential-type or locally analytical schemes. These schemes use as interpolating curve the exact solution of a linear equation that approximates the equation of interest. Such interpolating curve allows to simultaneously approximate the advective and the diffusive or viscous fluxes. In general, these schemes have robust stability. In addition to the simple exponential scheme (Spalding, 1972; Raithby and Torrance, 1974; Patankar, 1980) and its approximations as the hybrid scheme (Spalding, 1972; Patankar, 1980) and the power-law scheme (Patankar, 1980), the category also presents more sophisticated and accurate exponential-type schemes such as LOADS (Locally Analytic Differencing Scheme) (Wong and Raithby, 1979; Prakash, 1984), Flux-Spline (Varejão, 1979) and UNIFAES (Unified Finite Approaches Exponential-Type Scheme) (Figueiredo, 1997; Figueiredo and Llagostera, 1999; Llagostera and Figueiredo, 2000a,b; Figueiredo and Oliveira, 2009a,b, 2011).

This paper and its companion (Rodrigues *et al.*, 2018) present a systematic testing of several finite volume method schemes in the case of the transport equation of a scalar property in uniform velocity flow. This linear equation is solved by the method of separation of variables, leading to elementary solutions whose linear combination provides the general solution. The present investigation provides a testing of the above referred schemes, sweeping through these elementary solutions.

2. FINITE VOLUME INTERPOLATION SCHEMES

The schemes will be derived with respect to the convective-diffusive transport equation in Cartesian coordinates of a scalar property $\phi(x, y, t) \equiv \phi$, without source term, through a two-dimensional field of uniform velocity which is represented by the homogeneous linear equation of constant coefficients:

$$\frac{\partial(\rho c\phi)}{\partial t} + \frac{\partial(\rho cu\phi)}{\partial x} + \frac{\partial(\rho cv\phi)}{\partial y} - \frac{\partial}{\partial x}\left(\Gamma\frac{\partial\phi}{\partial x}\right) - \frac{\partial}{\partial y}\left(\Gamma\frac{\partial\phi}{\partial y}\right) = 0 \tag{1}$$

The Eq. (1) is written in non-dimensional form by dividing the spatial coordinates (x, y) by a characteristic dimension L and the velocity components (u, v) by a characteristic velocity V, considering the constant Γ case and without change of notation:

$$\frac{\partial\phi}{\partial t} + \frac{\partial(\mathrm{Pe}u\phi)}{\partial x} + \frac{\partial(\mathrm{Pe}v\phi)}{\partial y} - \frac{\partial^2\phi}{\partial x^2} - \frac{\partial^2\phi}{\partial y^2} = 0 \tag{2}$$

where Pe is the global Peclet number $\mathrm{Pe} = \rho V Lc/\Gamma$. The variable t now represents the non-dimensional time, given by the dimensional time multiplied by $\Gamma/(\rho c L^4)$.

Integrating Eq. (2) over the control volume shown in Fig. 1 and employing the divergence theorem, it can be expressed in a discrete way according to the finite volume method, obtaining:

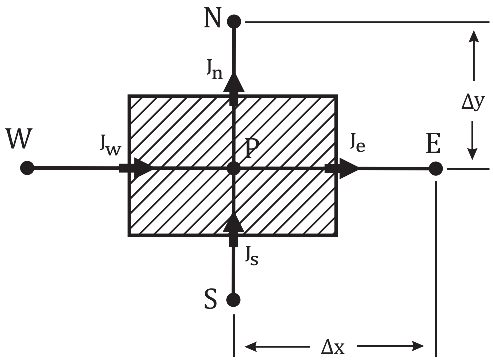


Figure 1. Two-dimensional sketch for finite volume discretization

$$\frac{\partial\phi}{\partial t}\Delta x\Delta y + (J_e - J_w)\Delta y + (J_n - J_s)\Delta x = 0 \tag{3}$$

where J_e is the combined convective and diffusive flux considered constant at the cell boundary e of the control volume:

$$J_e = \mathrm{Pe}u_e\phi_e - \left.\frac{\partial\phi}{\partial x}\right|_e \tag{4}$$

and so on to the other cell boundaries.

The following is a summary of the second order upwind, QUICK, LOADS and UNIFAES discretization schemes. Algebraic details of UNIFAES can be found in Figueiredo (1997) and Figueiredo and Llagostera (1999). The other classical schemes used in this paper are not presented, since they are consolidated in the literature.

2.1 Second Order Upwind Scheme

In the second order upwind (SOU) scheme, presented by Shyy (1985), the face value of ϕ is approximated by a linear extrapolation from two upstream neighboring nodes (see Fig. 2a). The solution uses a piecewise linear profile. Considering the flow always in the positive direction, one gets for the convective terms:

$$\phi_e = \frac{3}{2}\phi_P - \frac{1}{2}\phi_W \tag{5}$$

$$\phi_w = \frac{3}{2}\phi_W - \frac{1}{2}\phi_{WW} \tag{6}$$

For the diffusive terms, the central differencing scheme (piecewise linear profile) is maintained.

2.2 QUICK Scheme

The scheme proposed by Leonard (1979), QUICK (Quadratic Upstream Interpolation for Convective Kinetics), employs a parabolic interpolation to account for the value of ϕ in each face of the control volume. The quadratic function for a given face is adjusted to three neighboring nodes, two upstream and one downstream (see Fig. 2b). This interpolation curve is used for the convective terms. The diffusive terms can be evaluated using the gradient of the same quadratic function. It is interesting to note that, for a face-centered control volume, this practice results in the same expression of the central differencing scheme for diffusion. Again, considering the positive direction of the flow by QUICK:

$$\phi_e = \frac{3}{8}\phi_E + \frac{3}{4}\phi_P - \frac{1}{8}\phi_W \tag{7}$$

$$\phi_w = \frac{3}{8}\phi_P + \frac{3}{4}\phi_W - \frac{1}{8}\phi_{WW} \tag{8}$$

