Numerical Dissipation Effects on Detached Eddy Simulation of Turbomachinery Flows

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ABSTRACT
Detached eddy simulation (DES) is a high-resolution method for predicting complex unsteady flows in turbomachinery. Recent researches have shown that in DES the numerical dissipation from the spatial discretization scheme should be limited to a reasonable extent. Through the test-case of decaying isotropic turbulence, the impact of the Roe scheme is assessed with three reconstruction approaches: the 3rd-order MUSCL, the 5th-order WENO, and the 4th-order minimized dispersion and controllable dissipation (MDCD) scheme. From the results, however, even with the least dissipative 4th-order MDCD scheme, the Roe scheme possesses high numerical damping for the small-scale turbulent structures. To further decrease the dissipation, the Roe scheme is modified via an adaptive factor. This adaptive scheme has small dissipation in the LES region to capture multiscale turbulent structures and returns to the original Roe scheme near shock waves to suppress numerical oscillations. The scheme with adaptive dissipation is also used to calculate flows in a centrifugal compressor. The resolution of small vortex structures, such as the tip leakage vortices and the wake vortices, is well improved.

INTRODUCTION
Turbulence dominates the complex unsteady flows in high-speed turbomachinery. The flows are composed of several vortex structures such as the tip leakage vortices, the corner separation vortices and the wake vortices. High-resolution and efficient analytical tools are required to capture such flows accurately. Conventional Reynolds-averaged Navier-Stokes (RANS) methods have difficulties in modelling unsteady vortical flows, while large eddy simulation (LES) methods are too costly to simulate flows with high Reynolds number. Detached eddy simulation (DES), as a hybrid method of RANS and LES, is a feasible choice to simulate the turbulent flows in turbomachinery for both academic and industry communities.

Numerous researchers have applied DES-type methods to simulate the flows in turbomachinery. Shi and Fu investigated the unsteady flows in a transonic compressor rotor with the improved delayed DES (IDDES) method. The interaction of passage shock, blade tip leakage vortex and the blade boundary layer was considered to be the sources of the unsteadiness (Shi and Fu, 2013). Using DES, Yamada et al. calculated the flow field of the first seven stages of an axial compressor to recognize the flow physics of rotating stall inception. The hub corner separation appearing in a passage of the sixth stator induced the leading-edge separation, which rapidly developed to the rotating stall (Yamada et al., 2017). Fujisawa et al. performed DES analysis to reveal the generation mechanism of rotating stall in a centrifugal compressor with the volute. The diffuser stall fluctuation magnitude varied circumferentially, and the boundary layer separations on the shroud and hub wall played important roles on the stall generation (Fujisawa et al., 2020).

The numerical dissipation associated with the spatial discretization scheme for the inviscid fluxes of the N-S equations can have a significant influence on DES results. Gao et al. reviewed the applications of DES-type methods in
turbomachinery and indicated that the most popular spatial scheme is the approximate Riemann solver, like the Roe scheme, with the 2nd- and 3rd-order MUSCL reconstruction (Gao et al., 2017). However, such low-order MUSCL reconstruction is too dissipative to capture the small scale turbulent structures in DES (Xiao et al., 2012). Large numerical viscosity associated with the spatial discretization is likely to overshadow the turbulent viscosity in LES regions, and only very large-scale vortices can be resolved. The use of high-resolution spatial schemes with low dissipation enables finer capture of small coherent structures, which can improve the understanding of the flow mechanisms in turbomachinery. Marty et al. compared the 3rd-order MUSCL reconstruction with the 5th-order one in DES or LES of three turbomachinery cases. The higher-order scheme leads to the better resolution of small vortex structures, including the tip leakage vortices and the wake vortices (Marty et al., 2015). Lin et al. applied a newly developed low-dissipation numerical scheme coupled with DDES to study the wake shedding vortex of a turbine guide vane. The results well predicted the flow details including the shock, the pressure wave, and the wake vortices. The resolution was comparable to that of LES results (Lin et al., 2018). However, as far as the authors know, few researchers have applied high-resolution numerical schemes in DES-type investigations of turbomachinery, and the efficiency, accuracy and robustness of high-resolution schemes still need further research.

