Karadeniz Fen Bilimleri Dergisi, 12(2), 1069-1080, 2022. DOI: 10.31466/kfbd.1165640

KFBD

Karadeniz Fen Bilimleri Dergisi
The Black Sea Journal of Sciences
ISSN (Online): 2564-7377

Araştırma Makalesi / Research Article

An Innovative Approach for Numerical Solution of the Unsteady Convection-Dominated Flow Problems

Osman UNAL[1*], Nuri AKKAS[2]

Abstract

In this study, convection-diffusion equation is solved numerically using four different space discretization methods namely first-order upwinding, second-order central difference, cubic (partially upwinded) and cubic-TVD (Total Variation Diminishing) techniques. All methods are compared with the analytical solution. The first-order method is not close to the analytical solution due to the numerical dispersion. The higher-order techniques reduce numerical dispersion. However, they cause another numerical error, unphysical oscillation. This study proposes an innovative approach on cubic-TVD method to eliminate undesired oscillations. Proposed model decreases numerical errors significantly compared to previously developed techniques. Moreover, numerical results of presented model quite close to the analytical solution. Finally, all Matlab codes of numerical and analytical solutions for convection-diffusion equation are added to Appendix in order to facilitate other researchers' work.

Keywords: Convection-dominated flow, Numerical dispersion, Unphysical oscillation.

Kararsız Konveksiyon Ağırlıklı Akış Problemlerinin Sayısal Çözümü için Yenilikçi bir Yaklaşım

Öz

Bu çalışmada, konveksiyon-difüzyon denklemi; birinci dereceden yukarı yelpaze, ikinci dereceden merkezi fark alma, kübik (kısmen yukarı yelpaze uygulanmış) ve kübik-TVD (Toplam Varyasyon Azaltma) teknikleri olmak üzere dört farklı uzay ayrıklaştırma yöntemi kullanılarak sayısal olarak çözülmüştür. Tüm yöntemler analitik çözümle karşılaştırılmıştır. Birinci dereceden yöntem, sayısal dağılım nedeniyle analitik çözüme yakın değildir. Daha yüksek mertebeden teknikler sayısal dağılımı azaltmaktadır, ancak bir diğer sayısal hataya, fiziksel olmayan salınımlara sebep olmaktadırlar. Bu çalışma, istenmeyen salınımları ortadan kaldırmak için kübik-TVD yöntemine yenilikçi bir yaklaşım önermektedir. Önerilen model, daha önce geliştirilen tekniklere kıyasla sayısal hataları önemli ölçüde azaltır. Ayrıca sunulan modelin sayısal sonuçları analitik çözüme oldukça yakındır. Son olarak, diğer araştırmacıların işini kolaylaştırmak için konveksiyon-difüzyon denklemi için sayısal ve analitik çözümlerin tüm Matlab kodları Ek'e dahil edilmiştir.

Anahtar Kelimeler: Konveksiyon ağırlıklı akış, Sayısal dağılım, Fiziksel olmayan salınım.

[1]Sakarya University of Applied Sciences, Department of Mechanical Engineering , Sakarya, Turkey, osman92unal@gmail.com
[2]Sakarya University of Applied Sciences, Department of Mechanical Engineering , Sakarya, Turkey, nuriakkas@subu.edu.tr

[1]https://orcid.org/0000-0003-1101-6561 [2]https://orcid.org/0000-0001-7477-7777

[*]**Sorumlu Yazar/Corresponding Author** **Geliş/Received:** 23.08.2022 **Kabul/Accepted:** 06.12.2022

1. Introduction

Convection-dispersion equation has been broadly utilized in basic disciplines for instance mechanical engineering, environmental engineering, chemical engineering and civil engineering. The contaminant and sediment movement in the atmosphere, lakes, rivers, as well as groundwater aquifers are just a few examples of specific disciplines where the convection-diffusion equation is employed to explain the transport process (Peng et. al., 2013). In addition, convection–diffusion equations are critical for simulating flow and transport in oil and gas reservoirs, particularly in two-phase flow (Kurganov and Tadmor, 2000). Furthermore, the convection–diffusion equation is particularly useful in simulating miscible displacement, immiscible displacement, chemical displacement and non-isothermal injection techniques (Kamalyar et. al., 2014). In short, this equation has a substantial role in modeling many physical systems. The convection-diffusion problems are solved by commercial and non-commercial simulator for these different physical systems. These simulators use the numerical techniques to solve complex and multi-dimensional physical problems, because these sophisticated systems don't have any analytical solution yet. On the other hand, some one-dimensional and simple physical problems have analytical solution. The numerical simulator engineers validate their numerical methods with analytical solution for uncomplicated and one-dimensional physical problems. After that, they apply their numerical techniques to the multi-dimensional and advanced problems. In this study, four different numerical methods to solve following convection-diffusion equation have been compared with its analytical solution.

