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RETRACTED ARTICLE: Numerical Methods for Unsteady Convection-diffusion Problems Based on Combining Compact Difference Schemes with Runge-Kutta Methods

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ABSTRACT: *The convection-diffusion equation is of primary importance in understanding transport phenomena within a physical system. However, the currently available methods for solving unsteady convection-diffusion problems are generally not able to offer excellent accuracy in space and time. The one-dimensional unsteady convection-diffusion equation was solved by combing a compact difference scheme with the Runge-Kutta method. The combined method has fourth-order accuracy in space and time. To check the accuracy of the combined method, numerical experiments were carried out and comparisons were performed with the Crank-Nicolson method. The analysis results indicated that the combined method is numerically stable at low wave numbers and small Courant-Friedrichs-Lewy numbers. The combined method has higher accuracy than the Crank-Nicolson method.*

Keywords: compact difference schemes, Runge-Kutta methods, convection-diffusion equations, high-order accuracy, Crank-Nicolson methods

1. INTRODUCTION

The convection-diffusion equation is a combination of the diffusion and convection equations, and describes physical phenomena where particles, energy, or other physical quantities are transferred inside a physical system due to convection and diffusion processes.[1,2] This equation is of primary importance in understanding

transport phenomena within a physical system.[3,4] For a transport variable u, the one-dimensional unsteady convection-diffusion equation is given by

$$\frac{\partial u(x,t)}{\partial t} + c\,\frac{\partial u(x,t)}{\partial x} = \alpha\,\frac{\partial^2 u(x,t)}{\partial x^2},\ (x,t) \in (0,L) \times (0,T) \tag{1}$$

where c is the convection intensity and α is the diffusion coefficient.

The boundary and initial conditions are given by

$$u(0,t) = g_0(t),\ \ u(L,t) = g_1(t),\ \ t \in (0,T),\ \ u(x,0) = \phi(x) \tag{2}$$

where g_0 and g_1 are smooth functions.

A variety of finite difference schemes have been presented to solve unsteady convection-diffusion problems approximately.[5] Typically, these schemes usually have first-order or second-order accurate in space, but have fallen short of expectations for convection-dominated flows if the mesh is not sufficiently refined.[5] Discretisation with a higher order in space is usually associated with large stencils, thereby increasing the band-width of the resulting matrix.[5,6] A class of compact difference approximations have been recently developed to solve convection-diffusion problems.[7–9] These compact difference schemes have fourth-order accuracy in space, but fail when accuracy in time is most needed.[10,11] Additionally, most of these schemes have to compute the inverse of the block matrix.[10,11] It is therefore entirely necessary to develop an effective numerical scheme in order to obtain satisfactory results with a higher order accuracy in time and reasonable computational cost.

The objective is to develop an effective method to achieve higher accuracy in time by combining a high-order compact difference scheme and the Runge-Kutta method. This combined method is used to solve the unsteady convection-diffusion equation. The Runge-Kutta method is introduced briefly in Section 2. The compact difference scheme is presented in Section 3. The stability of the combined method is checked in Section 4. Some numerical examples are presented in Section 5 and the conclusions are summarised in Section 6.

2. RUNGE-KUTTA METHODS

The most widely known member of the Runge-Kutta family is generally referred to as the classic Runge-Kutta method.[12] When the classic Runge-Kutta method is used to solve the convection-diffusion equation, time is treated as an independent variable in an ordinary differential equation,

$$\frac{dQ}{dt} = R(t, Q) \tag{3}$$

where Q is an unknown function of time, and R denotes the numerical approximation to the spatial derivatives. The Runge-Kutta method is specified as follows:

$$Q^{n+1} = Q^n + \Delta t \hat{R}(Q^n, \Delta t) \tag{4}$$

where Δt is the time increment. The increment function $\hat{R}\,(Q^n, \Delta t)$ is subdivided into number of steps (N) on the interval $t^n \leq t \leq t^{n+1}$

