Effect of numerical truncation error on implicit finite difference methods in groundwater transport models

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A correction for truncation errors associated with implicit finite difference method (FDM) of the groundwater transport equation with reaction term, which is generally used in groundwater transport models, is developed here from a Taylor series analysis. An application example is formulated to illustrate the effect of truncation errors on the numerical solution of implicit FDM. The study compares the effect of truncation error on numerical model accuracy of implicit FDM and explicit FDM for groundwater transport equation with reaction term. The explicit FDM constitutes large deviation from analytical solution without truncation error correction. The relative error analysis reveals that error reduces from 75% to 30% after truncation error correction. Therefore, we can conclude that numerical truncation error correction has significant impact on accuracy of groundwater transport models based on explicit FDM than those based on implicit FDM.

Keywords: Groundwater transport, finite difference method, implicit and explicit models, numerical truncation error.

THE credible study of solute transport/advection–dispersion processes in hydrogeological systems has stimulated the development of various numerical methods for groundwater transport equations (advection dispersion equation; ADE). However, requirements regarding the accuracy and efficiency for these methods are constantly becoming stricter and therefore there is a still need to find better numerical schemes[1]. Therefore, understanding of theoretical truncation error is necessary, when concrete numerical schemes are applied.

The ADE of a solute transport is approximated by discretization, which generally suffers from the presence of truncation errors in the predictions[2]. The most recognized form of truncation error in the ADE is the numerical dispersion error[3]. This was first quantified as a second-order error through the analysis of truncated Taylor series approximation of a simple, explicit finite difference solution of the one-dimensional transport equation[4,5]. Although for this type of transport model, the truncation error results only from numerical dispersion. But in general form of ADE with reaction term, truncation error arises from other physical parameter terms also.

Many of the previous studies have considered the effect of numerical dispersion errors on the solution of ADE[6–10]. The previous studies presented a numerical model for chemical species (phosphorus) transport in soils and groundwater with two consecutive reactions[9]. The studies addressed the effect of numerical dispersion in the explicit finite difference method (FDM) despite the fact that the effects of zero- and first-order truncation errors were ignored. Later, these truncation errors in the ADE with reaction were quantified[11,12]. An explicit FDM was presented to calculate unsteady one-dimensional ADE and volatilization of toxic organic compounds in soils based on the formulation of an integrated mass flux approach[7]. In addition, numerical formulations for truncation error were extended for two-dimensional ADE by applying Taylor series expansion[13].

The previous studies were mainly focused on application of estimated numerical truncation error on explicit FDM and Crank–Nicolson method. They did not present any application related to truncation error analysis of implicit FDM. Therefore, the present study emphasizes on the numerical truncation error formulation for implicit FDM, its applications and implications on the accuracy of numerical solution of groundwater transport models.

Materials and methods

The partial differential equation describing one-dimensional transport of solute through homogeneous medium is written as

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - U\frac{\partial C}{\partial x} - kC, \qquad (1)$$

where C is the solute concentration [ML^{-3}], t the time [T], x the horizontal coordinate [L], U the Darcy flux [LT^{-1}],

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D is the physical dispersion coefficient [L^2 T^{-1}] and k is the reaction coefficient [T^{-1}].

The present study applies forward time and implicit centred FDM in space, and eq. (1) can be approximated as

$$\frac{C_i^{n+1}-C_i^n}{\Delta t}=D\left[\frac{C_{i+1}^{n+1}-2C_i^{n+1}+C_{i-1}^{n+1}}{\Delta x^2}\right]$$

$$-U\left[\frac{C_{i+1}^{n+1}-C_{i-1}^{n+1}}{2\Delta x}\right]-kC_i^{n+1}, \quad (2)$$

where the superscript n refers to time level, the subscript i refers to the node point, Δx is the spatial increment of grid [L] and Δt is the temporal increment [T]. Here, we consider uniform time and space increment.