$$D\nabla^2 C - u.\nabla C = \frac{\partial C}{\partial t} \tag{1}$$

Equation 1 indicates multi multi-dimensional form of convection-diffusion equation. The first and second terms in equation 1 are diffusion and convection terms respectively. The last term is accumulation term. C, D and u are concentration, diffusivity coefficient and velocity respectively. Equation 2 shows one-dimensional form of general convection-diffusion equation.

$$D\frac{\partial^2 C}{\partial x^2} - u\frac{\partial C}{\partial x} = \frac{\partial C}{\partial t} \tag{2}$$

The analytical solution of one-dimensional convection-diffusion equation is indicated by following equation (Peaceman, 2000).

$$C = \frac{1}{2} erfc\left(\frac{x - u\,t}{2(D\,t)^{0.5}}\right) + \frac{1}{2}\exp(u\,x/D)\, erfc\left(\frac{x + u\,t}{2(D\,t)^{0.5}}\right) \tag{3}$$

If physical dispersion coefficient is zero, equation 3 is undefined. In that case, following equation is obtained.

$$-u\frac{\partial C}{\partial x}=\frac{\partial C}{\partial t} \tag{4}$$

Equation 4 is called as advection equation or transport equation. It can be solved analytically using method of characteristics. It is required to know initial condition of equation 4 to solve it. The initial condition can be defined by equation 5.

$$C(0)=F(x_0) \tag{5}$$

In equation 4, u is a constant. The constant u is referred to as the velocity of propagation. This is the rate at which the solution will propagate along the characteristics. All points on the solution will propagate at the same speed u because of constant velocity. The method of characteristics implies that solution of transport equation is a function of initial condition. The solution of advection equation is shown following equation 6 (Sarra, 2002).

$$C(x,t)=F(x_0)=F(x-u\,t) \tag{6}$$

2. Materials and Methods

The convection-diffusion equation and transport equation can be solved numerically using different space and time discretization techniques. In this study, explicit time discretization method is used to simplify calculations. The equations 7 and 8 show full discretization of convection-diffusion equation and advection equation respectively.

$$D\frac{C_{i+1}^{n}-2C_{i}^{n}+C_{i-1}^{n}}{\Delta x^{2}}-u\frac{C_{i+1/2}^{n}-C_{i-1/2}^{n}}{\Delta x}=\frac{C_{i}^{n+1}-C_{i}^{n}}{\Delta t} \tag{7}$$

$$-u\frac{C_{i+1/2}^{n}-C_{i-1/2}^{n}}{\Delta x}=\frac{C_{i}^{n+1}-C_{i}^{n}}{\Delta t} \tag{8}$$

In equation 7 and 8, the subscript i values refer to nodes or grid blocks. The superscript n means time steps. Ci and Ci+1/2 refer to grid block central values and grid block face values respectively. The central difference method is used for space discretization of the diffusion term which depends only on the central grid block values. The central grid block values are determined at each time steps. Thus, there is no problem to calculate numerical expression of diffusion term. On the other hand, the space discretization of convection term depends on grid block face values, and there is no any exact information about face values in numerical calculations. The faces values can be predicted by various space discretization techniques, for instance first-order upstream method, second-order central difference technique, cubic method and cubic-TVD (Total Variation Diminishing) method. However, these all techniques are not certain values. They are only assumption, and main numerical errors arise from these approximations. The first objective of this study is to minimize these numerical errors using small change on cubic-TVD method. Second aim of this study is to compare numerical results of space discretization methods. Finally, this study is to present all Matlab codes for numerical and exact solutions as a simulator. This simulator can be used for different time interval, desired total simulation time, different space interval, and several space discretization methods by other researchers.