$$Q^1 = Q^n + \Delta t(\alpha_{11} R^n) \tag{5}$$

$$Q^2 = Q^n + \Delta t(\alpha_{21} R^n + \alpha_{22} R^1) \tag{6}$$

$$Q^3 = Q^n + \Delta t(\alpha_{31} R^n + \alpha_{32} R^1 + \alpha_{33} R^2) \tag{7}$$

$$Q^{n+1} = Q^n + \Delta t(\alpha_{N1} R^n + \alpha_{N2} R^1 + \ldots + \alpha_{NN} R^{N-1}) \tag{8}$$

where the superscript n, 1, 2, ..., and $n + 1$ denote the time steps on the time interval $t^n \leq t_1 \leq t_2 \leq \ldots \leq t_N \leq t^{n+1}$, and α is the weighting factor for the step i and term j.

A four-step algorithm is given by

$$Q^1 = Q^n + \frac{\Delta t}{4} R^n \tag{9}$$

$$Q^2 = Q^n + \frac{\Delta t}{3} R^1 \tag{10}$$

$$Q^3 = Q^n + \frac{\Delta t}{2} R^2 \tag{11}$$

$$Q^{n+1} = Q^n + \Delta t R^3 \tag{12}$$

This algorithm is convenient to program and no intermediate solution needs to be stored.[13]

3. COMPACT DIFFERENCE SCHEMES

The differential equation is specified as follows:

$$\alpha \frac{\partial^2 u(x)}{\partial x^2} - c \frac{\partial u(x)}{\partial x} = f(x), x \in (0, L) \tag{13}$$

with the boundary conditions

$$u(0) = g_0, u(L) = g_1 \tag{14}$$

The interval $0 \leq x \leq 1$ is subdivided into n equal subintervals by the grid points $x_i = ih$, where $h = \frac{1}{n}$.[14] The mesh function $u(ih)$ is written as u_i at grid point x_i. The second-order central difference schemes for second and first derivatives of u can be written as $\delta_x^2 u = \frac{(u_{i+1} - 2u_i + u_{i-1})}{h^2}$ and $\delta_x u = \frac{(u_{i+1} - u_{i-1})}{2h^2}$, respectively. The following relation can be derived from Equation (13) at point x_i:

$$\alpha \delta_x^2 u_i - c\delta_x u_i - \tau_i = f_i \tag{15}$$

$$\tau_i = \frac{h^2}{12} \left(\alpha \frac{d^4 u}{dx^4} - 2c \frac{d^3 u}{dx^3} \right) + O(h^4) \tag{16}$$

The fourth and third derivatives of u in the above equation should be approximated in order to obtain a compact difference scheme with fourth-order accuracy. Equation (13) gives:

$$\frac{d^3 u}{dx^3}\Big|_i = \frac{1}{\alpha} \left(\frac{df}{dx} + c \frac{d^2 u}{dx^2} \right)\Big|_i = \frac{1}{\alpha} (\delta_x f_i + c\delta_x^2 u_i) + O(h^2) \tag{17}$$

From Equations (13) and (17), it follows that

$$\frac{d^4 u}{dx^4}\Big|_i = \frac{1}{\alpha} \left(\frac{d^2 f}{dx^2} + c \frac{d^3 u}{dx^3} \right)\Big|_i = \frac{1}{\alpha} \delta_x^2 f_i + \frac{c}{\alpha^2} \delta_x f_i \frac{c^2}{\alpha^2} \delta_x^2 u_i) + O(h^2) \tag{18}$$

The following formula can then be derived:

$$\tau_i = \frac{h^2}{12}\left(\delta_x^2 f_i - \frac{c}{\alpha}\,\delta_x f_i - \frac{c^2}{\alpha}\,\delta_x^2 u_i\right) + O(h^4) \tag{19}$$

