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Research
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Numerical Simulation of Convection-Diffusion Equation Using a Novel Flux Limiter

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ABSTRACT: CFD (Computational Fluid Dynamics) researchers encounter some substantial problems such as numerical dispersion and unphysical oscillation. The first order space discretization technique causes large numerical dispersion, leading to inaccurate prediction of the flow behavior of fluids. Therefore, numerical simulation engineers apply some high-resolution schemes such as QUICK (Quadratic Upstream Interpolation for Convective Kinematics) and TCDF (Third-order Continuously Differentiable Function) to reduce the impacts of the numerical dispersion. However, the higher order methods lead to undesirable and unphysical oscillations at large Courant number. First objective of this study is to propose a novel flux limiter obtained by modifying TCDF. The modified TCDF flux limiter function works at large Courant number without any unphysical oscillation contrary to the previously improved TCDF flux limiter. Second purpose of this study is to present a numerical simulator for solution of convection-diffusion equation. The Matlab codes and Google drive links related to this numerical simulator were included in the Appendix to make other researchers' works easy.

KEYWORDS: Finite difference method, High-resolution scheme, Flux limiter.

1. INTRODUCTION

In numerical solution of convection-diffusion equation (Peng et. al., 2013, Kurganov & Tadmor, 2000, Kamalyar et. al., 2014, Morton, 2019), there are two alternatives to minimize numerical errors. The first one is to decrease time step intervals, but it increases total simulation time. Secondly, higher-order techniques are recommended to reduce numerical errors (Wolcott et. al., 1996). Although, there exist a lot of higher-order techniques in literature, some of them lead to unphysical and unacceptable oscillation at large Courant numbers. For instance, third-order accurate QUICK (Quadratic Upstream Interpolation for Convective Kinematics) technique proposed by Leonard (Leonard, 1979), is an extremely good technique to diminish numerical dispersion. However, it causes unphysical oscillation at some critical points for large time step intervals.

In 2015, the TCDF (Third-order Continuously Differentiable Function) method was proposed by Zhang (Zhang et. al., 2015) in order to suppress the oscillations occurring in the QUICK method. TCDF is a smooth multi-component function and it consists of three different functions which are smoothly connected each other with same gradient. In spite of the advantage of TCDF over QUICK method, TCDF technique causes unphysical oscillation at flood front for large Courant number due to the upper limiter of TCDF flux limiter.

In this study, a new polynomial-ratio expression was developed to decrease upper limit of TCDF method. The sharper flood front and more accurate results without any unphysical oscillation were obtained using the modified TCDF technique. The main contribution of this study is the suppression of unphysical oscillation of previously developed TCDF method using this novel flux limiter. Second contribution of this study is the introduction of a numerical simulator in Matlab environment for numerical solution of convection-diffusion equation.

2. MATERIALS AND METHODS

The general form of convection-diffusion equation (Peaceman, 2000) includes diffusion, convection and accumulation terms. The unsteady convection-diffusion equation is shown in following Equation 1.

$$D\nabla^2 U - v \cdot \nabla U = \frac{\partial U}{\partial t} \quad (1)$$

In Equation 1, U is variable of interest which can be supposed as concentration for miscible displacement fluid flow or it may be considered as temperature for heat transfer. D is diffusion coefficient (also called physical dispersion coefficient) and v refers to velocity of interested variable. The one dimensional form of convection-diffusion equation is given in Equation 2.

$$D \frac{\partial^2 U}{\partial x^2} - v \frac{\partial U}{\partial x} = \frac{\partial U}{\partial t} \quad (2)$$

The first, second and third terms in Equation 2 refer to diffusion, convection and accumulation terms respectively. The space discretization of Equation 2 is indicated in following Equation 3.

$$D \frac{U_{i+1} - 2U_i + U_{i-1}}{\Delta x^2} - v \frac{U_{i+\frac{1}{2}} - U_{i-\frac{1}{2}}}{\Delta x} = \frac{\partial U}{\partial t} \tag{3}$$

In this study, explicit time discretization numerical technique (Versteeg & Malalasekera, 2007, Lundgren & Mattsson, 2020) was used to simplify calculations. The full discretization (time and space discretization) form of one dimensional convection-diffusion equation can be expressed in following equation.

$$D \frac{U_{i+1}^n - 2U_i^n + U_{i-1}^n}{\Delta x^2} - v \frac{U_{i+\frac{1}{2}}^n - U_{i-\frac{1}{2}}^n}{\Delta x} = \frac{U_i^{n+1} - U_i^n}{\Delta t} \tag{4}$$

