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Data-Driven RANS Turbulence Modeling for Compressor Stall

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Declaration of Originality

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Abstract

Compressor stall in an aero-engine can result in partial or total loss of power for the engine, leading to engine failure or shutdown. Hence, it is a critical parameter during the design stages of an aero-engine. The conventional method to predict the compressor stall margin at the design phase is to perform a Reynolds-Averaged Navier-Stokes (RANS) simulation with a turbulence model. However, this method often underpredicts the stall margin due to the deficiency of the turbulence model in predicting 3D separated flows. Recent research has demonstrated the capabilities of a data-driven turbulence modeling approach in 2D canonical flows. In this thesis, a data-driven turbulence model for better prediction of compressor stall margin is pursued.

The ingredients for a data-driven turbulence model include (1) data, (2) flow physics, and (3) a data-driven framework. To address each of these issues for turbomachinery applications, this thesis is organized accordingly, with each one of the three major parts of the thesis corresponding to one issue.

In the first part of the thesis, an upgraded delayed detached eddy simulation (DDES) method is devised for compressor tip leakage flows, which provides a cost-effective means to generate a turbomachinery turbulence database. The method is validated and verified in a backward-facing step and a low-speed axial compressor rotor. Afterward, the method is applied to generate a turbulence database of compressor tip leakage flows. By analyzing the mean flows, the turbulence statistics, and the modal behavior, the understanding of turbulence modeling for compressor tip leakage flows is advanced. The proposed upgraded DDES method is promising for generating a larger turbomachinery turbulence database.

In the second part of the thesis, comprehensive uncertainty quantification and evaluation studies have been performed on the model coefficients and the model forms of the Spalart-Allmaras turbulence model. Results indicate that a data-driven correction at the transport equation level is most promising for compressor stall prediction. However, established empirical corrections fail to capture the flow features of 2D transonic flows and 3D separated flows. To tackle these limitations, two novel flow features namely baroclinicity and vortical pressure gradient are proposed, respectively. Modified turbulence model forms (i.e., SA-B and SA-PG $_{\omega}$) are proposed with respect to each of these new flow features, and the newly emerged model coefficients are calibrated with relevant flow data. The calibrated models demonstrate great improvement in prediction accuracy in similar but unseen flow cases. In particular, the SA-PG $_{\omega}$ model demonstrates adequate accuracy in predicting the stall boundary of a range of compressors. This modified model is the most useful contribution of the thesis.

In the last part of the thesis, a data-driven turbulence modeling framework is established and demonstrated in 2D transonic flows. Methods that improve the explainability of the trained machine learning model are applied, and the causal link between the input flow features and the output eddy viscosity difference of the trained machine learning model is explained. It is found that the trained machine learning model re-discovered (1) the scaling between the eddy viscosity and its source term and (2) the effect of shear and rotation on the eddy viscosity source term, which are well-known for human turbulence model developers. The presented method is transferable to a general data-driven turbulence model, and it can help industrial users build trust in the data-driven turbulence model.

The methods and knowledge obtained from the thesis provide engineering solutions for compressor stall prediction.

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“夫夷以近，則遊者眾；險以遠，則至者少。而世之奇偉瑰怪非常之觀，常在於險遠，而人之所罕至焉。故非有志者不能至也。”

— 王安石,《遊褒禪山記》

“It is regrettable that numerous are excursionists visiting places which are near and easily accessible, but few are travelers who come to places far and dangerous, which, nevertheless, command the most sublime, grotesque and unique views, scarcely enjoyed by ordinary folks. One can never reach such places unless one has strong willpower.”

— Anshi Wang, *A Visit to Baochan Mountain*

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1. Introduction

1.1 Motivation of Research

Axial compressors and fans are essential components of an aero-engine in the modern aviation industry. When the compressor operates beyond its flow stability boundary, the engine stalls, surges and eventually breaks down, leading to catastrophic outcomes. Thus, a reliable method to predict the occurrence of compressor flow instability is of great interest to compressor aero-designers.

The challenge of predicting compressor flow instability using computational fluid dynamics (CFD) lies in the turbulent flow across scales in compressor passages. Resolving full scales of turbulence via direct numerical simulation (DNS) is intractable due to the limited computation capacity and the tremendous cost. The conventional engineering approach is to solve the Reynolds-Averaged Navier-Stokes (RANS) equations with a turbulence model, which is based on a combination of flow physics, intuition, and empiricism. Through this approach, the compressor performance can be better predicted compared to empirical equations and inviscid simulations, and the mean flow physics of compressors can be visualized. When it comes to the operating conditions near the stability limit, however, existing RANS turbulence models often predict the compressor stability boundary at a higher mass flow rate (i.e., a lower incidence angle) than the experimentally measured stall line [1], especially at low speeds. This deficiency of turbomachinery RANS simulations is illustrated in the compressor map of Fig. 1.1, where the outlet-to-inlet total pressure ratio is plotted against the mass flow rate at constant speeds. The underlying reason is deduced to be the ineffectiveness of RANS turbulence models in 3D separated flows [1, 2], which were not considered in the development phase of these models.

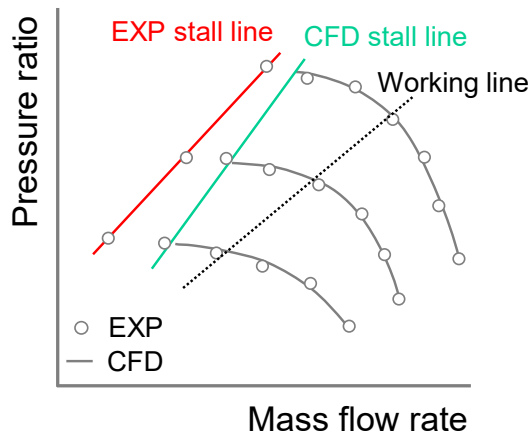


Figure 1.1: Illustration of the compressor stall line.

Recently, data science tools such as uncertainty quantification and machine learning have achieved great success in many applications. It is natural to expect that data science can also

play a role in the complex non-linear regression problem of turbulence modeling. Previous research [3] has proved this concept in a range of canonical 2D separated flows with different approaches. *Is it possible to push this concept towards higher technology readiness level and improve the prediction accuracy of compressor stall boundary?*

This thesis will present novel concepts, original methods, and efficient data generation algorithms for the development of a predictive, reusable, and explainable data-driven turbulence model for better prediction of compressor stall. It is among the very first works that explore a data-driven turbulence model solution for turbomachinery flows.

1.2 Hypothesis and Objectives

The hypothesis of the thesis is that: the deficiency of the established RANS turbulence models in compressor stall prediction can be alleviated by using a data-driven correction model with a high-fidelity turbulence database. It should be reminded that other factors such as grid resolution and boundary conditions can also affect the compressor stall prediction. These factors are mitigated by using fine grid resolution and realistic boundary conditions throughout this research.

To prove the above hypothesis, the following objectives need to be met:

1. Devise a cost-effective scale-resolving CFD method for turbomachinery based on the understanding of turbomachinery flows.
2. Evaluate the effects of empiricism in the turbulence model coefficients and the turbulence model forms on compressor stall prediction.
3. Propose mean flow features that capture the physics of compressor stall.
4. Prove the concept of a data-driven correction model and justify the model using physical explanations.

These objectives highlight the importance of physical understanding, which from the perspective of the author is the key to its successful application to industrial flows.

1.3 Thesis Outline

In an attempt to achieve the aforementioned objectives, the thesis is structured as follows:

- Chapter 2 presents an essential literature review of compressor flow instability, turbulence modeling from first principles, and turbulence modeling in the age of data. It provides the necessary background knowledge for the thesis.
- Chapter 3 introduces the RANS flow solver algorithms and the machine learning models used in this thesis. It also presents a collection of canonical cases, airfoil cases, and compressor cases in ascending order of flow complexity. These flow cases will be used for the development or validation of turbulence models in the following chapters.

- Chapter 4 presents the development of an upgraded delayed detached eddy simulation (DDES) solver tailored for compressor tip leakage flows. This upgraded DDES method provides a cost-effective means of scale-resolving simulation of turbomachinery flows. In the first place, the method is validated for a backward-facing step and a low-speed axial compressor rotor. Then, it is used to generate a turbulence database of the low-speed compressor rotor. Based on this database, an in-depth analysis of the mean flow, turbulence statistics, and modal behavior of compressor tip leakage flow is performed, which provides hints for turbulence model developments.
- Chapter 5 presents a comprehensive uncertainty quantification (UQ) study on the parametric uncertainty of the Spalart-Allmaras turbulence model. The parametric uncertainty is quantified in mildly separated 2D canonical flows, 2D subsonic airfoil stall, and 3D transonic compressor stall in ascending order of flow complexity. This study explores the potential of using a data-driven correction to the turbulence model coefficients. It also provides an understanding of the effect of different turbulence model transport equation terms (i.e., production, destruction, diffusion) in predicting mild/strong separations in 2D/3D flows.
- Chapter 6 evaluates established empirical modifications to the Spalart-Allmaras turbulence model for compressor stall prediction. This is intended to explore whether using a data-driven correction in the constitutive equation or in the transport equation will lead to a better prediction of compressor stall. The evaluation is performed in a range of compressor-like canonical flows and a transonic compressor. Results show that established modifications fail to improve the prediction accuracy in transonic flows and 3D-separated flows. To tackle these inaccuracies, novel modifications to the turbulence model are proposed, which are based on baroclinicity and vortical pressure gradients. The coefficients of the models are calibrated from relevant high-fidelity mean flow data. The proposed new models show great improvement in predicting similar but unseen flows. These novel modifications provide new input flow features for a data-driven turbulence model.
- Based on the understanding from Chapter 4, 5 and 6, Chapter 7 establishes a data-driven turbulence model framework and proves its concept in 2D transonic flows. The framework introduces a data-driven correction term that provides a functional mapping between the input flow features and the output eddy viscosity difference between the high-fidelity and the low-fidelity data. Based on this framework, methods that can improve the explainability of a machine learning model are applied, and the causal link between the input and the output of the trained machine learning turbulence model is explained.
- Finally, Chapter 8 concludes the major findings of the thesis and proposes follow-up future works.

1.4 Publications

The work presented in the thesis has been partially published in multiple peer-reviewed journals and conferences. A complete list of the publication in reverse chronological order is provided below. In this list, a paper that has been both presented at a conference and published in a journal is counted as one item; the notation “*” represents “corresponding author”, and “†” indicates “equal contribution”.

1. **He, X.***, Zhao, F., and Vahdati, M., “A Turbo-Oriented Data-Driven Modification to the Spalart-Allmaras Turbulence Model,” *ASME Journal of Turbomachinery*, 2022, 144(12), 121007.

He, X.*, Zhao, F., and Vahdati, M., “A Turbo-Oriented Data-Driven Modification to the Spalart-Allmaras Turbulence Model,” *Proceedings of the ASME Turbo Expo 2022: Turbomachinery Technical Conference and Exposition*. Volume 2D: Turbomachinery. Rotterdam, Netherlands. June 13–17, 2022. ASME Paper No. GT2022-80456. **ASME IGTI Committee Best Paper Finalist**.
2. **He, X.***, Tan, J., Rigas, G., and Vahdati, M., “On the Explainability of Machine-Learning-Assisted Turbulence Modeling for Transonic Flows,” *International Journal of Heat and Fluid Flow*, 2022, 97, 109038.

Tan, J.†, **He, X.*†**, Vahdati, M., and Rigas, G., “Towards Explainable Machine Learning Assisted Turbulence Modelling for Transonic Flows,” *Proceedings of the 14th European Conference on Turbomachinery Fluid Dynamics & Thermodynamics*. Virtual, Online. April 12-14, 2021. ETC Paper No. ETC2021-490.
3. **He, X.***, Zhao, F., and Vahdati, M., “Detached Eddy Simulation: Recent Development and Application to Compressor Tip Leakage Flow,” *ASME Journal of Turbomachinery*, 2022, 144(1), 011009.

He, X.*, Zhao, F., and Vahdati, M., “Detached Eddy Simulation: Recent Development and Application to Compressor Tip Leakage Flow,” *Proceedings of the ASME Turbo Expo 2021: Turbomachinery Technical Conference and Exposition*. Volume 2C: Turbomachinery. Virtual, Online. June 7–11, 2021. V02CT34A011. ASME Paper No. GT2021-59077. **ASME IGTI Committee Best Paper Recommendation**.
4. **He, X.***, Fang, Z., Rigas, G., and Vahdati, M., “Spectral Proper Orthogonal Decomposition of Compressor Tip Leakage Flow,” *Physics of Fluids*, 2021, 33(10), 105105.

He, X.*†, Fang, Z.†, Vahdati, M., and Rigas, G., “Spectral Proper Orthogonal Decomposition of Compressor Tip Leakage Flow,” *Proceedings of the 14th European Conference on Turbomachinery Fluid Dynamics & Thermodynamics*. Virtual, Online. April 12-14, 2021. ETC Paper No. ETC2021-491.
5. **He, X.***, Zhao, F., and Vahdati, M., “Evaluation of Spalart-Allmaras Turbulence Model Forms for a Transonic Axial Compressor,” *Proceedings of the Global Power and Propulsion Society Chania Conference 2020*. Virtual, Online. September 7-9, 2020. GPPS Paper No. GPPS-CH-2020-0013.
6. **He, X.***, Zhao, F., and Vahdati, M., “Uncertainty Quantification of Spalart-Allmaras Turbulence Model Coefficients for Compressor Stall,” *ASME Journal of Turbomachinery*, 2021, 143(8), 081007.

He, X.*, Zhao, F., and Vahdati, M., “Uncertainty Quantification of Spalart-Allmaras Turbulence Model Coefficients for Compressor Stall,” *Proceedings of the ASME Turbo Expo 2020: Turbomachinery Technical Conference and Exposition*. Volume 2C: Turbomachinery. Virtual, Online. September 21–25, 2020. V02CT35A028. ASME Paper No. GT2020-15014. **ASME IGTI Committee Best Paper Recommendation**.
7. **He, X.***, Zhao, F., and Vahdati, M., “Uncertainty Quantification of Spalart-Allmaras Turbulence Model Coefficients for Simplified Compressor Flow Features,” *ASME Journal of Fluids Engineering*, 2020, 142(9), 091501.

He, X.^{*}, Zhao, F., and Vahdati, M., “Machine Learning Uncertainty Quantification of Spalart-Allmaras Turbulence Model for Compressors,” Proceedings of the Global Power and Propulsion Society Beijing Conference 2019. Beijing, China. September 16-18, 2019. GPPS Paper No. 2019-BJ-0050.

In addition to the above publications, part of the methods and the data from this thesis were transferred to other research projects, yielding the following joint publications. These works are excluded from the current thesis.

1. He, X.^{*†}, Zhu, M.[†], Xia, K., Klausmann, F., Teng, J., and Vahdati, M., “Validation and Verification of RANS Solvers for TUDa-GLR-OpenStage Transonic Axial Compressor,” Journal of the Global Power and Propulsion Society, 2023, 7, 13-29.
Zhu, M., He, X.^{*}, Klausmann, F., Teng, J., and Vahdati, M., “Validation and Verification of RANS Solvers for TUDa-GLR-OpenStage Transonic Axial Compressor,” Proceedings of the Global Power and Propulsion Society Xi’an Conference 2021. Virtual, Online. April 11-13, 2022. GPPS Paper No. GPPS-TC-2021-0050.
2. Xia, K., He, X.^{*}, Zhu, M., Klausmann, F., Teng, J., and Vahdati, M., “Endwall Geometric Uncertainty and Error on the Performance of TUDA-GLR-OpenStage Transonic Axial Compressor,” 2023, Journal of the Global Power and Propulsion Society. (accepted).
Xia, K., He, X.^{*}, Zhu, M., Klausmann, F., Teng, J., and Vahdati, M., “Endwall Geometric Uncertainty and Error on the Performance of TUDA-GLR-OpenStage Transonic Axial Compressor,” Proceedings of the Global Power and Propulsion Society Chania Conference 2022. Chania, Greece. September 12-14, 2022. GPPS Paper No. GPPS-TC-2022-0126.
3. Wang, R.[†], He, X.[†], and Yan, X., “Spectral Proper Orthogonal Decomposition of Trailing Edge Cutback Film Cooling Flows,” Physics of Fluids, 2022, 34(10), 105106.
4. He, X.[†], Rauseo, M.[†], Rendu, Q.[†], Salles, L.[†], Vahdati, M.[†] and Zhao, F.[†], “Turbomachinery Aerodynamic and Aeromechanic Prediction in the Age of Data”, Proceedings of the 16th International Symposium on Unsteady Aerodynamics, Aeroacoustics and Aeroelasticity of Turbomachines. Toledo, Spain. September 19-23, 2022. ISUAAAT Paper No. ISUAAAT16-053.
5. Wang, J., He, X., Wang, B., and Zheng, X., “Shapley Additive Explanations of Multi-Geometrical Variable Coupling Effect in Transonic Compressor,” ASME Journal of Engineering for Gas Turbines and Power, 2022, 144(4), 041015.

2. Literature Review

“If I have seen further, it is by standing upon the shoulders of giants.”

— Isaac Newton, Letter to Robert Hooke

2.1 Compressor Flow Instability

2.1.1 Flow Physics

When reducing the compressor mass flow rate at a constant rotational speed, the incidence of the compressor blade increases. On the one hand, it increases the compressor work input and thus the pressure ratio. On the other hand, it also enlarges the separation in the compressor passage, reducing the compressor isentropic efficiency and thus the pressure ratio. Due to the trade-off effect of the two mechanisms, a peak pressure ratio must exist. By convention, the peak pressure ratio condition is defined as the compressor stall condition.

The compressor undergoes a series of flow instability when throttling from the peak efficiency condition to the post-stall condition. In ascending order of spatial and temporal scales, these flow instabilities include rotating instability, rotating stall, and surge, as illustrated in Fig. 2.1. A brief introduction to each type of flow instability is given as follows.

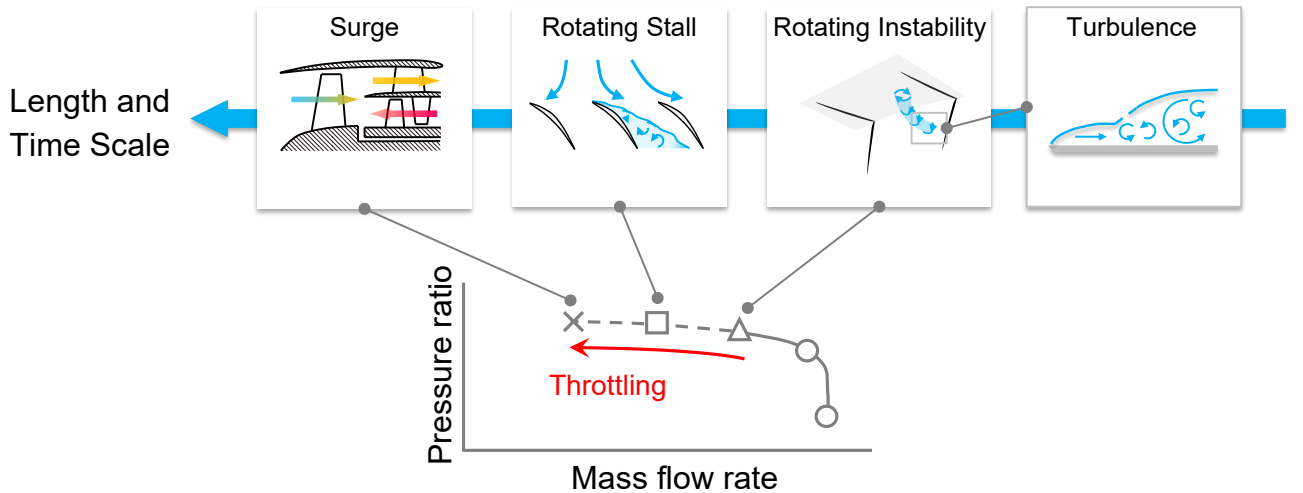


Figure 2.1: Evolution of the compressor flow instability.

Rotating instability, also known as rotating disturbance, is a pre-stall disturbance that can occur before the maximum pressure rise of the compressor is reached. The nature of

rotating instability is a large-scale coherent vortical structure. Specifically, it corresponds to the circumferential movement of a tornado-shape vortex, which connects the blade suction surface and the casing wall (see Fig. 2.1) [4, 5]. It only exists near the tip section of a rotor with a large tip gap (i.e., over 3% of the tip chord length [2]). The spatial and temporal scales of rotating instability are in the same order of magnitude as the rotor pitch and the blade passing period, respectively. These scales continually vary in time, creating a hump in the frequency spectrum. From an aerodynamic perspective, rotating instability is actually a stable state, because the compressor can stably operate at this condition without evident fluctuations in pressure ratio and mass flow. The outcome of rotating instability is only an increased level of noise and vibration [6], which is difficult to detect without intrusive pressure transducers. Hence, there is still some debate on the use of “instability” in this terminology [2]. From an aeroelastic perspective, however, rotating instability can trigger non-synchronized vibration, which increases the risk of high cycle fatigue [7].

Rotating stall describes the rotation of single or multiple stall cells (i.e., low-momentum blockage cells) around the compressor circumference, which limits the maximum pressure rise of the compressor. Its spatial and temporal scales are in the same order of magnitude as the compressor circumference and the rotor passing period, respectively. The well-known phenomenological model of rotating stall was proposed by Emmons [8]: when the first stall cell is formed in an arbitrary blade passage, the incoming flow of the current blade passage is blocked, leading to a sudden increase of incidence in the next blade passage opposite to the blade rotation direction; thus the stall cell rotates in the opposite direction of blade rotation when observing from the relative frame (see Fig. 2.1).