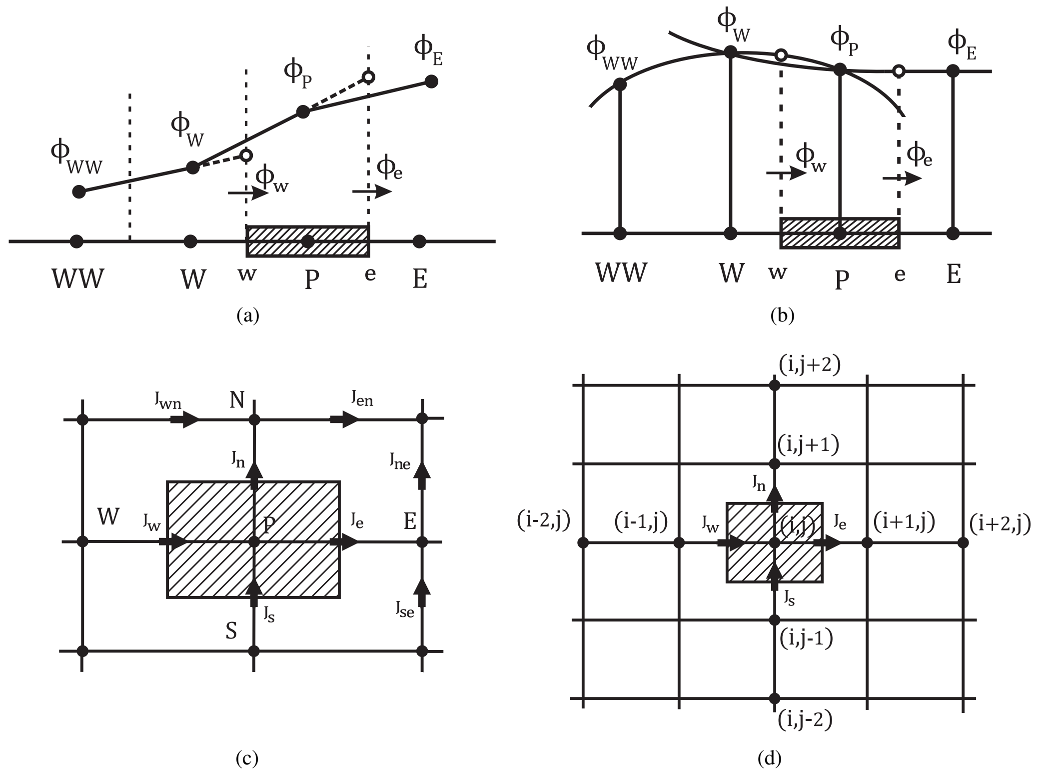


Figure 2. (a) Second order upwind velocity extrapolation. (b) QUICK interpolation curve. (c) LOADS control volume. (d) UNIFAES computational molecule

2.3 LOADS Scheme

Most exponential-type schemes use as the interpolating curve the solution of the one-dimensional differential equation, e.g. in the x direction:

$$\text{Pe}u\frac{d\phi}{dx} - \frac{d^2\phi}{dx^2} = K_x \tag{9}$$

which approximates the advective and diffusive terms given in Eq. (4) by assuming the velocity component u locally as constant, as well as the non-homogeneous term K_x, that represents all the terms of the original equation, Eq. (2), not explicitly included in Eq. (9). The general solution of Eq. (9) is:

$$\phi = c_1 + \frac{K_x}{\text{Pe}u}x + c_3\exp(\text{Pe}ux) \tag{10}$$

The determination of the non-homogeneous term K_x is not trivial in the context of finite volume. The various exponential schemes differ from one another in the determination of K_x. In fact, the simple exponential scheme (Raithby and Torrance, 1974) assumes K_x null, losing much of the similarity between the generating and original equations.

After the solution of the non-homogeneous equation, Eq. (9), and using Eq. (10) as an interpolating curve between the nodes P and E (see Fig. 1), the flux given by Eq. (4) can be written as:

$$J_e = \text{Pe}u_e\phi_P + \frac{\phi_P - \phi_E}{\Delta x}\frac{\text{Pe}u_e\Delta x}{\exp(\text{Pe}u_e\Delta x) - 1} + K_e\Delta x\left[\frac{1}{\exp(\text{Pe}u_e\Delta x) - 1} - \frac{1}{\text{Pe}u_e\Delta x} + \frac{1}{2}\right] \tag{11}$$

Analogous expressions can be obtained for the other boundaries.

The first exponential-type finite volume scheme to include the term K_x was LOADS (Locally Analytic Differencing Scheme) (Wong and Raithby, 1979), in which K_x is computed by comparing Eq. (2) and Eq. (9):

$$K_x = -\left(\frac{\partial\phi}{\partial t} + \text{Pe}v\frac{\partial\phi}{\partial y} - \frac{\partial^2\phi}{\partial y^2}\right) \tag{12}$$

LOADS determines K_x accounting the total flux, by convection and diffusion, through their respective faces, according to Fig. 2c. Thus, the terms of Eq. (12) are evaluated:

$$\frac{\partial\phi}{\partial t} = \frac{(\partial\phi/\partial t)_{i,j} + (\partial\phi/\partial t)_{i+1,j}}{2} \tag{13}$$

$$\text{Pe}v\frac{\partial\phi}{\partial y} - \frac{\partial^2\phi}{\partial y^2} = \frac{1}{\Delta y}\left[\frac{(J_n - J_s) + (J_{ne} - J_{se})}{2}\right] \tag{14}$$

with the K's for the other directions calculated by an analogous procedure. The computation of the convective and diffusive cross-fluxes in Eq. (14) is done by means of the simple exponential scheme, where the terms K are neglected.

2.4 UNIFAES Scheme

The UNIFAES (Unified Finite Approaches Exponential-Type Scheme) discretization scheme, idealized and developed by Figueiredo (1997), brings in its original formulation a new alternative for the calculation of the source term of the generating Eq. (9). UNIFAES gets its name from the fact that the information about K required by the finite volume treatment is provided by the finite difference approach of Allen and Southwell (1955).