In Equation 4, i subscripts and n superscripts refer to space and time steps respectively. In numerical calculations, all grid block central values (... , U_{i-1} , U_i , U_{i+1} , ...) are calculated for each time step. On the other hand, there is no exact knowledge about grid block face values (... , $U_{i-1/2}$, $U_{i+1/2}$, ...). The main numerical errors arise from the approximation of these face values. Therefore, the problematic term in convection-diffusion equation is convection term especially for convection-dominated fluid flow. These face values must be predicted properly to obtain stable and accurate results. Otherwise, it causes large numerical dispersion and huge unphysical oscillation. There are some techniques in literature to predict grid block face values namely first-order method, QUICK technique and TCDF method.

2.1. FIRST ORDER METHOD

The conventional and simplest technique to approximate grid block face values is first-order method. The assumption of the face value as previous grid block central value can be defined as first-order method or first-order upstream technique (also called first-order upwinding method) (Ertekin et. al., 2001). Equation 5 shows mathematical expression of first-order method.

$$U_{i+\frac{1}{2}}^n \approx U_i^n \tag{5}$$

Despite the simplicity of first-order method, it causes large numerical dispersion. Nevertheless, first-order method never causes unphysical oscillation. Figure 1 shows numerical solution of convection-dominated flow equation using first-order method.

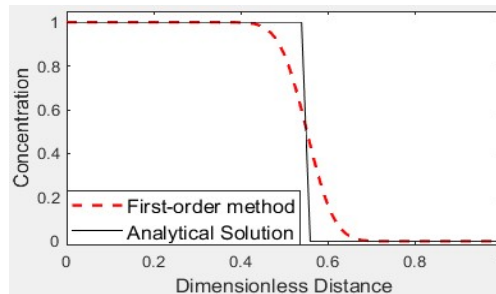


Figure 1. First-order method.

According to Figure 1, there is no unphysical oscillation of first-order method. It is an advantage of first-order upstream method, but numerical result of first-order method is far away from the analytical solution (Sarraf, 2002) due to the large numerical dispersion. Therefore, the higher-order numerical solution should be used to minimize numerical dispersion.

2.2. QUICK METHOD

The QUICK method is a quite useful technique to decrease numerical dispersion because it has third order accuracy in space discretization. Equation 6 indicates QUICK method to approximate grid block right face value.

$$U_{i+\frac{1}{2}}^n \approx \frac{U_{i+1}^n + U_i^n}{2} - \frac{U_{i+1}^n - 2U_i^n + U_{i-1}^n}{8} \tag{6}$$

According to QUICK method, face value depends not only on previous grid block central value but also on current and next grid block central values. Hence, it yields more accurate results compared to first-order upwinding technique. In spite of the advantages of QUICK method, it has a weakness. QUICK method causes large unphysical oscillation when physical dispersion coefficient approaches to zero and Courant number comes closer to one (Liu, 1993). It is

recommended to combine TVD (Total Variation Diminishing) method with the QUICK method to suppress this oscillation (Harten, 1984, Sweby, 1984). The general form of TVD formulation is given by following equation.

$$U_{i+\frac{1}{2}}^n \approx U_i^n + \frac{1}{2} \varphi(r) [U_i^n - U_{i-1}^n] \tag{7}$$

The first term at left-hand side in Equation 6 is upstream or upwinding term. The second term at left-hand side in Equation 6 is anti-diffusive term which prevents numerical dispersion. In Equation 6, φ is a flux limiter and it is a function of interested variable or concentration gradient ratio (r). The formulation of gradient ratio is shown in Equation 8.

$$r = \frac{U_{i+1}^n - U_i^n}{U_i^n - U_{i-1}^n} \tag{8}$$

Equations 9 and 10 imply pure QUICK method and QUICK-TVD method respectively.

$$\varphi(r) = \frac{3r + 1}{4} \tag{9}$$

$$\varphi(r) = \min \left(2, 2r, \frac{3r + 1}{4} \right) \tag{10}$$

Figure 2 shows general schematic of TVD area and relationship of flux limiter with gradient ratio for pure QUICK method and QUICK method with piecewise linear flux limiter function. The unphysical oscillations of pure QUICK method are suppressed thanks to this piecewise linear function. QUICK-TVD flux limiter consists of three parts. If concentration gradient ratio is small, the results are two times of gradient ratio. If gradient ratio so high, the results are restricted to 2 by limiter function so as to prevent oscillations. Otherwise, it's same as pure QUICK.

