Contemporary Mathematics
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Research Article

Numerical Solution to Unsteady One-Dimensional Convection-Diffusion Problems Using Compact Difference Schemes Combined with Runge-Kutta Methods

Zhenwei Zhu, **Junjie Chen***

Department of Energy and Power Engineering, School of Mechanical and Power Engineering, Henan Polytechnic University, Jiaozuo, Henan, China
E-mail: cjjtpj@163.com

Received: 22 September 2021; **Revised:** 9 November 2021; **Accepted:** 12 November 2021

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 both time and space variables. A procedure was given in detail to solve the unsteady one-dimensional convection-diffusion equation through a combination of Runge-Kutta methods and compact difference schemes. The combination method has fourth-order accuracy in both time and space variables. Numerical experiments were conducted and the results were compared with those obtained by the Crank-Nicolson method in order to check the accuracy of the combination method. The analysis results indicated that the combination method is numerically stable at low wave numbers and small CFL numbers. The combination method has higher accuracy than the Crank-Nicolson method.

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

MSC: 60J60, 65L06, 76E06, 76R50

1. Introduction

The convection-diffusion equation is a combination of the convection and diffusion 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 arises in numerous models of flows and other physical phenomena. This equation is of primary importance in understanding transport phenomena within a physical system [3, 4]. This equation is also a fundamental sub-problem for models of incompressible flow. Depending on the context, the same equation can be called the advection-diffusion equation, drift-diffusion equation, or scalar transport equation. Computers are often used to numerically approximate the solution to the convection-diffusion equation, typically using the finite element method. In this study, the convection-diffusion equation is solved by a combination of Runge-Kutta methods and high-order compact finite difference discretization schemes.

DOI: https://doi.org/10.37256/cm.2420211167

For a transport variable u, the unsteady one-dimensional advection-diffusion equation is usually written as

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

with the initial condition

$$u(x,0)=\phi(x), \tag{2}$$

and the boundary conditions

$$u(0,t)=g_0(t), u(L,t)=g_1(t), t\in(0,\ T), \tag{3}$$

in which c is an arbitrary constant indicating the intensity of the convection, the diffusion coefficient α is positive constant, and g_0 and g_1 are assumed in this study to be smooth functions.

A variety of finite difference schemes have been presented to solve unsteady convection-diffusion problems approximately [5]. These schemes usually have first-order or second-order accuracy in space variables but have fallen short of expectations for convection-dominated flows if the mesh is not sufficiently refined [5]. Discretization with a higher order in space variables is usually associated with large stencils, thereby increasing the bandwidth of the resulting matrix [5, 6]. A class of compact finite difference approximations has been recently developed to solve convection-diffusion problems [7-9]. These compact finite difference schemes have fourth-order accuracy in space variables, but fail when accuracy in time variables 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 variables and reasonable computational cost.

The primary focus of this study is on developing an effective method to achieve higher accuracy in time variables by a combination of Runge-Kutta methods and high-order compact finite difference discretization schemes. This combination method is then used to solve the unsteady one-dimensional convection-diffusion equation and has fourth-order accuracy in both time and space variables. The Runge-Kutta methods are introduced briefly in Section 2. A fourth-order compact finite difference approximation scheme is presented in Section 3 for the unsteady convection-diffusion equation. A stability analysis is performed on the fully discretized equation in Section 4 to check the stability of the combination method. Some numerical examples are presented in Section 5 and concluding remarks are finally given in Section 6.