A Taylor series expansion of C about any grid point is used to determine the form of the truncation errors[4,5]. If the third- and higher-order spatial derivatives are neglected, then the following formulation is obtained

$$C_i^{n+1}\approx C_i^n+\sum_{m=1}^{\infty}\frac{\Delta t^m}{m!}\frac{\partial^m C}{\partial t^m}, \quad (3)$$

$$C_{i+1}^{n+1}\approx C_i^{n+1}+\Delta x\frac{\partial C^{n+1}}{\partial x}+\frac{\Delta x^2}{2}\frac{\partial^2 C^{n+1}}{\partial x^2}, \quad (4)$$

$$C_{i-1}^{n+1}\approx C_i^{n+1}-\Delta x\frac{\partial C^{n+1}}{\partial x}+\frac{\Delta x^2}{2}\frac{\partial^2 C^{n+1}}{\partial x^2}. \quad (5)$$

The second and higher-order temporal derivatives of C are written in terms of spatial derivatives using the differentiated form of eq. (1) as

$$\frac{\partial^2 C}{\partial t^2}=\frac{\partial}{\partial t}\left(\frac{\partial C}{\partial t}\right), \quad (6)$$

$$\frac{\partial^2 C}{\partial t^2}=D\frac{\partial^2}{\partial x^2}\left(\frac{\partial C}{\partial t}\right)-U\frac{\partial}{\partial x}\left(\frac{\partial C}{\partial t}\right)-k\left(\frac{\partial C}{\partial t}\right). \quad (7)$$

To express eq. (6) only in spatial terms, we eliminate the temporal terms. For this, substitute eq. (1) into eq. (6) as

$$\frac{\partial^2 C}{\partial t^2}=D\frac{\partial^2}{\partial x^2}\left(D\frac{\partial^2 C}{\partial x^2}-U\frac{\partial C}{\partial x}-kC\right)$$

$$-U\frac{\partial}{\partial x}\left(D\frac{\partial^2 C}{\partial x^2}-U\frac{\partial C}{\partial x}-kC\right)-k\left(D\frac{\partial^2 C}{\partial x^2}-U\frac{\partial C}{\partial x}-kC\right). \quad (8)$$

Neglect the higher-order derivative terms

$$\frac{\partial^2 C}{\partial t^2}\approx(U^2-2kD)\frac{\partial^2 C}{\partial x^2}+2kU\frac{\partial C}{\partial x}+k^2C. \quad (9)$$

Similarly, the higher-order temporal derivative can be formulated as

$$\frac{\partial^3 C}{\partial t^3}\approx(-3kU^2+3k^2D)\frac{\partial^2 C}{\partial x^2}-3k^2U\frac{\partial C}{\partial x}-k^3C, \quad (10)$$

$$\frac{\partial^4 C}{\partial t^4}\approx(6k^2U^2-4k^3D)\frac{\partial^2 C}{\partial x^2}+4k^3U\frac{\partial C}{\partial x}+k^4C, \quad (11)$$

$$\frac{\partial^5 C}{\partial t^5}\approx(-10k^3U^2+5k^4D)\frac{\partial^2 C}{\partial x^2}-5k^4U\frac{\partial C}{\partial x}-k^5C. \quad (12)$$

From eqs (9)–(12), it can write a general formula, i.e. for $m\geq 2$

$$\frac{\partial^m C}{\partial t^m}\approx(-1)^m\left(\frac{m(m-1)}{2}k^{m-2}U^2-mk^{m-1}D\right)\frac{\partial^2 C}{\partial x^2}$$

$$+(-1)^m mk^{m-1}U\frac{\partial C}{\partial x}+(-1)^m k^m C. \quad (13)$$

Therefore, eq. (3) can be written as

$$C_i^{n+1}\approx C_i^n+\Delta t\frac{\partial C}{\partial t}+\sum_{m=2}^{\infty}\frac{\Delta t^m}{m!}$$

$$\times\left[\begin{array}{l}(-1)^m\left(\dfrac{m(m-1)}{2}k^{m-2}U^2-mk^{m-1}D\right)\dfrac{\partial^2 C}{\partial x^2}\\ +(-1)^m mk^{m-1}U\dfrac{\partial C}{\partial x}+(-1)^m k^m C\end{array}\right]. \quad (14)$$