The formation of the first stall cell is of particular interest in the following research. Two types of stall inception mechanisms have been identified so far, namely modal-type stall inception and spike-type stall inception. Modal-type stall inception is a two-dimensional, low amplitude, and long-length scale perturbation that takes over tens of rotor revolutions to develop into a mature stall cell [9]. It usually exists at a zero or slightly positive slope of the compressor pressure rise characteristics. The evolution of the modal perturbation can be theoretically modeled [10, 11] and thus can be suppressed under an active control framework [12]. Spike-type stall inception is a three-dimensional, high amplitude, and short-length scale perturbation that develops into a mature stall cell within five rotor revolutions [13]. It normally occurs at a negative slope of the compressor pressure rise characteristics. The nature of spikes is the formation of a near-tip tornado-shape vortex that induces sudden blockage of the passage [14], which is an ephemeral version of the vortex related to rotating instability. Because of its fast growth rate, the spike-type stall inception cannot be actively controlled yet. For modern multi-stage high-speed compressor design, rotating stall is mostly triggered by spikes [13]. The stall inception location can be either in a rotor or a stator and either near-hub or near-tip [15, 16], depending on the design, the matching, and the operating speed of the compressor.

Surge is the streamwise flow breakdown of the compression system accompanied by large oscillations of flow properties. Its spatial and temporal scales are in the same order of magnitude as the compressor axial length and the Helmholtz oscillation period of the compression system, respectively. The nature of surge can be well-explained via a lumped parameter model proposed by Gretizer [17], where the dynamic response of a compression system is modeled in a similar fashion to a mass-spring-damper system. Therefore, the filling and the discharge of flow in a compression system can be physically viewed as the vibration of a mass attached to a damper and a spring. The form and the strength of surge oscillations can be further determined by the

non-dimensional B parameter, which is the ratio of the pressure force to the inertia force as deduced from the lumped parameter model. A low value of B indicates that rotating stall is first reached when throttling the compressor; a medium value corresponds to mild surge without reverse flow; a high value corresponds to deep surge with reverse flow. The outcome of surge is often disastrous. The engine cold section will be damaged by the reverse high-temperature flow from the engine hot section. Such a flow reversal is often visible when an engine spits out a fire, where the air-fuel mixture reverses back from the core engine, enters the bypass duct, and finally burns at the exhaust duct (see Fig. 2.1). Moreover, a violent periodic axial force will be induced during the surge cycles, which damages the shaft system. A violent radial force will also be induced at the axisymmetric surge onset, leading to the blade rubbing and the deformation of the casing [18].

2.1.2 Role of Turbulence

Turbulence is a chaotic state of fluid motion that involves violent fluctuations of flow velocity and pressure. It is composed of multi-scale swirling vortices leading to enhanced mixing of mass, momentum, and energy. Flow regimes of laminar flow and turbulent flow can be distinguished by the non-dimensional Reynolds number (Re), which is the ratio of the inertia force to the viscous force. When the Reynolds number surpasses a critical value, the laminar-to-turbulent transition occurs.

The effect of turbulence on the stall inception was first noticed in early-time wind tunnel tests of airfoils. In Fig. 2.2, the stall angle of attack of various airfoils is plotted against the Reynolds number based on the experimental data [19–21]. At low Reynolds numbers, laminar separation occurs near the leading edge of the airfoil, resulting in an airfoil stall at a relatively small angle of attack. Increasing the Reynolds number over a critical value (i.e. 10^5 to 10^6) will produce turbulence before the separation point, which energizes the boundary layer, pushes the separation point rearward towards the trailing edge, and thus delays the stall inception to a much higher angle of attack.

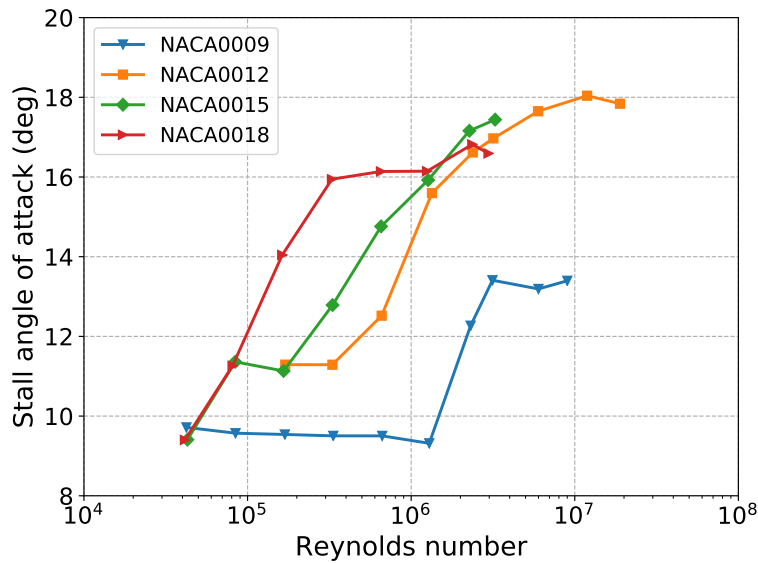


Figure 2.2: Effect of Reynolds number on stall angle of attack of NACA airfoils at free transition and subsonic conditions.

The effect of turbulence on the stall inception of compressors is more complex than that of airfoils because the evolution of compressor flow instability usually involves large-scale 3D vortical structures. In numerical simulations, different levels of turbulence intensity can be achieved by using different RANS turbulence models. Effects of RANS turbulence models on predicting the tip leakage flow [22] and the hub corner separation [23, 24] in compressors have been examined. It was concluded that the trajectory of the tip leakage vortex and the size of the corner separation are both very sensitive to the choice of turbulence model. Considering the importance of tip leakage flow and hub corner separation to the evolution of compressor flow instability, a significant effect of turbulence on the compressor stall margin is expected.

Performance characteristics of two typical axial compressors, namely NASA Rotor 37 and NASA Rotor 67, are presented in Fig. 2.3 based on experimental data [25, 26] and simulation data [27, 28]. It is illustrated that turbulence models have a crucial effect on predicting the compressor near-stall performances, and the predicted stability boundary can vary significantly. Table 2.1 summarizes the variation of stall mass flow of both NASA rotors and other compressors. In axial compressors, it is generally found that a different choice of turbulence model yields a 10% to 20% variation of stall mass flow normalized by the stable mass flow range. Such a variation is even stronger in radial compressors where the secondary flow is more pronounced.

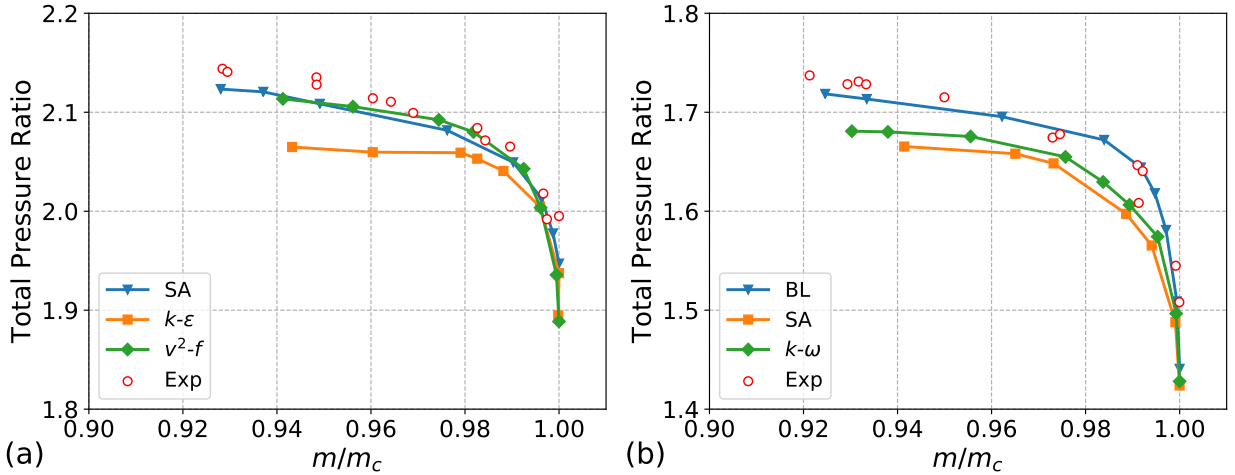


Figure 2.3: Effect of different turbulence models on predicting the pressure characteristics of (a) NASA Rotor 37 and (b) NASA Rotor 67.

Table 2.1: Sensitivity of turbulence models to compressor stall mass flow.

Case Description	Turbulence Models	$\Delta m_s / (m_c - m_s)$	Reference
Axial Rotor	SA, $k-\epsilon$, v^2-f	18.3%	Haase et al. [27]
Axial Rotor	BL, SA, $k-\omega$	20.8%	Schneider et al. [28]
Axial 1-Stage	$k-\omega$, $k-l$	13.2%	Gourdain [29]
Axial 8-Stage	$k-\omega$, SST, EARSM	10.8%	Wang et al. [30]
Radial 1-Stage	$k-\epsilon$, SST, RSM	72.6%	Bourgeois et al. [31]

2.2 Turbulence Modeling from First Principles

2.2.1 Direct Numerical Simulation

The motion of fluid, regardless of turbulent or laminar flow regimes, is governed by the Navier-Stokes (NS) equations. The momentum component of the three-dimensional NS equation writes as Eq. (2.1):

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \quad (2.1)$$

where τ_{ij} denotes the shear stress tensor induced by molecular viscosity. For a Newtonian fluid with the Stokes hypothesis, τ_{ij} can be calculated by Eq. (2.2):

$$\tau_{ij} = 2\rho\nu S_{ij}^* \quad (2.2)$$

with the traceless strain rate tensor S_{ij}^* defined in Eq. (2.3):

$$S_{ij}^* = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{1}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij} \quad (2.3)$$

Noticing that the momentum equation together with the continuity equation, the energy equation, and the equation of state have 6 unknown variables (i.e., p, ρ, T, u_x, u_y and u_z) and 6 independent equations, there is no closure issue in the NS equations. Thus, it is possible to solve this set of equations directly to simulate turbulent flow. Such an approach is known as direct numerical simulation (DNS).

Although DNS is conceptually simple, its application is rather difficult due to the range of turbulence scales to be resolved. It was demonstrated by Pope [32] that the numerical resource needed for DNS is proportional to Re^3 based on the smallest turbulence length scale (i.e., Kolmogorov length scale) of $\text{Re}^{-\frac{3}{4}}$. For boundary layer flows, the grid point required by DNS is proportional to $\text{Re}^{37/14}$ [33], resulting in the required numerical resource being scaled to $\text{Re}^{3.5}$ when considering the Courant–Friedrichs–Lewy (CFL) condition. The typical Reynolds number of an aero-engine compressor ranges from 10^6 to 10^7 [34], which is far too expensive for DNS applications. The state-of-the-art practice of DNS is restricted to part-span low-speed compressor cascades at mildly separated operating conditions [35–39]. To provide a rule of thumb for the numerical resources required by DNS, detailed numerical setups of these studies are summarized in Table 2.2.

Table 2.2: Summary of state-of-the-art practices of DNS for compressor applications.

Case	Re_c	Span	Grid No.	Spatial accuracy	Year	Ref.
NACA65 cascade	1.4×10^5	20% c_x	8.5×10^7	2 nd order	2010	[35]
SMURF stator	3.4×10^5	10% c_x	6.3×10^7	4 th order	2018	[36]
NACA65 cascade	1.4×10^5	10% c_x	1.0×10^8	4 th order	2021	[37]
NACA65 cascade	1.4×10^5	10% c_x	1.3×10^8	4 th order	2020	[38]
CDA cascade	2.5×10^5	15% c_x	1.7×10^8	4 th order	2020	[38]
TU Dresden cascade	2.2×10^5	82% c_x	3.5×10^8	2 nd order	2021	[39]

2.2.2 Reynolds-Averaged Navier-Stokes Simulation

For engineering applications, it is often the mean flow quantities, such as the pressure ratio and the isentropic efficiency of a compressor, that are of most interest. The small-scale turbulence resolved by DNS is often not needed from this perspective. To reduce the computation cost of DNS, a solution is to decompose the flow quantity into a mean term and a fluctuation term, such as the Reynolds decomposition of Eq. (2.4) and the Favré decomposition of Eq. (2.5):

$$\phi(\mathbf{x}, t) = \bar{\phi}(\mathbf{x}, t) + \phi'(\mathbf{x}, t) \quad (2.4)$$

$$\phi(\mathbf{x}, t) = \tilde{\phi}(\mathbf{x}, t) + \phi''(\mathbf{x}, t) \quad (2.5)$$

$$\bar{\phi}(\mathbf{x}, t) = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \phi^{(n)}(\mathbf{x}, t) \quad (2.6)$$

$$\tilde{\phi}(\mathbf{x}, t) = \frac{\overline{\rho\phi}(\mathbf{x}, t)}{\bar{\rho}} \quad (2.7)$$

where $\bar{(\cdot)}$ and $\tilde{(\cdot)}$ denote the ensemble-averaged quantity and the density-weighted ensemble-averaged quantity, respectively. Applying the Favré decomposition to the NS equation of Eq. (2.1), the general compressible Reynolds-Averaged Navier Stokes (RANS) equation is obtained as Eq. (2.8):

$$\frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i \tilde{u}_j}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \bar{\tau}_{ij}}{\partial x_j} + \frac{\partial (-\overline{\rho u_i'' u_j''})}{\partial x_j} \quad (2.8)$$

where the symmetric Reynolds stress tensor $\tau_{ij}^{RANS} \equiv -\overline{\rho u_i'' u_j''}$ arises due to the non-linear nature of the advection term $u_i u_j$. This tensor represents the shear stress induced by turbulent fluctuations, and it has six independent elements that need to be closed via a turbulence model.

A straightforward way to model τ_{ij}^{RANS} is to introduce six transport equations for each independent element of τ_{ij}^{RANS} . Such a model is called a Reynolds stress model (RSM). The pioneering work from Chou [40] obtained these transport equations by manipulating the transport equations of the mean flow and the fluctuation. However, there are still higher order non-linear terms (i.e., $\overline{\rho u_i'' u_j'' u_k''}$) that must be modeled with assumptions. Later, a complete RSM was proposed by Launder et al. [41]. This model is conceptually predictive because it rigorously considers the effects of turbulence anisotropy, streamline curvature and rotation. However, the accuracy of the RSM is not always superior to its counterparts [34]. Besides, the RSM is still computationally expensive as more than ten partial differential equations (PDE) need to be solved at the same time. Therefore, the RSM is not widely applied to turbomachinery flows.

A more efficient and popular approach to model τ_{ij}^{RANS} is based on the concept of eddy viscosity (or turbulent viscosity), which assumes the effect of turbulent fluctuations on the mean flow is similar to that of molecular viscosity. Therefore, a linear constitutive relation similar to Eq. (2.2) can be used, as shown in Eq. (2.9):

$$\tau_{ij}^{RANS} = 2\rho\nu_t S_{ij}^* - \frac{2}{3}\rho k \delta_{ij} \quad (2.9)$$

which is also known as the Boussinesq assumption. Here, the symbols $\bar{(\cdot)}$ and $\tilde{(\cdot)}$ of mean flow quantities are removed for simplicity. This equation introduces six independent equations but

also two extra scalar variables namely the eddy viscosity ν_t and the turbulence kinetic energy k . Thus, the RANS closure problem has been simplified to the modeling of ν_t and k .

The easiest approach to do so is to directly calculate the eddy viscosity from the flow variables without solving a transport equation. Examples include the pioneering mixing length model from Prandtl [42] and later a zonal version named the Baldwin-Lomax (BL) model [43]. The other approach involves the construction of one or several transport equations, such as the transport equation of the modified turbulent viscosity for the one-equation Spalart-Allmaras (SA) model [44], the turbulence kinetic energy and the turbulence dissipation rate for the two-equation k - ϵ model [45], and the turbulence kinetic energy and the specific turbulence dissipation rate for the two-equation k - ω model [46] and shear stress transport (SST) model [47].

Increasing the number of the transport equation conceptually enables more flow physics to be considered, which potentially improves the prediction accuracy. This hypothesis is partially supported by the investigation of airfoil flows [48], where the two-equation SST model showed a closer agreement with the experimental results than the one-equation SA model. However, both the SA and the SST model show deficiencies in compressor flow: regarding the tip leakage flow, the SA model predicts the most accurate tip leakage vortex trajectory at the design condition, but the SST model provides the best result at the near-stall condition [22]; regarding the hub corner separation, both the SA model and the SST model over-predict the separation size [23, 24]. Thus, there is not yet a best RANS turbulence model for compressor applications.

The linear correlation in the Boussinesq assumption of Eq. (2.9) enforces the anisotropy of the Reynolds stress tensor to be the same as that of the strain rate tensor, which is not exactly true when there are sudden changes in mean strain rate (e.g., flow with rotation, curvature, strong three-dimensionality or boundary layer separation, etc.) [49]. Thus, efforts toward a nonlinear eddy viscosity model have been made, including the SA model with a quadratic constitutive relation (SA-QCR) [50], the v^2 - f model [51] developed from the k - ϵ model, and the explicit algebraic Reynolds stress (EARS) model [52, 53] developed from the k - ω model. These models are more capable in flows with strong anisotropy, but they run at a higher computational cost than their predecessors.

A summary of the RANS turbulence models is given in Fig. 2.4. Detailed introductions to most of the models can be found in the book of Wilcox [49], the Turbulence Modeling Resource website [54] and the CFD-Wiki website [55].

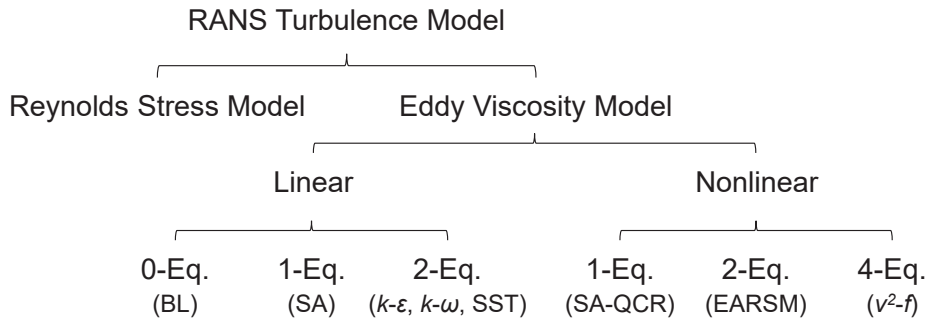


Figure 2.4: Classification of RANS turbulence models.

2.2.3 Large Eddy Simulation

Although the RANS simulation has become the workhorse in fluids engineering, it showed unsatisfactory results when the turbulent mixing process is of most concern (e.g., turbulent combustion, turbine film cooling, etc.). There is a natural glass ceiling for the accuracy of RANS models due to the loss of information during the Reynolds averaging process. To conquer that limit, large eddy simulation (LES) was developed. The core idea of LES is to filter out small-scale vortices using a given length scale: the effect of small scales on the mean flow is modeled by a subgrid-scale (SGS) model, whereas the large scales are directly resolved. Thus, a flow quantity can be decomposed into a resolved part and an unresolved part, such as the filter decomposition of Eq. (2.10) and the density-weighted filter decomposition of Eq. (2.11):

$$\phi(\mathbf{x}, t) = \bar{\phi}(\mathbf{x}, t) + \phi'(\mathbf{x}, t) \quad (2.10)$$

$$\phi(\mathbf{x}, t) = \tilde{\phi}(\mathbf{x}, t) + \phi''(\mathbf{x}, t) \quad (2.11)$$

$$\bar{\phi}(\mathbf{x}, t) = \int_{-\infty}^{+\infty} \phi(\mathbf{r}, t) G(\mathbf{x} - \mathbf{r}, t) d\mathbf{r} \quad (2.12)$$

$$\tilde{\phi}(\mathbf{x}, t) = \frac{\bar{\rho}\phi(\mathbf{x}, t)}{\bar{\rho}} \quad (2.13)$$

where $(\bar{\cdot})$ and $(\tilde{\cdot})$ denote the resolved component of a quantity, and $G(\cdot)$ denotes the filter function. A typical choice of the filter function is the box filter:

$$G(x) = \begin{cases} \frac{1}{\Delta}, & |x| \leq \frac{\Delta}{2} \\ 0, & |x| > \frac{\Delta}{2} \end{cases} \quad (2.14)$$

with Δ denotes the grid length scale. When Δ is infinitely small, the LES result becomes comparable to DNS.

Applying the density-weighted filter decomposition to the NS equation of Eq. (2.1), the filtered compressible Navier-Stokes equation is obtained as Eq. (2.15):

$$\frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i \tilde{u}_j}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \bar{\tau}_{ij}}{\partial x_j} + \frac{\partial (-\bar{\rho} \widetilde{u_i u_j} + \bar{\rho} \tilde{u}_i \tilde{u}_j)}{\partial x_j} \quad (2.15)$$

where a residual tensor term is generated after the filter operation. This tensor is called the SGS stress tensor. Similar to the RANS equation in Eq. (2.8), the filtered Navier-Stokes equation in Eq. (2.15) also has a closure problem, and an SGS turbulence model is required for closure. The physical relevance of an SGS turbulence model is to model the dissipation of vortices with subgrid scales, rather than the influence of the subgrid scales on the resolved scales. The accuracy of LES is mainly dependent on the grid size rather than the SGS turbulence model. Thus, most SGS turbulence models are comparatively simple based on the Boussinesq assumption with zero or one transport equation to be solved [32].