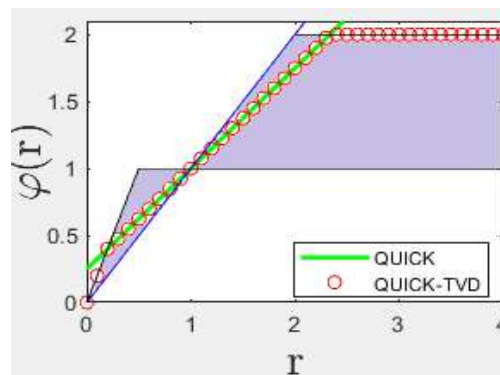


Figure 2. QUICK method and QUICK-TVD method.

The limiter functions must pass through the grayscale area of Figure 2 to obtain second order accurate scheme (Wolcott et. al., 1996). Numerical result of QUICK-TVD method is shown in Figure 3. The pure QUICK method doesn't give logical and meaningful numerical result for this condition (convection-dominated flow and high Courant number).

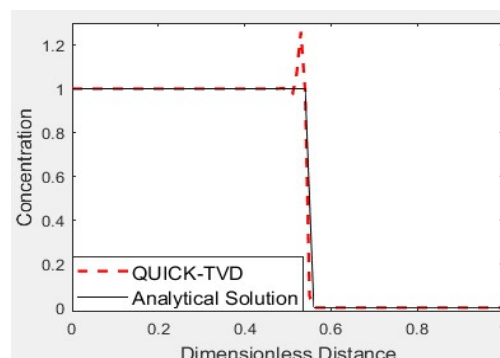


Figure 3. QUICK-TVD method.

In Figure 3, the QUICK-TVD technique decreases numerical dispersion, but it has some unphysical oscillation at flood front. Consequently, smooth flux limiter should be used instead of piecewise linear flux limiter to minimize the unphysical oscillations at flood front.

2.3. TCDF METHOD

The TCDF method is a smooth flux limiter function. It comprises three different functions which are linked each other with the same slope. The formula of the TCDF method is given in Equation 11 (Zhang et. al., 2015).

$$\varphi(r) = \begin{cases} r^3 - 2r^2 + 2r & \text{if } 0 \leq r < 0.5 \\ 0.75r + 0.25 & \text{if } 0.5 \leq r < 2 \\ \frac{2r^2 - 2r - 9/4}{r^2 - r - 1} & \text{if } 2 \leq r < \infty \end{cases} \quad (11)$$

Firstly, the third-order QUICK scheme is stuck to over the interval $0.5 \leq r \leq 2$, which corresponds to the relatively smooth regions. Hence,

$$\varphi(r) = 0.75r + 0.25 \quad \text{if } 0.5 \leq r < 2 \quad (12)$$

Secondly, in the region of $0 \leq r < 0.5$, a cubic polynomial is selected to get a smooth function.

$$\varphi(r) = a r^3 + b r^2 + c r + d \quad (13)$$

It passes through two points: (0, 0) and (0.5, 0.625). The slope of TCDF method at the first point is 2 (two) and it has same gradient (0.75) with the third-order QUICK scheme at the second point. There are four equations and there are four unknowns, so this equation system can be solved (a=1, b=-2, c=2, d=0).

$$\varphi(r) = r^3 - 2r^2 + 2r \quad \text{if } 0 \leq r < 0.5 \quad (14)$$

Thirdly, the general polynomial ratio expression is applied for the last part of the TCDF, $2 \leq r < \infty$.

$$\varphi(r) = \frac{M r^2 + a r + b}{r^2 + c r + d} \quad (15)$$

In equation 15, M can be defined as maximum target of flux limiter. It is selected as 2 (two) for the TCDF flux limiter. In order to simplify calculation, c and d are selected as -1 (Zhang et. al., 2015). This last function passes through the point (2, 1.75) with the same slope of third-order QUICK scheme (0.75). There are two unknowns with two equations, so this equation system can be solved (a=-2, b=-9/4).

$$\varphi(r) = \frac{2 r^2 - 2 r - 9/4}{r^2 - r - 1} \quad (16)$$

Figure 4 shows the schematic for the TCDF method on TVD region using Equation 16.