As exponential based scheme, the initial mathematical procedures are similar to those in the LOADS scheme. Thus, by fitting the interpolating curve, Eq. (10), to the three neighboring nodes W, P and E, according to Fig. 1, one obtains:

$$\phi_W = c_1 - \frac{K_x}{\text{Pe}u}\Delta x + c_3\exp(-\text{Pe}u\Delta x) \tag{15}$$

$$\phi_P = c_1 + c_3 \tag{16}$$

$$\phi_E = c_1 + \frac{K_x}{\text{Pe}u}\Delta x + c_3\exp(\text{Pe}u\Delta x) \tag{17}$$

Solving the system of equations above for K_x, one obtains the finite difference analog of the combined convective-diffusive flux in the considered direction. This finite difference analog is equal to the generating equation's source term K, as expressed in Eq. (18). Therefore, Allen's methodology is employed as a way to determine the generating equation's source term K as described below:

$$\text{Pe}u\frac{d\phi}{dx} - \frac{d^2\phi}{dx^2} = K_x = (\phi_P - \phi_E)\Pi^+ + (\phi_P - \phi_W)\Pi^- \tag{18}$$

where, for the case of regular grid:

$$\Pi^+ = \frac{\text{Pe}u_P\Delta x}{\Delta x^2\left[\exp(\text{Pe}u_P\Delta x) - 1\right]} \tag{19}$$

$$\Pi^- = \frac{-\text{Pe}u_P\Delta x}{\Delta x^2\left[\exp(-\text{Pe}u_P\Delta x) - 1\right]} \tag{20}$$

In UNIFAES, the source term $K_e^{i,j}$, for example, is obtained by a linear interpolation from the values computed with the immediate nodes (i,j) and $(i+1,j)$. Due to the form of the source term of Eq. (18), the UNIFAES computational molecule involves extra nodes in each direction (see Fig. 2d).

$$K_e^{i,j} = 0.5\left(K_x^{i,j} + K_x^{i+1,j}\right) \tag{21}$$

Although the Allen and Southwell (1955) scheme is not numerically conservative, its use in UNIFAES ensures numerical conservation since $K_e^{i,j} = K_w^{i+1,j}$, so that $J_e^{i,j} = J_w^{i+1,j}$. In the neighboring cells of the domain boundaries, K is extrapolated linearly from the nearest inner nodes.

3. CONVECTIVE-DIFFUSIVE TRANSPORT IN PARALLEL FLOW

The convective and diffusive transport in Cartesian coordinates of a scalar property $\phi(x, y) \equiv \phi$, in steady state, without source term, through a uniform velocity field is represented by the homogeneous linear equation of constant coefficients in its non-dimensional form:

$$\mathrm{Pe}u\frac{\partial \phi}{\partial x} + \mathrm{Pe}v\frac{\partial \phi}{\partial y} - \frac{\partial^2 \phi}{\partial x^2} - \frac{\partial^2 \phi}{\partial y^2} = 0 \tag{22}$$

where the velocity components are $u = V\cos\theta$ e $v = V\sin\theta$, with modulus V and angle θ with the x-axis. To determine the exact solution, Eq. (22) is rewritten as a function of the coordinate system (s, n), respectively parallel and normal to the flow streamline, as shown in Fig. 3, resulting:

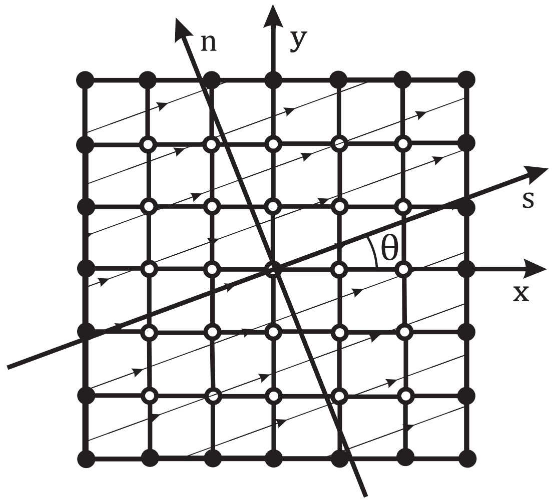


Figure 3. Sketch the analytical and numerical coordinate system

$$\mathrm{Pe}\frac{\partial \phi}{\partial s} - \frac{\partial^2 \phi}{\partial s^2} - \frac{\partial^2 \phi}{\partial n^2} = 0 \tag{23}$$

The Eq. (23) can be solved by the method of separation of variables, assuming solutions of type $\phi(s, n) = \xi(s)\zeta(n)$, as presented by Figueiredo (1992, 1997):

$$\xi = c_1 \exp\left(\frac{\mathrm{Pe} + \sqrt{\mathrm{Pe}^2 \pm 4\lambda^2}}{2}s\right) + c_2 \exp\left(\frac{\mathrm{Pe} - \sqrt{\mathrm{Pe}^2 \pm 4\lambda^2}}{2}s\right) \tag{24}$$

$$\zeta = c_3 \exp\left(\sqrt{-(\pm 1)}\lambda n\right) + c_4 \exp\left(-\sqrt{-(\pm 1)}\lambda n\right) \tag{25}$$

where the eigenvalue λ belongs to the set of non-negative real numbers and the c_i are constants. Taking the positive signals before λ in Eqs. (24) e (25), since all the essential characteristics of the sine or cosine functions are featured by any of them, the sine-shaped solutions appear in the form:

$$\phi_A = \exp\left(\frac{\mathrm{Pe} - \sqrt{\mathrm{Pe}^2 + 4\lambda^2}}{2}s\right)\sin(\lambda n) \tag{26}$$

$$\phi_B = \exp\left(\frac{\mathrm{Pe} + \sqrt{\mathrm{Pe}^2 + 4\lambda^2}}{2}s\right)\sin(\lambda n) \tag{27}$$

Now, functions with the negative signal before the eigenvalue are considered. Observe that, because the origin of the coordinate system coincides with the center of the numerical domain, negative and positive exponentials will appear symmetrically. Thus, without loss of generality, only the solution $\exp(\lambda n)$ may be considered. Therefore, in the case of $\lambda/\mathrm{Pe} \leq 0.5$, the solutions are:

$$\phi_C = \exp\left(\frac{\mathrm{Pe} - \sqrt{\mathrm{Pe}^2 - 4\lambda^2}}{2}s\right)\exp(\lambda n) \tag{28}$$