The current study is motivated by the lack of simulations with high-resolution numerical schemes in turbomachinery. The numerical dissipation of different spatial schemes are assessed through the test-case of decaying isotropic turbulence (DIT). A low-dissipation numerical scheme is applied in a transonic centrifugal compressor. The results show a well improved resolution of small coherent structures compared with that of the conventional Roe scheme coupled with the 3rd-order MUSCL reconstruction.

**NUMERICAL METHODS**

An in-house computational fluid dynamics (CFD) solver named UNITs, which was developed to solve the three-dimensional compressible N-S equations based on a cell-central finite volume formulation, is applied in this study. The governing equations are solved in a rotating Cartesian frame fixed on the compressor rotor to avoid using moving mesh. The details of the equations can be found in the paper of Shi and Fu (Shi and Fu, 2013). The shear stress transport (SST) k-ω turbulence model is used in the present code and expended to IDDES. The IDDES method can be easily constructed by the substitution of a hybrid length scale for the RANS length in the dissipation term of the k-transport equation. The detailed formulations and model parameters of IDDES based on the SST k-ω model can be found in the article of Shur et al. (Shur et al., 2008). For both N-S and turbulence transport equations, the viscous fluxes are evaluated by the second-order central scheme. The implicit lower-upper symmetric Gauss–Seidel (LU-SGS) scheme with sub-iterations in pseudo time is employed for time integration, which has 2nd-order precision for unsteady predictions. The inviscid fluxes of the turbulence transport equations are discretized by the 2nd-order upwind scheme. The inviscid fluxes of the N-S equations are discretized with different schemes to explore the effects of different levels of numerical dissipation on DES.

The current study mainly investigates the impact of the adaptive-dissipation rotated Roe scheme coupled with the MDCD reconstruction on IDDES calculations. MDCD is a newly developed 4th-order scheme of reconstruction in which the numerical dissipation and dispersion are controlled by two independent coefficients (Wang et al., 2013). In each dimension, the MDCD scheme uses the information of six neighboring grid cells to interpolate variables at the cell interface, but only 4th-order accuracy is achieved. Thus, there remain two independent coefficients and they control the numerical dissipation and dispersion respectively. The MDCD technique optimizes the coefficients to obtain minimized numerical dispersion and reasonable numerical dissipation from the scheme of reconstruction. To capture the shock waves, the nonlinear mechanism of the WENO scheme is introduced into MDCD. The interpolation of the MDCD scheme at the grid interface i+1/2 is as follows:

\[
W^L_{i+1/2} = \sum_{k=0}^{1} \omega_k W_{i+1/2}^{(k)}
\]

where \( W^L \) represents the vector of primitive variables at the left side of the grid interface i+1/2, and \( W^{(k)} \) is calculated by a 2nd-degree polynomial reconstructed on the kth substencil:

\[
\begin{align*}
W_{i+1/2}^{(0)} &= \frac{2}{6} W_{i+1} - \frac{7}{6} W_{i} + \frac{11}{6} W_{i-1} \\
W_{i+1/2}^{(1)} &= -\frac{1}{6} W_{i+1} - \frac{5}{6} W_{i} + \frac{2}{6} W_{i-1} \\
W_{i+1/2}^{(2)} &= \frac{5}{6} W_{i+1} + \frac{1}{6} W_{i+2} - \frac{1}{6} W_{i} \\
W_{i+1/2}^{(3)} &= \frac{11}{6} W_{i+1} - \frac{7}{6} W_{i+2} + \frac{2}{6} W_{i+3}
\end{align*}
\]