A fourth-order compact difference scheme can be obtained, given by

$$\left(\alpha + \frac{c^2h^2}{12\alpha}\right)\delta_x^2 u_i - c\delta_x u_i = f_i + \frac{h^2}{12}\left(\delta_x^2 f_i - \frac{c}{\alpha}\,\delta_x f_i\right) + O(h^4) \tag{20}$$

Here, two difference operators are defined as follows:

$$L_x = 1 + \frac{h^2}{12}\left(\delta_x^2 - \frac{c}{\alpha}\,\delta_x\right), \quad A_x = -\left(\alpha + \frac{c^2h^2}{12\alpha}\right)\delta_x^2 + c\delta_x \tag{21}$$

Equation (20) can be formulated symbolically as

$$L_x^{-1} A_x u_i = f_i + O(h^4) \tag{22}$$

The combined method is used to solve the convection-diffusion equation.

4. STABILITY ANALYSIS

The stability of the combined method is checked by performing a von Neumann linear stability analysis. Let $u_i^n = b^n e^{Ikhi}$ to be the value of u_i^n at x_i, where $I = \sqrt{-1}$, b^n is the amplitude at time level n, and k is the wave number. The amplification factor is defined as

$$g = \frac{b^{n+1}}{b^n} \tag{23}$$

The amplification factor of Equation (12) discretised by the Runge-Kutta method is given by

$$g = 1 + Z + \frac{1}{2}\,Z^2 + \frac{1}{6}\,Z^3 + \frac{1}{24}\,Z^4 \tag{24}$$

The variable Z represents the spatial discretisation applied to the convection-diffusion terms.[13] The explicit, discretised form is given by

$$Z = \left[\left(24\,\frac{F}{Pe} + 2F \bullet Pe\right)(1 - \cos k) - 12\mathrm{I}F \sin k\right] / (10 + 2\cos k - 1Pe \sin k) \tag{25}$$

The CFL (Courant-Friedrichs-Lewy) number F is defined as

$$F = \frac{c\Delta t}{h} \tag{26}$$

The Péclet number Pe is defined as

$$Pe = \frac{ch}{\alpha} \tag{27}$$

When the Péclet number is low the diffusion term dominates.[15,16] When the Péclet number is high, the convection term dominates.[15,16] For stability, the amplification factor has to satisfy the relation $|g| \leq 1$. When $|g| > 1$, the combined method is numerically unstable. The contour of amplification factor is plotted in Figures 1–4, respectively, in the plane of CFL number and wave number with various Péclet numbers such as 1, 10, 100 and 1000. The absolute value of amplification factor is presented in the following contours. The results indicate that the combined method is numerically stable at small Courant-Friedrichs-Lewy numbers and low wave numbers.

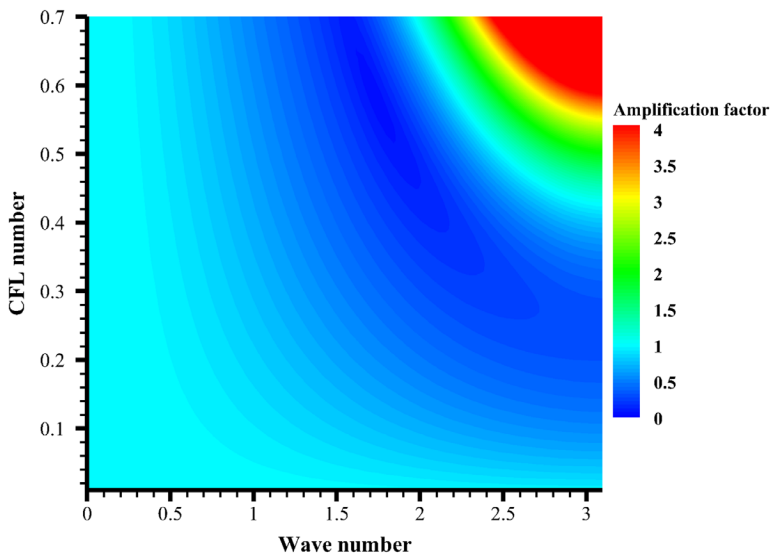

Figure 1: Contour of amplification factor in the plane of CFL number and wave number with a Péclet number of 1.