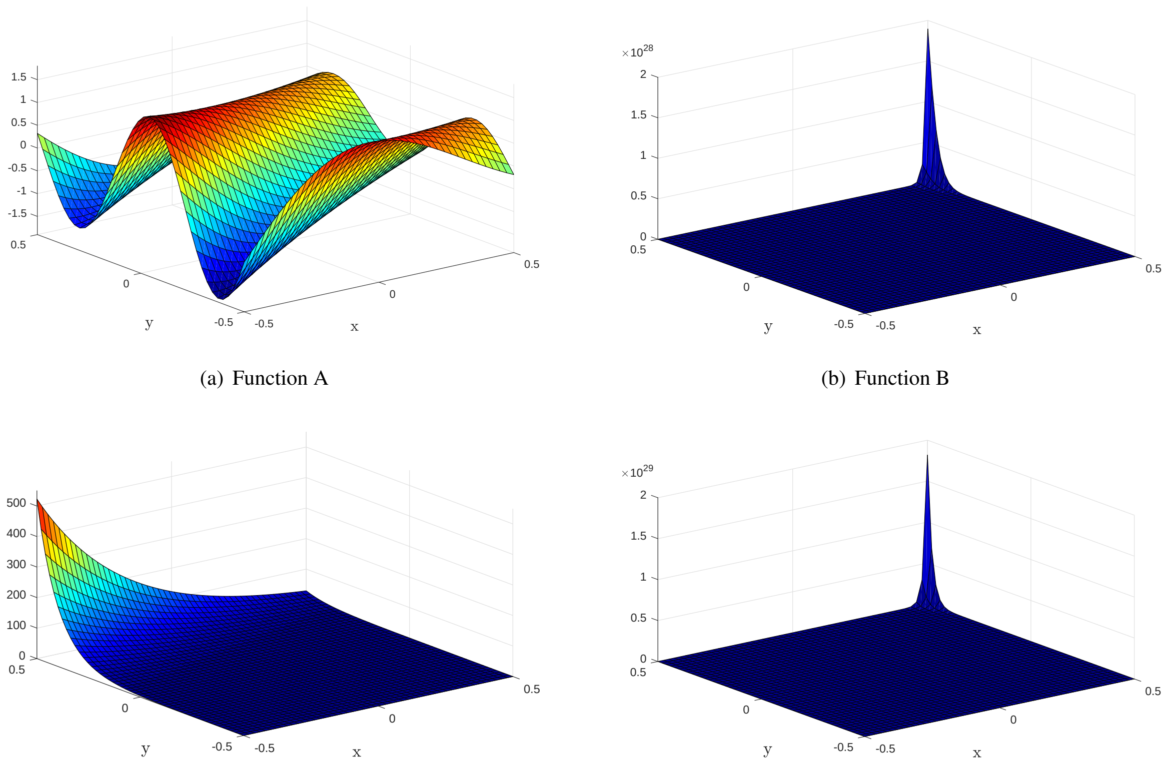
$$\phi_D = \exp\left(\frac{\mathrm{Pe} + \sqrt{\mathrm{Pe}^2 - 4\lambda^2}}{2}s\right)\exp(\lambda n) \tag{29}$$

For the case $\lambda/\mathrm{Pe} > 0.5$, the discriminant within the square root can be negative, being, therefore, a complex exponential. Thus, the elementary solutions are found in real form as:

$$\phi_{CD} = \exp\left(\frac{\mathrm{Pe}}{2}s\right)\sin\left(\sqrt{\lambda^2 - \frac{\mathrm{Pe}^2}{4}}s\right)\exp(\lambda n) \tag{30}$$

$$\phi_{DC} = \exp\left(\frac{\mathrm{Pe}}{2}s\right)\cos\left(\sqrt{\lambda^2 - \frac{\mathrm{Pe}^2}{4}}s\right)\exp(\lambda n) \tag{31}$$

The investigation of the present paper is restrict to analysis with low ratios $\lambda/\mathrm{Pe}(\leq 0.1)$ for functions of types A, B, C and D, as shown in Fig. 4. Here, the eigenvalue-Peclet ratios mentioned at the title of this paper refer to λ/Pe. Higher ratios λ/Pe, which include also CD and DC functions, are considered in the companion paper (Rodrigues *et al.*, 2018).



(a) Function A

(b) Function B

(c) Function C

(d) Function D

Figure 4. Analytical solutions found for $\mathrm{Pe} = 100$, $\lambda = 10$, $\theta = 22.5$ degrees.

Functions A and B, which are sinusoidal in the normal flow direction and exponential in the streamline flow direction, differ from one another in the smoother or abrupt nature of the exponential. This difference comes from taking either more or less the square root of the discriminant in the exponential. An analogous difference occurs between functions C and D, both exponential in the cross direction.