2. Runge-Kutta methods

In numerical analysis, Runge-Kutta methods are a family of implicit and explicit iterative methods [12]. When Runge-Kutta methods are used to solve the convection-diffusion equation, time is treated as an independent variable in an ordinary differential equation, for example,

$$\frac{dQ}{dt}=R(t,Q), \tag{4}$$

in which Q is an unknown function of time, and R denotes the numerical approximation to the spatial derivatives. The Runge-Kutta method used in this study is given in the following form

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

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

$t \le t^{n+1}$

$$Q^1 = Q^n + \Delta t(\alpha_{11} R^n), \tag{6}$$

$$Q^2 = Q^n + \Delta t(\alpha_{21} R^n + \alpha_{22} R^1), \tag{7}$$

$$Q^3 = Q^n + \Delta t(\alpha_{31} R^n + \alpha_{32} R^1 + \alpha_{33} R^2), \tag{8}$$

$$Q^{n+1} = Q^n + \Delta t(\alpha_{N1} R^n + \alpha_{N2} R^1 + \cdots + \alpha_{NN} R^{N\text{-}1}), \tag{9}$$

in which the superscript n, 1, 2, ..., and $n + 1$ denote the time steps on the time interval $t^n \le t_1 \le t_2 \le \cdots \le t_N \le t^{n+1}$, and α_{ij} is the weighting factor for the step i and term j.

A four-step algorithm is given by

$$Q^1 = Q^n + \frac{\Delta t}{4} R^n, \tag{10}$$

$$Q^2 = Q^n + \frac{\Delta t}{3} R^1 \tag{11}$$

$$Q^3 = Q^n + \frac{\Delta t}{2} R^2, \tag{12}$$

$$Q^{n+1} = Q^n + \Delta t R^3. \tag{13}$$

For the four-step Runge-Kutta method, ten coefficients are constrained by seven equations, which are tabulated in the literature [13]. This algorithm is convenient to program and no intermediate solution needs to be stored [14].

3. A fourth-order compact finite difference scheme

The differential equation considered here takes the form

$$\alpha \frac{\partial^2 u(x)}{\partial x^2} - c\frac{\partial u(x)}{\partial x} = f(x), x \in (0, L), \tag{14}$$

with the boundary conditions

$$u(0) = g_0, u(L) = g_1. \tag{15}$$

A compact difference scheme with fourth-order accuracy can be obtained for Equation (14) as follows [15]: the interval $0 \le x \le 1$ is subdivided into n equal subintervals by the grid points $x_i = ih$, in which $h = \frac{1}{n}$. 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 for Equation (14) at point x_i:

$$\alpha\delta_x^2 u_i - c\delta_x u_i - \tau_i = f_i, \tag{16}$$

in which

$$\tau_i = \frac{h^2}{12}\left(\alpha\frac{d^4u}{dx^4} - 2c\frac{d^3u}{dx^3}\right) + O(h^4). \tag{17}$$

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 (14) gives:

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

From Equation (14) and Equation (18), it follows that

$$\frac{d^4u}{dx^4}\Big|_i = \frac{1}{\alpha}\left(\frac{d^2f}{dx^2} + c\frac{d^3u}{dx^3}\right)\Big|_i = \frac{1}{\alpha}\left(\delta_x^2 f_i + \frac{c}{\alpha^2}\delta_x f_i + \frac{c^2}{\alpha^2}\delta_x^2 u_i\right) + O(h^2). \tag{19}$$

By substituting Equations (18) and (19) for the corresponding terms used in Equation (17), the solution is given by

$$\tau_i = \frac{1}{12}\left(\delta_x^2 f_i - \frac{c}{\alpha}\delta_x f_i - \frac{c^2}{\alpha}\delta_x^2 u_i\right) + O(h^4). \tag{20}$$

A fourth-order compact finite difference scheme for Equation (14) can be obtained by substituting Equation (20) in Equation (16). This gives

$$\left(\alpha + \frac{c^2h^2}{12\alpha}\right)\delta_x^2 u_i - c\delta_x u_i = f_i + \frac{h^2}{12}\left(\delta_x^2 f_i - \frac{c}{\alpha}\delta_x f_i\right) + O(h^4). \tag{21}$$

Here, two difference operators are defined as follows:

$$L_x = 1 + \frac{h^2}{12}\left(\delta_x^2 - \frac{c}{\alpha}\delta_x\right),\ A_x = -\left(\alpha + \frac{c^2h^2}{12\alpha}\right)\delta_x^2 + c\delta_x. \tag{22}$$

Equation (21) can be formulated symbolically as

$$L_x^{-1} A_x u_i = f_i + O(h^4). \tag{23}$$

The above compact finite difference scheme is combined with the Runge-Kutta method described earlier to solve the one-dimensional advection-diffusion equation.