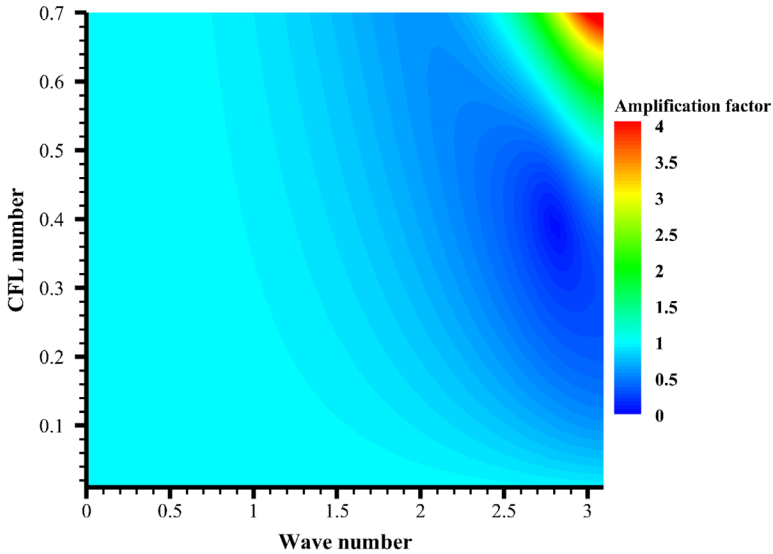

Figure 2: Contour of amplification factor in the plane of CFL number and wave number with a Péclet number of 10.

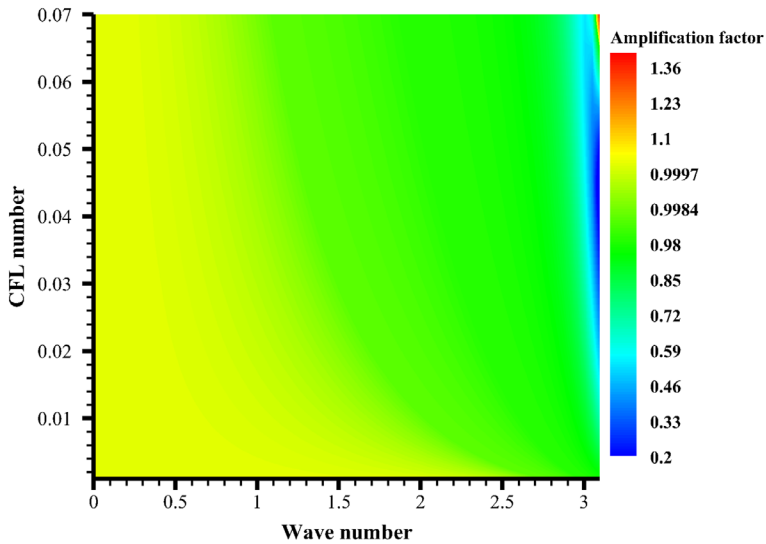

Figure 3: Contour of amplification factor in the plane of CFL number and wave number with a Péclet number of 100.