In numerical calculation, the improper approximation of grid block face values leads to numerical errors: numerical dispersion and unphysical oscillation. If first-order method is used to predict face values, it causes numerical dispersion. This method is a non-oscillatory technique, but it is far from exact solution especially for large time steps and wide space intervals. Equation 9 shows the mathematical expression of first-order upstream space discretization method (Ertekin et. al., 2001).

$$C_{i+1/2} \approx C_i \tag{9}$$

Equation 9 implies right face value is equal to central value of previous grid block. Similarly, left face value is determined by decreasing the sub-index value by one. Figure 1 shows numerical result of first-order upwinding method and exact solution.

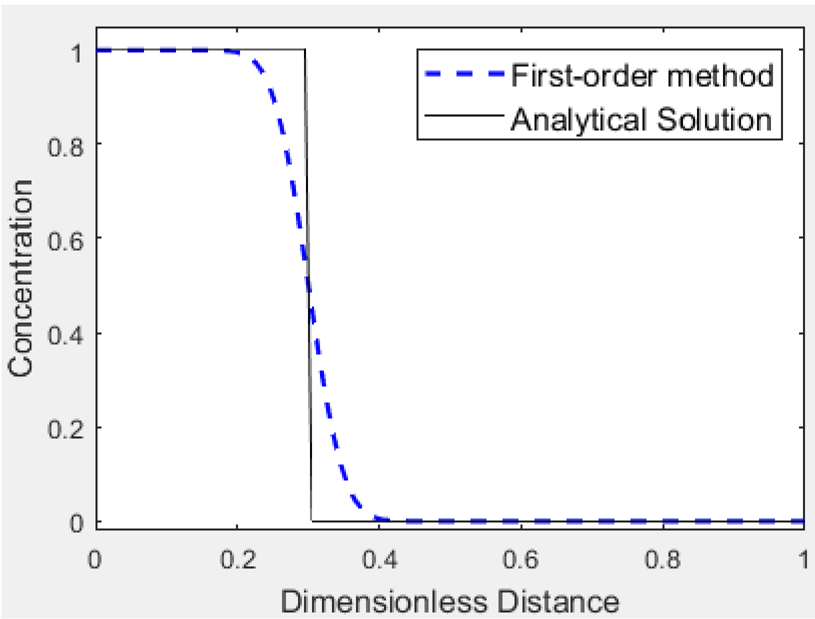

Figure 1. First-order method.

According to figure 1, the numerical result is not close to analytical solution. The advantage of first-order technique is that it hasn't any unphysical oscillation and it is the simplest method to predict face values. However, it has significant numerical dispersion. It is exactly known that grid block face values are greater than central values of previous grid block for upwinding or upstream flow or heat transfer. The assumption of single-point upstream technique means that flow or heat transfer propagates easily through the opposite direction of the upstream region without any obstacle on grid block face. There is no any excessive accumulation in interested grid block due to this assumption. That's why first-order technique doesn't have any unphysical oscillation, but this case leads to numerical dispersion which is main problem for numerical simulator engineers. The higher-order techniques should be used in order to decrease numerical dispersion (Wolcott et. al., 1996). The second-order central finite difference method is used to increase accuracy of the numerical calculation and it reduces numerical dispersion (Mazumder, 2015). The mathematical formula of central difference method can be expressed as following equation 10.

$$C_{i+1/2} \approx \frac{C_{i+1} + C_i}{2} \tag{10}$$

The central difference method means that face value is equal to half of summation of previous and next grid block central values. If this supposition is greater than real values for grid block face, it causes excessive accumulation in interested grid block and it leads to unphysical oscillation. Figure 2 shows numerical solution for second-order central difference method and analytical solution.