The drawback of LES is still the intensive numerical resources required. Due to the small-scale vortices of near-wall flows, the total number of grid points required by a wall-resolved LES (WRLES) is proportional to $\text{Re}^{13/7}$ [33], leading to the required numerical resource of $\text{Re}^{2.5}$ considering the CFL condition. It was estimated by Spalart [50] that the WRLES for an airliner would not be ready until the year 2045, which is even an optimistic estimation

considering Moore's law [56] may fail by 2025 [57]. Thus, a massive practice of WRLES on compressor flows is likely not realistic in the foreseeable future.

A solution to relieve the numerical cost of WRLES is to model the near-wall region while keeping the far-wall region resolved out (i.e., wall-modeled LES, or WMLES). WMLES can reduce the required total number of grid points to be proportional to Re [33], which results in the required numerical resource of $Re^{4/3}$ considering the CFL condition. In general, there are three types of methods to model the near-wall flow, namely the wall function method, the thin boundary layer method, and the hybrid RANS/LES method in ascending order of accuracy and required computational resources [58]. A detailed classification of the LES methods is given in Fig. 2.5.

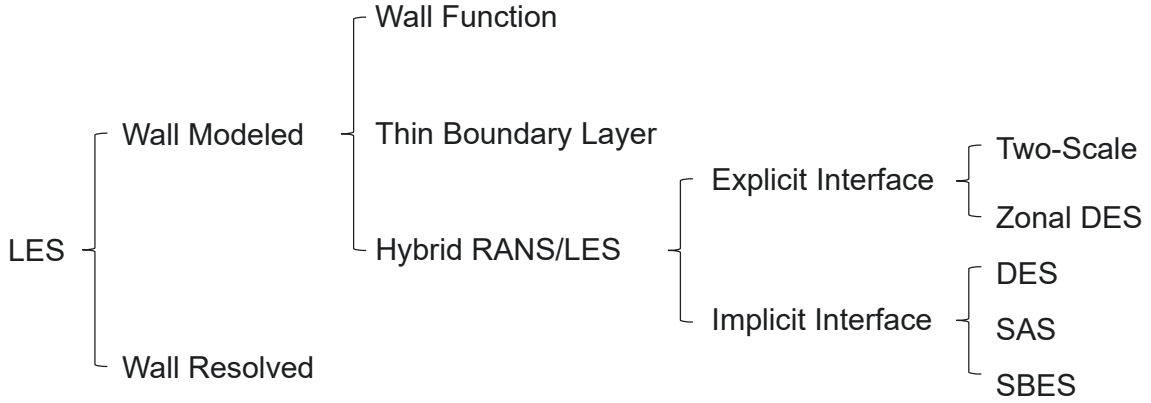


Figure 2.5: Classification of LES methods.

The wall function method presumes the near-wall velocity distribution based on the boundary layer log-law, by which the wall shear stress can be directly calculated to serve as the boundary condition. For this approach, the first layer of the mesh can be set away from the wall (i.e., $y^+ > 10$) as illustrated in Fig. 2.6(a). Thus, the number of grid points is reduced. The weakness of the wall function method is twofold. Firstly, the boundary layer log-law does not hold true when there are strong pressure gradients, 3D mean flows, or flow separations [58], which induces near-wall error that propagates to the whole flow field. Secondly, the wall function enforces the wall-normal component of velocity to be zero, which is physically wrong at $y^+ \sim 10^2$ due to the existence of three-dimensional vortex structures (i.e., boundary layer streaks) [59].

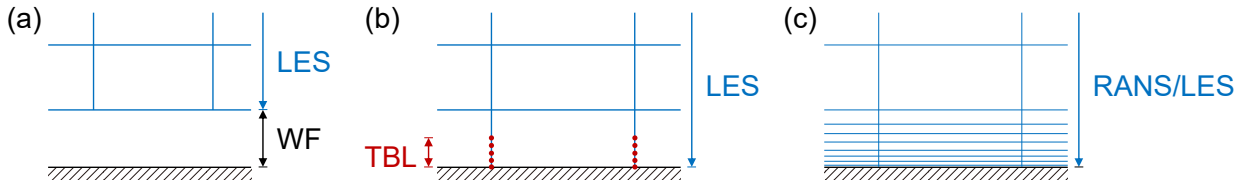


Figure 2.6: Illustration of near-wall mesh for (a) the wall function (WF) method, (b) the thin boundary layer (TBL) method and (3) the hybrid RANS/LES method.

The thin boundary layer method takes a step further from the wall function method. Instead of presuming the near-wall velocity profile, the thin boundary layer method resolves it by solving the RANS turbulent boundary layer equations based on the embedded mesh grids.

A typical mesh for this method is presented in Fig. 2.6(b). The challenge of this method is to determine the thickness of the thin boundary layer in advance, which should be close to the wall so that the approximation of a constant stress layer still holds true. Otherwise, the predicted velocity profile will be shifted upward (i.e., log-layer mismatch) [59].

The most trending WMLES method is the hybrid RANS/LES method. Depending on how the RANS/LES interface is determined, this branch of methods can be further classified into an explicit interface branch and an implicit interface branch.

The hybrid RANS/LES methods with an explicitly assigned RANS/LES interface require knowledge of the flow physics beforehand. The advantage of these methods is that the grids in the RANS region and the LES region can be generated separately, following the best practice of RANS meshing and LES meshing, respectively. Thus, the obtained result can achieve good quality with minimal numerical cost. The disadvantage of these methods is that it requires several rounds of trial-and-error pre-simulations to understand the flow physics, which increases the human workload. An early example of this branch of methods is the Zonal Detached Eddy Simulation (ZDES) proposed by Deck [60], where the attached boundary layer and the detached wake are explicitly enveloped in a RANS zone and an LES zone, respectively. A more recent example is the two-scale method proposed by He [61]. In this approach, only one turbomachinery blade passage is solved in the LES mode, and the Reynolds stresses obtained from this passage are broadcast to the rest blade passages solved in the RANS mode. Note that the broadcast stresses are considered exact. Therefore, no additional RANS turbulence model is needed for the RANS zone.

The hybrid RANS/LES methods with an implicit RANS/LES interface automatically recognize the RANS region and the LES region by using the local flow quantities. Specifically, this is usually achieved by implementing a length scale switch in the destruction term of RANS turbulence models. The choice of the switch can be based on either the wall distance as in the Detached Eddy Simulation (DES) method [62], or the local flow quantity as in the Scale-Adaptive Simulation (SAS) method [63], or both as in the Stress-Blended Eddy Simulation (SBES) [64].

The advantage of this branch of methods is clear: they can enable the heritage of existing RANS solvers to have LES capability with only tens of lines of changes in the source code. This is possible because the PDEs solved by RANS and LES essentially share the same form, as shown in Eq. (2.8) and Eq. (2.15). The implemented length scale switch can change the turbulence model between a RANS turbulence model mode and an LES SGS turbulence model mode, and thus the physical interpretation behind the same PDEs changes accordingly. Another merit of this branch of methods is that it allows RANS and LES to be solved in the same mesh (see Fig. 2.6(c)), which reduces human workload.

The disadvantage of this branch of methods is twofold [65]. The first issue is the uniqueness of the solution. Since both the pure-RANS solution and the pure-LES solution are consistent with the governing equations, the initial condition should be defined carefully in order to converge to the desired solution mode. The second issue is related to the interface between the RANS region and the LES region, which is also referred to as the grey area. When the grey area is pushed close to the wall due to the inadequate near-wall streamwise grid spacing, it induces modeled-stress depletion and thus incipient separations. This is amendable by either tuning the near-wall mesh or modifying the definition of the length scale switch so that it properly shields the near-wall RANS region [66]. When the grey area is located in the boundary layer

log-law region, the phenomena of log-layer mismatch can occur, where the velocity is shifted upward by three wall units in the LES region. The remedy of log-layer mismatch requires more modeling to constrain the log-layer behavior [67]. A refinement of the mesh is not helpful to relieve the mismatch.

2.2.4 State-of-the-Art Practice for Compressor Flows

From the brief review above, a hierarchy of turbulence modeling methods is presented: turbulence can be treated by RANS, WMLES, WRLES or DNS in ascending order of accuracy and cost. It is meaningful to review the state-of-the-art practice in compressor applications so that the capability and the required numerical resources for each method can be better understood.

A survey of turbulence modeling methods used for compressor research is presented in Fig. 2.7, where the number of journal papers using each turbulence modeling method is plotted chronologically. In general, the RANS method has been and still will be serving as the workhorse of compressor research. The one-equation SA model [44] and two-equation SST model [47] are among the most popular RANS models, taking 37.4% and 33.0% of the RANS share respectively in recent five years. The LES method has come into play since 2010, and it continues to contribute roughly 10% of journal publications in the last five years. However, most of these papers used hybrid RANS/LES methods that also involve RANS turbulence models. Lastly, the application of DNS is still in its infancy, with only a couple of groups around the world capable of running DNS for compressor research.

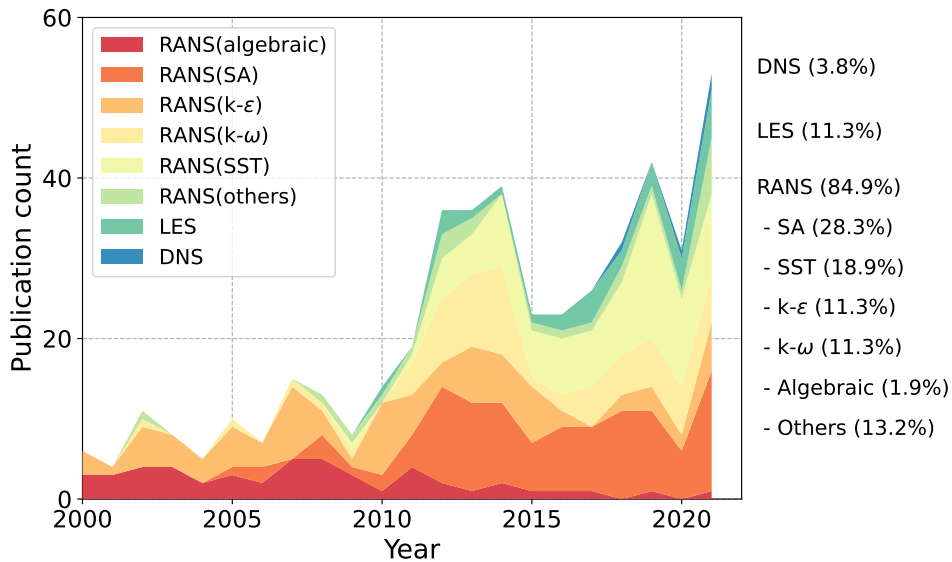


Figure 2.7: Review of turbulence models applied to compressors; data extracted from ASME Journal of Turbomachinery by searching keywords “compressor” and “CFD”.

A more recent survey of RANS turbulence model usage for compressors has been conducted in the GPPS CFD Workshop series. The theme of the two workshops is the validation and verification of turbomachinery RANS solvers in predicting the performances and flow fields of TUDa-GLR-OpenStage compressor. In total, 60 performance characteristic curves were

received from 11 institutes by using 12 different flow solvers, and the usage of the RANS turbulence model is summarized in Fig. 2.8. It shows that the SA-branch models and the SST-branch models are used by 62.7% and 30.5% of the submissions, respectively. These results again show that the SA model and the SST model are the most popular for compressor applications.

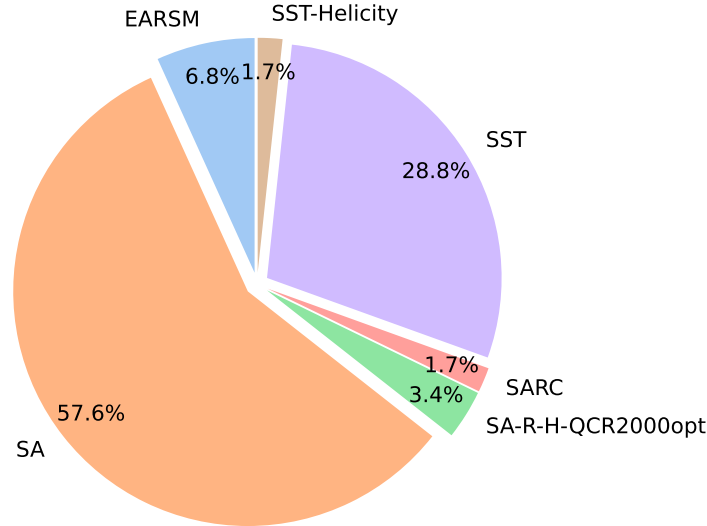


Figure 2.8: Summary of RANS turbulence model usage in the GPPS CFD Workshops in 2021 and 2022.

Regarding the applications to compressor near-stall and post-stall flows, detailed numerical settings of the relevant papers are summarized in Table 2.3.

The simulation of the large-scale surge phenomenon requires a large simulation domain not only includes the compressor stages but also the inlet and outlet piping system. Thus, even using a relatively coarse mesh with only 0.3 million grid points per blade passage, the total number of grid points for an 8-stage axial compressor still reaches 300 million, which requires over 2.3×10^5 CPU core hour to simulate one deep surge cycle [68]. Scale-resolving methods seem not feasible for surge simulations unless the geometry is simple and the flow is assumed circumferentially periodic. For example, the surge cycle of a single-stage and one-third annulus radial compressor was simulated using WRLES, and the simulation time for one surge cycle is about 1.0×10^5 CPU core hour [69].

The simulation of the rotating stall phenomenon also requires a large simulation domain, because which compressor stage initializes the stall cell is unknown beforehand. Therefore, the simulation domain usually contains multiple full-annulus stages, leading to the total number of grid points comparable to that in the surge prediction. The majority of rotating stall predictions used the URANS method. A typical example is from the URANS study of the same 8-stage axial compressor, where over 7.7×10^4 CPU core hour is needed to simulate the full stalling process [16]. The state-of-the-art practice of LES-type simulation for rotating stall is reported in Yamada et al. [70]. In this study, a total of 2×10^9 grid points were used to discretize a full-annulus 7-stage axial compressor, and the DES method from the WMLES branch is used.

The simulation of the full stalling process takes over 5.5×10^6 CPU core hour, which is two-order of magnitude larger than the URANS counterpart. Although emerging techniques such as GPU-based CFD simulations are potentially an order of magnitude faster than the conventional CPU-based ones [71], it is still not enough to cover the gap between the cost of URANS and WMLES in multi-stage compressor geometries.

Lastly, there are a couple of WRLES studies on laboratory-level compressor stages and cascades, such as that of Hah [72] for tip leakage flow and Gao [73] for corner separation. Although the investigated geometries are simpler than the industrial machines, these studies provide insights into flow physics which nevertheless are difficult to obtain from industrial machines.

Table 2.3: State-of-the-art practices of CFD simulations for compressor instabilities.

Nature	Domain	Method	Grid No.	Time Step	Year	Ref.
Surge	Full-Ann. Axial 15-Stage	URANS	1×10^9	1500/rev.	2021	[74]
Surge	Full-Ann. Axial 8-Stage	URANS	3×10^8	1500/rev.	2018	[68]
Surge	Part-Ann. Radial 1-Stage	WRLES	9.6×10^6	420/rev.	2015	[69]
Surge	Part-Ann. Axial 3.5-Stage	URANS	2.8×10^7	4800/rev.	2014	[75]
Rot. Stall	Part-Ann. Axial 1.5-Stage	WRLES	3.6×10^8	8000/rev.	2019	[76]
Rot. Stall	Full-Ann. Radial 1-Stage	DES	8×10^7	10000/rev.	2019	[77]
Rot. Stall	Full-Ann. Axial 1-Stage	URANS	1×10^8	2880/rev.	2019	[78]
Rot. Stall	Full-Ann. Axial 7-Stage	DES	2×10^9	10000/rev.	2017	[70]
Rot. Stall	Full-Ann. Radial 1-Stage	URANS	6×10^7	1680/rev.	2016	[79]
Rot. Stall	Part-Ann. Axial 8-Stage	URANS	7×10^7	1200/rev.	2015	[16]
Rot. Stall	Full-Ann. Axial Rotor	URANS	7.4×10^7	3888/rev.	2015	[14]
Rot. Stall	Part-Ann. Axial 3.5-Stage	URANS	2.8×10^7	4800/rev.	2014	[80]
Rot. Stall	Part-Ann. Axial 1.5-Stage	DES	3.1×10^7	4800/rev.	2013	[81]
Tip Sep.	Part-Ann. Axial 1.5-Stage	WRLES	9.8×10^8	6000/rev.	2017	[72]
Tip Sep.	Full-Ann. Radial 1-Stage	URANS	6×10^7	1680/rev.	2016	[82]
Corner Sep.	Part-Span Cascade	DDES	2.2×10^7	-	2018	[83]
Corner Sep.	Part-Span Cascade	WRLES	6.9×10^7	-	2017	[84]

From the above discussions, it can be concluded that the RANS method and the hybrid RANS/LES method are feasible tools to predict compressor near-stall and post-stall flows, while other methods with higher levels of fidelity are intractable due to their high cost. Thus, a predictive RANS turbulence model is crucial for the industry in the foreseeable future.

2.3 New Horizon in the Age of Data

2.3.1 Introduction of Machine Learning Application to CFD

With the rapid development of machine learning (ML) algorithms and the accumulation of high-fidelity (Hi-Fi) data, data-driven simulation methods have brought new horizons in the

fluid mechanics community [85]. Depending on which PDE the ML algorithm is implemented in, previous research can be categorized into the following three types:

- **ML correction of RANS turbulence model equations.**

In this branch of research, ML has been applied to correct the linear constitutive relation of the Reynolds stress tensor, the equilibrium turbulence assumption used in the turbulence model transport equations, and the model coefficients that were calibrated using small data [3]. However, this approach is still based on the RANS assumption that the mean flow quantities can uniquely determine the macroscopic state of turbulence without the information of the microscopic state. This assumption sets up a ceiling for RANS prediction accuracy.

- **ML correction of discretized NS equations.**

In this branch of research, ML has been applied to correct the discretization error and the subgrid-scale turbulence modeling error induced by using a coarse mesh, and initial success has been achieved in 1D and 2D simple canonical flows [86, 87]. However, the method at its current stage assumes periodicity in the flow problem to be solved, i.e., the dynamic state obtained from Hi-Fi fine-mesh simulation at a periodic unit can be simultaneously broadcast to the rest Lo-Fi coarse-mesh domain. This assumption hinders the application of this method to a general flow problem.

- **PDE-free ML prediction of flow field.**

In this branch of research, ML is used as a surrogate model of the NS equations, and the physics constraints from the boundary conditions and the conservation laws are implicitly enforced in the training cost function of the ML model [88, 89]. However, this approach is geometry dependent, i.e., an ML model trained in one geometry cannot be reused in another. Therefore, this method is often used for data assimilation and reduced-order modeling rather than prediction.

In the context of this work, the ML correction to the RANS turbulence models is of the most interest. The following sections will provide a further literature review on this topic.

2.3.2 Uncertainty Quantification of RANS Turbulence Modeling

Rapid progress on RANS turbulence models was made until around the year 2000, from which the research focus of the turbulence modeling community was shifted to the hybrid RANS/LES methods. With the emergence of uncertainty quantification (UQ) in turbulence modeling around the year 2010, the interest in RANS turbulence models has been renewed, and a new path of research has been initiated. The purpose of conducting UQ studies on turbulence models is not to design a perfect model form that best describes the nature of turbulence; instead, it is to evaluate the confidence level in results obtained from an existing model which has intrinsic flaws.

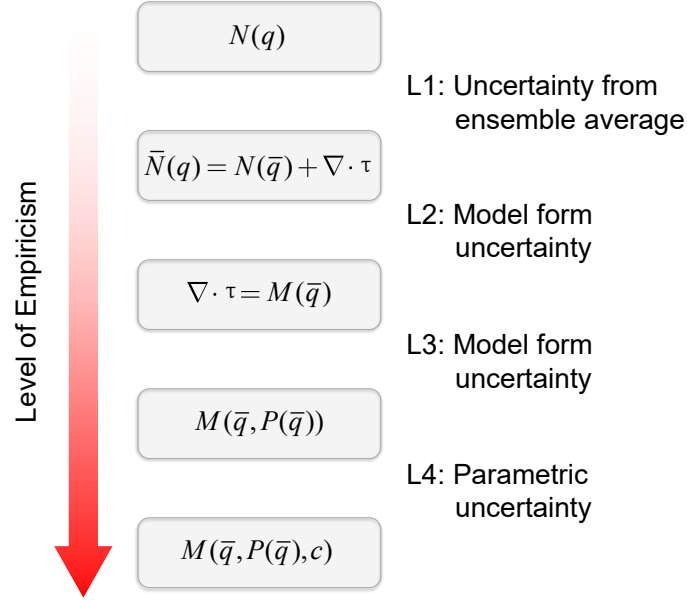


Figure 2.9: Illustration of the source of uncertainties in RANS turbulence models at different levels of empiricism

2.3.2.1 Source of Uncertainty in RANS Turbulence Modeling

Following the analysis of Duraisamy et al. [3], the source of uncertainties in RANS turbulence models can be grouped into four levels, as illustrated in Fig. 2.9.

The Level 1 (L1) uncertainty comes from the loss of information during the ensemble averaging process. When calculating the ensemble-averaged Navier-Stokes equation ($\bar{N}(\cdot)$) from the original Navier-Stokes equation ($N(\cdot)$), only the mean values of unknown quantities ($\bar{q}$) are left, whereas the fluctuation values are dropped out. This type of uncertainty is fundamentally not recoverable, and it sets up a ceiling on the accuracy of RANS models.

The Level 2 (L2) uncertainty occurs when assumptions are made for the constitutive relation ($M(\cdot)$), which correlates the ensemble-averaged flow quantities to the Reynolds stress tensor. An example of L2 uncertainty is the uncertainty induced by the Boussinesq linear constitutive relation.