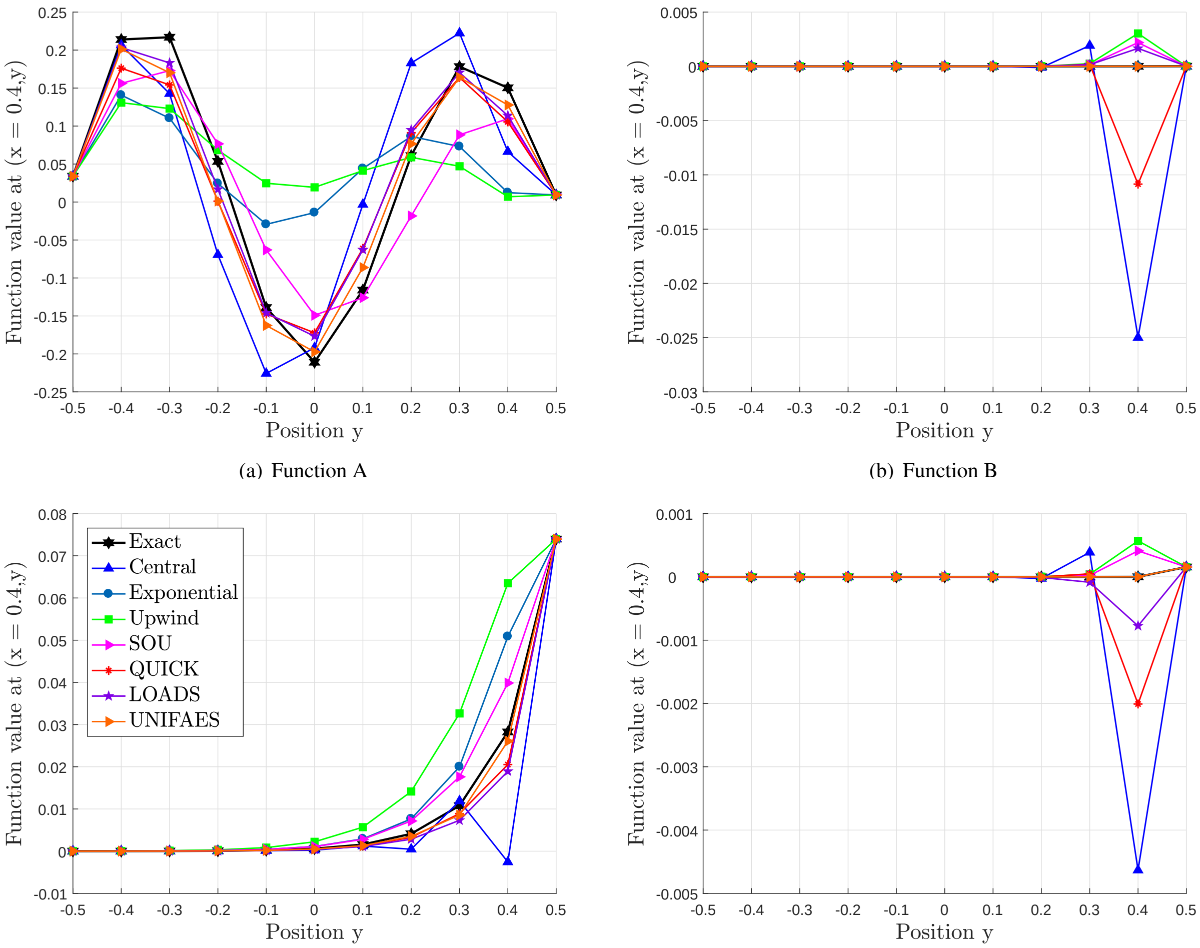
4. RESULTS AND DISCUSSIONS

The elementary solutions above are employed to compare several finite volume discretizations: central differencing, upwind, simple exponential, second order upwind, QUICK, LOADS and UNIFAES. The exact solution, Eq. (23), is imposed as Dirichlet condition at the boundaries of the square domain (see Fig. 3). For the QUICK and second order upwind schemes, at the inlet boundaries of the domain where terms related to nodes outside the calculation domain would appear, the central differencing scheme formulation was used. This decision was made so that all nodes involved in the system equations were contained within the domain.

The time is just used to control the iterative process from which the problem solution is obtained. Only the steady state solution is achieved. The algebraic linear system from the discretization of Eq. (2) is solved with the ADI (Alternating Direction Implicit) method (Peaceman and Rachford, 1955) for the five-node schemes. The extra terms of the second order upwind, QUICK, UNIFAES and LOADS are computed explicitly.

The numerical behavior of the several discretization schemes used to solve the convective-diffusive transport equation, Eq. (22), will now be discussed. The rms errors of each scheme are comparatively presented and related to their respective exact solutions. For all tests, the numerical solution was considered to converged whenever the maximum rate of variation of the function ϕ with time was less than 10^{-5}. The errors are presented by the quadratic mean (rms error) and normalized by the maximum distance between the values of ϕ within the domain, including the values of the boundary.

Most of the computations to be presented refer to a standard set of parameters given by $\lambda = 10$ e $\theta = 22.5$ degrees. Figure 5 presents the profiles of the exact and numerical solutions for functions A, B, C and D with Pe $= 100$ and 10×10 spacing grid.



(a) Function A (b) Function B (c) Function C (d) Function D

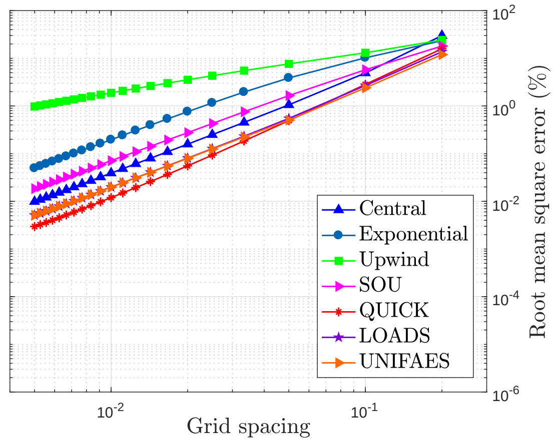
Figure 5. Exact and numerical profiles for functions A, B, C and D at $x = 0.4$, 10×10 grid, Pe $= 100$, $\lambda = 10$, $\theta = 22.5$ degrees.

Considering such low ratios $\lambda/\text{Pe}(= 0.1)$, functions A and C feature low derivatives along the stream direction and moderate in the normal direction, so that they tend to represent situations of diffusion on the cross-flow direction. Meanwhile, functions B and D have very high derivatives on the exit boundary, where there is relevant counter-flow diffusion, the function being practically null upwind that boundary region.

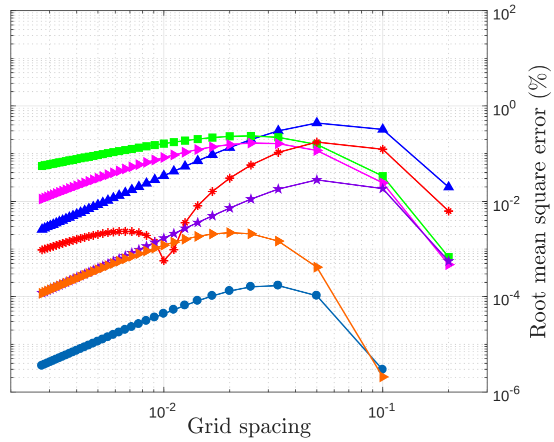
For the type A and C functions, the upwind and simple exponential schemes, although highly stable and free of oscillations, confirms themselves as strongly diffusive schemes. On the other hand, in functions B and D, the simple exponential alongside UNIFAES present results that visually coincide with the exact solution. In these cases, LOADS shows some wiggles, but they are smaller than those wiggles featured by central differencing and QUICK. In his investigation of LOADS, Prakash (1984) also identified some cases of wiggly behavior. Due to its unboundedness to the moderate Peclet number, the central differencing scheme shows wiggly behavior in all functions.

Both schemes that employ the generating equation's source term, *i.e.* UNIFAES and LOADS, alongside the QUICK scheme present the best performances in nearly all functions. In function A, their rms errors are 2.16%, 2.42% and 2.55%, respectively. Similarly, the rms errors in function C are 0.11%, 0.44% and 0.24%, respectively. However, in functions B and D, QUICK is bested by UNIFAES and LOADS. UNIFAES behaves satisfactorily in all functions. In function C it is clearly the best for the set of adopted parameters .