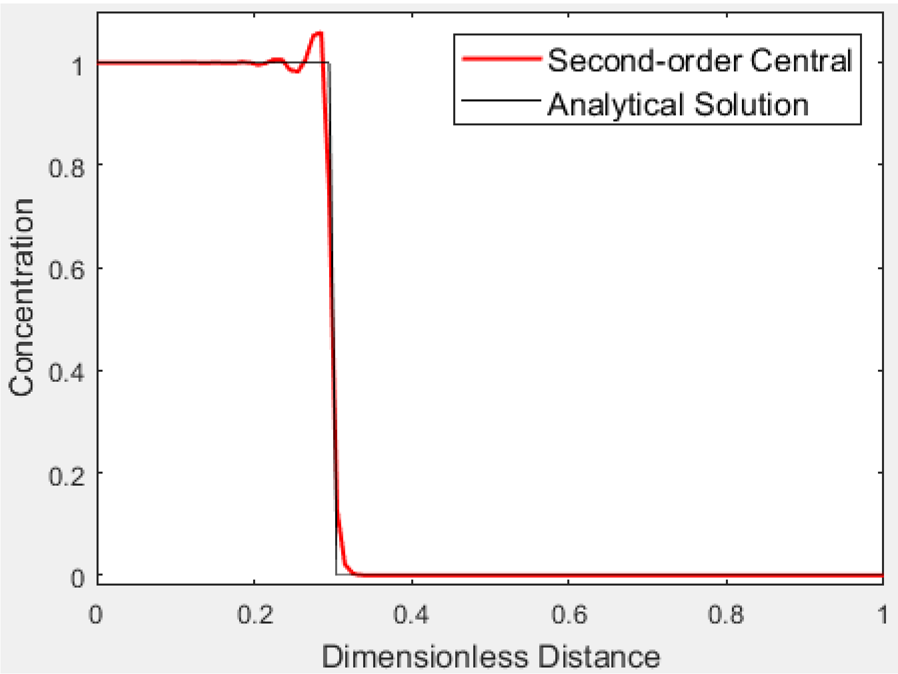

Figure 2. Second-order central difference technique.

The numerical dispersion decreases using second-order central difference method according to figure 2. Nevertheless, incorrect prediction of face values causes unphysical oscillation. This undesired oscillation can be vanished using other higher-order techniques. Equation 11 indicates cubic method proposed by Leonard many years ago (Leonard, 1979).

$$C_{i+1/2} \approx \frac{C_{i+1} + C_i}{2} - \frac{C_{i+1} - 2C_i + C_{i-1}}{6} \tag{11}$$

Equation 11 is a higher-order technique called as partially upwinding or upstream method. Although the main advantage of higher-order technique is to reduce numerical dispersion, some higher-order techniques give unreasonable oscillation due to high Courant number and low physical dispersion coefficient.

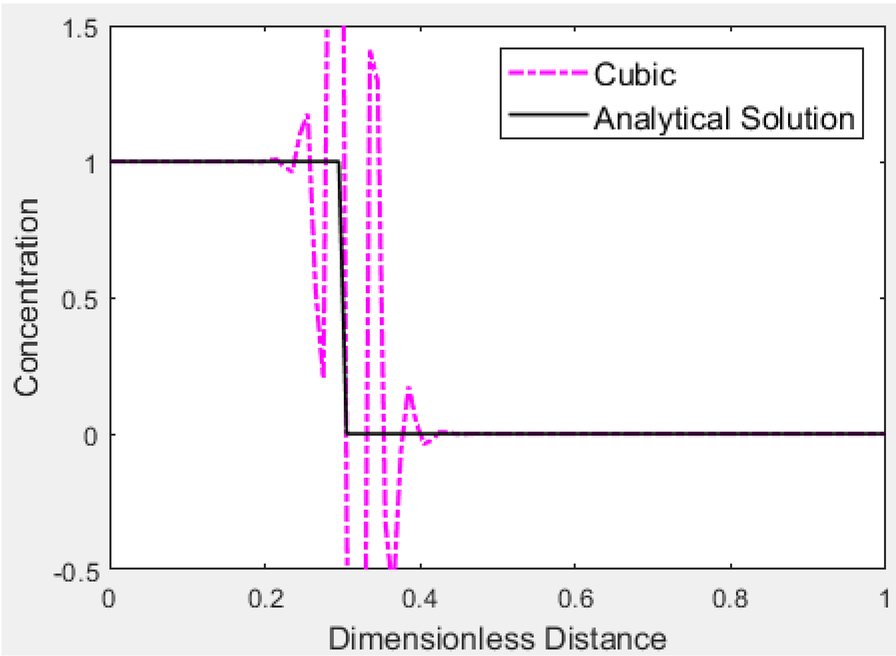

Figure 3. Partially upwinding cubic technique.