The Level 3 (L3) uncertainty appears when assumptions are made for the transport equations ($P(\cdot)$) of a turbulence model. An example is the mathematical form of the ϵ equation in the k - ϵ turbulence model, which empirically mimics the form of the k equation in the same model.

Finally, the Level 4 (L4) uncertainty is generated when deterministic values are assigned to the model coefficients. These values are usually calibrated from canonical flow cases (e.g., homogeneous turbulence, zero-pressure gradient flat plate, etc.), which may not apply to more general flows.

2.3.2.2 Uncertainty Quantification of the Spalart-Allmaras Turbulence Model

The readers are redirected to Xiao and Cinnella [90] for a comprehensive turbulence modeling UQ review. In the following, a brief review of UQ studies on the SA model is made. In terms of the UQ methodology, previous research applied either a forward propagation approach or a backward propagation approach.

The forward approach pre-assumes the probability density function (PDF) of model terms or model coefficients and then propagates it through RANS equations to obtain the PDF of the quantity of interest (QoI). An example of the forward approach is from Han and Hosder [91], where the model-form uncertainty of the SA model was investigated by multiplying the eddy viscosity by a random variable with a uniform PDF. In their study, the measured velocity profiles of the synthetic jet actuator case could be enveloped by the 95% confidence interval. Another example is from Schaefer et al. [92, 93] and Stephanopoulos et al. [94], where the non-intrusive polynomial chaos method was applied to investigate the parametric uncertainty of the SA model. The idea was to train a metamodel of RANS equations based on the response surface and then propagate the SA model coefficients with uniform PDFs through the metamodel. Their test cases included the transonic axisymmetric bump, the RAE 2822 transonic airfoil, the subsonic flat plate, and the subsonic backward-facing step. It was generally found that the discrepancy between the experiment and the simulation was most evident in the separation regions, and the predicted results were sensitive to the SA model coefficients σ , κ , c_{v1} , c_{b1} and c_{w2} .

The backward approach first solves a calibration problem in a Bayesian framework, which utilizes experiment or high-fidelity simulation results to infer a proper PDF of model terms or model coefficients. The calibrated PDF is then propagated to predict the PDF of the QoI. Oliver and Moser [95] calibrated the SA model coefficients and compared the SA model with other turbulence models in a fully developed channel flow. Results showed that the calibrated SA model coefficients σ and κ have very similar values to their defaults, and the SA model predicted a comparable velocity profile to the k - ϵ model and the v^2 - f model but with higher uncertainty. Cheung et al. [96] performed a similar calibration of SA model coefficients in a subsonic flat plate under different pressure gradients. An evident difference between the default values and the calibrated values of the SA model coefficients was observed for all calibration scenarios. Papadimitriou and Papadimitriou [97] adopted an adjoint method to optimize the posterior Gaussian distribution of the SA model coefficients. In the investigated cases of the subsonic flat plate and the subsonic backward-facing step, the SA model was found accurate except for the separation region.

2.3.3 Machine Learning Assisted RANS Turbulence Modeling

An ML-assisted turbulence model can reduce different levels of uncertainties in a RANS turbulence model depending on its implementation. The ML correction term can be used to reduce either the parametric uncertainty or the model-form uncertainty. It is also possible to build a pure ML turbulence model given an extensive training database. The hierarchy of ML-assisted turbulence modeling is illustrated in Fig. 2.10.

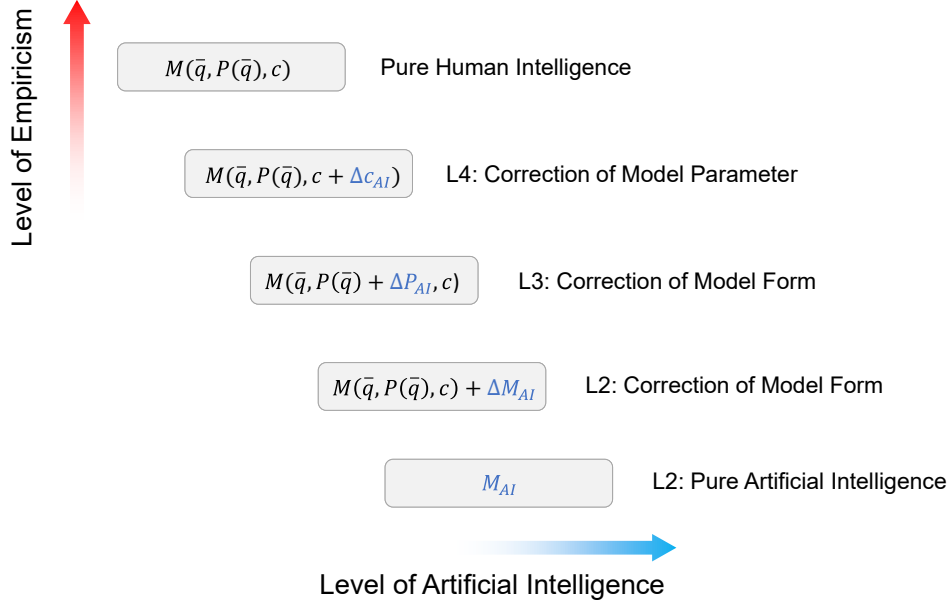


Figure 2.10: Illustration of machine learning turbulence modeling research framework

2.3.3.1 Pure Machine Learning Turbulence Modeling

Research towards a pure ML turbulence model (i.e., without solving transport equations of an established turbulence model) started by mimicking existing RANS turbulence models. When using a shallow neural network, it was found capable of replicating the source term of the SA model [98]. Later, a radial basis function shallow neural network was found to replicate the full SA model [99].

The milestone work of Ling et al. [100] applied a deep neural network to construct the Reynolds stress tensor directly. Specifically, the deep neural network predicts the coefficients multiplied to the ten invariant tensor basis functions [101]. After training the neural network with DNS data, it was demonstrated that the neural network model outperformed the conventional RANS models in predicting turbulence anisotropy. Following this approach, similar results were obtained by later researchers, and further improvement of the model accuracy was achieved by modifications of the neural network structure to avoid overfitting [102], input feature selection [103], training with mean flow data via the adjoint method [104], and online training within CFD iterations [105]. Although this approach has demonstrated good accuracy in a range of canonical flows, it may be argued as a black-box system because the causal link between the input flow features and the output Reynolds stresses remains unclear. Knowledge obtained from existing turbulence modeling can hardly be plugged into this framework either.

2.3.3.2 Machine Learning Correction to the Constitutive Relation

To take advantage of existing turbulence models, an alternative approach is to introduce an ML correction term to reduce the L2 uncertainty.

Sandberg and co-workers [106] applied the gene expression programming (GEP) algorithm to build up an anisotropy correction tensor, which is added to the Reynolds stress tensor calculated from the Boussinesq assumption. This algorithm performs symbolic regression: it

takes the basis tensors and invariants [101] as input, and the outcome is an explicit mathematical expression of the anisotropy term. Based on this approach, the ML-assisted SST model showed better accuracy than the original SST model in a broad range of flows, including backward-facing step [106], periodic hill [106], rectangular duct [107], asymmetric diffuser [107] and trailing edge wake [108]. More recently, the authors improved the input data pre-processing via phase-lock averaging [109] and triple decomposition [110] to tackle the deterministic unsteadiness (e.g., blade passing, vortex shedding, etc.); the training process is also changed from offline frozen training to online real-time training [111], which is more realistic and allows the use of mean flow quantities in the training cost function. Following this symbolic regression approach, a novel deterministic symbolic regression method named sparse regression of turbulent stress anisotropy (SpaRTA) was introduced by Schmelzer et al. [112]. Compared to the GEP algorithm, the SpaRTA method narrowed down the range of the candidate model form so that the models trained from different databases are more consistent with each other. The obtained model showed improved prediction accuracy in periodic hill flows [112] especially when the model was trained online with CFD iterations [113].

Concurrently, Xiao and co-workers [114,115] used the random forest algorithm to construct a correction tensor added to the Reynolds stress tensor modeled from an established turbulence model. Unlike the gene expression programming algorithm, the random forest algorithm generates a complex implicit expression of the correction tensor rather than an interpretable explicit form. The input variables of the random forest include not only the strain rate and the vorticity but also flow-specific variables like pressure gradient, turbulence kinetic energy gradient, turbulence time and length scale, and dimensionless wall distance. The output variables of the random forest represent the magnitude, shape, and orientation of the Reynolds stress discrepancy tensor. Certain success has been achieved in flows like periodic hill [115], square duct [115], and supersonic flat plate [116]. However, the explicit modeling of the Reynolds stress tensor may result in considerable errors in mean flow quantities due to the ill-conditioned RANS equations [117].

Following the spirit of Ling et al. [100], Jiang et al. [118] constructed a correction tensor based on the invariant tensor basis of Pope [101], and the coefficients of each tensor basis are determined by a deep neural network. In the later form of this framework [119], an independent neural network is used to determine the form of the tensor basis, which removes the constraint on Pope’s tensor basis. Based on a similar idea, Mandler [120] converts the multivariate regression problem of the tensor basis coefficients to a set of univariate regression problems by using field inversion and tensor projection, which potentially improves prediction accuracy and model explainability.

2.3.3.3 Machine Learning Correction to the Transport Equations

In addition to the correction of the Boussinesq assumption, the ML correction term can also be introduced to reduce L3 uncertainty.

Duraisamy and co-workers [121,122] combined Bayesian field inversion and the ML algorithm to construct an ML correction term, which is multiplied by the production term of an established turbulence model. The purpose of performing the field inversion is to infer the spatial distribution of the true production term, which is hidden beneath the Hi-Fi data (i.e., either turbulence statistics or mean flow quantities). It was demonstrated in flows including

channel [121], airfoil [122] and shock-boundary layer interaction [123] that the ML-assisted model performs better than the original model. The same approach is adopted by the following researchers, and improved prediction accuracy was obtained in the transitional flow of a low-pressure turbine [124] and an iced airfoil [125].

A more straightforward formulation of the L3 correction is to approximate the eddy viscosity from the Hi-Fi turbulence statistics data, and then use ML to correct the eddy viscosity difference between the Hi-Fi results and the Lo-Fi RANS results. This is the approach adopted in this work (as will be shown later in Chapter 7), and it is also concurrently investigated by a broad range of groups [126–129].

It should be emphasized that corrections at L3 only still imply the alignment of the Reynolds stress anisotropy tensor with the mean strain rate (i.e., Boussinesq assumption). Therefore, it cannot improve highly anisotropic flows such as corner flows [130].

2.3.3.4 Machine Learning Correction to the Turbulence Model Coefficients

Finally, the ML correction term can be added to the model coefficients to reduce L4 uncertainty. Similar to the approach of reducing L3 uncertainty, an extra step of field inversion is needed in order to infer the spatial distribution of the true model coefficients. Duraisamy and co-workers [123] applied the field inversion and the Adaptive Boosting algorithm to correct the c_{w2} coefficient of the SA model. This approach not only improved the model accuracy in the transonic bump flow but also maintained the model accuracy in the boundary layer log-law region. Durbin and co-workers [131] applied the field inversion and the decision tree algorithm to set a zonal value of the k - ω model coefficient $C_{\omega1}$. The decision trees serve as a classifier of zones, where different values of $C_{\omega1}$ are assigned. It was demonstrated in a series of bump flows that the ML-assisted k - ω model showed better accuracy than the conventional model.

2.3.3.5 Summary

From the above overview of different ML-assisted turbulence modeling methods, a broad range of possibilities has been presented. However, it should be emphasized that the research toward an ML-assisted turbulence model is still in its infancy. For one thing, the universality of the trained model is still limited, as the prediction error increases when the underlying physics of the test case is evidently different from that of the training case. As a result, the training and test flows are still limited to simple canonical flows rather than complex industrial flows. For another, the trained model is sometimes hardly interpretable, which lowers the confidence of users. More research is needed in the near future.

3. Methodology

“A craftsman who wishes to practice his craft well must first sharpen his tools.”

— Confucius, *Analects*

3.1 Introduction

In this chapter, the CFD methods and the machine learning methods used in this thesis are introduced in detail. These methods will serve as the building blocks for the investigations of the following chapters. Moreover, the test cases which will be used in the following chapters for validation and investigation are also introduced here.

3.2 Reynolds-Averaged Navier-Stokes Flow Solver

3.2.1 Governing Equations

A typical RANS flow solver for turbomachinery applications solves the three-dimensional, unsteady, compressible Favre-averaged Navier-Stokes equations in the reference frame attached to the blade. In conservative form, the equations can be lumped as Eq. (3.1):

$$\frac{d}{dt} \int_{\Omega} \mathbf{U} d\Omega + \oint_{\partial\Omega} (\mathbf{F} - \frac{1}{Re} \mathbf{G}) \cdot \mathbf{n} d\Gamma = \int_{\Omega} \mathbf{S} d\Omega \quad (3.1)$$

where Ω denotes the control volume and Γ denotes its boundary; $\mathbf{U}$, $\mathbf{F}$, $\mathbf{G}$ and $\mathbf{S}$ represents the solution vector of conservative variables, the inviscid flux vector, the viscous flux vector and the source vector, respectively, which are written as Eq. (3.2):

$$\mathbf{U} = \begin{bmatrix} \rho \\ \rho \mathbf{u} \\ \rho e \end{bmatrix}, \quad \mathbf{F} = \mathbf{U} \otimes \mathbf{w} + \begin{bmatrix} 0 \\ p\delta_{ij} \\ u_j p \end{bmatrix}, \quad \mathbf{G} = \begin{bmatrix} 0 \\ \sigma_{ij} \\ u_k \sigma_{ik} + k \frac{\partial T}{\partial x_i} \end{bmatrix}, \quad \mathbf{S} = \begin{bmatrix} 0 \\ \rho \boldsymbol{\omega} \times \mathbf{u} \\ 0 \end{bmatrix} \quad (3.2)$$

Here, δ_{ij} is the Kronecker delta function; $\mathbf{u}$, $\mathbf{w}$ and $\boldsymbol{\omega}$ denotes the vector of absolute velocity, relative velocity and blade angular velocity, respectively; ρ , p , T and e represent density, pressure, temperature and internal energy, respectively; σ_{ij} and k denote the viscous stress tensor and the effective thermal conductivity, both of which are dependent on the properties of the working fluid.

To close Eq. (3.1) and Eq. (3.2), further assumptions about the thermodynamic equation of state $f(\rho, p, T) = 0$, the viscous stress tensor σ_{ij} and the effective thermal conductivity k are required. The following assumptions are often used by a turbomachinery flow solver:

- The working fluid is assumed to be an ideal gas.
- The working fluid is assumed to be a Newtonian fluid.
- The laminar viscosity is assumed to follow Sutherland's law.
- The bulk viscosity is assumed to be zero (i.e., Stokes' hypothesis).
- The effect of turbulent fluctuations is modeled based on the concept of eddy viscosity.
- The viscous stress due to turbulent fluctuations is assumed to be linearly correlated with the strain rate tensor (i.e., Boussinesq assumption).
- The thermal conductivity is assumed to be linearly correlated with viscosity.

These assumptions yield the following equations:

$$p = \rho RT \quad (3.3)$$

$$\sigma_{ij} = (\mu_l + \mu_t) \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right) \quad (3.4)$$

$$\mu_l = \mu_{l,ref} \left(\frac{T}{T_{ref}} \right)^{3/2} \frac{T_{ref} + T_s}{T + T_s} \quad (3.5)$$

$$k = \frac{\gamma}{\gamma - 1} \left(\frac{\mu_l}{Pr_l} + \frac{\mu_t}{Pr_t} \right) \quad (3.6)$$

where the constants are $R = 287 J/(kg \cdot K)$, $\mu_{l,ref} = 1.716 \times 10^{-5} kg/(m \cdot s)$, $T_{ref} = 273.15 K$, $T_s = 110.4 K$, $\gamma = 1.4$, $Pr_l = 0.72$ and $Pr_t = 0.90$; the eddy viscosity μ_t needs to be closed by a turbulence model.

The Spalart-Allmaras (SA) one-equation turbulence model [44] is the most widely used RANS turbulence model for compressor applications (Sec. 2.2.4). Therefore, detailed analysis and data-driven modifications of the SA model are pursued throughout this thesis.

The SA model solves the modified eddy viscosity $\tilde{\nu}$ via a transport equation, which was constructed step-by-step. Firstly, the form of the production term was proposed based on homogeneous turbulence. Then, the diffusion term inspired by the classical diffusion operator was added, and the model coefficients in both the production and the diffusion terms were calibrated using free-shear flow data. Lastly, the form of the destruction term was proposed based on the assumption of equilibrium turbulence and dimensional analysis, and the corresponding model coefficients were calibrated using zero pressure gradient flat plate data. The final formulation is shown in Eq. (3.7):

$$\begin{aligned} \frac{\partial \tilde{\nu}}{\partial t} + u_j \frac{\partial \tilde{\nu}}{\partial x_j} = & \underbrace{\left[c_{b1}(1 - f_{t2})\hat{S}\tilde{\nu} \right]}_{\text{production}} - \underbrace{\left[c_{w1}f_w - \frac{c_{b1}}{\kappa^2}f_{t2} \right] \left(\frac{\tilde{\nu}}{d} \right)^2}_{\text{destruction}} \\ & + \underbrace{\frac{1}{\sigma} \left[\frac{\partial}{\partial x_j} \left((\nu + \tilde{\nu}) \frac{\partial \tilde{\nu}}{\partial x_j} \right) + c_{b2} \frac{\partial \tilde{\nu}}{\partial x_i} \frac{\partial \tilde{\nu}}{\partial x_i} \right]}_{\text{diffusion}} \end{aligned} \quad (3.7)$$

with additional functions calculated in the following:

$$\begin{aligned}
\mu_t &= \rho \hat{\nu} f_{v1} & \hat{S} &= \Omega + \frac{\nu}{\kappa^2 d^2} \chi f_{v2} & c_{w1} &= \frac{c_{b1}}{\kappa^2} + \frac{1 + c_{b2}}{\sigma} & f_{v1} &= \frac{\chi^3}{\chi^3 + c_{v1}^3} \\
g &= r + c_{w2}(r^6 - r) & f_{v2} &= 1 - \frac{\chi}{1 + \chi f_{v1}} & f_w &= g \left[\frac{1 + c_{w3}^6}{g^6 + c_{w3}^6} \right]^{1/6} & \chi &= \frac{\hat{\nu}}{\nu} \\
r &= \min \left[\frac{\hat{\nu}}{\hat{S} \kappa^2 d^2}, 10 \right] & f_{t2} &= c_{t3} \exp(-c_{t4} \chi^2)
\end{aligned} \tag{3.8}$$

where d is wall distance, and $\sigma = 0.667$, $\kappa = 0.41$, $c_{v1} = 7.1$, $c_{b1} = 0.1355$, $c_{b2} = 0.622$, $c_{w2} = 0.3$, $c_{w3} = 2.0$, $c_{t3} = 1.2$ and $c_{t4} = 0.5$ are model coefficients. To improve the numerical stability, $\hat{S}$ is limited to be greater than zero.

3.2.2 Numerical Schemes

The RANS flow solver used in this work uses a node-centered finite volume scheme with an edge-based data structure. The fluxes of the RANS equations are solved by the Jameson-Schmidt-Turkel (JST) scheme [132] with artificial dissipation based on Roe's matrix [133]. The spatial accuracy is second-order accurate in most parts of the computation domain, but it reduces to first-order accuracy to stabilize shocks by using a pressure switch. The fluxes of the SA transport equation are calculated based on the first-order upwind scheme. The spatial gradients are calculated based on the Green-Gauss method. For steady flows, the block Jacobi preconditioner is used for the linear solver, and the residual smoothing method is employed to accelerate convergence. For unsteady flows, the second-order accurate implicit time integration method via Newton iterations is adopted. These numerical schemes are representative of typical turbomachinery flow solvers used in both academia and industry.

3.3 Machine Learning Model

3.3.1 Fully Connected Neural Network

Fully connected neural network (FCNN) [134] is a classic regression model in machine learning. It is composed of multiple layers of artificial neurons, with neurons in one layer fully connected to the neurons in the previous and the next layer, as illustrated in Fig. 3.1. The input variables, the intermediate values, and the outputs are stored in the input layer, hidden layers and output layer, respectively.

The FCNN predicts the outputs with forwarding propagation. Firstly, the inputs are normalized by their maximum and minimum values (i.e., min-max normalization) in the learning database. The values at the l^{th} layer are then propagated to the $(l+1)^{th}$ layer using Eq. (3.9):

$$\mathbf{a}^{(l+1)} = g(\mathbf{w}^{(l+1)} \mathbf{a}^{(l)} + \mathbf{b}^{(l+1)}) \tag{3.9}$$

where $\mathbf{w}$ is the weight matrix, $\mathbf{b}$ is the bias vector, and $g(\cdot)$ is the non-linear activation function (e.g., sigmoid function, hyperbolic tangent function, etc.). In this work, the activation function

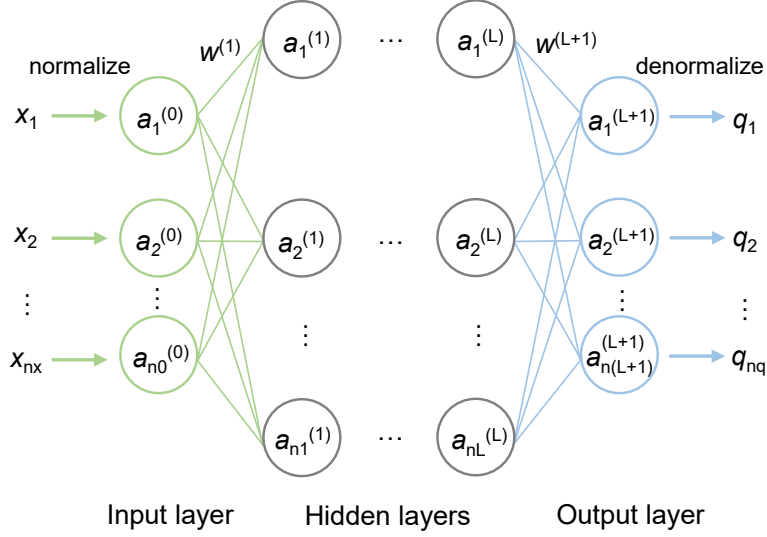


Figure 3.1: Illustration of a fully connected neural network.

of the output layer uses a sigmoid function, which is bounded between 0 and 1. Therefore, the values at the output layer need to be denormalized back to the original values of the outputs. Considering the outputs from the test database may fall out of the training database range, the outputs are normalized to the range of $0.5 \pm 0.5\omega^{-1}$ where ω is a scaling factor. When $\omega = 1$, it turns back to the min-max normalization.