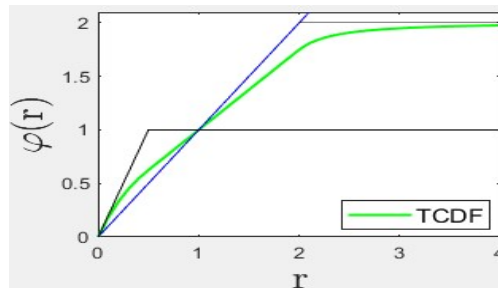


Figure 4. TCDF method and TVD region.

The numerical solution of convection-dominated fluid flow using TCDF method is shown in Figure 5.

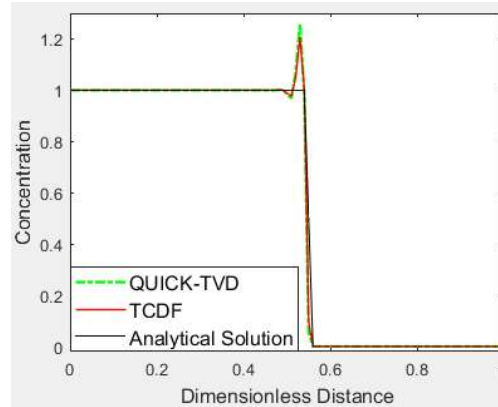


Figure 5. Numerical solution using TCDF method.

The oscillation of TCDF method is less than that of QUICK-TVD method, but still it is not acceptable. The TCDF method may be modified to suppress unphysical oscillations.

2.4. MODIFIED TCDF METHOD

In this study, it has been observed that unphysical oscillation of TCDF method arises from upper limit of the flux limiter. The last part of TCDF flux limiter has been modified to decrease upper limit of flux limiter and minimize unphysical oscillations. The new upper limit was selected as 1.6 instead of 2. It is assumed that, the new polynomial ratio expression passes through the two points (1.6, 1.45) and (5, 1.6) with the 0.75 and 0.1 gradients respectively. In that case, there are four equations and four unknowns, so this equation system can be solved. The modified part of the TCDF method is given by Equation 17. The modified TCDF method on TVD area is shown by Figure 6 using Equation 17.

$$\varphi(r) = \frac{1.6r^2 - \frac{292963}{28150}r + \frac{324943}{28150}}{r^2 - \frac{18256}{2815}r + \frac{20038}{2815}} \tag{17}$$

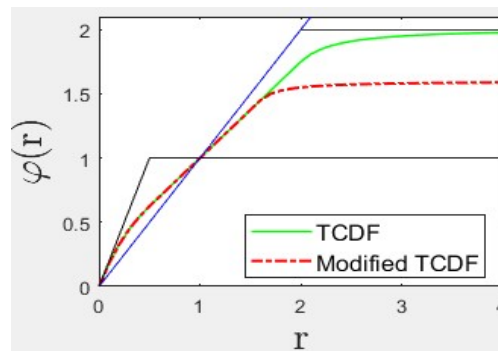


Figure 6. TCDF method and modified TCDF method.

3. RESULTS

In this study, it is supposed that Courant number is equal to 0.55, velocity is 1 and physical dispersion is 0 (zero) in order to compare all spatial discretization techniques properly. In addition to these assumptions, explicit time discretization technique is applied to all numerical technique. Figure 7 shows numerical results with exact (analytical) solution. According to the Figure 7, the first-order upstream method gives large numerical dispersion. The TCDF method has huge unphysical oscillation at flood front and it is not close to analytical solution. The modified TCDF flux limiter function has no oscillations and is the closest numerical solution to the analytical solution.

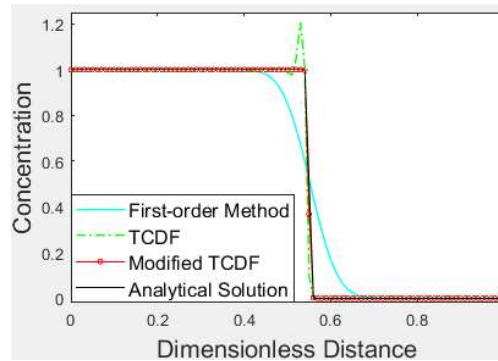


Figure 7. The numerical result of modified TCDF method.

It is important note that Courant number must be less than 1 (one) to get stable numerical solution due to the inherent of explicit scheme. The modified TCDF method works up to Courant number is equal to 0.55 without unphysical oscillation. This novel technique extends the limitation of explicit solution. If Courant number is greater than 0.55 and less than 1, the small unphysical oscillation may be observed. If Courant number is greater than 1, this numerical solution is unstable and unmeaningful results are obtained. This is the limitation of explicit numerical solution.