Figure 3 indicates that the partially upstream cubic method results in simulation with excessive unphysical oscillation. It arises from inaccurate prediction of the face values. The numerical estimation of face values should be optimized using TVD technique (Harten, 1984) to obtain meaningful numerical results from partially upwinding cubic method. TVD method can be defined as following equation.

$$C_{i+1/2} \approx C_i + \frac{1}{2}\varphi(r)[C_i - C_{i-1}] \tag{12}$$

Equation 12 consists of upwinding term (first term at right-hand side) and anti-diffusive term (second term at right-hand side). Anti-diffusive term is used to decrease numerical dispersion. If it is greater than actual value, it causes unphysical oscillation. If it is lesser than real face value, it leads to numerical dispersion. The main objective of TVD technique is to optimize anti-diffusive term according to different conditions. Anti-diffusive term depends on flux limiter that is a function of following gradient ratio (Sweby, 1984).

$$r = \frac{C_{i+1} - C_i}{C_i - C_{i-1}} \tag{13}$$

The definition of pure-cubic method and cubic-TVD technique using flux limiter functions can be expressed by equations 14 and 15 respectively (Wolcott et. al., 1996).

$$\varphi(r) = \frac{2r+1}{3} \tag{14}$$

$$\varphi(r) = \min\left(2, 2r, \frac{2r+1}{3}\right) \tag{15}$$

The relationship between flux limiter function and gradient ratio for pure-cubic and cubic-TVD methods is shown in Figure 4.

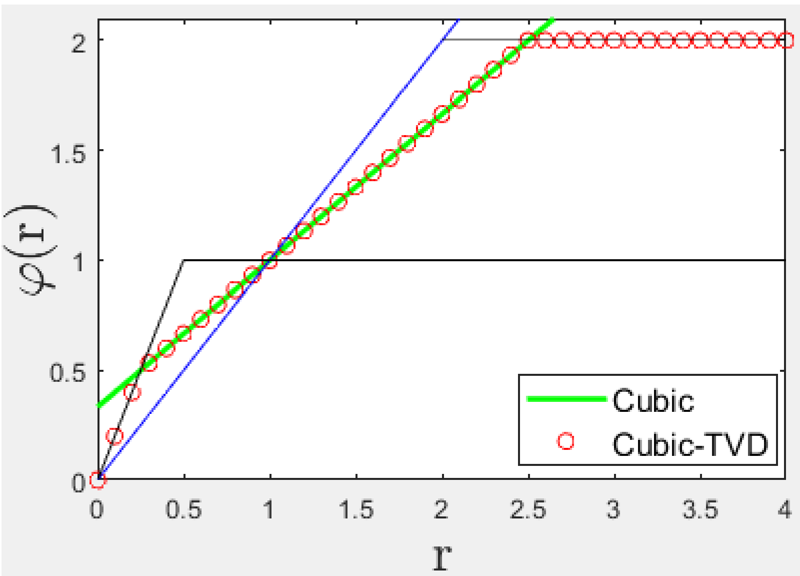

Figure 4. Cubic and cubic-TVD methods at TVD region.

The pure-cubic method (green line) isn't restricted by any upper limit. Hence, it may lead unphysical oscillation when gradient ratio of interested variable is greater than 2.5. In addition, the pure-cubic method may cause undesired oscillation at the flood front due to its high values for small gradient ratios compared to cubic-TVD technique.