\( \omega_k \) is the nonlinear weight of the kth substencil:

\[
\omega_k = \alpha_k \left( \sum_{k=0}^{1} \alpha_k \right), \quad \alpha_k = \frac{C_k}{(\xi + IS_k)^2}, \quad \xi = 10^{-6}
\]
where ISk is the smoothness measurement of the WENO scheme (Jiang and Shu, 1996). Equations (1) to (3) are the same as the WENO scheme, and the MDCD technique is performed by optimizing the linear weight Ck:

\[
C_0 = \frac{3}{2} \gamma_{disp} + \frac{3}{2} \gamma_{diss}, \quad C_1 = \frac{1}{2} (1-3\gamma_{disp} + 9\gamma_{diss}) \quad (4)
\]

\[
C_s = \frac{1}{2} (1-3\gamma_{disp} - 9\gamma_{diss}), \quad C_3 = \frac{3}{2} \gamma_{diss} - \frac{3}{2} \gamma_{diss}
\]

where \(\gamma_{disp}\) is the coefficient of dispersion and \(\gamma_{diss}\) is the coefficient of dissipation, which can independently control the numerical dispersion and dissipation of the MDCD scheme. In this study, \(\gamma_{disp}\) is set as 0.0463783 and \(\gamma_{diss}\) is set as 0.012. In smooth regions, it is expected that the MDCD reconstruction is linear. That is, the linear weight is active, \(\omega_k=C_k\). The spectral properties of this linear MDCD reconstruction have been proved better than the WENO reconstruction. However, the nonlinear adaptation of MDCD reconstruction may deteriorate the spectral properties even in smooth regions. For further improvement, a shock detector proposed by Ren et al. is applied to combine the linear and nonlinear MDCD scheme (Ren et al., 2003):

\[
W_{i+1/2}^{\text{hybrid}} = \beta W_{i+1/2}^{\text{linear}} + (1-\beta) W_{i+1/2}^{\text{nonlinear}} \quad (5)
\]

The detector \(\beta\) reaches zero near the discontinuities and equals to one in smooth regions.

Besides the scheme of reconstruction, the numerical dissipation from the approximate Riemann solver also plays an important role in DES-type simulations. The rotated Roe scheme is an improved approximate Riemann solver based on the original Roe scheme, which is more robust than the latter while the numerical dissipation keeps similar (Ren, 2003). Xiao et al. suggested to reduce the dissipation of the Roe scheme through multiplying the upwind term by an adaptive parameter \(\phi\) (Xiao et al., 2012):

\[
F_{\text{mixed}} = \frac{1}{2} \left[ F(W^L) + F(W^R) \right] - \phi \times \frac{1}{2} |\Delta_{\text{up}}| (W^R - W^L) \quad (6)
\]

On the one hand, in the regions of RANS calculations, far fields or discontinuities, the adaptive parameter \(\phi\) is expected to be one so that the large numerical dissipation can suppress the numerical oscillations. On the other hand, in the regions of LES calculations, \(\phi\) is expected small enough to maintain the high resolution of LES for small coherent structures. The current study follows the formulations suggested by Xiao et al. (Xiao et al., 2015):

\[
\phi = \max \left[ 1 - (1-\sigma_1)(1-\sigma_2), \phi_{\text{min}} \right] \quad (7)
\]

where \(\sigma_1\) is a detector of RANS and LES, which approaches zero in LES regions and returns to one in RANS regions or far fields. It is first proposed by Travin et al. for the SST-based DES method (Travin et al., 2002):

\[
\sigma_1 = \tanh \left( A^\Omega \right); \quad A = CH_z \cdot \max \left( \left[ \left| l_{\text{grid}} / l_{\text{sub}} \right| \right] / g_0 - 0.5, 0 \right)
\]

\[
l_{\text{grid}} = C_{\text{DES}} \Delta_{\text{grid}}, \quad l_{\text{sub}} = \left( \left( \mu + \mu_t \right) / \left( \rho K_e C_{\mu}^{1.5} \right) \right)^{0.5}
\]

\[
g_0 = \tanh B_0; \quad B_0 = CH_3 \cdot \Omega \cdot \max \left( \Omega, S \right) / \max \left( \left( S^2 + \Omega^2 \right) / 2, 10^{-20} \right)
\]

\[
K_s = \max \left( \left( S^2 + \Omega^2 \right) / 2 \right), 0.1; \quad \Delta_{\text{grid}} = \max \left( \Delta_x, \Delta_y, \Delta_z \right)
\]

\[
S = \sqrt{2S_{\rho g} S_{\rho g}}, \quad \Omega = \sqrt{\Omega_{\rho g} \Omega_{\rho g}}, \quad \Omega_{\rho g} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right); \quad \Omega = \sqrt{2} \frac{\partial u_i}{\partial x_j} \Omega_{\rho g}
\]

\[
CH_1 = 3; CH_2 = 1; CH_3 = 2; \quad C_{\text{DES}} = 0.61; C_{\text{DES}} = 0.78; C_{\mu} = 0.09
\]