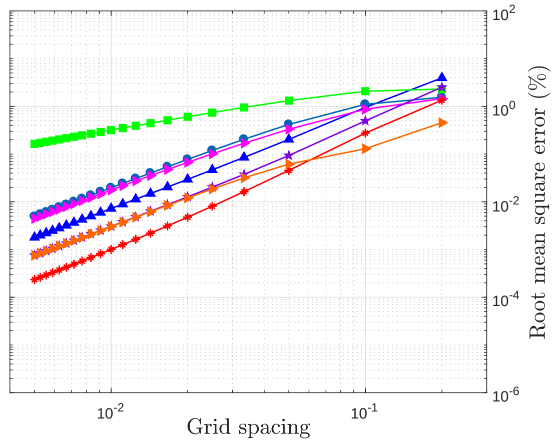
Figure 6 shows the error against refinement for all schemes. The errors are presented by the quadratic mean, expressed as a percentage of the difference between maximum and minimum of each function.



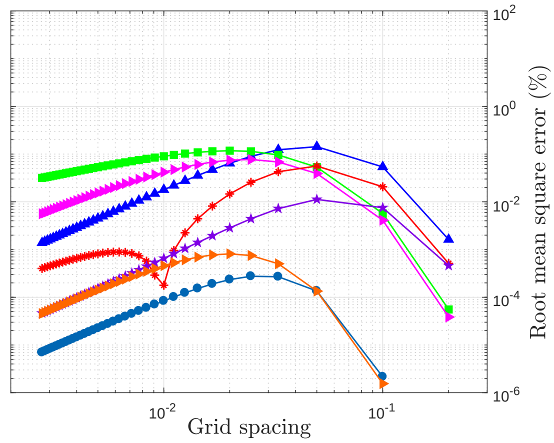
(a) Function A



(b) Function B



(c) Function C



(d) Function D

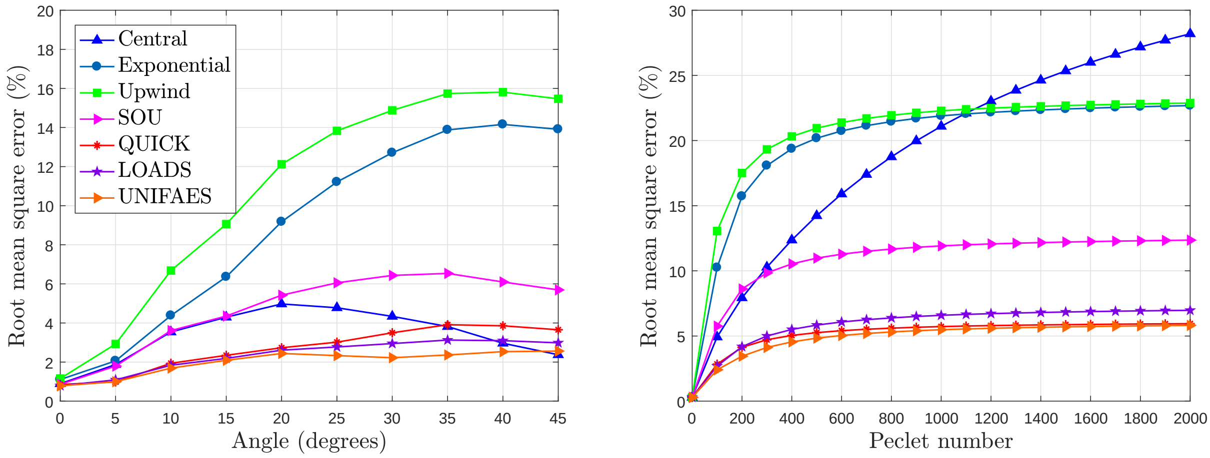
Figure 6. Root mean square error against grid refinement for function A, B, C and D, Pe $= 100$, $\lambda = 10$, $\theta = 22.5$ degrees.

The upwind scheme presents the worst results on all the functions, except at the coarse grids. In functions A and C, the quadratic behavior of the decrease of the error with the refinement is generally reached for a mesh 40×40 control volumes. It is also observed, in function B and D, non-monotonic behavior of the schemes for coarse meshes. QUICK is the only one to present for moderately refined meshes. Absence of monotonicity caused the asymptotic quadratic error to be reached only for meshes with refinement starting from 400×400 control volumes. As can be seen Fig. 6, QUICK shows itself as a second order accurate scheme. This is proven by Taylor series error analysis in Appendix A.

The second order upwind exhibits intermediate performance in all cases. UNIFAES, LOADS and QUICK schemes present the best results for the great majority of functions. The asymptotic errors of UNIFAES and LOADS seem to coincide in all cases. In functions A and C, QUICK overcomes UNIFAES and LOADS in acuity.

The evaluation of effect of the angle between the flow and the grid lines, at the various schemes, is shown in Fig. 7a, which presents the rms error as a function of the angle θ. It is important to mention that solutions converged with all schemes are obtained for any angle θ. Yet, the exact solution is best represented by all schemes for the angle $\theta = 0$ degrees with errors in the range from 0.7% to 1.04%. UNIFAES has the lowest dependence on the angle, as well as the smallest errors, being closely followed by LOADS. The maximum error of each scheme is: central differencing = 4.97% for $\theta = 20$ degrees, simple exponential = 14.15% for $\theta = 40$ degrees, upwind = 15.81% for $\theta = 40$ degrees, second order upwind = 6.53% for $\theta = 35$ degrees, QUICK = 3.91% for $\theta = 35$ degrees, LOADS = 3.12% for $\theta = 35$ degrees, UNIFAES = 2.56% for $\theta = 45$ degrees.

Figure 7b shows the behavior of the numerical solutions of the schemes for a wide range of Peclet numbers. UNIFAES is the least affected by the increase in the Peclet number, alongside the QUICK and LOADS scheme, presenting the smallest errors. The rms errors of the simple exponential and upwind tend to coincide as the Peclet number increases. It can be observed that the errors of most of the schemes become constant as the Peclet number increases, except for central differencing in which the errors continues to grow with the increase of the Peclet number.