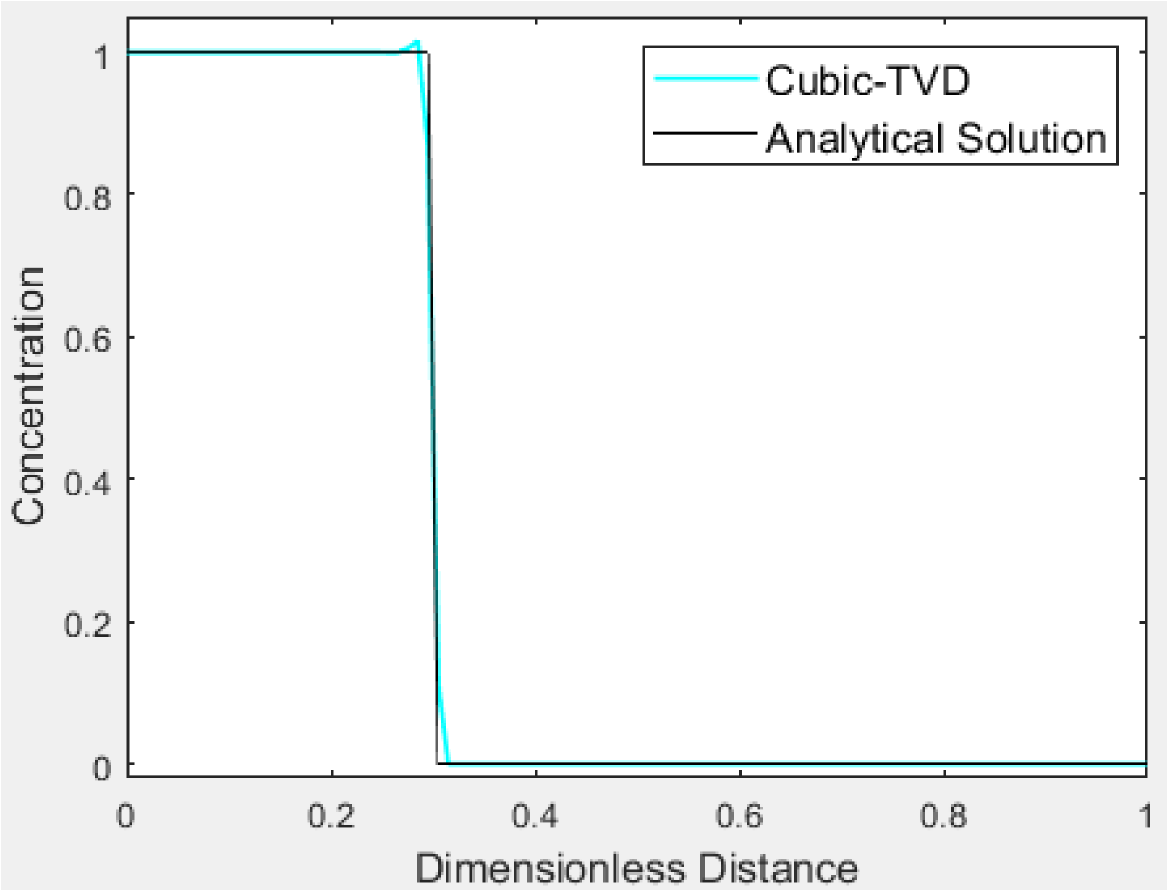

Figure 5. Cubic TVD method.

Figure 5 demonstrates numerical results for cubic-TVD method. Even though, cubic-TVD method reduces both numerical dispersion and unphysical oscillation, still it has small unphysical oscillation at flood front. This undesired oscillation may be eliminated by small adjustment on cubic-TVD technique.

3. Findings and Discussion

In this study, it's observed that the small unphysical oscillation in figure 5 results from upper limit of cubic-TVD method and decreasing upper limit leads suppressing of unphysical oscillations. The upper limit of cubic-TVD method may be changed by 1.7 instead of 2 in order to remove all unphysical oscillation for this study. The value of 1.7 is obtained by trial and error method. This upper limit is not deterministic and it may change for different cases. However, it's well known that reducing upper limit suppresses unphysical oscillations. The highest value that does not cause unphysical oscillations must be selected in order not to diminish order of convergence.

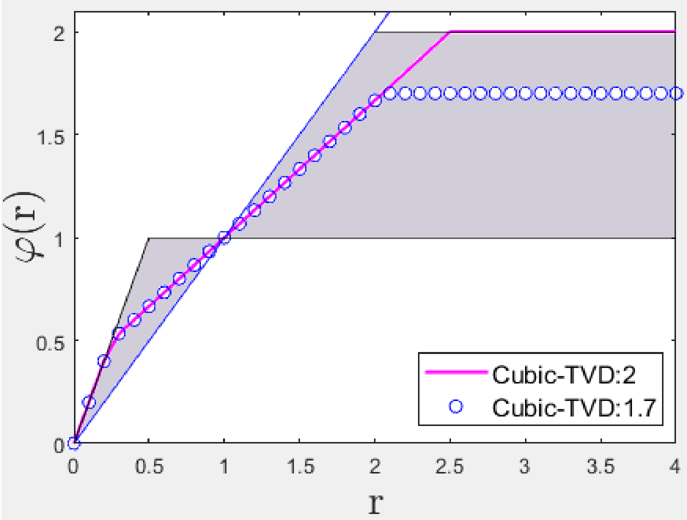

Figure 6. Cubic-TVD method for 1.7 upper limit.