The accuracy of the FCNN depends on the network parameters $\mathbf{w}^{(l)}$ and $\mathbf{b}^{(l)}$, which are initialized randomly before training. Calibration of these parameters, or training of the FCNN, is achieved by solving an optimization problem that minimizes the cost function J defined by Eq. (3.10):

$$J(w_{i,k}^{(l)}, b_i^{(l)}) = \frac{1}{2m} \sum_{j=1}^m \sum_{i=1}^{n_{L+1}} (q_i^{(j)} - \hat{q}_i^{(j)})^2 + \frac{\lambda}{2m} \sum_{l=1}^{L+1} \sum_{i=1}^{n_l} \sum_{k=1}^{n_{l-1}} (w_{i,k}^{(l)})^2 \quad (3.10)$$

where $\hat{\mathbf{q}}$ and $\mathbf{q}$ are the vector of the training data and the corresponding FCNN predictions in the output layer, respectively; m , n and L denote the number of training samples, the number of neurons in a layer and the number of hidden layers, respectively; λ is a regularization factor that penalizes large-valued weights in order to avoid overfitting.

In this work, the FCNN is self-programmed based on the PYTHON library NUMPY, and the gradient-based Broyden-Fletcher-Goldfarb-Shanno (BFGS) optimizer [135] from the PYTHON library SCIPY is applied for training.

3.3.2 Random Forest

Random forest (RF) [136] is a classic regression and classification model in machine learning. An RF regressor is an ensemble of decision trees (DT), which takes the average prediction of all DTs as its output. An illustrative diagram of an RF is shown in Fig. 3.2(a). For each DT, it produces its prediction by going through layers of if-then-else decision rules based on a subset of inputs, as illustrated in Fig. 3.2(b). During the training of the RF model, the DT is

allowed to grow to full depth without pruning to maximize its capability. The RF algorithm from the PYTHON library SCIKIT-LEARN [137] is adopted in this work.

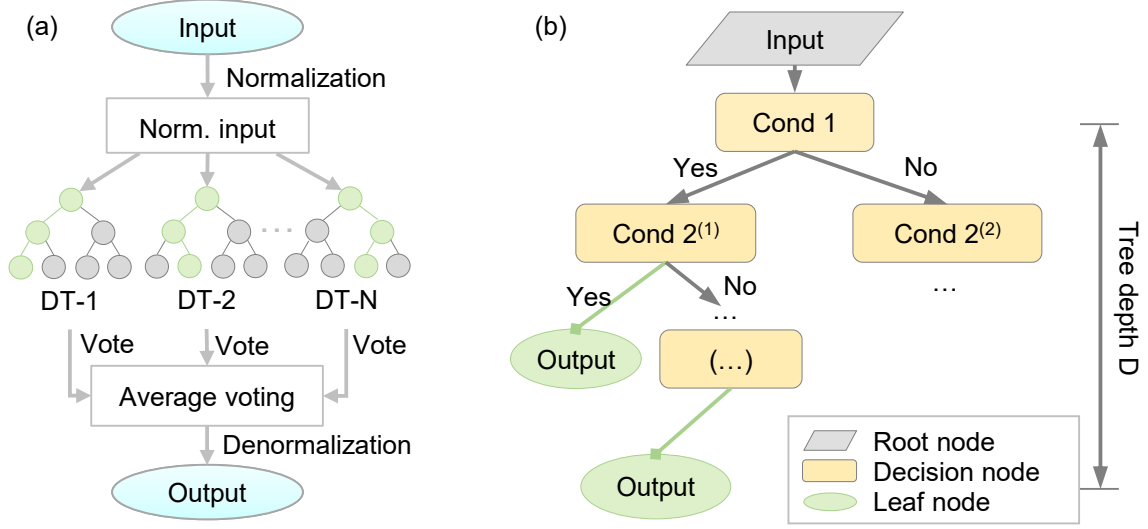


Figure 3.2: Illustration of (a) a random forest and (b) a decision tree.

3.4 Collection of Flow Cases

3.4.1 Canonical Cases

In this work, three canonical flow cases from NASA Turbulence Modeling Resource (TMR) website [54] are investigated, namely the supersonic square duct, the axisymmetric transonic bump and the backward-facing step. These flow cases are featured by endwall corner blockage, shock-induced separation and geometry-induced flow separation, respectively, which resemble part of the flow physics of compressor tip leakage flow. The resemblance between these canonical flows and the compressor tip leakage flow is illustrated in Fig. 3.3.

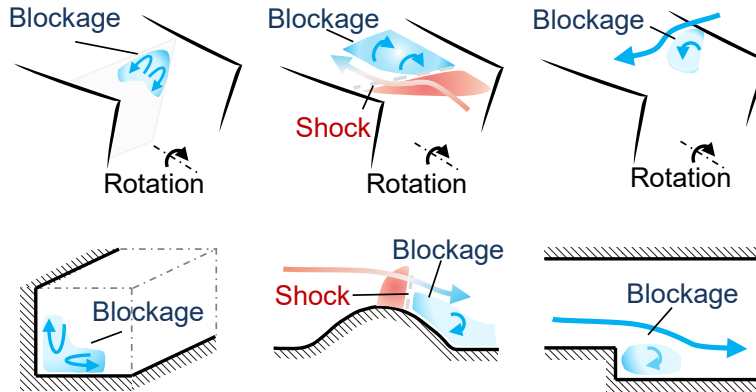


Figure 3.3: Illustration of compressor tip flow features and selected canonical flow cases.

3.4.1.1 Supersonic Square Duct

In this work, the supersonic square duct flow of Davis and Gessner [138] from the University of Washington is investigated. This square duct (25.4×25.4 mm) was tested within an outer square duct (50.8×50.8 mm) so that the boundary layers of the tested duct surfaces were allowed to develop naturally from scratch. The operating condition is at $T_\infty \approx 288.89$ K, $M_\infty = 3.9$ and $Re_D = 5.08 \times 10^5$, where D denotes the edge length of the square. The available measured data include the wall surface pressure, wall skin friction and cross-sectional distribution of total pressure, static pressure, Mach number and velocity components, all of which were obtained from probe measurements. More details about the experiment can be found in Davis and Gessner [138].

The flow domain and the boundary conditions of the supersonic square duct are illustrated in Fig. 3.4(a). Compared to the measured geometry, the numerical model corresponds to only one-quarter of the duct with symmetry boundary conditions, which reduces the computational cost. Another difference is that the duct length of the numerical model is longer than the measured geometry (i.e., $52D$ versus $50D$) so as to alleviate the outlet boundary condition effect on predicting the flows at $x/D = 50$.

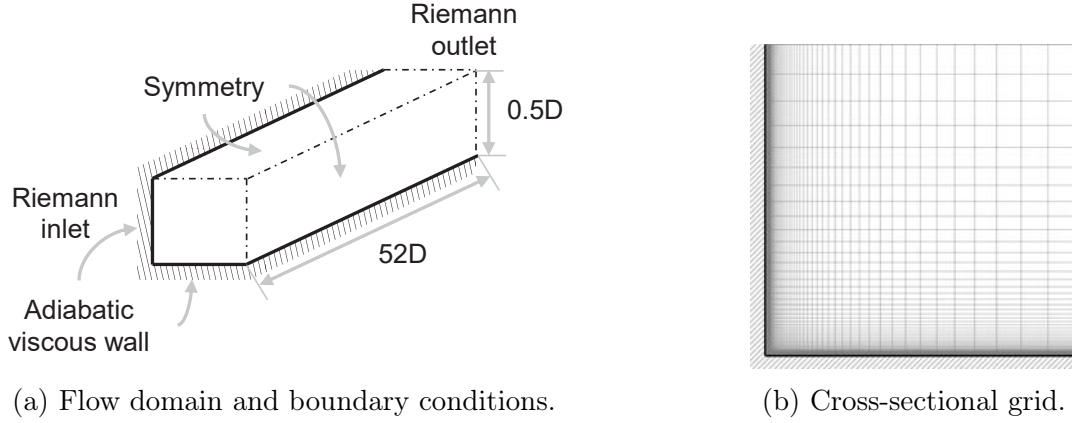


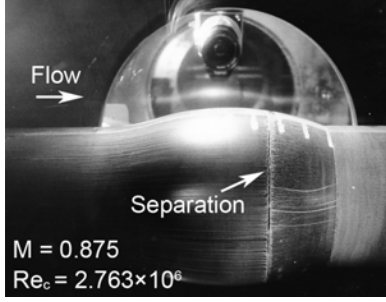
Figure 3.4: Illustration of the numerical model of the supersonic square duct.

The grid of the supersonic square duct is the second-finest grid from NASA TMR [54], which has 481 and 81 grid points on the streamwise and wall-normal direction, respectively (i.e., $481 \times 81 \times 81$). The total number of grid points is 3.16 million. The y^+ value of the near-wall grid layer is kept below 1. A cross-sectional view of the grid is shown in Fig. 3.4(b).

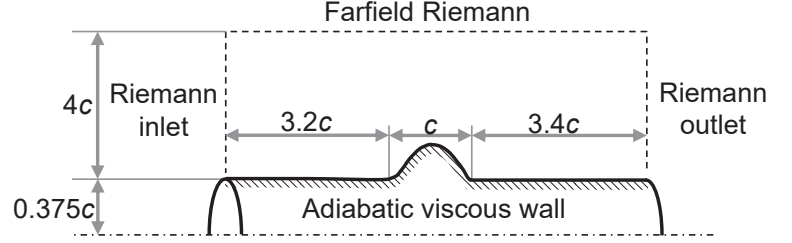
3.4.1.2 Axisymmetric Transonic Bump

The axisymmetric transonic bump investigated in this work was measured at NASA Ames Research Center [139, 140]. It was also known informally as the “Bachalo-Johnson” flow. The measurement was firstly performed in a 6×6 ft supersonic wind tunnel with solid walls, where the surface pressure distribution and oil-flow visualization were acquired [139]. The test condition is at $T_\infty \approx 300$ K, $M_\infty = 0.6, 0.8, 0.85, 0.875, 0.9, 0.925$ and $Re_c = 2.763 \times 10^6$, where c denotes the chord of the bump. Later, the same bump geometry at $M = 0.875$ was measured in a 2×2 ft transonic wind tunnel with partially open walls. In addition to the surface pressure

distribution and oil-flow visualization, velocity profiles and Reynolds stress profiles were also obtained by using a laser Doppler velocimeter [140]. A photo of the later test scheme and the oil-flow visualization is shown in Fig. 3.5(a). Recently, Hi-Fi simulations such as LES [141] and DNS [142] were also performed on the bump case at $M = 0.875$.



(a) Surface oil-flow visualization.



(b) Flow domain and boundary conditions.

Figure 3.5: Illustration of flow physics and numerical model of the axisymmetric transonic bump (photo courtesy of Dr. Dennis Johnson).

The flow domain and the boundary conditions of the axisymmetric transonic bump are illustrated in Fig. 3.5(b). This flow domain is comparable to the one used in the 6×6 ft tunnel experiment and the Hi-Fi simulations. Therefore, these data will be regarded as ground truth in later investigations. Experimental data from the 2×2 ft tunnel are subjected to pronounced wall effects (note the diameter of the base cylinder is 1 ft). Thus, they are expected to differ from the predictions of the current numerical model. For completeness, the velocity and Reynolds stress profiles measured in this tunnel will still be presented for reference.

The grids of the axisymmetric transonic bump are the second, third and fourth-finest grids from NASA TMR [54]. All these grids have an H-grid topology, and the y^+ value of the near-wall grid layer is kept below 1. The details of the grid points are summarized in Table 3.1. To reduce the computational cost, only two layers of grids are used in the circumferential direction, and the periodic boundary condition is used at both boundaries.

Table 3.1: Details of axisymmetric transonic bump grids.

Grid topology	Coarse	Medium	Fine
Streamwise grid point	181	361	721
Transverse grid point	81	161	321
Total grid point (thousand)	14.66	58.12	231.44
Usage	-	Ch. 7	Ch. 5

3.4.1.3 Backward-Facing Step

The backward-facing step is a classic flow model featured by flow separation and reattachment, as illustrated in Fig. 3.6(a). In this work, the backward-facing step of Driver and

Seegmiller [143] from NASA Ames Research Center is investigated. The measurement was performed on the floor of a low-speed wind tunnel at $T_\infty \approx 298.33\text{K}$, $M = 0.128$, $Re_H = 3.6 \times 10^4$ and $ER = 9/8$. Here, M is measured at the location $4H$ above the step (i.e., the center line of the inlet duct), H denotes the step height, and ER represents the expansion ratio. The acquired quantities of interest include the surface pressure distribution from pressure taps, the surface skin friction distribution from an oil-flow laser interferometer and the velocity and Reynolds stress components from a laser Doppler velocimeter. Hybrid RANS/LES simulation was also performed on the same configuration in previous research [144].

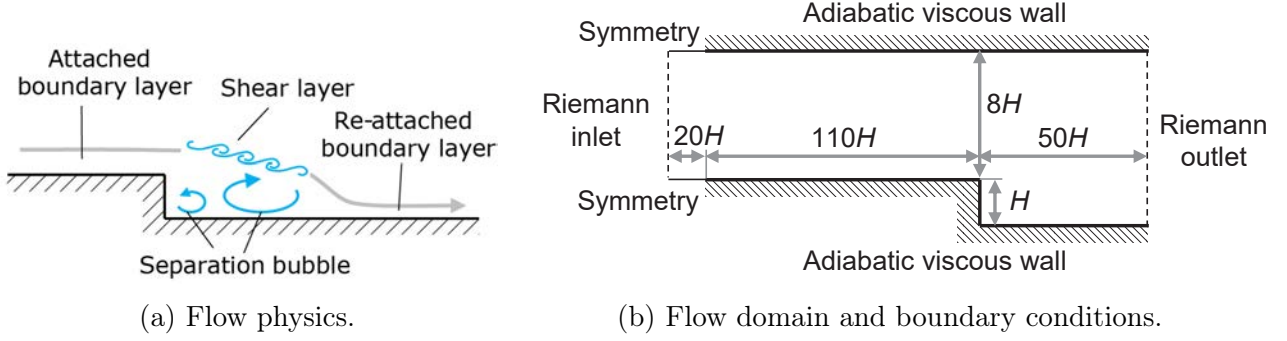


Figure 3.6: Illustration of flow physics and numerical model of the backward-facing step.

The flow domain and the boundary conditions of the backward-facing step are illustrated in Fig. 3.6(b). Here, the duct length upstream of the step has been adjusted so that the naturally developed boundary layer can produce approximately the same skin friction and boundary layer thickness as the experiment at the location $4H$ upstream of the step. To achieve the prescribed M value, the static pressure value at the outlet boundary needs to be adjusted by trial and error.

The grids of the backward-facing step are the second, third and fourth-finest grids from NASA TMR [54], all of which have an H-grid topology. The y^+ value of the near-wall grid layer is kept below 1 for the horizontal walls, but that for the vertical wall is kept around 3 for better grid quality. The details of the grid points are summarized in Table 3.2. To reduce the computational cost, only two layers of grids are used in the spanwise direction, and the periodic boundary condition is used at both boundaries.

Table 3.2: Details of backward-facing step grids.

Grid topology	Coarse	Medium	Fine
Streamwise grid point (inlet duct)	89	177	353
Transverse grid point (inlet duct)	65	129	257
Streamwise grid point (outlet duct)	129	257	513
Transverse grid point (outlet duct)	113	225	449
Total grid point (thousand)	20.30	80.53	320.80
Usage	Ch. 4	Ch. 4	Ch. 5

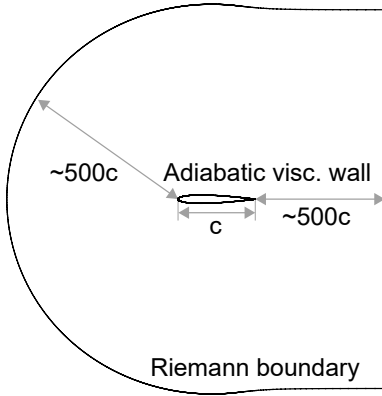
3.4.2 Airfoil Cases

A turbomachinery blade can be viewed as the stacking of a series of 2D airfoils. A typical aeroengine compressor blade operates under subsonic conditions at the hub section and transonic conditions at the tip section, which triggers flow separation and thus compressor stall with different flow mechanisms. In this work, the subsonic NACA 0012 airfoil and the transonic RAE 2822 airfoil will be studied.

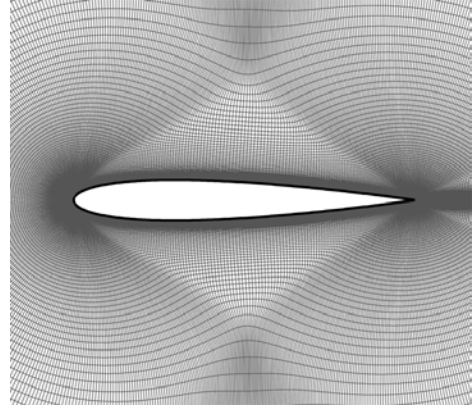
3.4.2.1 NACA 0012 Airfoil

The NACA 0012 airfoil is a classic subsonic airfoil that has extensive applications in both internal and external flow studies. In this study, the operating condition at $T_\infty \approx 300$ K, $Re_c = 6 \times 10^6$, $M_\infty = 0.15$ and different values of AoA is investigated. The corresponding measurement was performed in a wind tunnel at NASA Langley Research Center [145], where the characteristics of lift coefficient and drag coefficient were obtained.

The computational domain and the boundary conditions of the NACA 0012 airfoil are illustrated in Fig. 3.7(a). The farfield boundary of the domain is extended approximately $500c$ away from the airfoil, which alleviates the sensitivity of the simulation results to the point vortex correction [146] at the farfield boundary.



(a) Flow domain and boundary conditions.



(b) Near-wall grid.

Figure 3.7: Illustration of the numerical model of the NACA 0012 airfoil.

The grid of NASA 0012 airfoil used in this work is the second-finest grid from NASA TMR [54]. It uses a C-grid topology with 257, 897 and 513 grid points on the wall-normal direction, the circumferential direction and the airfoil surface, respectively. A near-wall view of the grid is presented in Fig. 3.7(b), and the y^+ value of the near-wall grid layer is kept below 1. To reduce the computational cost, only two layers of grids are considered in the spanwise direction, and the periodic boundary condition is used for both boundaries. The total number of grid points is 0.46 million.

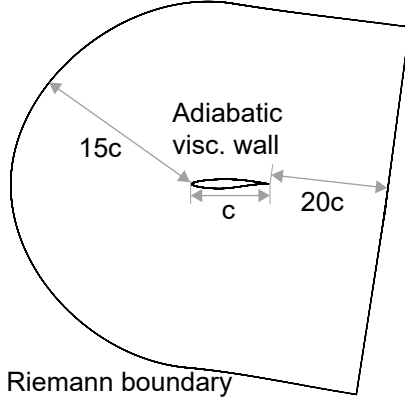
3.4.2.2 RAE 2822 Airfoil

The RAE 2822 airfoil is a classic transonic airfoil widely used in CFD validation and verification. It was measured by Royal Aircraft Establishment (RAE) in a 6×8 ft wind tunnel, where the surface pressure distribution, the surface skin friction distribution and the velocity profiles in the boundary layer and the wake were acquired [147]. In total, 13 operating conditions with different M_∞ , Re_c and AoA were measured, and Case 6, Case 9 and Case 10 are investigated in this work. The operating conditions after corrections of wind tunnel wall effects [148, 149] are summarized in Table 3.3.

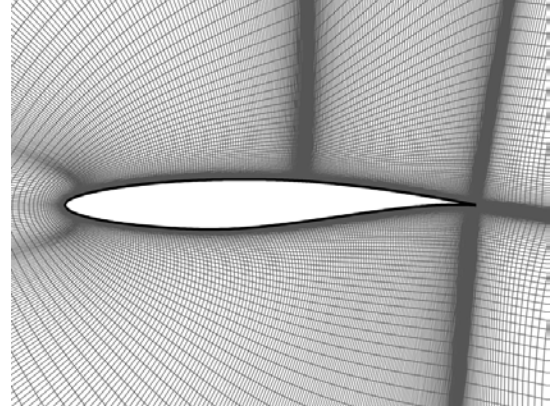
Table 3.3: Operating conditions of RAE 2822 airfoil.

Case ID	Re_c	M_∞	AoA (deg)	T_∞ (K)
6	6.5×10^6	0.729	2.31	273.15
9	6.5×10^6	0.730	2.80	273.15
10	6.2×10^6	0.750	2.80	273.15

The computational domain and the boundary conditions of the RAE 2822 airfoil are illustrated in Fig. 3.8(a). The farfield boundary of the domain is extended approximately $15c$ away from the airfoil. Despite the flow domain is relatively small, it will not induce a visible difference in the surface pressure distribution compared to a larger domain (i.e., farfield boundary extended $100c$ away) [150]. It should be noted that the laminar-to-turbulent flow transition in the experiment was triggered immediately after the leading edge (i.e., $0.03c$ downstream). Thus, the experimental data are comparable to fully turbulent RANS simulations without using a transition model.