\(\sigma_2\) is a detector of discontinuities which is close to one near discontinuities and reaches zero in smooth regions (Xiao et al., 2015):

\[
\sigma_2 = \left( \frac{\partial u_i}{\partial x_j} \right)^2 / \left( \left( \frac{\partial u_i}{\partial x_j} \right)^2 + \Omega^2 \right) \quad (8)
\]

\(\phi_{\text{min}}\) is the minimum value of the adaptive parameter \(\phi\) to limit the minimal numerical dissipation for suppressing numerical oscillations. According to the following results of DIT simulation, \(\phi_{\text{min}}\) is set as 0.05.
DECAYING ISOTROPIC TURBULENCE

DIT is the simplest turbulent flow where both the transport and the production vanish in the equation for the evolution of turbulent kinetic energy (Pope, 2000):

\[ \frac{dk}{dt} = -\epsilon \] (10)

For IDDES computation of DIT, only the LES branch is active as there exists no wall boundary. The origin of total dissipation in the simulation can be divided into three parts: the molecular viscosity, the turbulent viscosity and the numerical viscosity.

\[ \epsilon = \epsilon_{\text{molecular}} + \epsilon_{\text{turbulent}} + \epsilon_{\text{numerical}} \] (11)

The turbulent viscosity is quite large in RANS, so the low-order numerical schemes are appropriate due to the better efficiency and robustness. However, the turbulent viscosity is relatively small in LES, and the numerical dissipation from the low-order schemes can be comparable to the turbulent dissipation of the LES model. The small scale turbulent structures will be eliminated by the large numerical dissipation. Numerical schemes with lower dissipation level are required to obtain more resolved turbulence when LES acts.

According to equation (10), the effects of numerical dissipation can be quantitatively explored through simulating DIT. Considering the in-house code is a compressible solver, a DIT test-case with the initial turbulent Mach number of 0.3 is selected (Santamay et al., 2001). The computational domain is a cube with the side length of \( 2\pi \), containing \( 64^3 \) uniform grids. The periodical boundary conditions are set in all three directions, and the turbulence is statistically homogeneous. To get the reasonable magnitude of the subgrid stress, the initial time of IDDES computation is chosen as the first large-eddy-turnover time of the direct numerical simulation (DNS) results. Different spatial schemes are investigated to assess the effects of different numerical dissipation on the turbulent energy spectra, including the 4th-order central scheme, the rotated Roe scheme with the third-order MUSCL, the fifth-order WENO, and the fourth-order MDCD reconstruction. The upwind term of the rotated Roe scheme with MDCD reconstruction is further adjusted by a fixed coefficient of 100% or 5%. The IDDES results are compared with DNS results.

![Energy spectra at time=1.0](image1)

![Energy spectra at time=3.0](image2)