Substituting eq. (14) in eqs (4) and (5) and neglecting the higher-order spatial derivative yields the following expressions for C_{i+1}^{n+1} and C_{i-1}^{n+1}

$$C_{i+1}^{n+1}\approx C_i^n+\Delta t\frac{\partial C}{\partial t}+\sum_{m=2}^{\infty}\frac{\Delta t^m}{m!}$$

$$\times\left[\begin{array}{l}(-1)^m\left(\dfrac{m(m-1)}{2}k^{m-2}U^2-mk^{m-1}D\right)\dfrac{\partial^2 C}{\partial x^2}\\ +(-1)^m mk^{m-1}U\dfrac{\partial C}{\partial x}+(-1)^m k^m C\end{array}\right]$$

$$+\Delta x\frac{\partial C}{\partial x}+\Delta t\Delta x\left(-U\frac{\partial^2 C}{\partial x^2}-k\frac{\partial C}{\partial x}\right)$$

$$+\Delta x\sum_{m=2}^{\infty}\frac{\Delta t^m}{m!}\begin{bmatrix}(-1)^m mk^{m-1}U\dfrac{\partial^2 C}{\partial x^2}\\ +(-1)^m k^m\dfrac{\partial C}{\partial x}\end{bmatrix}$$

$$+\frac{\Delta x^2}{2}\frac{\partial^2 C}{\partial x^2}-\frac{\Delta x^2\Delta t}{2}k\frac{\partial^2 C}{\partial x^2}$$

$$+\frac{\Delta x^2}{2}\sum_{m=2}^{\infty}\frac{\Delta t^m}{m!}\left[(-1)^m k^m\frac{\partial^2 C}{\partial x^2}\right], \tag{15}$$

$$C_{i-1}^{n+1}\approx C_i^n+\Delta t\frac{\partial C}{\partial t}+\sum_{m=2}^{\infty}\frac{\Delta t^m}{m!}$$

$$\times\begin{bmatrix}(-1)^m\left(\dfrac{m(m-1)}{2}k^{m-2}U^2-mk^{m-1}D\right)\dfrac{\partial^2 C}{\partial x^2}\\ +(-1)^m mk^{m-1}U\dfrac{\partial C}{\partial x}+(-1)^m k^m C\end{bmatrix}$$

$$-\Delta x\frac{\partial C}{\partial x}-\Delta t\Delta x\left(-U\frac{\partial^2 C}{\partial x^2}-k\frac{\partial C}{\partial x}\right)$$

$$-\Delta x\sum_{m=2}^{\infty}\frac{\Delta t^m}{m!}\begin{bmatrix}(-1)^m mk^{m-1}U\dfrac{\partial^2 C}{\partial x^2}\\ +(-1)^m k^m\dfrac{\partial C}{\partial x}\end{bmatrix}$$

$$+\frac{\Delta x^2}{2}\frac{\partial^2 C}{\partial x^2}-\frac{\Delta x^2\Delta t}{2}k\frac{\partial^2 C}{\partial x^2}$$

$$+\frac{\Delta x^2}{2}\sum_{m=2}^{\infty}\frac{\Delta t^m}{m!}\left[(-1)^m k^m\frac{\partial^2 C}{\partial x^2}\right]. \tag{16}$$

Substituting eqs (14)–(16) into eq. (2), and rearranging yields the following equation

$$\frac{\partial C}{\partial t}=\frac{\partial^2 C}{\partial x^2}\left\{\begin{matrix}D-2D\Delta tk+D\displaystyle\sum_{m=2}^{\infty}\frac{\Delta t^m}{m!}[(-1)^m k^m]\\ +U^2\Delta t-U\displaystyle\sum_{m=2}^{\infty}\frac{\Delta t^m}{m!}[(-1)^m mk^{m-1}U]\\ +(-1-k\Delta t)\displaystyle\sum_{m=2}^{\infty}\frac{\Delta t^{m-1}}{(m-1)!}\\ \left[(-1)^m\left(\dfrac{(m-1)}{2}k^{m-2}U^2-k^{m-1}D\right)\right]\end{matrix}\right\}$$

$$-\frac{\partial C}{\partial x}\begin{bmatrix}U-2U\Delta tk+U\displaystyle\sum_{m=2}^{\infty}\frac{\Delta t^m}{m!}[(-1)^m k^m]\\ +\displaystyle\sum_{m=2}^{\infty}\frac{\Delta t^{m-1}}{(m-1)!}[(-1)^m k^{m-1}U](1+k\Delta t)\end{bmatrix}$$

$$-C\left(k-k^2\Delta t+(1+k\Delta t)\sum_{m=2}^{\infty}\frac{\Delta t^{m-1}}{m!}[(-1)^m k^m]\right). \tag{17}$$

Comparing eq. (17) and the original governing equation shows that even in implicit method discretization introduces three forms of truncation error. It can be formulated as given below.