(a) Flow domain and boundary conditions.



(b) Near-wall grid.

Figure 3.8: Illustration of the numerical model of the RAE 2822 airfoil.

The grid of RAE 2822 airfoil used in this work is the finest grid from NASA High-Order CFD Workshop [151], which uses a C-grid topology with 177, 737 and 512 grid points on the wall-normal direction, the circumferential direction and the airfoil surface, respectively. A near-wall view of the grid is presented in Fig. 3.8(b), and the y^+ value of the near-wall grid layer is kept below 1. To reduce the computational cost, only two layers of grids are considered in the spanwise direction, and the periodic boundary condition is used for both boundaries. The total number of grid points is 0.26 million.

3.4.3 Compressor Cases

The flow topologies leading to compressor rotating stall include the free tip separation and the fixed corner separation [152], as illustrated in Fig. 3.9. In this work, four compressor cases summarized in Table 3.4 are studied. Within these cases, the LMFA NACA65 cascade and the BUAA Stage B rotor have laboratory-level M and Re , whereas the NASA Rotor 67 and the TUDa-GLR-OpenStage have industrial-level M and Re ; the LMFA NACA65 cascade is featured by corner separation, whereas the rest three cases are featured by tip separation. Further details of each compressor case will be introduced in the following subsections.

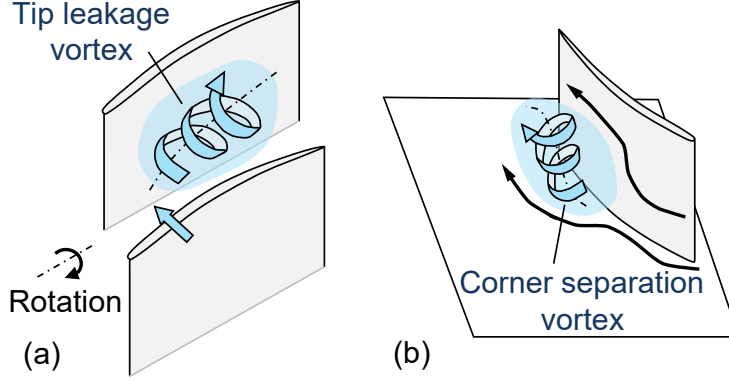


Figure 3.9: Illustration of detached flow topology in compressors: (a) tip separation and (b) corner separation.

Table 3.4: Summary of investigated compressor cases.

Case	Type of Geometry	Flow feature	$M_{1t/\infty}$	$Re_{c,t}$
LMFA NACA65 cascade	Linear cascade	Corner separation	0.12	3.82×10^5
BUAA Stage B rotor	Axial rotor	Tip separation	0.17	7.78×10^5
NASA Rotor 67	Axial rotor	Tip separation	1.38	2.75×10^6
TUDa-GLR-OpenStage	Axial 1.5-stage	Tip separation	1.17	2.55×10^6

3.4.3.1 LMFA NACA65 Cascade

LMFA NACA65 cascade is a low-speed linear compressor cascade featured by corner separation. Its design specification is summarized in Table 3.5. The cascade has been measured extensively by aerodynamic probes, and the available data include the cascade inlet and exit profiles of pressure and velocity components, the blade surface pressure and the endwall surface pressure [153–155]. The test rig and the measurement planes are presented in Fig. 3.10(a). Concurrently, scale-resolving simulations were also performed on this case under 4 degrees of incidence [73, 83, 156, 157].

The computational domain and boundary conditions of LMFA NACA65 cascade are illustrated in Fig. 3.10(b). It considers 50% span of the blade with a symmetry boundary condition, and it uses an extended duct of 5 chord length attached to the outlet of the experiment to damp

Table 3.5: Design specifications of LMFA NACA65 cascade.

Parameter	Symbol	Value
Freestream velocity (m/s)	u_1	40.0
Chord (mm)	c	150.0
Solidity	s/c	1.12
Aspect ratio	h/c	2.47
Camber angle (deg)	ϕ	23.22
Stagger angle (deg)	γ	42.70
Mach number	M_{1t}	0.12
Reynolds number	Re_c	3.82×10^5

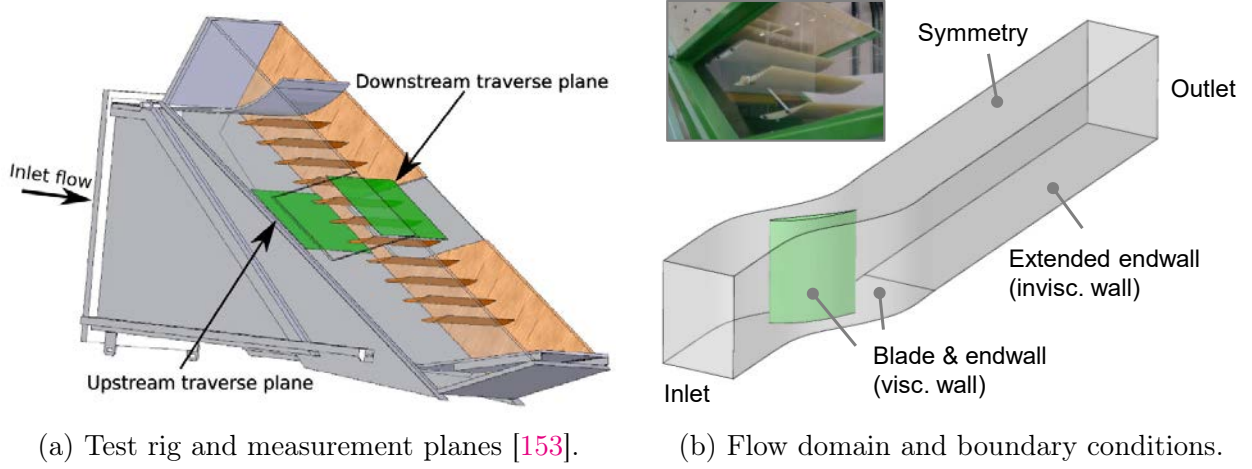


Figure 3.10: Illustration of test and numerical model of LMFA NACA65 cascade (photo courtesy of Dr. Wei Ma).

out the outlet pressure waves. At the inlet, the total pressure, total temperature and ν_t/ν profiles from a zero pressure gradient flat plate are assigned, which matches with the measured velocity profile at the inlet; the flow angle is determined by the operating incidence of the compressor cascade. At the outlet, the mass flow boundary condition is used based on the measured inlet mass flow. It should be noted that the laminar-to-turbulent flow transition in the experiment was triggered by sandpapers near the leading edge. Therefore, the experimental data are comparable to the fully turbulent RANS simulations without using a transition model.

To discretize the flow domain of LMFA NACA65 cascade, five sets of grids are generated by using AUTOGRID [158]. These grids have an O4H-type grid topology with hexahedra elements. The average y^+ value of the near-wall grid layer is kept around 1. The grid refinement was performed uniformly so that the number of grid points in each dimension is approximately 1.5 times that of a coarser grid. Details of the number of grid points in each dimension are summarized in Table 3.6. In the following investigation, the medium mesh will be used for RANS simulations.

Table 3.6: Details of LMFA NACA65 cascade grids.

Grid name	Ultracoarse	Coarse	Medium	Fine	Ultrafine
Total radial grid point	49	69	101	149	201
Total tangential grid point	41	65	89	141	181
Total axial grid point	97	129	193	289	385
Boundary layer grid point	13	17	25	37	49
Total grid point (million)	0.37	0.98	2.74	9.10	19.96
Usage	-	-	Ch. 6	-	-

3.4.3.2 BUAA Stage B Rotor

BUAA Stage B rotor is a laboratory-level low-speed axial compressor rotor. The whole stage is composed of an inlet guide vane, a rotor and a stator. The design specification of this rotor is summarized in Table 3.7. Extensive measurement campaigns were performed on this compressor stage with different rotor tip gap sizes and different stator configurations, and the available data include the rotor inlet and exit radial profiles from aerodynamic probes and the near-tip velocity field from the stereoscopic particle image velocimetry (SPIV) [159–162]. The SPIV measurement planes are illustrated in Fig. 3.11(a), including 10 slices between 10% and 100% of the blade tip chord near the suction surface and 11 slices between 5% and 105% of the blade tip chord near the pressure surface. For the rotor-only configuration with a 1.8% tip gap-to-chord ratio, scale-resolving simulations were also conducted [163]. The same rotor-only configuration will be investigated in this work.

Table 3.7: Design specifications of BUAA Stage B rotor.

Parameter	Symbol	Value
Hub-to-tip radius ratio	r_h/r_t	0.6
Tip gap to chord ratio	τ/c_t	1.8%
Tip aspect ratio	h/c_t	1.2
Flow coefficient	u_{x1}/U_m	0.58
Loading coefficient	$\Delta p_t/\rho_1 U_m^2$	0.52
Rotor design speed (RPM)	N	1100
Tip Mach number	M_{1t}	0.17
Reynolds number	Re_τ	1.4×10^4
Number of blade	Z	17

The computational domain and boundary conditions of BUAA Stage B rotor are illustrated in Fig. 3.11(b), which consists of a rotor blade passage with periodic boundary conditions and an extended nozzle with a buffer zone. At the inlet, the measured total pressure, total temperature and flow angle profiles are prescribed; the inlet ν_t/ν profiles are extracted from zero pressure gradient flat plate flows at the same boundary layer thickness. At the exit, the operating condition is controlled by a choked nozzle [164]. Euler equations are solved in the nozzle domain to reduce the calculation cost. A mixing plane model is used at the interface between the rotor domain and the nozzle domain.

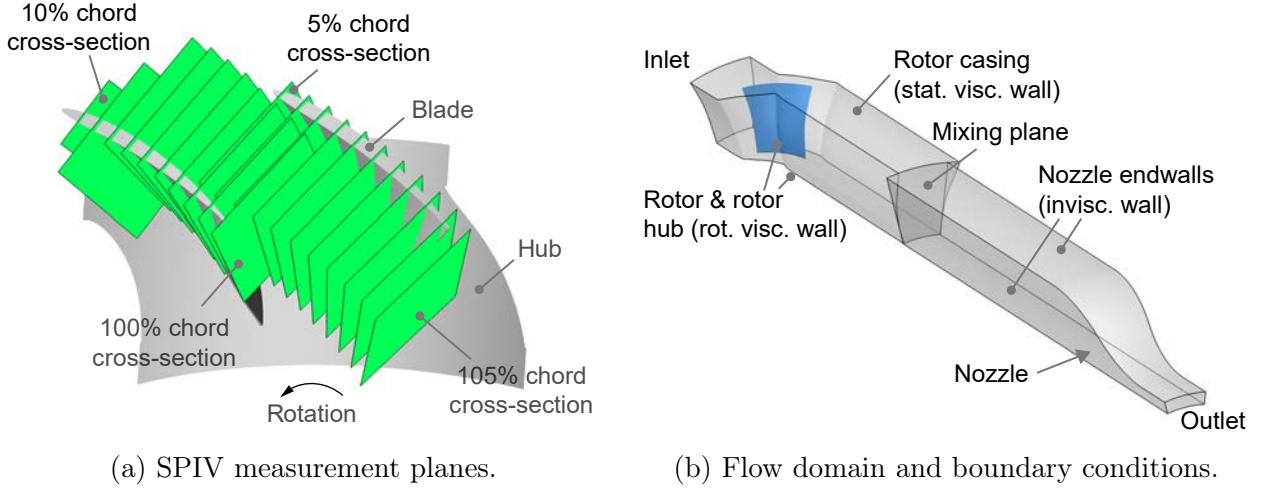


Figure 3.11: Illustration of measurement planes and numerical model of BUAA Stage B rotor.

The rotor domain is discretized by hexahedral grids generated by AUTOGRID [158]. In total, five sets of grids are generated, whose details are summarized in Table 3.8. To enhance the grid capability of resolving the tip leakage flow, over 50% of the radial grid points are located above the 80% span. The average y^+ value of the near-wall first-layer grid points is about 1. The nozzle domain is meshed by a hexahedral grid with 0.2 million points, which is generated by an in-house PYTHON script.

Table 3.8: Details of BUAA Stage B rotor grids.

Grid name	Ultracoarse	Coarse	Medium	Fine	Ultrafine
Total radial grid point	57	77	117	177	233
Tip gap radial grid point	13	21	29	45	57
Total tangential grid point	49	65	97	145	193
Total axial grid point	45	61	89	133	121
Boundary layer grid point	13	17	25	37	49
Tip gap O-grid point	13	17	25	37	49
Total grid point (million)	0.42	1.02	3.33	11.21	23.41
Usage	-	-	Ch. 4	Ch. 4, 6	Ch. 4

3.4.3.3 NASA Rotor 67

NASA Rotor 67 is a high-speed first-stage rotor of a two-stage fan. Its design specification is summarized in Table 3.9. Detailed geometry data and extensive measurement data of this case can be found in Strazisar et al. [26], where measurements of compressor characteristics, rotor exit radial profiles, rotor exit circumferential profiles and chordwise profiles were reported. The corresponding measurement planes are illustrated in Fig. 3.12(a). More recent performance characteristics data can be found in Grosvenor [165] and Fidalgo et al. [166].

Table 3.9: Design specifications of NASA Rotor 67.

Parameter	Symbol	Value
Mean hub-to-tip radius ratio	r_h/r_t	0.427
Tip gap to chord ratio	τ/c_t	0.7%
Mean aspect ratio	$(r_t - r_h)/c_{x,m}$	1.56
Design speed (RPM)	N	16043
Tip Mach number	M_{1t}	1.38
Reynolds number	Re_τ	1.8×10^4
Flow coefficient	u_{x1}/U_m	0.50
Loading coefficient	$\Delta h_t/\rho_1 U_m^2$	0.46
Mass flow (kg/s)	m	33.25
Total pressure ratio	π	1.63
Number of blade	Z	22

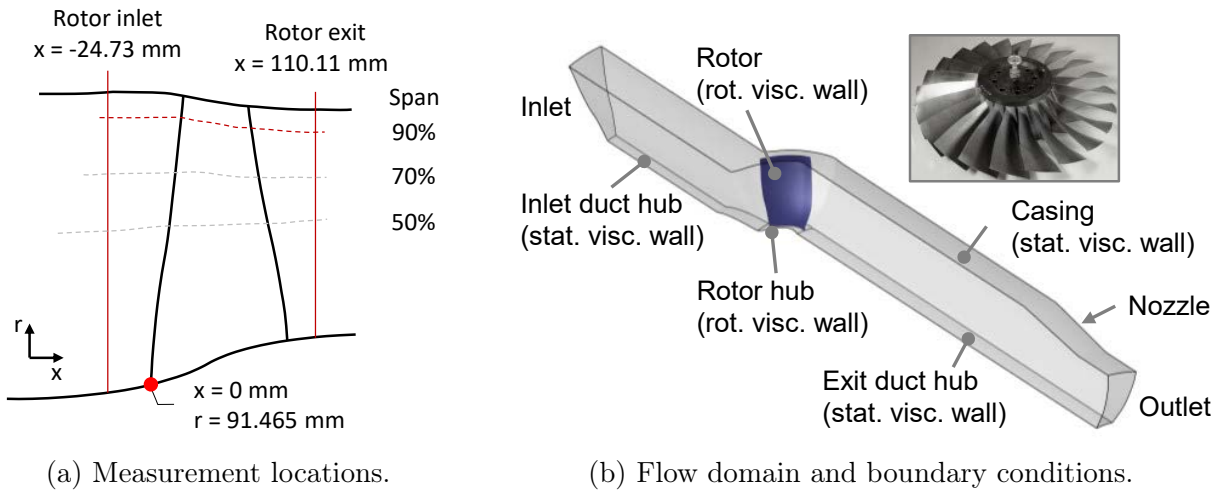


Figure 3.12: Illustration of measurement locations and numerical model of NASA Rotor 67 (photo courtesy of Daniel Laity).

The measured compressor performance characteristics were based on the pressure and temperature probe data at the rotor inlet and exit, and the mass flow was measured at the downstream orifice. The pressure was work-weighted averaged over each measurement plane, while the temperature was mass-weighted averaged. Since the difference between the two averaging methods is usually small [167] (e.g., $\pm 0.01\%$ in total pressure ratio in the current case), the mass-weighted average method is used throughout this work. Uncertainties of the total pressure ratio and the isentropic efficiency are calculated from the pressure probe uncertainty of 1 kPa and the temperature probe uncertainty of 0.6 K [26]. The radial profiles of total pressure, total temperature and absolute flow angle were also based on the probe data, and they were circumferentially mass-weighted averaged. The circumferential and chordwise profiles of relative Mach number and relative flow angle were based on the laser anemometer measurement, which was ensemble-averaged over 50 rotor passages.

The computational domain and boundary conditions of NASA Rotor 67 used in this research are illustrated in Fig. 3.12(b), which consists of an inlet duct, a rotor passage, an exit duct and a nozzle. At the inlet, radial profiles of total pressure, total temperature, flow angle and eddy viscosity are prescribed to match with the measured rotor inlet profiles, and the

freestream ν_t/ν is set as 0.7 [168]. At the exit, the compressor operating condition is controlled by a choked nozzle [164]. The mass flow rate difference between neighboring operating points is controlled within 0.2 kg/s when approaching stall.

The rotor domain is discretized by mixed-element unstructured meshes obtained from an in-house mesh generator. In total, five sets of meshes were generated with a refinement ratio of 1.5 in each dimension. The average y^+ value of the near-wall mesh is kept below 3. The tip gap and the hub fillet are considered in the grid.

Table 3.10: Details of NASA Rotor 67 grids.

Grid name	Ultracoarse	Coarse	Medium	Fine	Ultrafine
Total radial grid point	44	66	99	149	223
Tip gap radial grid point	9	13	20	30	45
Grid spacing (mm)	0.0675	0.045	0.03	0.02	0.0133
Boundary layer grid point	8	12	18	27	41
Total grid point (million)	0.15	0.48	1.44	5.00	14.54
Usage	-	-	Ch. 5, 6	-	-

3.4.3.4 TUDa-GLR-OpenStage

TUDa-GLR-OpenStage represents a typical front stage of a high-pressure compressor. It consists of a blisk rotor with radially stacked CDA airfoils, a stator with optimized 3D shapes, and an outlet guide vane (OGV) that straightens the flow. The rotor is originally designed by MTU and first tested in 1994, which has been investigated extensively in a series of experimental and numerical works [169–171]. The rotor blades are highly cambered near the hub and thin near the tip. The running tip gap size is approximately 0.75 mm at the design condition, and the hub fillet radius is 5 mm. The stator is designed conjointly between GLR and the German Aerospace Center (DLR). It is optimized via an automated multi-objective optimization process to suppress the separation size [172]. The stator blades have a forward sweep feature near both endwalls and a bow feature towards the pressure surface near the casing. The shapes of the fillets at both endwalls are prescribed by a digitized geometry file. The more detailed specification of the compressor stage is summarized in Table 3.11.

The TUDa-GLR-OpenStage was tested on the transonic compressor rig of GLR, which can measure the steady-state performance, the aerodynamic instabilities and the blade vibration levels of the compressors. The measurement sections of the compressor are presented in Fig. 3.13(a). At the stage inlet section (ME15), radial profiles of total pressure and total temperature are measured. At the rotor exit section (ME21), radial profiles of total pressure and absolute Mach number components are available. At the stage exit section (ME30), 2D distributions of total pressure and total temperature are acquired. The total pressure ratio and total temperature ratio characteristics are calculated by the area-averaged probe data at sections ME15 and ME30; the isentropic efficiency is calculated using the probe-based total pressure ratio and the shaft power. For a fair comparison between the experiment and CFD, the isentropic efficiency from CFD is calculated based on the area-averaged pressure ratio and

Table 3.11: Design parameters of TUDa-GLR-OpenStage.

Parameters	Symbols	Values
Rotor mean aspect ratio	$(r_t - r_h)/c_m$	0.94
Rotor hub-to-tip ratio	r_h/r_t	0.51
Rotor tip gap-to-chord ratio	τ/c_t	0.8%
Rotor tip radius (mm)	r_t	190
Rotor tip chord length (mm)	c_t	94
Rotor design speed (RPM)	N	20000
Rotor tip Mach number	M_t	1.17
Rotor Reynolds number	Re_τ	2.2×10^4
Stage flow coefficient	u_{x1}/U_m	0.52
Stage loading coefficient	$\Delta h_t/\rho_1 U_m^2$	0.36
Stage mass flow (kg/s)	m	16.0
Stage total pressure ratio	π	1.49
Number of blades	Z	16/29/5

the mass-averaged temperature ratio. Calculations of the measurement uncertainty along with the measured data are detailed in Klausmann et al. [173].