**Figure 1 DIT Turbulent Energy Spectra of IDDES Predictions with Different Spatial Schemes**

From the results shown on Fig. 1, the 4th-order central scheme with no numerical dissipation predicts a spurious energy accumulation at high wavenumbers because of the numerical dispersion and the truncation error. Such numerical error can easily cause serious oscillations and lead the calculation to diverge in more complex flows. On the contrary, the rotated Roe scheme with the 3rd-order MUSCL reconstruction is the most dissipative and the energy cascade cannot be well predicted. The large numerical dissipation eliminates most turbulent kinetic energy at high wavenumbers, which indicates only very large coherent structures can be resolved. The 5th-order WENO scheme and the 4th-order MDCD scheme with 100% dissipation demonstrates an improvement compared with the MUSCL results. The results of MDCD shows less dissipation than that of WENO. However, without modifying the upwind term of the Roe scheme, even the least dissipative MDCD scheme shows significant numerical damping on turbulent energy at high wavenumbers. The modified rotated Roe scheme with 5% dissipation remarkably reduces the gap between IDDES and DNS results, and well predicts the energy spectra at all wavenumbers. It indicates that the 5%-dissipation rotated Roe scheme with the MDCD reconstruction can resolve most turbulent structures when LES is active. In more complex situations like turbomachinery flows, however, the fixed 5% dissipation is too small to suppress numerical oscillations generally. The adaptive-
dissipation scheme introduced in equations (6) to (8) is the most reasonable to adapt the complex flows in turbomachinery. From DIT results, 0.05 is chosen as the minimum value of the adaptive factor.

**TRANSONIC CENTRIFUGAL COMPRESSOR**

The current study simulates the flow in a transonic centrifugal compressor, TTL, which is composed of an impeller and a vaneless diffuser (Niu et al., 2020). Table 1 shows the most important parameters of the compressor.

<table>
<thead>
<tr>
<th>PARAMETERS</th>
<th>VALUES</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of Impeller Blades</td>
<td>24</td>
</tr>
<tr>
<td>Rotational Speed</td>
<td>70500 r/min</td>
</tr>
<tr>
<td>Impeller Outlet Radius</td>
<td>50.0 mm</td>
</tr>
<tr>
<td>Diffuser Inlet Radius</td>
<td>55.0 mm</td>
</tr>
<tr>
<td>Diffuser Outlet Radius</td>
<td>86.0 mm</td>
</tr>
<tr>
<td>Diffuser Width</td>
<td>3.5 mm</td>
</tr>
</tbody>
</table>

**Table. 1 Characteristic Parameters of Centrifugal Compressor TTL**

The computational domain, as illustrated in Fig. 2, contains single passage of the impeller and vaneless diffuser. A step is set in the inlet to model the bolts in the real test rig. The number of grid cells is around 3.4 million in total. 91 grid points are used in the span direction, including 26 grid points in the blade tip clearance. The height of wall neighboring cells is 0.5µm, which guarantees that the parameter y+ is less than 1 on most solid walls. At the inlet boundary, the total pressure and total temperature are given, and purely axial flow is assumed. Empirical parameters of turbulent kinetic energy and turbulent viscosity ratio are given at the inlet for convenience. A uniform static pressure is fixed at the outlet of the computational domain. Different mass flow rates are obtained by varying the outlet pressure. For all solid walls, no-slip and adiabatic conditions are adopted. The periodic boundary conditions are imposed at the passage interfaces as only one of 24 passages is calculated. For unsteady simulations, 60 physical time steps are included in one period for a blade rotating through one passage.

**Figure 2 (i) Numerical Mesh of the Centrifugal Compressor and (ii) Distribution of y+**

For IDDES computations of the transonic centrifugal compressor, two different spatial schemes are applied: the original-dissipation rotated Roe scheme with 3rd-order MUSCL reconstruction, and the adaptive-dissipation rotated Roe scheme with 4th-order MDCD reconstruction. Converged steady RANS results are employed as the initial flow fields of unsteady IDDES calculations. The current study uses (i) mass flow rate at the diffuser outlet and (ii) the ratio between the averaged static pressure at the diffuser outlet and the averaged total pressure at the impeller inlet as the compressor characteristic parameters. The monitoring history of the mass flow rate and static-total pressure ratio for unsteady simulations are illustrated in Fig 3. Judging from the averaged value from beginning (solid lines), for both MDCD and MUSCL simulations, the averaged characteristic parameters reach a relatively steady state from about step=3000 on. The averaged characteristic parameters from step=3000 are calculated to show the compressor performance, and the unsteady flow fields after step=3000 are analyzed.
Comparisons are made between the CFD results and the experimental results on the compressor performance map, as is shown in Fig 4. The performance points predicted by MDCD and MUSCL methods differ slightly from each other though the same back pressure is given in the two simulations. The large numerical dissipation of the MUSCL method leads to more serious blending in flow fields, and exacerbates the losses induced by vortices. Thus, the MDCD method predicts higher mass flow rate, and agrees better with the experiment.