Derivation of truncation error formula

Second-order truncation error or numerical dispersion

$$D_{\text{num}}=-2D\Delta tk+D\sum_{m=2}^{\infty}\frac{\Delta t^m}{m!}[(-1)^m k^m]$$

$$+U^2\Delta t-U\sum_{m=2}^{\infty}\frac{\Delta t^m}{m!}[(-1)^m mk^{m-1}U]$$

$$+(-1-k\Delta t)\sum_{m=2}^{\infty}\frac{\Delta t^{m-1}}{(m-1)!}$$

$$\left[(-1)^m\left(\frac{(m-1)}{2}k^{m-2}U^2-k^{m-1}D\right)\right]. \tag{18}$$

First-order truncation error or numerical water velocity

$$U_{\text{num}}=-2U\Delta tk+U\sum_{m=2}^{\infty}\frac{\Delta t^m}{m!}[(-1)^m k^m]$$

$$+\sum_{m=2}^{\infty}\frac{\Delta t^{m-1}}{(m-1)!}[(-1)^m k^{m-1}U](1+k\Delta t). \tag{19}$$

Zero-order truncation error or numerical reaction coefficient

$$k_{\text{num}}=-k^2\Delta t+(1+k\Delta t)\sum_{m=2}^{\infty}\frac{\Delta t^{m-1}}{m!}[(-1)^m k^m]. \tag{20}$$

In order to eliminate the truncation error due to numerical dispersion, numerical velocity and numerical reaction coefficient, the derived formula for these terms is subtracted from the physical dispersion, velocity and reaction coefficient. New terms are substituted in eq. (1) as

$$\frac{\partial C}{\partial t}=D^*\frac{\partial^2 C}{\partial x^2}-U^*\frac{\partial C}{\partial x}-k^*C, \tag{21}$$

where D^*, U^* and k^* denote the truncation error corrected forms.

$$D^* = D - D_{\text{num}}, \tag{22}$$

$$U^* = U - U_{\text{num}}, \tag{23}$$

$$k^* = k - k_{\text{num}}. \tag{24}$$

Results and discussion

In order to study the effect of error due to numerical truncation (numerical dispersion, numerical velocity and numerical reaction coefficient) on forward time and implicit centred FDM, we compared the numerical simulation of truncation error-corrected and non-corrected truncation error scheme with the analytical solution adopted from the previous studies[12,14]. The analytical solution for solute transport equation for the following initial and boundary conditions, i.e.

$$C = C_i, \ t = 0, \ x > 0;$$

$$C = C_0, \ t > 0, \ x = 0;$$

$$C = 0, \ t > 0, \ x \to \infty;$$

is

$$C(x,t) = \left\{ \frac{C_0}{2} \left[\exp\left(\frac{(U-v)x}{2D} \right) \operatorname{erfc}\left(\frac{x - vt}{2(Dt)^{0.5}} \right) \right] + \left[\exp\left(\frac{(U+v)x}{2D} \right) \operatorname{erfc}\left(\frac{x + vt}{2(Dt)^{0.5}} \right) \right] \right\}, \tag{25}$$

where v is calculated as

$$v = (U^2 + 4kD)^{0.5}. \tag{26}$$

Also, the performance of the model is confirmed by estimating relative error (RE) as

$$\text{RE}(\%) = \frac{C_{\text{num}} - C_{\text{ana}}}{C_{\text{ana}}} \times 100, \tag{27}$$

where C_{num} and C_{ana} are numerical and analytical solute concentrations respectively.

In order to show that implicit centred FDM can yield a solution which is close to the analytical solution by applying numerical error terms in calculation, we provide an application example with the following input parameters. The numerical problem is composed of a semi-infinite column, where $U = 10$ cm/h; $D = 100$ cm^2/h; $k = 0.5$ h^{-1}; incoming concentration = 1000 mg/l and initial concentration = 0.0 mg/l. Here, a space increment of 20 cm and temporal increment of 1.0 h is applied (Figure 1). We compare the numerical solution with the analytical solution at time of 24 h.