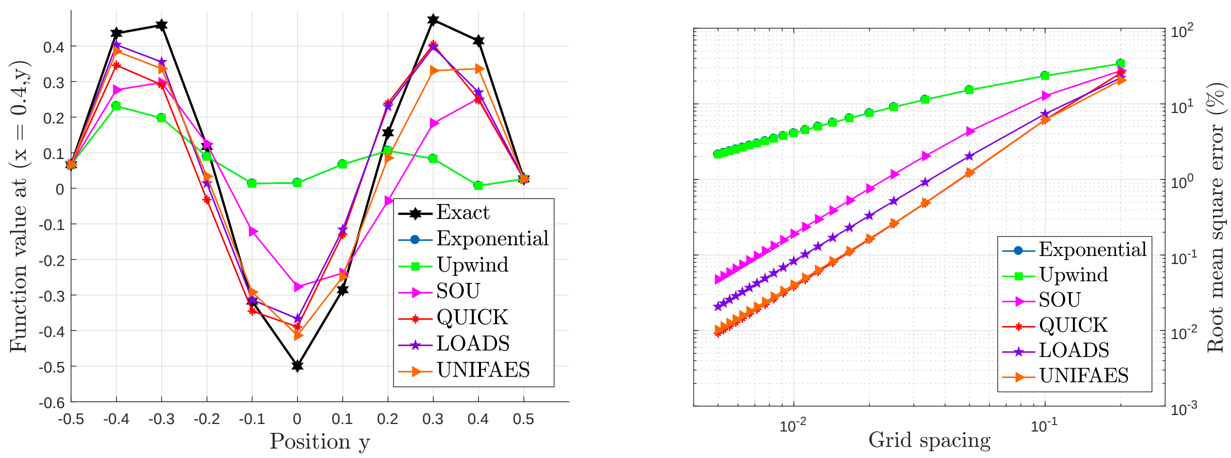


(a) 10×10 spacings grid, Pe $= 100$, $\lambda = 10$

(b) 10×10 spacings grid, $\lambda = 10$, $\theta = 22.5$ degrees.

Figure 7. (a) Root mean square error dependence on angle. (b) Root mean square error dependence on Peclet number. Both relative to function A

The performance of the schemes for a high Peclet number (10^9), except central differencing due to its restricted stability, is shown in Fig. 8a. Furthermore, Fig. 8b shows the curves of errors against refinement. Both curves refer to function A. It is clear that for high Peclet numbers, UNIFAES, LOADS and QUICK schemes present the best results, becoming more evident their differences with the results obtained by other schemes. Thus, UNIFAES, LOADS and QUICK schemes show excellent acuity for all function types throughout the Peclet number range.



(a) 10×10 spacings grid, Pe $= 10^9$, $\lambda = 10$, $\theta = 22.5$ degrees

(b) Pe $= 10^9$, $\lambda = 10$, $\theta = 22.5$ degrees.

Figure 8. (a) Exact and numerical profiles at $x = 0.4$. (b) Root mean square error against grid refinement. Both relative to function A

5. CONCLUSIONS

Although restricted to the constant velocity case, employed testing methodology, sweeping the spectrum of solutions, was able to reproduce many situations found in applied problems, such as the effects of the angle between the flow and the grid lines, Peclet number variations and the distinct levels of smoothness.

Clearly the performance of all schemes depends on the particular solution of the transport equation. Reaffirming conclusions of many previous studies, the central differencing shows wiggly behavior in all functions ϕ. For high Peclet numbers, one can see that the results of simple exponential tend to those of the upwind scheme. Although in functions B and D, the simple exponential displayed superb accuracy. As seen in all cases, the second order upwind exhibits intermediate performance. Summing up the results for the low ratios λ/Pe, the best global performances are obtained by UNIFAES, LOADS and QUICK, all three showing excellent acuity for all function types throughout the Peclet number range. On the other hand, the calculation of the source term by UNIFAES is simpler than that of LOADS. In transient and three-dimensional problems, the calculation of the source term by LOADS demands high computational cost. UNIFAES, on the other hand, is not computationally expensive. It should also be mentioned that UNIFAES has the advantage of being unconditionally stable for all Peclet numbers, while QUICK shows non-monotonic convergence for B and D function.

The relevance of monotonic spatial convergence is related to the need of spatial refinement for assessment of accuracy whatever scheme is employed. This is exemplified by the use of Richardson's extrapolation in some problems. This extrapolation was successfully employed by Figueiredo and Llagostera (1999) and Figueiredo and Oliveira (2009a,b, 2011) using central differencing and UNIFAES. However, some irregularities were observed when Richardson's extrapolation was employed to evaluate the performance of QUICK (Santos and Figueiredo, 2007). This can be attributed to its non-monotonic behavior.

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7. RESPONSIBILITY NOTICE

The authors are the only responsible for the printed material included in this paper.

APPENDIX A. QUICK SCHEME ORDER OF ACCURACY

There is some controversy in the literature as to the claim of the third order accuracy of the QUICK scheme. Thus, the present analysis will distinguish two possible cases in order to determine the order of accuracy of the scheme. First, consider the approximation given by the interpolation curve as a function whose value is defined in the control volume face. A generic expression can be applied to generate an entire family of formulas by defining a general interpolation rule for the face values of the control volume. The function value at the face e is defined from the mesh point values, following:

$$\phi_e = \phi_P + \alpha(\phi_E - \phi_P) + \beta(\phi_P - \phi_W) \tag{A.32}$$

General conditions can be written for this interpolation formula to be at least second order or third order accurate. An uniform mesh is assumed. The choice $\alpha = 1/2$ and $\beta = 0$ corresponds to the central differencing scheme. The choice $\alpha = \beta = 0$ reproduces the upwind scheme. Selecting $\alpha = 0$ and $\beta = 1/2$ leads to the second order upwind scheme. The QUICK scheme is obtained by choosing the parameters $\alpha = 3/8$ and $\beta = 1/8$ resulting in Eq. (7).