4. Stability analysis

A von Neumann linear stability analysis is performed to check the stability of the combination method. Let $u_i^n =$

$b^n e^{Ikhi}$ to be the value of u_i^n at x_i, in which $I = \sqrt{-1}$, b^n is the amplitude at time level n, and k is the wave number. The amplification factor is defined as

$$g = \frac{b^{n+1}}{b^n}. \tag{24}$$

The amplification factor of Equation (13) discretized by the Runge-Kutta method can be obtained as follows [14]:

$$g = 1 + Z + \frac{1}{2}Z^2 + \frac{1}{6}Z^3 + \frac{1}{24}Z^4. \tag{25}$$

The variable Z represents the spatial discretization applied to the convection-diffusion terms. The explicit, discretized form is given by

$$Z = \left[\left(24\frac{F}{Pe} + 2F \cdot Pe\right)(1 - \cos k) - 12IF\sin k\right] / (10 + 2\cos k - IPe\sin k). \tag{26}$$

in which F is the CFL number and is defined as

$$F = \frac{c\Delta t}{h}, \tag{27}$$

In Equation (26), Pe is the Péclet number and is defined as

$$Pe = \frac{ch}{\alpha}. \tag{28}$$

When the Péclet number is high, the convection term dominates [16, 17]. When the Péclet number is low the diffusion term dominates [16, 17].

The amplification factor, as defined above, is rather complex. For stability, the amplification factor has to satisfy the relation $|g| \leq 1$. When $|g| > 1$, the combination method for solving the advection-diffusion equation is numerically unstable. Contours of the absolute value of the amplification factor are plotted in the k-F plane in Figures 1-4, respectively, with various Péclet numbers such as 1, 10, 100, and 1000. The results indicate that the combination method for solving the advection-diffusion equation is numerically stable at low wave numbers and small CFL numbers.

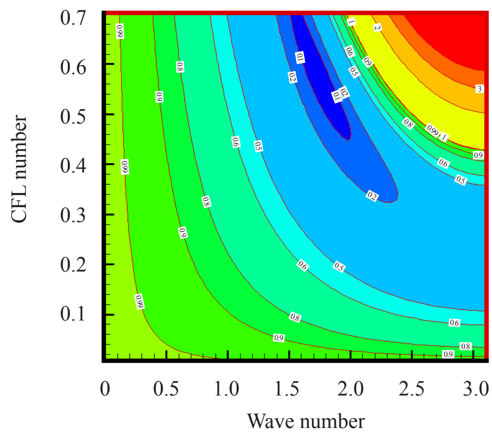

Figure 1. Contours of the absolute value of the amplification factor in the k-F plane with a Péclet number of 1

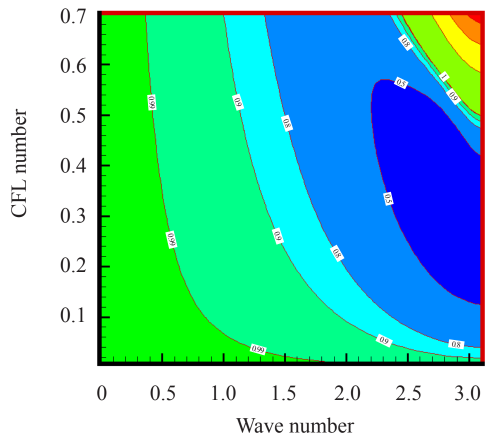

Figure 2. Contours of the absolute value of the amplification factor in the *k*-*F* plane with a Péclet number of 10