The limiter function must be in grayscale region (in figure 6) to achieve minimum second-order numerical schemes (Sweby, 1984). The proposed limiter function is in the grayscale area. Thus, it is minimum second-order accurate space discretization technique. Figure 7 shows numerical result of proposed model. The cubic-TVD method for 1.7 upper limit suppresses oscillations and it reduces numerical dispersion significantly. It has only 1.6% deviation from the analytical solution, which means it is almost the same as the exact solution. Consequently, the numerical result of the proposed model in figure 7 is the most suitable method and it is nearest to analytical solution compared to others.

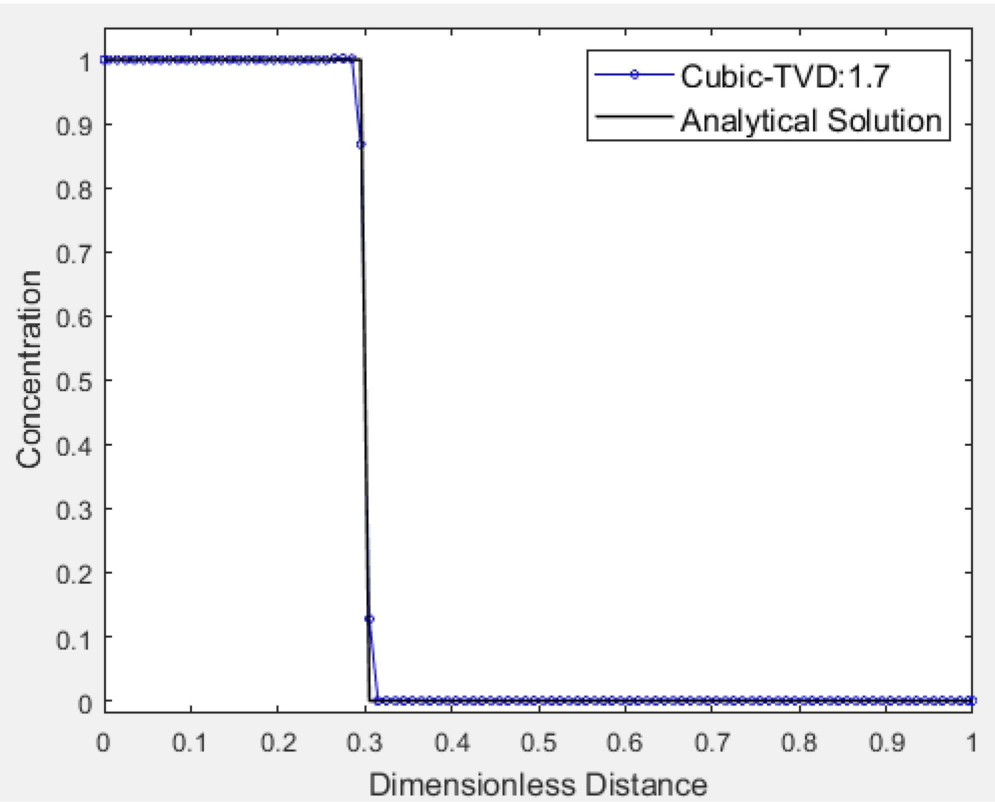

Figure 7. Cubic-TVD method for 1.7 upper limit.

4. Conclusion

This study deals with numerical solution of convection-diffusion equation using different space discretization techniques. Previously developed methods lead numerical errors especially for convection-dominated flow. It is observed that decreasing of upper limit of cubic-TVD method eliminates unphysical oscillation at flood front. This innovative approach reduces numerical errors substantially. Furthermore, proposed model is the nearest numerical solution to analytical solution compared to other numerical space discretization methods. Secondly, this study is to present a numerical simulator to solve transport equation and convection-diffusion equation. The Matlab codes and a Google drive link of this numerical simulator have been attached to Appendices. The developed numerical simulator is suitable for any grid dimension, several space discretization techniques, any space interval and time interval.

Statement of Research and Publication Ethics

The author declares that this study complies with Research and Publication Ethics.