Therefore, the first case focuses on the derivation of the conditions for the Eq. (A.32) to be at least third order accurate. For this, the error analysis requires that the terms of the left and right sides at Eq. (A.32) be expanded in Taylor series around node P. Assuming that the function ϕ is sufficiently differentiable, one will have according to Fig. 2b:

$$\phi_e = \phi_P + \frac{\partial \phi_P}{\partial x}\left(\frac{\Delta x}{2}\right) + \frac{\partial^2 \phi_P}{\partial x^2}\frac{1}{2!}\left(\frac{\Delta x}{2}\right)^2 + \frac{\partial^3 \phi_P}{\partial x^3}\frac{1}{3!}\left(\frac{\Delta x}{2}\right)^3 + \cdots \tag{A.33}$$

$$\phi_E = \phi_P + \frac{\partial \phi_P}{\partial x}(+\Delta x) + \frac{\partial^2 \phi_P}{\partial x^2}\frac{1}{2!}(+\Delta x)^2 + \frac{\partial^3 \phi_P}{\partial x^3}\frac{1}{3!}(+\Delta x)^3 + \cdots \tag{A.34}$$

$$\phi_W = \phi_P + \frac{\partial \phi_P}{\partial x}(-\Delta x) + \frac{\partial^2 \phi_P}{\partial x^2}\frac{1}{2!}(-\Delta x)^2 + \frac{\partial^3 \phi_P}{\partial x^3}\frac{1}{3!}(-\Delta x)^3 + \cdots \tag{A.35}$$

Substituting Eqs. (A.33), (A.34) and (A.35) into (A.32) leads to:

$$\begin{aligned}\frac{\partial \phi_P}{\partial x}\frac{\Delta x}{2} + \frac{\partial^2 \phi_P}{\partial x^2}\frac{\Delta x^2}{8} + \frac{\partial^3 \phi_P}{\partial x^3}\frac{\Delta x^3}{48} + \cdots = {} & \frac{\partial \phi_P}{\partial x}(\alpha+\beta)\Delta x + \frac{\partial^2 \phi_P}{\partial x^2}\left(\frac{\alpha}{2} - \frac{\beta}{2}\right)\Delta x^2 \\ & + \frac{\partial^3 \phi_P}{\partial x^3}\left(\frac{\alpha}{6} + \frac{\beta}{6}\right)\Delta x^3 + \cdots\end{aligned} \tag{A.36}$$

Thus, the conditions that the above expression must respect in order to be at least third order accurate are:

$$\begin{cases}\alpha + \beta = 1/2 \\ \alpha - \beta = 1/4\end{cases} \tag{A.37}$$

Solving the system (A.37), one finds the parameters $\alpha = 3/8$ and $\beta = 1/8$. Note that these parameters correspond to the QUICK scheme. Thus, as proven by Eqs. (A.32) to (A.37), Eq. (7) is indeed a third order approximation for the function value ϕ_e at the control volume face. However, when considering the $\partial/\partial x$ operator to be discretized from a transport equation, *i.e.* the control volume analog of the first derivative $(\phi_e - \phi_w)/\Delta x$, based solely on the mesh point values, the QUICK scheme approximation of the first derivative is only second order accurate, as shown below.

As described in section 2.2, a parabolic interpolation curve is used to approximate the convective term, while for the diffusive term the central differentiation is maintained. Thus, attention is focused only on the convective term. By integrating and applying the divergence theorem to the convective term, one obtains the analogue, in the context of the finite volume approach, of the first derivative, in the form:

$$\frac{1}{\Delta x}\int_w^e \frac{\partial\left(\rho u\phi\right)}{\partial x}dx \cong \frac{1}{\Delta x}\left[\left(\rho u\phi\right)_e - \left(\rho u\phi\right)_w\right] \tag{A.38}$$

The second case employs a classical procedure, using the concept of representation of the first derivative $\partial\phi_P/\partial x$ at the central node P (see Fig. 2b) and employing the parabolic interpolation curve ϕ, which is used for the error analysis by Taylor series at an unidirectional control volume with regular spacing. This interpolation curve ϕ takes the generic form:

$$\phi = a + bx + cx^2 \tag{A.39}$$

By adjusting the expression (A.39), for example, to the nodes WW, W and P (see Fig. 2b), it follows that:

$$\phi = \phi_P + \left(\frac{3\phi_P - 4\phi_W + \phi_{WW}}{2\Delta x}\right)x + \left(\frac{\phi_P - 2\phi_W + \phi_{WW}}{2\Delta x^2}\right)x^2 \tag{A.40}$$

Thus, for $x = -\Delta x/2$ it is possible to evaluate the value of ϕ at the west face w, given by Eq. (8). Proceeding in a similar way, one can compute ϕ at the east face e, resulting in Eq. (7). In the present analysis, the coefficient ρu is assumed constant. Thus, attention is focused only on the liquid convective flux. Substituting Eqs. (7) and (8) into (A.38) results:

$$\frac{\phi_e - \phi_w}{\Delta x} = \frac{1}{\Delta x}\left[\frac{3}{8}\phi_E + \frac{3}{8}\phi_P - \frac{7}{8}\phi_W + \frac{1}{8}\phi_{WW}\right] \tag{A.41}$$

Substituting Eqs. (A.34), (A.35) and the Taylor series expansion of ϕ_{WW} into (A.41) results:

$$\frac{\phi_e - \phi_w}{\Delta x} = \frac{\partial\phi_P}{\partial x} + \frac{\partial^3\phi_P}{\partial x^3}\frac{\Delta x^2}{24} + \frac{\partial^4\phi_P}{\partial x^4}\frac{\Delta x^3}{16} + \cdots \tag{A.42}$$

Therefore, it is concluded that the QUICK scheme produces an estimate of the convective term $\partial\phi_P/\partial x$ (where the coefficient ρu was suppressed for simplicity), within the finite volume approach, of second order accuracy. The QUICK scheme leads to a dominating truncation error equal to $-(\partial^3\phi_P/\partial x^3)\Delta x^2/24$.

The piecewise constant approximation in finite volume approaches the value of the function at cell boundary with first order error and the derivative also with first order error. Analogously, the piecewise linear approaches the function at cell boundary and the derivative with second order error. However, the same analogy cannot be applied to QUICK. This result can be proved indirectly through the Lax equivalence theorem (Richtmyer and Morton, 1994), which states that for the numerical solution of a linear problem, by using a consistent discretization, the stability of the numerical method is a necessary and sufficient condition for convergence. The consistency error of a numerical method is obtained from the Taylor series error analysis, yet the convergence error is the result of the refinement of the mesh. Thus, by the Lax theorem, if a numerical scheme has second order consistency error and is stable, then, it also has second order convergence error. This statement further reinforces the analysis of the accuracy order of the QUICK scheme performed here at Appendix A.