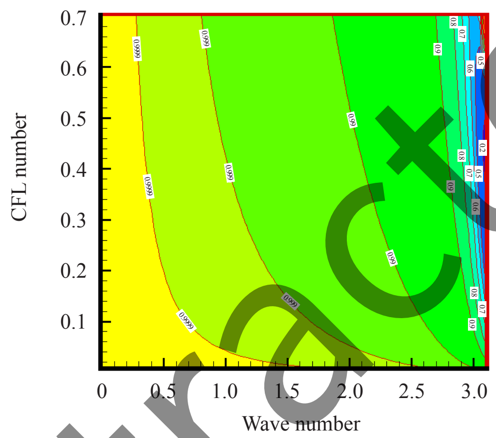

Figure 3. Contours of the absolute value of the amplification factor in the *k*-*F* plane with a Péclet number of 100

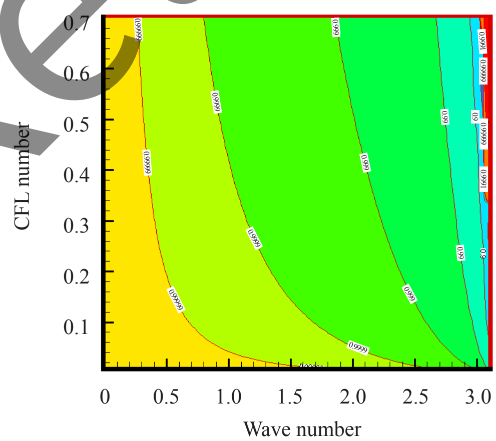

Figure 4. Contours of the absolute value of the amplification factor in the *k*-*F* plane with a Péclet number of 1000

Despite the apparent simplicity of the problem, its numerical solution is still a challenge when convection is strongly dominant. The basic difficulty is that, in this case, the solution of the problem typically possesses interior and boundary layers, which are small subregions where the derivatives of the solution are very large [18]. The widths of these layers are usually significantly smaller than the mesh size and hence the layers cannot be resolved properly. This leads to unwanted spurious oscillations in the numerical solution, the attenuation of which has been the subject of extensive research for more than three decades [19, 20]. The issue of spurious oscillations is not addressed in this study.

5. Numerical experiments

In numerical analysis, the Crank-Nicolson method is a finite difference method used for numerically solving the heat equation and similar partial differential equations [21, 22]. It is a second-order method in time. It is implicit in time, can be written as an implicit Runge-Kutta method, and it is numerically stable. The Crank-Nicolson method is based on the trapezoidal rule. This method is often applied to diffusion problems. Some numerical results are presented in Examples 5.1-5.3 to compare the present method, denoted by P.M, with the Crank-Nicolson method, denoted by C-N. M. It is assumed that all exact solutions of the convection-diffusion equations given below are known.

Example 5.1 The following convection-diffusion equation is considered here

$$\frac{\partial u}{\partial t}+0.1\frac{\partial u}{\partial x}=0.01\frac{\partial^2 u}{\partial x^2},(x,t)\in(0,1)\times(0,T), \tag{29}$$

the exact solution of the above equation is given by

$$u(x,t)=e^{5x-(0.25+0.01\pi^2)t}\sin\pi x. \tag{30}$$

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

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

t	$x = 0.1$		$x = 0.3$		$x = 0.5$		$x = 0.7$		$x = 0.9$	
	P.M	CN.M	P.M	CN.M	P.M	CN.M	P.M	CN.M	P.M	CN.M
0.2	6.579E-010	1.897E-005	1.623E-009	3.636E-005	2.108E-009	1.409E-005	2.725E-009	2.066E-004	5.991E-008	1.645E-003
0.4	1.134E-009	3.239E-005	3.028E-009	6.781E-005	3.932E-009	2.630E-005	5.146E-009	3.854E-004	2.455E-007	1.645E-003
0.6	1.474E-009	4.170E-005	4.232E-009	9.472E-005	5.501E-009	3.679E-005	8.038E-009	5.380E-004	5.145E-007	2.105E-003
0.8	1.720E-009	4.820E-005	5.248E-009	1.173E-004	6.838E-009	4.576E-005	1.294E-008	6.654E-004	8.263E-007	2.418E-003
1	1.896E-009	5.268E-005	6.088E-009	1.357E-004	7.951E-009	5.335E-005	2.11E-008	7.685E-004	1.158E-006	2.628E-003