Fig. 5 depicts the instantaneous fields of entropy near the midspan of blade trailing edge. The periodic shedding wake vortices can be clearly observed in MDCD results, while the shedding vortices almost disappear in MUSCL results. The wake vortices are seriously dissipated so that the wake flows appear nearly steady. The black lines in Fig. 5 are contour lines where the IDDES length scale equals to the RANS length scale, which divides RANS regions and LES regions. As is expected, RANS is active near the solid walls and LES is active in the main part of blade wake flows for both MDCD and MUSCL calculations. In the lower-dissipation MDCD simulations, the high resolution of LES for turbulence can be preserved well. However, the resolution of LES is heavily limited due to the large numerical dissipation in MUSCL simulations. The numerical dissipation has similar effects on the behavior of tip leakage vortices, as illustrated in Fig. 6. MDCD results predict the periodic oscillation of the tip leakage vortex on the side of blade section surface, while the MUSCL results show an almost steady tip leakage vortex.

Fig. 7 indicates the difference of resolution between MDCD and MUSCL results from the view of three-dimensional vortices near the blade trailing edge, recognized by the Q criterion (Hunt et al., 1988). The MUSCL results resolve only very large vortices. The MDCD method predicts a similar overall vortex structures with MUSCL results, but contains a large number of small vortices. Details of the vortex development, breakdown and interaction can be described by MDCD results. It is consistent with the analysis of DIT that the low-dissipation spatial scheme significantly improves the resolution of small coherent structures in LES regions.
Figure 5 Contours of Entropy near the Midspan of Blade Trailing Edge (black lines: contour lines where the IDDES length scale is equal to the RANS length scale)

Figure 6 Tip Leakage Vortices at Blade Leading Edge

Figure 7 Three-Dimensional Vortices near the Blade Trailing Edge
CONCLUSIONS

The effects of the numerical dissipation from spatial discretization schemes on IDDES calculations are investigated in decaying isotropic turbulence and in a transonic centrifugal compressor. The results can be summarized as follows:

(1) The original-dissipation Roe scheme with the 3rd-order MUSCL reconstruction eliminates most turbulent kinetic energy at high wavenumbers in the IDDES calculation of DIT. The 5%-dissipation Roe scheme with the 4th-order MDCD reconstruction shows a remarkable improvement and relatively well predicts the energy spectra at all wavenumbers.

(2) Large numerical dissipation of spatial discretization schemes significantly suppresses the resolution of small coherent structures in turbomachinery flows. The original-dissipation Roe scheme with the 3rd-order MUSCL reconstruction can resolve only very large vortices. Almost steady blade wake vortices and tip leakage vortices are predicted.

(3) The adaptive-dissipation Roe scheme with the 4th-order MDCD reconstruction performs high-resolution simulations for small coherent structures. Multiscale vortices are visible in MDCD results. The periodic oscillation of blade wake vortices and tip leakage vortices is clearly captured.

NOMENCLATURE

- $C$: linear weight of the MDCD scheme
- $F$: inviscid fluxes of the N-S equations
- $k$: turbulent kinetic energy [$m^2/s^2$]
- $t$: time [s]
- $u$: velocity [m/s]
- $W$: vector of primitive variables
- $x$: spatial coordinate [m]
- $σ_1$: detector of RANS and LES regions
- $σ_2$: detector of discontinuities
- $β$: blending factor of linear and nonlinear MDCD scheme
- $ε$: rate of dissipation of turbulent kinetic energy [$m^2/s^3$]
- $γ_{disp}$: coefficient of dispersion
- $γ_{diss}$: coefficient of dissipation
- $ϕ$: adaptive factor of upwind terms
- $ω$: nonlinear weight of the MDCD scheme
- $ρ$: density [$kg/m^3$]
- $μ$: molecular viscosity [$Pa·s$]
- $μ_T$: turbulent viscosity [$Pa·s$]

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