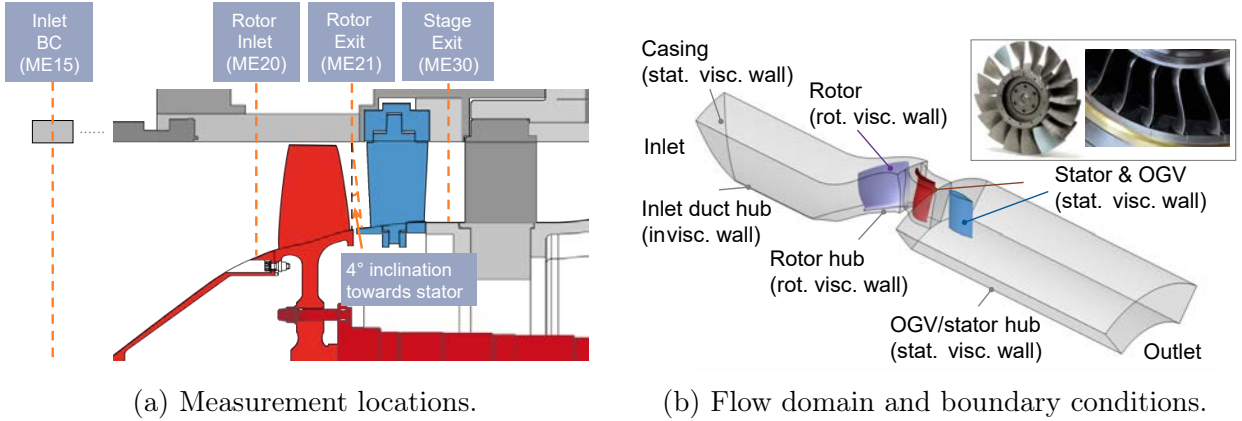


Figure 3.13: Illustration of measurement locations and numerical model of TUDa-GLR-OpenStage (photo courtesy of GLR, TU Darmstadt).

The computational domain and boundary conditions of TUDa-GLR-OpenStage are illustrated in Fig. 3.13(b). The flow domain corresponds to one blade passage of the compressor. At the inlet, the measured total pressure and total temperature profiles, the flow direction (axial flow without swirl), and a uniform $\nu_t/\nu = 35$ are prescribed. At the outlet, a static pressure boundary condition is used when operating away from stall, while a nozzle characteristics boundary condition (i.e., the outlet static pressure is updated iteratively according to a prescribed nozzle characteristic curve) [82] is used when approaching the stall limit. The mass flow rate difference between neighboring operating points is controlled within 0.2 kg/s when approaching stall.

The flow domain of TUDa-GLR-OpenStage is discretized by hexahedral grids generated by AUTOGRID [158]. In total, five sets of grids are generated for the rotor and stator, where

the grid refinement was performed uniformly in each dimension with a refining ratio of about 1.5. The tip gap and the fillets of the blades are considered in the grid. The OGV is discretized by 0.9 million grid points, which has a grid density similar to the medium grid of the rotor and stator. The average y^+ value of the near-wall mesh is kept below 3.

Table 3.12: Details of TUDa-GLR-OpenStage grids.

Grid name		Ultracoarse	Coarse	Medium	Fine	Ultrafine
Rotor	Total radial grid point	37	53	81	121	181
	Tip gap radial grid point	9	13	21	33	49
	Hub fillet radial grid point	9	13	17	29	45
	Total tangential grid point	29	41	65	93	145
	Total axial grid point	41	61	97	141	213
	Boundary layer grid point	9	13	21	29	45
	Tip gap O-grid point	5	9	13	21	29
	Total grid point (million)	0.12	0.28	1.08	3.36	11.77
Stator	Total radial grid point	41	65	93	137	201
	Tip/hub fillet radial grid point	9	13	21	29	49
	Total tangential grid point	17	29	41	69	101
	Total axial grid point	37	53	85	129	189
	Boundary layer grid point	9	13	21	29	45
	Tip gap O-grid point	5	9	13	21	29
	Total grid point (million)	0.04	0.16	0.53	1.80	5.81
Usage		-	-	Ch. 6	-	-

3.4.3.5 Grid Independence Study

Minimizing the grid-induced discretization error is essential for turbulence model development. Following the procedures in Ref. [174], a flow quantity of interest q can be written as:

$$q = C\Delta^n + q_{ideal} \quad (3.11)$$

where $C\Delta^n$ is the discretization error with C a constant, $\Delta = (1/N_g)^{1/3}$ the grid spacing and n the order of spatial accuracy; q_{ideal} is the ideal value of q free of discretization error. By running CFD simulations with a series of uniformly refined grids, a dataset of $q(\Delta)$ is obtained, and the n_{th} order polynomial function in Eq. (3.11) can be fitted through the data to obtain k and q_{ideal} . The relative discretization error can therefore be calculated as:

$$\epsilon_q = \left| \frac{q - q_{ideal}}{q_{ideal}} \right| \times 100\% \quad (3.12)$$

For the four compressor cases investigated in this work, the above procedures are performed based on the RANS-SA simulation data obtained from the aforementioned five sets of grids. The flow quantities of interest are static pressure rise coefficient for LMFA NACA65 cascade and BUAA Stage B rotor, rotor total pressure ratio for NASA Rotor 67 and stage total pressure ratio

for TUDa-GLR-OpenStage. The derived relative discretization errors of all the investigated grids are plotted against the number of grid points in Fig. 3.14. Results show that using the medium grid for NASA Rotor 67 and TUDa-GLR-OpenStage and the fine grid for LMFA NACA65 cascade and BUAA Stage B rotor can achieve a discretization error of less than 1%, which is sufficiently small for the purpose of the study. Considering the fine mesh steady RANS simulation results of LMFA NACA65 presented inherent unsteadiness in the wake region, the medium mesh is used instead.

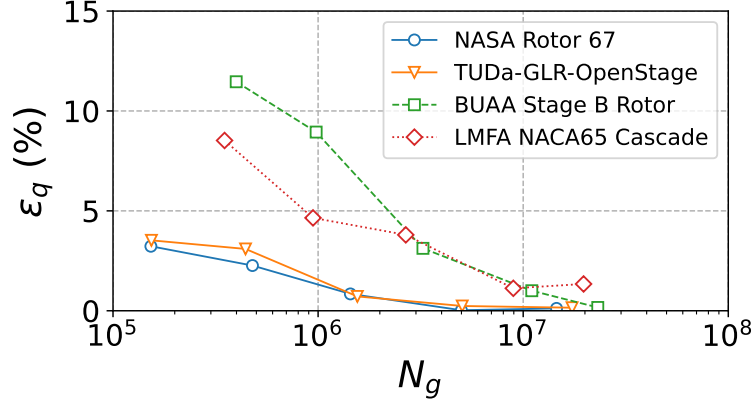


Figure 3.14: Discretization error versus number of grid points

The final adopted grids for each compressor case and the corresponding relative discretization errors are summarized in Table 3.13.

Table 3.13: Summary of discretization error of validation cases

Case	q	Grid name	N_g (million)	ϵ_q (%)
LMFA NACA65 cascade	C_p ($i = 4$ deg)	Medium	2.74	3.80
BUAA Stage B rotor	C_p ($\phi = 0.61$)	Fine	11.21	1.00
NASA Rotor 67	π_{1t-2t} (NS)	Medium	1.44	0.84
TUDa-GLR-OpenStage	π_{1t-4t} (NS)	Medium	1.61	0.72

4. Turbulence Database of Compressor Tip Leakage Flow

“Science can only be created by those who are thoroughly imbued with the aspiration toward truth and understanding.”

— *Albert Einstein, Science and Religion*

4.1 Introduction

High-fidelity turbulence data is the prerequisite for data-driven turbulence modeling. Due to the high Reynolds number and the complex flow domain of industrial turbomachines, DNS and wall-resolved LES are prohibitively expensive. Hybrid RANS/LES methods such as DES achieves a compromise in both accuracy and cost. In this chapter, a DES-type method will be established to generate a database of compressor tip leakage flow.

This chapter is organized as follows. To start with, the recent developments of DES will be reviewed, and the recommended DES upgrades for predicting compressor tip leakage flow will be given. Then, the updated DES method will be validated and verified in a backward-facing step and a low-speed compressor rotor. Following that, a turbulence database of compressor tip leakage flow will be generated. Lastly, the transient flow features, the mean flow quantities, the turbulence statistics and the modal components of the database will be analyzed.

4.2 Detached Eddy Simulation for Turbomachinery

4.2.1 Formulation and Recent Development

DES [62] is originally proposed based on the Spalart-Allmaras (SA) turbulence model [44], which solves a transport equation for the modified turbulent viscosity $\tilde{\nu}$. In the logarithmic region of the boundary layer, the SA model assumes the turbulent viscosity ν_t to be proportional to the wall distance d (i.e., $\nu_t \propto Sd^2$), which resembles the Smagorinsky subgrid-scale (SGS) turbulent viscosity ν_{SGS} proportional to the grid spacing Δ (i.e., $\nu_{SGS} \propto S\Delta^2$). Therefore, the scale-resolving capability of the SA model can be achieved by replacing d with $\tilde{d}$ in Eq. (4.1):

$$\tilde{d} = \min(d, C_{DES}\Delta) \quad (4.1)$$

where the model coefficient $C_{DES} = 0.65$ is calibrated in homogeneous isotropic turbulence [175], and the grid spacing Δ is by default the longest cell edge length (i.e., Δ_{max}). By using the term

$\tilde{d}$ in the turbulent viscosity destruction term, the near-wall region is solved in RANS mode, and the far-wall region is resolved in LES mode.

The RANS-to-LES switch of the original DES purely depends on the grid but not the flow field, which may lead to grid-induced separation (GIS) [65]. An update to alleviate this issue is the DDES method [66], which uses a flow-dependent shielding function f_d to preserve the RANS mode near the boundary, as given by Eq. (4.2):

$$\begin{aligned}\tilde{d} &= d - f_d \max(0, d - C_{DES} \Delta) \\ f_d &= 1 - \tanh\left(\left[\frac{C_{d1} \tilde{\nu}}{\kappa^2 d^2} \left(\frac{\partial u_i}{\partial x_j} \frac{\partial u_i}{\partial x_j}\right)^{-\frac{1}{2}}\right]^{C_{d2}}\right)\end{aligned}\quad (4.2)$$

where the Karman constant $\kappa = 0.41$ and the model coefficients $C_{d1} = 8$ and $C_{d2} = 3$ were calibrated in flat plate boundary layer based on Δ_{max} [66]. DDES is now the standard version of the DES-type methods since it conceptually outperforms the original DES. DDES is also implemented with other RANS models such as the SA-RC [176] and SST [177] models.

As the application of DDES accumulates, some shortcomings of the method have become apparent. These limits are fundamentally caused at the RANS-to-LES interface, where no mechanism of converting between the modeled and resolved turbulence kinetic energy exists. Flow solutions near the interface are neither RANS nor LES, hence referred to as “gray area”. The gray area not only leads to the slow LES development (SLD) in shear layers but also causes the modeled stress depletion (MSD) or even the GIS in attached boundary layers [65].

Although the gray area issue cannot be solved completely (without using zonal treatments), there are some numerical strategies that mitigate its harmful effects. The SLD issue can be alleviated by improving the baseline LES model of Smagorinsky, i.e., $\nu_{SGS} = (C_{DES} \Delta)^2 S$, which cannot predict the turbulence transition (i.e., laminar-to-turbulent transition in terms of physics; RANS-to-LES transition in terms of CFD) correctly. The improvement involves either an alternative definition of the grid spacing (e.g., $\Delta_{\omega, vol}$ [178], $\tilde{\Delta}_\omega$ [179], $F_{KH} \tilde{\Delta}_\omega$ [180]), or an alternative definition of the velocity differential operator (e.g., S_W^* for the WALE model and S_σ^* for the σ model [179]), or a dynamic C_{DES} constant [181] in Eq. (4.2). The MSD issue can be alleviated by improving the shielding function to push the grey area away from the boundary layer. Examples of the improved shielding functions include f_e of the Improved DDES (IDDES) [67], f_s of the shielded DES (SDES) [64] and $f_d(G_{\tilde{\nu}})$ of the Zonal DES (ZDES) [182]. In addition, minor modifications such as removal of the f_{t2} term [183] and correction of the low-Reynolds number term [66] in the SA model can reduce the risk of MSD further.

The aforementioned evolution of DES-type methods is summarized in Fig. 4.1.

4.2.2 Recommendation for Turbomachinery Flow Solver

4.2.2.1 Compressor Detached Flow Topology

Detached flow topologies leading to compressor rotating stall include the free tip separation and the fixed corner separation [152].

The free-tip separation is caused by the abrupt expansion of the geometry. After the pressure-driven tip leakage flow detaches from the blade tip, it forms a shear layer between itself

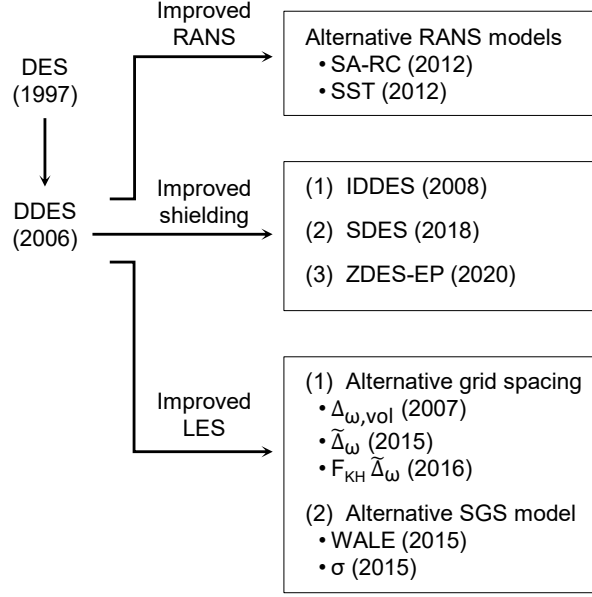


Figure 4.1: Evolution of Detached Eddy Simulation.

and the main flow, which induces multi-scale vortical structures (i.e., Kelvin–Helmholtz instability) [82]. The challenge in simulating this case is the correct prediction of the Kelvin–Helmholtz instability, which requires an improved LES capability in the DES-type methods. To the best knowledge of the authors, no previous research has attempted it yet.

The fixed corner separation is caused by the adverse pressure gradient and the boundary layer development. The key to predicting the separation size accurately relies on the correct prediction of both the separated flow and the development of the boundary layer before separation. For the DES-type methods, it requires both an improved LES prediction in the separation region and an improved RANS prediction in the attached boundary layer. Previous research has investigated the effects of the baseline RANS model [23, 184] and the LES model [157] on this case.

This chapter focuses on the free tip separation and hence pursues an improved LES model for DES. Past research (summarized in Fig. 4.1) has demonstrated that modifying the grid spacing definition achieves a similar level of accuracy as modifying the SGS model, but it is simpler and more universal [180]. Using an alternative grid spacing definition is also compatible with other upgrades in the baseline RANS model and the shielding function. Thus, it is adopted in this work.

4.2.2.2 Alternative Grid Spacing Definition

Available grid spacing definitions for DES are summarized in Table 4.1, which includes a general version for an arbitrary cell and a more interpretable version for a cuboid cell. Here, the arbitrary cell has n_n nodes, n_l edges and n_s surfaces, and its node coordinates, edge length, surface area and volume are denoted by $\mathbf{x}$, $\mathbf{l}$, $\mathbf{A}$ and V ; $\mathbf{n}_\omega$ denotes the local unit vorticity vector and is assumed to be on the z-direction in the cuboid cell.

The default grid spacing Δ_{max} was proposed based on the observation of a boundary layer mesh for RANS simulations, which features a large streamwise grid spacing of the same order as the boundary layer thickness [62]. Although Δ_{max} is a reasonable estimation of the RANS/LES interface location, it may over-dissipate the turbulent fluctuations in shear layers if the local mesh is anisotropic. Another definition Δ_{vol} is based on the cell volume, which is inherited from LES [185]. However, it may under-predict the SGS turbulent viscosity (i.e., MSD) in highly anisotropic cells. The defects of Δ_{max} and Δ_{vol} originate from the lack of information on the vortices to be resolved. For a local vortex spinning around an arbitrary axis, it is the grid spacing in the plane normal to the spinning axis that determines the resolved scale. A handy indicator of the spinning axis is the local vorticity vector. Based on this idea, $\Delta_{\omega,vol}$ (originally termed as Δ_{ω} [178]) and $\Delta_{\omega,max}$ are proposed, which conceptually mimic Δ_{vol} and Δ_{max} . A more recent proposal is $\tilde{\Delta}_{\omega}$ [179], which initially projects the 3D grid cell to a 2D plane normal to the vorticity vector and then takes the longest distance in the projected area.

Table 4.1: Summary of grid spacing definition.

Symbol	Arbitrary cell	Cuboid cell
Δ_{max}	$\max_{i=1,n_l} \Delta \mathbf{l}_i $	$\max (\Delta x, \Delta y, \Delta z)$
Δ_{vol}	$V^{1/3}$	$(\Delta x \Delta y \Delta z)^{1/3}$
$\Delta_{\omega,max}$	$\max_{i=1,n_l} \Delta \mathbf{l}_i \times \mathbf{n}_{\omega} $	$\max (\Delta x, \Delta y)$
$\Delta_{\omega,vol}$	$(\sum_{i=1}^{n_s} \mathbf{A}_i \cdot \mathbf{n}_{\omega} / 2)^{1/2}$	$(\Delta x \Delta y)^{1/2}$
$\tilde{\Delta}_{\omega}$	$\frac{1}{\sqrt{3}} \max_{i,j=1,n_n} (\mathbf{x}_i - \mathbf{x}_j) \times \mathbf{n}_{\omega} $	$\frac{1}{\sqrt{3}} \sqrt{\Delta x^2 + \Delta y^2}$

To compare different grid spacing definitions with each other, their values are calculated and depicted for a hexahedron and a triangular prism in Fig. 4.2, which are commonly used in unstructured turbomachinery solvers. The boundary layer mesh of a turbomachinery blade passage contains mostly hexahedra. In the scenario of Fig. 4.2(a), the hexahedron is located in the boundary layer of a blade, and the streamwise, pitchwise and spanwise directions are aligned with the x , y and z axis respectively. Thus, the unit vorticity vector is in the z direction. Triangular prisms are commonly used to fill in the turbomachinery passage except for the boundary layers. In the scenario of Fig. 4.2(b), the triangular prism is located near the tip span, and it shares the same coordinate system with that of the hexahedron. The unit vorticity vector coincides with the trajectory of the TLV.

Results in Fig. 4.2 show that Δ_{vol} , $\Delta_{\omega,vol}$ and $\tilde{\Delta}_{\omega}$ all lead to a smaller grid spacing compared to Δ_{max} , which helps alleviate the SLD issue. However, Δ_{vol} and $\Delta_{\omega,vol}$ are an order of magnitude smaller than Δ_{max} in hexahedra with high aspect ratios and highly skewed prisms, which increases the risk of MSD. Despite the merit of $\tilde{\Delta}_{\omega}$, it is not recommended for turbomachinery flow solvers because: (1) the vorticity vector no longer indicates the spinning axis of the local vortex in a strong shear flow [186] or in a rotating reference frame, both of which are the case for the tip leakage flow of a compressor rotor; (2) the constant $1/\sqrt{3}$ of $\tilde{\Delta}_{\omega}$ is designed for hexahedron only but not universal for a mixed-element mesh.

Based on the above discussions, the recommended grid spacing is a hybrid definition between Δ_{max} and Δ_{vol} firstly proposed by Deck [187], where $\Delta_{hyb} = \Delta_{vol}$ in the LES region

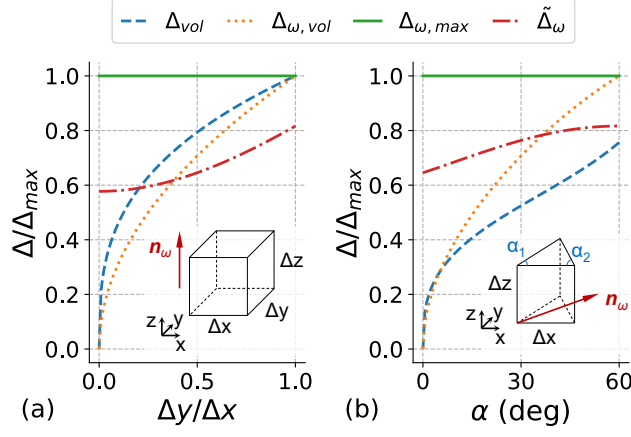


Figure 4.2: Comparison of grid spacing definitions: (a) hexahedron and (b) triangular prism; the plot assumes $\Delta_z = \Delta_x$, $\alpha_1 = \alpha_2 = \alpha$ and $\langle \mathbf{n}_\omega, \mathbf{n}_x \rangle = 30\text{deg}$ for better visualization.

and $\Delta_{hyb} = \Delta_{max}$ in the RANS region. This definition addresses both the SLD and the MSD issues like $\tilde{\Delta}_\omega$ does, but it is more computationally efficient and more compatible with a turbomachinery unstructured solver. To inform the local flow physics to the SGS model, the Kelvin-Helmholtz instability unlocker F_{KH} from Shur et al. [180] is multiplied by the grid spacing. Thus, the final grid spacing definition is denoted by Eq. (4.3):

$$\Delta = F_{KH} \Delta_{hyb} = \begin{cases} \Delta_{max}, & (f_d < f_{d0}) \\ F_{KH} \Delta_{vol}, & (f_d \geq f_{d0}) \end{cases} \quad (4.3)$$

where the threshold $f_{d0} = 0.99$, and the term F_{KH} is calculated using Eq. (4.4) based on the Vortex Tilting Measure (VTM). The constants are $F_{KH}^{max} = 1.0$, $F_{KH}^{min} = 0.1$, $a_1 = 0.15$ and $a_2 = 0.3$.

$$F_{KH} = \max\{F_{KH}^{min}, \min\{F_{KH}^{max}, \frac{F_{KH}^{max} - F_{KH}^{min}}{a_2 - a_1}(\langle \text{VTM} \rangle - a_1)\}\}$$

$$\text{VTM} = \frac{\sqrt{6} |(\mathbf{S} \cdot \boldsymbol{\omega}) \times \boldsymbol{\omega}|}{\omega^2 \sqrt{3 \text{tr}(\mathbf{S}^2) - [\text{tr}(\mathbf{S})]^2}} \max\{1, 0.2\nu/\nu_t\} \quad (4.4)$$

4.2.2.3 Modification to the Numerical Scheme

A typical turbomachinery flow solver is capable of handling mixed elements meshes and uses a second-order accurate spatial scheme. This type of scheme is robust in RANS simulations but is too dissipative for LES simulations. Meanwhile, high-order schemes on unstructured meshes are difficult to formulate and hence are not commonly used. To maximize the scale-resolving capabilities of the second-order schemes, a simple modification is to use a hybrid definition of artificial dissipation. Take the artificial dissipation term based on Roe's matrix [133] for example. Considering the flux between node i and j , the artificial dissipation is written in Eq. (4.5):

$$D_{ij} = |A_{i,j}| [\epsilon_2 \sigma_p (\Phi_i - \Phi_j) + \epsilon_4 (1 - \sigma_p) (L(\Phi_j) - L(\Phi_i))] \quad (4.5)$$

where A is the standard Roe's matrix, Φ is the solution vector of conservative variables, σ_p is a pressure-based sensor, and L is a pseudo-Laplacian operator. The sensor σ_p only switches on

in the vicinity of shock waves to damp numerical oscillations, and its corresponding dissipation coefficient ϵ_2 is kept unchanged for numerical stability concerns. The artificial dissipation in the rest of the flow domain is dominated by the dissipation coefficient ϵ_4 , which needs to be large in the RANS regions for stability and small in the LES regions for accuracy. Hence, a hybrid fourth-order dissipation coefficient $\epsilon_{4,hyb}$ based on a flow region sensor σ_ϵ was proposed [144], as shown in Eq. (4.6):

$$\epsilon_{4,hyb} = \epsilon_{4,RANS}(1 - \sigma_\epsilon) + \epsilon_{4,LES}\sigma_\epsilon \quad (4.6)$$

where $\epsilon_{4,RANS} = 1/64$ is kept unchanged as the base RANS solver and $\epsilon_{4,LES} = 1/1024$ is adopted following the calibration in Probst et al. [144].