Figures 2–4 show numerical results. Figure 2 shows the results with and without correction of numerical error for implicit centred finite difference scheme. The numerical results showed a close match with the analytical solution irrespective of the numerical truncation correction. Also, it should be pointed out that as the depth increases, the corrected numerical solution is closer to the analytical solution compared to solution without correction. However, numerical solution without correction from implicit scheme does not show a significant deviation from the analytical solution. A comparison between numerical result of explicit scheme and analytical solution shows that the numerical solution without numerical error correction deviates comparatively larger from analytical solution compared to implicit FDM (Figure 3). The numerical solution with error correction matches well with the analytical solution in case of explicit scheme. This indicates the smallest truncation error associated with numerical solution of implicit centred FDM compared to explicit FDM (Figure 3). Therefore, Figures 2 and 3 illustrates that explicit FDM improves by application of numerical error term, while implicit FDM shows less improvement in the accuracy of numerical solution.

Moreover, the study illustrates the effect of increase in the number of terms used in the series (m) on solution accuracy in the case of implicit FDM. The number of terms used in the series (m) controls the error between numerical solution and analytical solution[12]. The truncation error can be minimized by increase in the number of terms in the series. But at certain m value, the numerical solution fully converges with the analytical solution (Figure 4). Therefore, increase in m value after this value cannot contribute to significant improvement in the accuracy of the numerical result[12].

The study estimated the relative error for truncation error corrected and non-corrected numerical solution of different FDMs by applying eq. (27). Our results reveal that numerical error decreases drastically by removal of truncation error from FDM (Figure 5). The maximum error limit is reduced from 75% to 30% after truncation error correction (Figure 5). Therefore, it is significant to study the truncation error correction of FDM because the groundwater model such as MT3D applies FDM to solve the numerical problems. Application of truncation error correction term can reduce error from the numerical results of these FDM. The present study could shed light on the truncation error due to the advection term, dispersion and reaction term.

According to the present study, it is clear that numerical truncation error correction has a significant impact on

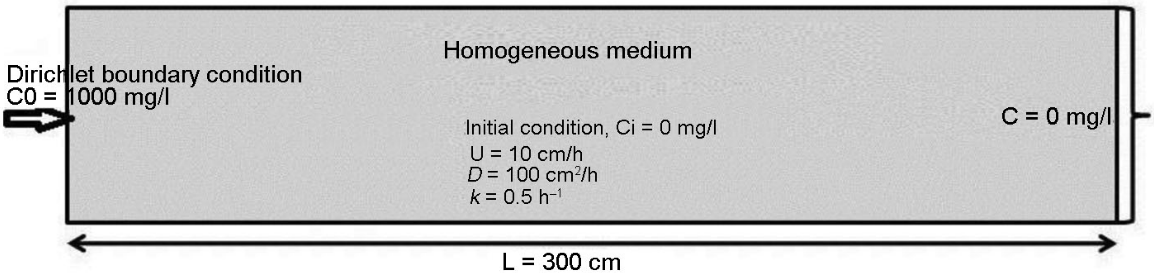

Figure 1. Numerical experimental set-up and initial and boundary conditions.

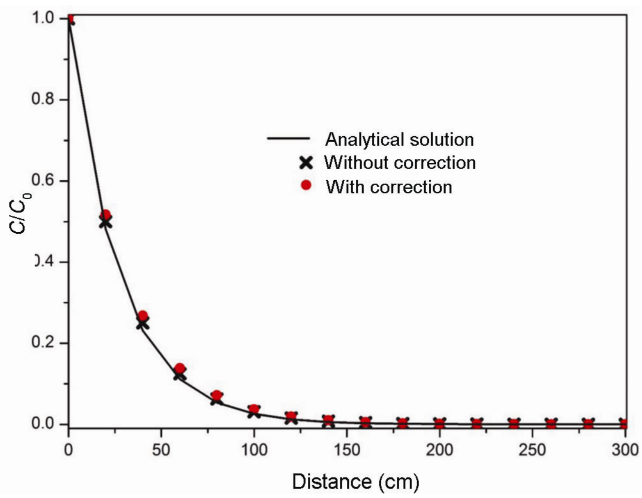

Figure 2. Comparison of numerical solution with correction and without correction in the case of implicit centred finite difference scheme.