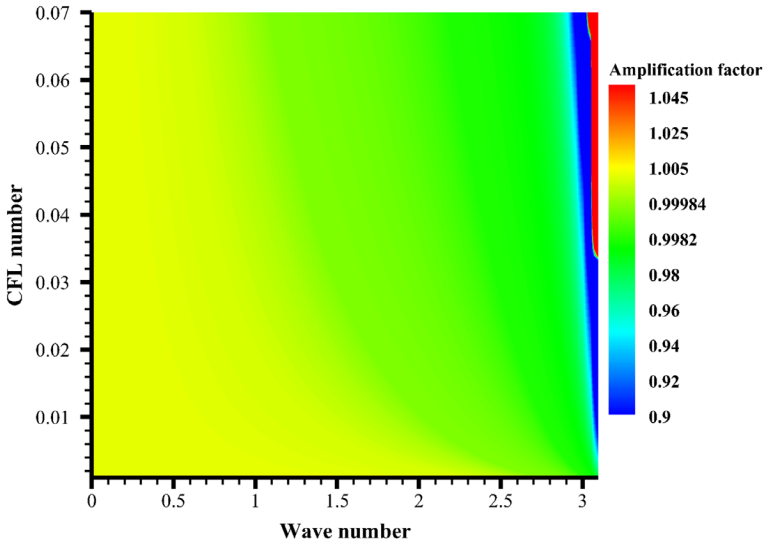

Figure 4: Contour of amplification factor in the plane of CFL number and wave number with a Péclet number of 1000.

5. NUMERICAL EXPERIMENTS

The Crank-Nicolson method can be written as an implicit Runge-Kutta method.[17,18] The numerical results are presented by comparing the combined method (C.M), with the Crank-Nicolson method (CN.M).

Example 5.1. The convection-diffusion equation is

$$\frac{\partial u}{\partial t} + 0.1\,\frac{\partial u}{\partial x} = 0.01\,\frac{\partial^2 u}{\partial x^2},\ (x,t) \in (0,1) \times (0,T) \tag{28}$$

The exact solution is given by

$$u(x,t) = e^{5x - (0.25 + 0.01\pi^2)t} \sin \pi x \tag{29}$$

The initial and boundary conditions are defined so that the results are agreed well with the exact problem solution. The accuracy of the combined method is compared with that of the Crank-Nicolson method. The results are presented in Table 1 for various values of t. The absolute error is obtained along the x direction. In addition, h is 0.005 and Δt is 0.001.

Table 1: The absolute error for various values of t, in which h is 0.005 and Δt is 0.001.

t	$x = 0.1$		$x = 0.3$		$x = 0.5$		$x = 0.7$		$x = 0.9$	
	CN.M	C.M	CN.M	C.M	CN.M	C.M	CN.M	C.M	CN.M	C.M
0.2	1.90×10^{-5}	0.66×10^{-9}	3.64×10^{-5}	1.62×10^{-9}	1.41×10^{-5}	2.11×10^{-9}	2.07×10^{-4}	2.73×10^{-9}	1.65×10^{-3}	5.99×10^{-8}
0.4	3.24×10^{-5}	1.13×10^{-9}	6.78×10^{-5}	3.03×10^{-9}	2.63×10^{-5}	3.93×10^{-9}	3.85×10^{-4}	5.15×10^{-9}	1.65×10^{-3}	2.46×10^{-7}
0.6	4.17×10^{-5}	1.47×10^{-9}	9.47×10^{-5}	4.23×10^{-9}	3.68×10^{-5}	5.50×10^{-9}	5.38×10^{-4}	8.04×10^{-9}	2.11×10^{-3}	5.15×10^{-7}
0.8	4.82×10^{-5}	1.72×10^{-9}	1.17×10^{-5}	5.25×10^{-9}	4.58×10^{-5}	6.84×10^{-9}	6.65×10^{-4}	1.29×10^{-8}	2.42×10^{-3}	8.26×10^{-7}
1	5.27×10^{-5}	1.90×10^{-9}	1.36×10^{-5}	6.09×10^{-9}	5.34×10^{-5}	7.95×10^{-9}	7.69×10^{-4}	2.11×10^{-8}	2.63×10^{-3}	1.16×10^{-6}

Example 5.2. The convection-diffusion equation is

$$\frac{\partial u}{\partial t} + 0.22\ \frac{\partial u}{\partial x} = 0.5\ \frac{\partial^2 u}{\partial x^2},\ (x,t) \in (0,1) \times (0,T) \tag{30}$$

The exact solution is given by

$$u(x,t) = e^{0.22x - (0.0242 + 0.5\pi^2)t} \sin \pi x \tag{31}$$

The initial and boundary conditions of the problem are defined so that the results are agreed well with the exact problem solution. The accuracy of the combined method is compared with that of the Crank-Nicolson method. The results are presented in Table 2 for various values of t. The absolute error is obtained along the x direction. In addition, h is 0.01 and Δt is $0.5h^2$.