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Symbols

C = *concentration*
D = *physical dispersion*
Nc = *courant number*
Δt = *timestep*
Δx = *space interval*
u = *velocity*

Subscripts

i = *index for blocks in the x direction*

$i-\frac{1}{2}$ = *index for left face values*

$i+\frac{1}{2}$ = *index for right face values*

Superscripts

n = *old timestep*
$n+1$ = *current timestep*

Appendices

Appendix A. Sub-function to run the numerical simulator.

```
function y=TVD(x)
% Select Space Discretization Method(SDM)
% For First Order Upstream Method -> SDO=1
% For Second Order Central Method -> SDO=2
% For Third Order Upwinding (Leonard-Cubic) Method -> SDO=30
% For Third Order Upwinding (TVD with Leonard-Cubic) -> SDO=31
SDO=31;
if SDO==1; y=0; %First Order Upstream
elseif SDO==2; y=x; %Second Order Central
elseif SDO==30; y=(2*x+1)/3; %Third Order Upwinding (Leonard-Cubic)
elseif SDO==31; y=max(0,min([1.7,2*x,(2*x+1)/3])); (TVD with Leonard-Cubic)
end
end
```

Appendix B. The numerical simulator.
Note: In order to run Matlab codes in APPENDIX B, it's required to get ''TVD.m'' Matlab file. It can be obtained using APPENDIX A. The name of the Matlab file must be ''TVD'' without quotes. Secondly, designed TVD.m Matlab file and the numerical simulator mfile (in Appendix B) must be at the same path. Thirdly, if you don't want to use Appendix A and B in order to run Matlab file, you can use Appendix C.

```
tic; clc; clearvars;
I=100;%Number of nodes at i-direction
dx=0.1;%Space interval
X=[0 dx/2:dx:I*dx-dx/2 I*dx];%Distance
t=3;%Total simulation time
dt=0.05;%Time interval
vf=1;%Velocity*(df/du)
L=vf*dt/dx;%Courant Number
```

```
D=0;%Physical dispersion
Up(1:I)=0;%Initial Condition
b1=1; bI=0;%Boundary Condition
Un(1:I)=NaN;
for n=1:t/dt%Time iteration
%%Numerical Solution
for i=1:I
if i==1
WW=NaN; W=2*b1-Up(i); P=Up(i); E=Up(i+1);
w=b1; e=P+0.5*max(0,TVD((E-P)/(P-W)))*(P-W);
elseif i==2
WW=2*b1-Up(i-1); W=Up(i-1); P=Up(i); E=Up(i+1);
w=W+0.5*max(0,TVD((P-W)/(W-WW)))*(W-WW); e=P+0.5*max(0,TVD((E-P)/(P-W)))*(P-W);
elseif 2<i && i<I
WW=Up(i-2); W=Up(i-1); P=Up(i); E=Up(i+1);
w=W+0.5*max(0,TVD((P-W)/(W-WW)))*(W-WW); e=P+0.5*max(0,TVD((E-P)/(P-W)))*(P-W);
elseif i==I
WW=Up(i-2); W=Up(i-1); P=Up(i); E=2*bI-Up(i);
w=W+0.5*max(0,TVD((P-W)/(W-WW)))*(W-WW); e=bI;
end
Un(i)=dt*(D*(E-2*P+W)/dx^2-vf*(e-w)/dx)+P;
end
Up=Un;
%%Analytical Solution
i=1; Ua(1:I)=NaN;
for x=X
if D==0
Ua(i)=1-heaviside(x-vf*dt*n); %Analytical Solution with MoC
else
Ua(i)=0.5*erfc((x-vf*dt*n)/(2*(D*dt*n)^0.5))+0.5*exp(vf*x/D)*erfc((x+vf*dt*n)/(2*(D*dt*n)^0.5));
end
i=i+1;
end
% Plot Solution
set(gcf, 'Units', 'Normalized', 'OuterPosition', [0 0 1 1]);
plot(X/I/dx,[b1 Un bI],'gv-','markerfacecolor','g');
hold on
plot(X/I/dx,Ua,'k-','linewidth',2);
xlabel('Dimensionless Distance','fontsize',12)
ylabel('Concentration','fontsize',12)
legend('Numerical Solution','Analytical Solution')
hold off; pause(0.001)
end
toc
```

Appendix C. Google Drive link.
In order to reach Matlab files, please use following Google Drive link:
https://drive.google.com/drive/folders/1nyO1gi3oBAKlMI4Zo8_kspIAwpZy-Qq1?usp=sharing