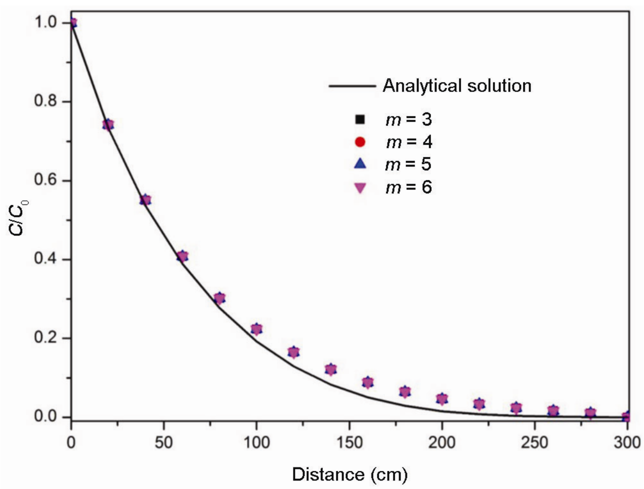

Figure 4. Comparison of the effect of number of terms in the series on numerical solution accuracy in the case of implicit centred finite difference scheme.

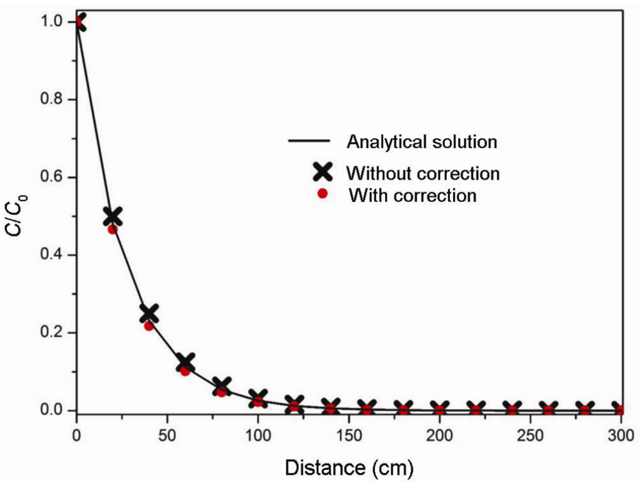

Figure 3. Comparison of numerical solution with and without correction in the case of explicit centred finite difference scheme.

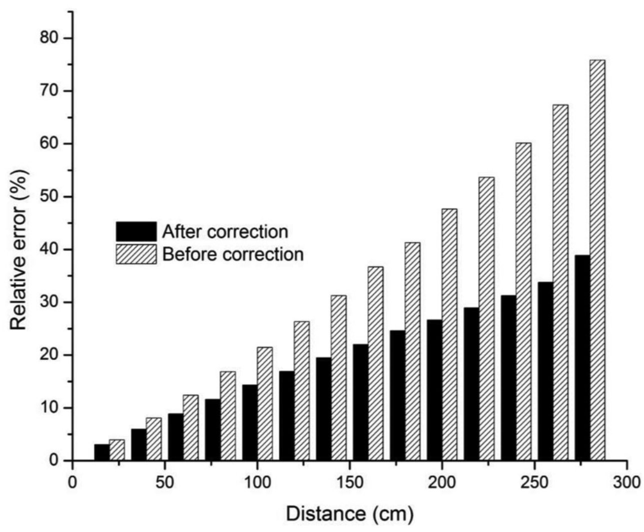

Figure 5. Relative error estimated before and after truncation error correction for explicit centred finite difference scheme.

improving solution accuracy of the FDM, especially in the case of explicit FDM. The numerical solution without error correction shows significant deviation from the analytical solution in case of explicit finite difference scheme. The implicit FDM shows less deviation from the analytical solution, even without error correction. Therefore, numerical error correction is most effective for explicit FDM than implicit FDM.

Conclusion

A simple modification or subtraction of the numerical truncation error term dramatically increases the solution accuracy of FDM. The present study compared the solution accuracy of implicit FDM with and without truncation error corrections. The results show that truncation error in implicit FDM is small. The study also compares the numerical solution of explicit centred FDM. It showed that truncation error correction can significantly improve the solution accuracy of explicit FDM. Also, the study shows that increase in the number of terms in series after a certain value cannot improve the numerical solution accuracy. In addition, the present study estimated the RE associated with explicit centred FDM before and after removal of truncation error. The results reveal that truncation error correction can improve the solution accuracy of explicit FDM significantly, which is obvious from RE estimation too. The observation of results from two FDM (i.e. explicit and implicit centred) shows that the application of truncation error formula is most effective on explicit FDM compared to implicit FDM.

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