Example 5.3. The convection-diffusion equation is

$$\frac{\partial u}{\partial t} + 0.1\ \frac{\partial u}{\partial x} = 0.2\ \frac{\partial^2 u}{\partial x^2},\ (x,t) \in (0,1) \times (0,T) \tag{32}$$

The exact solution is given by

$$u(x,t) = e^{0.25x - (0.0125 + 0.02\pi^2)t} \sin \pi x \tag{33}$$

The initial and boundary conditions are defined so that the results are agreed well with the exact problem solution. The accuracy of the combined method is compared with that of the Crank-Nicolson method. The results are presented in Table 3 for various values of t. The absolute error is obtained along the x direction. In addition, h is 0.01 and Δt is h^2.

The comparison results presented in Tables 1–3 indicate that the combined method has higher accuracy than the Crank-Nicolson method.

The combined method can effectively solve the one-dimensional unsteady convection-diffusion equation, with fourth-order accuracy in space and time. Additionally, the combined method has higher accuracy than the Crank-Nicolson method in all the cases studied. It is acknowledged that the combined method for solving the convection-diffusion equation has certain limitations. Specifically, the combined method is numerically stable at low wave numbers and small Courant-Friedrichs-Lewy numbers and may be prone to numerical instabilities at high wave numbers and large Courant-Friedrichs-Lewy numbers.

Table 2. The absolute error for various values of t, in which h is 0.01 and Δt is $0.5h^2$.

t	$x = 0.1$		$x = 0.3$		$x = 0.5$		$x = 0.7$		$x = 0.9$	
	CN.M	C.M	CN.M	C.M	CN.M	C.M	CN.M	C.M	CN.M	C.M
0.2	9.77×10^{-6}	1.55×10^{-9}	2.67×10^{-5}	6.24×10^{-9}	3.46×10^{-5}	1.66×10^{-8}	2.92×10^{-5}	3.94×10^{-8}	1.16×10^{-5}	8.45×10^{-8}
0.4	7.25×10^{-6}	6.33×10^{-9}	1.98×10^{-5}	2.19×10^{-8}	2.56×10^{-5}	4.49×10^{-8}	2.17×10^{-5}	8.00×10^{-8}	8.64×10^{-6}	1.31×10^{-7}
0.6	4.03×10^{-6}	1.05×10^{-8}	1.10×10^{-5}	3.43×10^{-8}	1.43×10^{-5}	6.42×10^{-8}	1.21×10^{-5}	1.03×10^{-7}	4.81×10^{-6}	1.51×10^{-7}
0.8	2.00×10^{-6}	1.30×10^{-8}	5.46×10^{-6}	4.15×10^{-8}	7.05×10^{-6}	7.46×10^{-8}	5.96×10^{-6}	1.14×10^{-7}	2.38×10^{-6}	1.59×10^{-7}
1	9.25×10^{-7}	1.43×10^{-8}	2.53×10^{-6}	4.50×10^{-8}	3.27×10^{-6}	7.97×10^{-8}	2.77×10^{-6}	1.18×10^{-7}	1.10×10^{-6}	1.63×10^{-7}

Table 3. The absolute error for various values of t, in which h is 0.01 and Δt is h^2.