4. DISCUSSION AND CONCLUSION

There are two significant problems of the numerical solution for convection-diffusion equation: numerical dispersion and unphysical oscillation. The easiest way to solve convection-diffusion equation numerically is through the use of first-order upwinding space discretization technique. However, it gives rise to large numerical dispersion. The higher-order technique should be utilized to minimize the effect of the numerical dispersion. When the large Courant number and the low physical dispersion coefficient are used, some higher-order techniques (such as QUICK and TCDF methods) lead to huge unphysical oscillations. This study is to propose the modified TCDF technique to suppress unphysical oscillation of previously developed TCDF method. Secondly, this study is to present a numerical simulator for solution of convection-diffusion equation. The all open source Matlab codes and Google drive links related to this numerical simulator were provided in the Appendices. The developed numerical simulator is convenient for any grid dimension, any space interval, any time interval and some space discretization techniques.

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Appendix

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 Third Order Upwinding (Leonard-Quick) Method -> SDO=30
% For Third Order Upwinding (TVD with Leonard-Cubic) -> SDO=31
% For Third Order Upwinding (TVD with Leonard-Quick) Method -> SDO=32
% For TCDF Method -> SDO=33
% For Modified TCDF Method -> SDO=34
SDO=34;
if SDO==1%First Order Upstream
y=0;
elseif SDO==30%Third Order Upwinding (Leonard-Quick)
y=(3*x+1)/4;
elseif SDO==31%Third Order Upwinding (TVD with Leonard-Cubic)
y=max(0,min([2,2*x,(2*x+1)/3]));
elseif SDO==32%Third Order Upwinding (TVD with Leonard-Quick)
y=max(0,min([2,2*x,(3*x+1)/4]));
elseif SDO==33%TCDF
if 0<=x && x<0.5
y=x^3-2*x^2+2*x;
elseif 0.5<=x && x<2
y=0.75*x+0.25;
elseif 2<=x
y=(2*x^2-2*x-9/4)/(x^2-x-1);
else
y=0;
end
elseif SDO==34%Modified TCDF
if 0<=x && x<0.5
y=x^3-2*x^2+2*x;
elseif 0.5<=x && x<1.6
y=0.75*x+0.25;
elseif 1.6<=x
y=(1.6*x^2-292963/28150*x+324943/28150)/(x^2-18256/2815*x+20038/2815);
else
y=0;
end
end
end
```

Appendix B. The numerical simulator.

Note: In order to run Matlab codes in APPENDIX B, it's required to obtain "TVD.m" Matlab file. It can be designed using APPENDIX A. The name of the Matlab file have to be "TVD" without quotes. Secondly, generated TVD.m Matlab file and the numerical simulator mfile (in Appendix B) have to 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+1;%Number of i-direction points
t=5.5;%Total simulation time
dx=0.1;%Space interval
dt=0.055;%Time interval
vf=1;%Velocity*(df/du)
L=vf*dt/dx;%Courant Number
D=0;%Physical dispersion
U00=0.5; Ui0=0;%Initial Condition
U0n=1; UIn=0;%Boundary Condition
Up(1)=U00; Up(2:I)=Ui0;
Un(1)=U0n; Un(2:I-1)=NaN; Un(I)=UIn;
for n=1:t/dt%Time iteration
%%Numerical Solution
for i=2:I-1
if i==2
rf=Up(i); lf=Up(i-1);
else
rf=Up(i)+0.5*max(0,TVD((Up(i+1)-Up(i))/(Up(i)-Up(i-1))))*(Up(i)-Up(i-1));
lf=Up(i-1)+0.5*max(0,TVD((Up(i)-Up(i-1))/(Up(i-1)-Up(i-2))))*(Up(i-1)-Up(i-2));
end
Un(i)=dt*(D*(Up(i+1)-2*Up(i)+Up(i-1))/dx^2-vf*(rf-lf)/dx)+Up(i);
end
Up=Un;
%%Analytical Solution
i=1; Ua(1:I)=NaN;
for x=0:dx:(I-1)*dx
```

```
if D==0
Ua(i)=1-heaviside(x-vf*dt*n); %Analytical Solution with Method of Characteristics
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(0:dx:(I-1)*dx,Un,'gv-','markerfacecolor','g');
hold on
plot(0:dx:(I-1)*dx,Ua,'k-','linewidth',2);
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/1e0MWNkUHjqJRpl7RrtJJdGLm73LciQoL?usp=sharing>