Example 5.2 Given a convection-diffusion equation

$$\frac{\partial u}{\partial t}+0.22\frac{\partial u}{\partial x}=0.5\frac{\partial^2 u}{\partial x^2},(x,t)\in(0,1)\times(0,T), \tag{31}$$

the exact solution is given by

$$u(x,t) = e^{0.22x-(0.0242+0.5\pi^2)t} \sin \pi x. \tag{32}$$

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

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

t	$x = 0.1$		$x = 0.3$		$x = 0.5$		$x = 0.7$		$x = 0.9$	
	P.M	CN.M	P.M	CN.M	P.M	CN.M	P.M	CN.M	P.M	CN.M
0.2	1.551E-009	9.770E-006	6.236E-009	2.674E-005	1.655E-008	3.456E-005	3.943E-008	2.921E-005	8.450E-008	1.162E-005
0.4	6.331E-009	7.250E-006	2.185E-008	1.984E-005	4.491E-008	2.563E-005	7.997E-008	2.167E-005	1.306E-007	8.636E-006
0.6	1.052E-008	4.034E-006	3.432E-008	1.104E-005	6.418E-008	1.426E-005	1.025E-007	1.205E-005	1.507E-007	4.807E-006
0.8	1.299E-008	1.995E-006	4.146E-008	5.460E-006	7.459E-008	7.054E-006	1.136E-007	5.963E-006	1.593E-007	2.378E-006
1	1.425E-008	9.253E-007	4.504E-008	2.531E-006	7.965E-008	3.270E-006	1.18E-007	2.765E-006	1.629E-007	1.102E-006

Example 5.3 Given a convection-diffusion equation

$$\frac{\partial u}{\partial t} + 0.1\frac{\partial u}{\partial x} = 0.2\frac{\partial^2 u}{\partial x^2}, (x,t) \in (0,1)\times(0,T), \tag{33}$$

the exact solution is given by

$$u(x,t) = e^{0.25x-(0.0125+0.02\pi^2)t} \sin \pi x. \tag{34}$$

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

t	$x = 0.1$		$x = 0.3$		$x = 0.5$		$x = 0.7$		$x = 0.9$	
	P.M	CN.M	P.M	CN.M	P.M	CN.M	P.M	CN.M	P.M	CN.M
0.2	3.677E-010	7.143E-006	1.143E-009	1.970E-005	2.687E-009	2.565E-005	9.496E-009	2.183E-005	3.559E-008	8.703E-006
0.4	9.510E-010	9.617E-006	3.896E-009	2.650E-005	1.115E-008	3.447E-005	2.988E-008	2.933E-005	7.205E-008	1.173E-005
0.6	2.363E-009	9.702E-006	9.198E-009	2.672E-005	2.285E-008	3.475E-005	5.017E-008	2.956E-005	9.962E-008	1.184E-005
0.8	4.306E-009	8.698E-006	1.565E-008	2.395E-005	3.480E-008	3.114E-005	6.758E-008	2.649E-005	1.197E-007	1.062E-005
1	6.350E-009	7.309E-006	2.205E-008	2.012E-005	4.558E-008	2.616E-005	8.167E-008	2.225E-005	1.342E-007	8.925E-006

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

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

6. Conclusions

The primary focus of this study is on developing an effective method to solve the unsteady one-dimensional convection-diffusion equation by a combination of Runge-Kutta methods and high-order compact finite difference discretization schemes. A high-order compact finite difference scheme is used to approximate the spatial derivatives, and Runge-Kutta methods are used to approximate the time derivative. This combination method has fourth-order accuracy in both time and space variables. The numerical results obtained by the combination method have been found to be in good agreement with the exact solutions. Additionally, the combination method has higher accuracy than the Crank-Nicolson method. The combination method has superiority over most of the other high-order compact finite difference schemes in terms of computational cost, and is highly efficient as there is no need to compute the inverse of the block matrix.

Acknowledgement

This work was supported by the National Natural Science Foundation of China (No. 51506048).

Conflict of interest statement

The authors declare no conflict of interest.

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