t	$x = 0.1$		$x = 0.3$		$x = 0.5$		$x = 0.7$		$x = 0.9$	
	CN.M	C.M	CN.M	C.M	CN.M	C.M	CN.M	C.M	CN.M	C.M
0.2	7.14×10^{-6}	0.37×10^{-9}	1.97×10^{-5}	1.14×10^{-9}	2.57×10^{-5}	2.69×10^{-9}	2.18×10^{-5}	9.50×10^{-9}	8.70×10^{-6}	3.56×10^{-8}
0.4	9.62×10^{-6}	0.95×10^{-9}	2.65×10^{-5}	3.90×10^{-9}	3.45×10^{-5}	1.12×10^{-8}	2.93×10^{-5}	2.99×10^{-8}	1.17×10^{-5}	7.21×10^{-8}
0.6	9.70×10^{-6}	2.36×10^{-9}	2.67×10^{-5}	9.20×10^{-9}	3.48×10^{-5}	2.29×10^{-8}	2.96×10^{-5}	5.02×10^{-8}	1.18×10^{-5}	9.96×10^{-8}
0.8	8.70×10^{-6}	4.31×10^{-9}	2.40×10^{-5}	1.57×10^{-8}	3.11×10^{-5}	3.48×10^{-8}	2.65×10^{-5}	6.76×10^{-8}	1.06×10^{-5}	1.20×10^{-7}
1	7.31×10^{-6}	6.35×10^{-9}	2.01×10^{-5}	2.21×10^{-8}	2.62×10^{-5}	4.56×10^{-8}	2.23×10^{-5}	8.17×10^{-8}	8.93×10^{-6}	1.34×10^{-7}

In contrast, for diffusion equations and many other equations, the Crank-Nicolson method is unconditionally stable.[19] However, the price one pays for the unconditional stability of the Crank-Nicholson method is having to invert a tridiagonal matrix equation at each time-step.[20] Furthermore, the Crank-Nicholson method has second order accurate in time, and therefore the overall accuracy depends also upon the spatial differencing practice.

6. CONCLUSIONS

The objective is to develop an effective method to solve the one-dimensional unsteady convection-diffusion equation by combing a high-order compact difference scheme with the Runge-Kutta method. The Runge-Kutta method is used to approximate the time derivative, and the compact difference scheme is used to approximate the spatial derivatives. This combined method has fourth-order accuracy in space and time. The predictions are in good agreement with the exact solutions. In addition, the combined method has higher accuracy than the Crank-Nicolson method. The combined method is highly efficient and has superiority over most of the other high-order compact difference schemes in terms of computational cost.

7. RECOMMENDATIONS FOR FUTURE RESEARCH

In many diffusion processes arising in physical problems, convection essentially dominates diffusion, and it is natural to seek numerical methods for such problems that reflect their almost hyperbolic nature.[21] Two types of high order compact schemes have been developed, including high order compact polynomial and exponential finite difference schemes. However, the existing high order compact polynomial finite difference schemes are not suitable for particular physical problems, for example, abrupt boundary layer in convection-dominated problems, unless a very fine mesh is used. This dilemma can be resolved by utilising local mesh refinement strategies or a non-uniform mesh.[22] However, in case of using a non-uniform mesh, the boundary layer location or the singularity region must be known before the construction of the non-uniform mesh.

In contrast, the high order compact exponential finite difference scheme has the noteworthy feature that it provides very accurate solution for singular perturbation problems characterised by boundary or transition layers where the gradients of the solution are large.[23–26] Tian and Dai have developed a fourth order compact exponential finite difference scheme for solving one-dimensional

and two-dimensional steady-state convection-diffusion equations with constant and variable convection coefficients on compact stencil.[27] Mishra and Yedida have developed a sixth order compact exponential finite difference scheme for solving one-dimensional convection-diffusion equations with constant convection coefficients and a fourth order compact exponential finite difference scheme for two-dimensional convection-diffusion equations.[28] In particular, Tian and Yu have developed a fourth order compact exponential finite difference scheme for solving one-dimensional unsteady convection-diffusion equations.[26] The fourth order compact exponential finite difference scheme is unconditionally stable with fourth-order accuracy in space and time, thereby providing an excellent solution to convection dominated problems.

Recommendations are made here for future research regarding convection dominated problems. Further study is needed to extend the present numerical methods to multi-dimensional cases by reference to the existing schemes with higher accuracy and stability.

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