A natural choice of σ_ϵ is the f_d shielding function from DDES, which is physically justified, computationally efficient and widely applied by previous researchers [188, 189]. However, when using this approach, numerical stability issues were reported for the simulation of some external flow cases [189]. Another candidate for σ_ϵ is the empirical function σ_{NTS} [190], which is also used extensively by researchers [144, 191, 192]. This function identifies both the far-wall inviscid region and the near-wall boundary layer as regions vulnerable to numerical instability. However, the detected boundary layer thickness will be thinner than that of the f_d function [144]. Considering the flows of interest are internal flows of turbomachinery blade passages, the advantage of σ_{NTS} for external flows [190] is irrelevant. Thus, f_d is recommended for σ_ϵ .

4.2.3 Implementation in the In-House Flow Solver

Following the recommendations in section 4.2.2, DES is implemented in the in-house flow solver by the following means:

1. SA-based DDES in Eq. (4.2) with $f_{t2} = 0$ and Ψ -based low-Re correction [66, 183].
2. Alternative grid spacing $\Delta = F_{KH}\Delta_{hyb}$ detailed in Eq. (4.3) and (4.4) [180, 187].
3. A hybrid low-dissipation scheme with $\sigma_\epsilon \equiv f_d$ in Eq. (4.6) [144].

In the next section, both the original and the recommended DDES settings are compared with each other, which are referred to as DDES(SA- Δ_{max}) and DDES(SA- $F_{KH}\Delta_{hyb}$) respectively. All calculations are based on the same low-dissipation scheme.

4.3 Detached Eddy Simulation of Backward-Facing Step

4.3.1 Case Description

To demonstrate the capability of the DES methods, the backward-facing step is investigated first. The backward-facing step is the simplest flow model that resembles part of the flow physics of compressor tip leakage flow. It is also an ideal case for DES validation because it contains attached, detached and reattached flow zones that are separated by clear boundaries. Both the SLD issue and the MSD issue are pronounced at these interfaces, as illustrated in Fig. 4.3. In this work, the backward-facing step at Reynolds number $Re_H = 3.6 \times 10^4$, Mach number

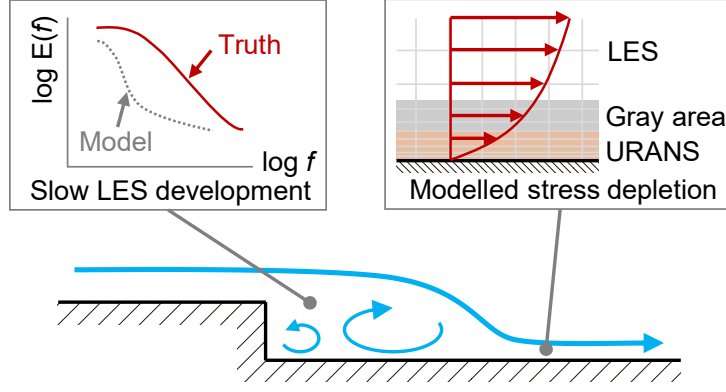


Figure 4.3: Illustration of flow physics and numerical issues in backward-facing step.

$M = 0.128$ and expansion ratio $ER = 9/8$ is studied. Extensive measured data of this case can be found in Driver and Seegmiller [143].

The size of the flow domain is $34H \times 9H \times 4H$ as shown in Fig. 4.4. At the inlet, profiles of total pressure, total temperature, velocity angles and turbulent viscosity are prescribed to match the measured velocity and Reynolds shear stress profiles [143]; at the top and the bottom walls, the adiabatic viscous wall condition is assigned; at the exit, the backpressure is set to match the prescribed Mach number; at the spanwise boundaries, the symmetry boundary condition is used.

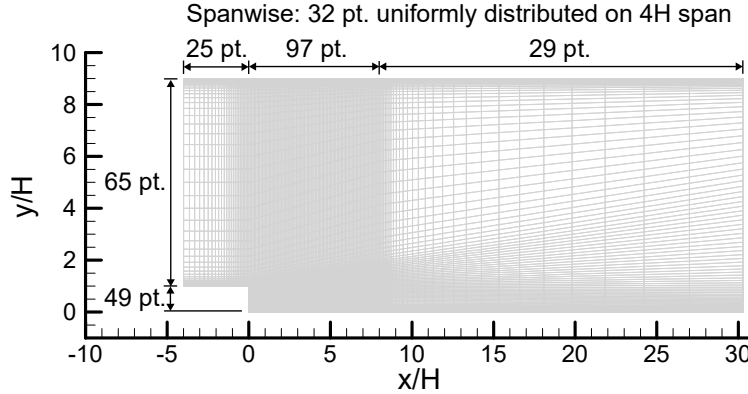


Figure 4.4: Illustration of backward-facing step coarse grid.

The flow domain is discretized by using hexahedral cells, and two grids with different mesh densities were used. The coarse grid has 0.5 million points, which is presented in Fig. 4.4. The medium grid has 4.0 million points and the grid refinement is performed by doubling the mesh point in all dimensions. The two meshes are truncated from the 3rd and 4th finest meshes provided by the NASA Turbulence Modeling Resource website [54]. The non-dimensional time step is set as $\Delta t/t_0 = 7.02 \times 10^{-2}$ and 3.51×10^{-2} for the two meshes, where $t_0 = H/U_\infty$ is the convective time unit. This time step leads to a local CFL number finer than the recommended value of unity [193]. Within each physical time step, 8 Newton iterations are performed, and the residual drops for over 2 orders of magnitude. The converged steady RANS simulation results were used as the initial condition for the DDES simulations. After the simulation achieves a statistically stationary state, the mean flow quantities and the turbulence statistics

are calculated via spanwise averaging over the middle half of the flow domain (i.e., $\Delta z/H = 2$) and time averaging over $400t_0$.

4.3.2 DES Verification

To verify the DES methods are implemented correctly, the f_d and F_{KH} functions are examined in Fig. 4.5. For the contour plot of f_d , the boundary layers before and after the step are well preserved in the RANS mode (i.e., $f_d \rightarrow 0$) while elsewhere in the domain is solved in the LES mode (i.e., $f_d \rightarrow 1$), which is conceptually correct. The contour plot of F_{KH} successfully captures the shear layer formed immediately after the step and lowers down the local modeled turbulent viscosity (i.e., $F_{KH} < 1.0$), which is the design intent. Since results from both meshes are similar, only the coarse grid results are shown here for brevity.

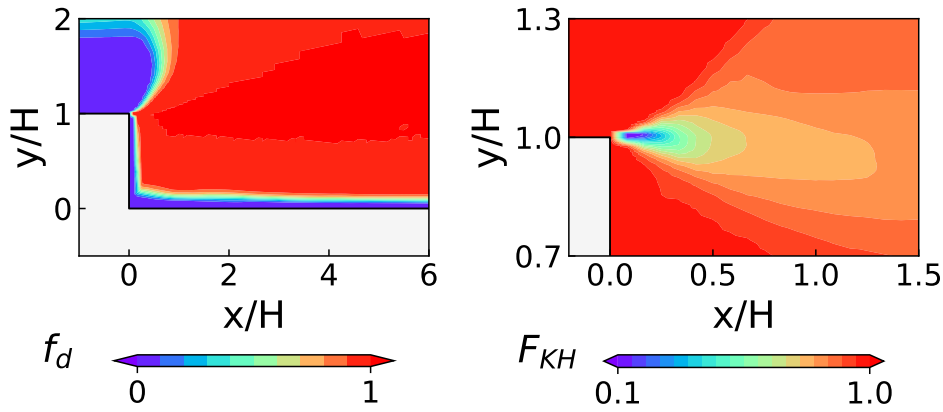


Figure 4.5: Contours of f_d and F_{KH} for the backward-facing step; coarse grid DDES(SA- $F_{KH}\Delta_{hyb}$) result.

The quality of the scale-resolving solution can be quantified by the IQ_ν index [194] shown in Eq. (4.7):

$$IQ_\nu = (1 + \alpha_\nu (\frac{\nu_{t,eff}}{\nu})^n)^{-1} \quad (4.7)$$

where the effective viscosity $\nu_{t,eff}$ includes both the modelled turbulent viscosity ν_t and the numerical viscosity ν_{num} induced by the discretization error, and the coefficients $\alpha_\nu = 0.05$ and $n = 0.53$. A higher IQ_ν implies a larger percentage of resolved turbulence. Specifically, an $IQ_\nu > 0.80$ indicates a good quality LES, and an $IQ_\nu > 0.95$ indicates a good quality DNS [194]. The calculation of ν_{num} requires a ground truth solution (e.g., high-resolution DNS) beforehand, which is not available for this case. In this work, the ν_{num} term is ignored and the IQ_ν index is calculated using $\nu_{t,eff} \approx \nu_t$. This form of IQ_ν is overestimated compared to the original definition, and the threshold values of 0.80 and 0.95 may not be valid. However, such a simplification will not degrade the comparison between different DES settings based on the same spatial discretization scheme.

The contours of IQ_ν obtained from different DES settings are compared in Fig. 4.6. Results show that DDES(SA- $F_{KH}\Delta_{hyb}$) resolves more turbulence (i.e., higher values of IQ_ν) than DDES(SA- Δ_{max}) does, especially in the shear layer and the reattached boundary layer. When the medium grid is used, the IQ_ν values for both methods increase, but DDES(SA- $F_{KH}\Delta_{hyb}$)

still outperforms DDES(SA- Δ_{max}) in a similar manner. These results are not shown for brevity.

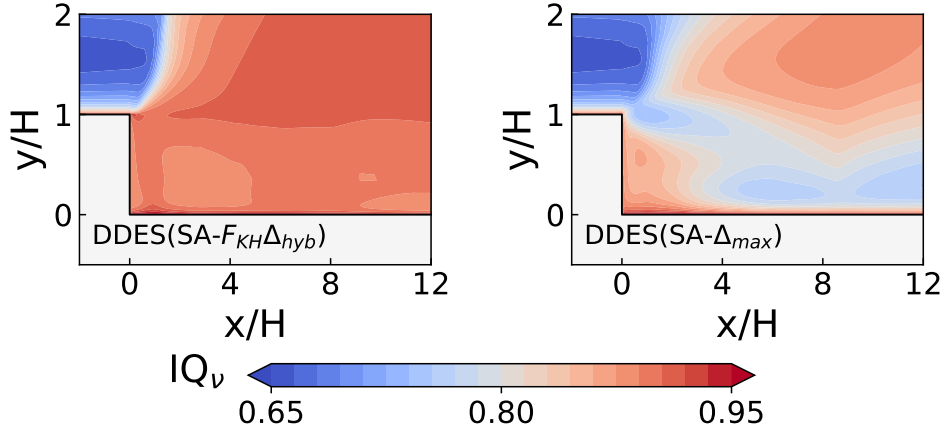


Figure 4.6: Contours of IQ_v for the backward-facing step; coarse grid result.

4.3.3 Mean Flow Quantities

The mean flow quantities of interest for the step case are the velocity profiles and the skin friction distribution at the bottom wall. In this section, simulation results from both DDES(SA- Δ_{max}) and DDES(SA- $F_{KH}\Delta_{hyb}$) are compared against RANS(SA) and measured data. The results obtained by the coarse and the medium grid are denoted by “C-” and “M-” in the following figures.

For the velocity profiles presented in Fig. 4.7, the measured data identify a flow separation bubble in the region $0 < x/H < 6$. Further downstream at $x/H > 6$, the flow reattaches to the bottom wall. Regarding the simulation results, DDES(SA- $F_{KH}\Delta_{hyb}$) with both meshes predicts the velocity profiles at all the axial locations accurately; RANS(SA) predicts stronger flow reversal in the separation bubble near the wall, but its predictions after the reattachment point are accurate; DDES(SA- Δ_{max}), however, presents the worst agreement with the measured data, where the deficiency originates from the shear layer near $0 < x/H < 4$ and $0.5 < y/H < 1$ and advects further downstream towards the bottom wall. Refining the coarse grid to the medium grid only reduces the deficiency of DDES(SA- Δ_{max}) in the reattached boundary layer, but the problem near the shear layer still persists.

For the skin friction distribution shown in Fig. 4.8, the measured reattachment point with local $C_f = 0$ is located around $x/H = 6.3$, which is predicted accurately by DDES(SA- $F_{KH}\Delta_{hyb}$) and RANS(SA). The skin friction in the separation region is also predicted well by DDES(SA- $F_{KH}\Delta_{hyb}$), but RANS(SA) predicts larger negative values that are consistent with the over-predicted flow reversal shown in Fig. 4.7. DDES(SA- Δ_{max}) predicts a more downstream separation bubble and hence shows the worst agreement with the measured data. When refining the coarse grid to the medium grid, the skin friction prediction of DDES(SA- $F_{KH}\Delta_{hyb}$) improves slightly in the separated region; the DDES(SA- Δ_{max}) prediction of the separation bubble size and the skin friction in the reattached boundary layer are improved, but they are still worse than the coarse grid DDES(SA- $F_{KH}\Delta_{hyb}$) results.

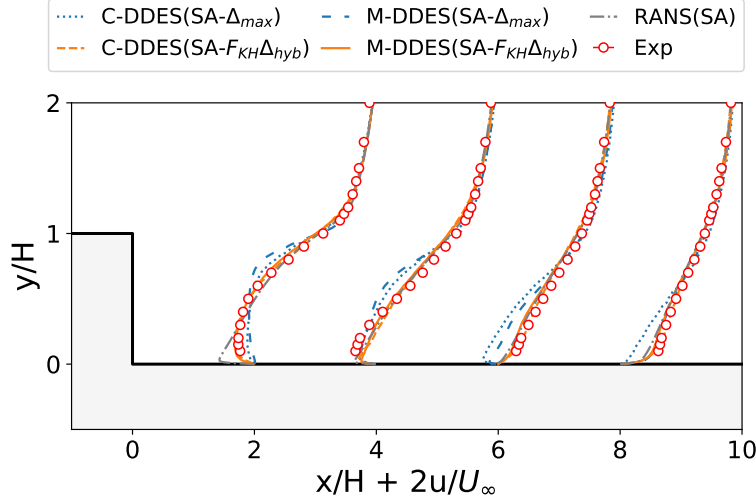


Figure 4.7: Velocity profiles of backward-facing step

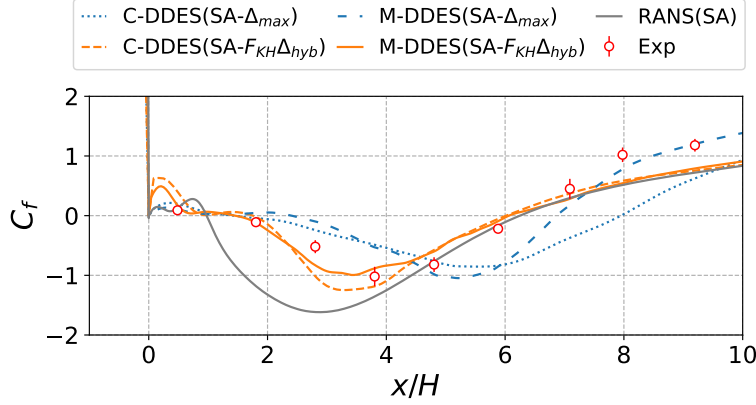


Figure 4.8: Skin friction of backward-facing step

4.3.4 Turbulence Statistics

From the perspective of turbulence modeling, the quantities of interest include the turbulence kinetic energy (TKE) and the anisotropy of the Reynolds stress tensor. This information will serve as the training data for RANS turbulence model development.

The two-component TKE profiles are shown in Fig. 4.9. DDES(SA- $F_{KH}\Delta_{hyb}$) predicts the most accurate profiles in comparison to RANS(SA) and DDES(SA- Δ_{max}). Despite some minor differences between the coarse mesh DDES(SA- $F_{KH}\Delta_{hyb}$) results and the experimental results, the discrepancy decreases with further mesh refinement. DDES(SA- Δ_{max}) predicts a delayed transition to turbulence where the TKE is underpredicted immediately after the step but overpredicted further downstream. Further mesh refinement attempted in this work does not help DDES(SA- Δ_{max}) unlock the physics of Kelvin-Helmholtz instability in the shear layer, but it increases the TKE further downstream which reduces the separation bubble size. RANS(SA) does not predict the TKE [44] and thus is not shown in the figure.

Turbulence anisotropy can be quantified by solving an eigenvalue problem of the Reynolds

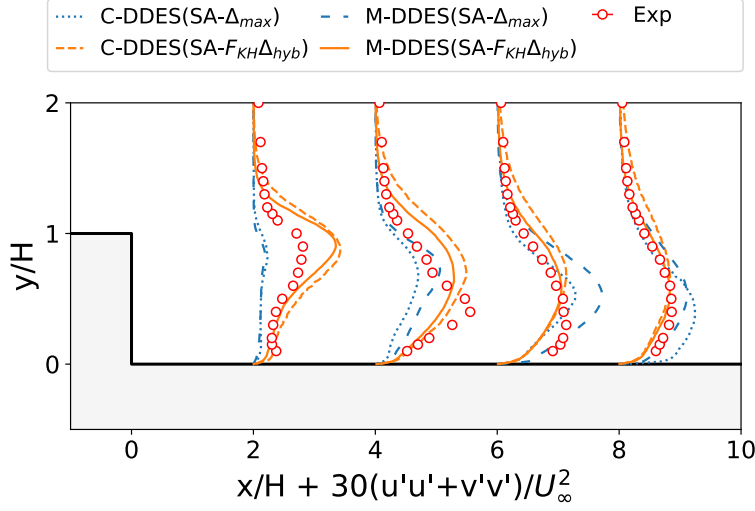


Figure 4.9: Two-component turbulence kinetic energy profiles of backward-facing step

stress anisotropy tensor, whose incompressible form is denoted by Eq. (4.8):

$$a_{ij} = \frac{\overline{u'v'}}{2k} - \frac{\delta_{ij}}{3} \quad (4.8)$$

where k is the turbulence kinetic energy, and a_{ij} has eigenvalues $\lambda_1 > \lambda_2 > \lambda_3$. Note that an arbitrary realizable turbulence state can be reconstructed by a linear combination of the three limiting turbulence states, namely one-component (1C), axisymmetric two-component (2C) and isotropic (3C). Hence, an arbitrary turbulence state can be visualized by a barycentric map using the coordinate system of Eq. (4.9) [195]:

$$\mathbf{x}_B = C_{1c}\mathbf{x}_{1c} + C_{2c}\mathbf{x}_{2c} + C_{3c}\mathbf{x}_{3c} \quad (4.9)$$

where the weights are $C_{1c} = \lambda_1 - \lambda_2$, $C_{2c} = 2(\lambda_2 - \lambda_3)$, $C_{3c} = 3\lambda_3 + 1$; the coordinates of the limiting states are $\mathbf{x}_{1c} = (1, 0)$, $\mathbf{x}_{2c} = (0, 0)$ and $\mathbf{x}_{3c} = (1/2, \sqrt{3}/2)$.

The turbulence anisotropy barycentric map of a profile within the separation bubble is illustrated in Fig. 4.10. For comparison with the RANS and the DES setups, the Direct Numerical Simulation (DNS) result of a similar backward-facing step case [196] is also depicted. The DNS result shows mostly axisymmetric two-component state (2C) close to the wall, indicating that the non-penetration condition of the wall has a stronger dissipation effect on turbulent fluctuations than the non-slip condition. This effect is not considered in the SA model, which leads to the deficiency of RANS(SA) near the wall. In the mainstream, the DNS result shows a compound state of turbulence componentality, indicating the difficulty in achieving the isotropic turbulence state (3C) in internal flows. However, the RANS(SA) result shows a 3C state in the mainstream enforced by the Boussinesq assumption, which again shows the deficiency of RANS(SA). All the DDES solutions show a qualitatively good agreement with DNS on the turbulence componentality profile except for DDES(SA- Δ_{max}) with the coarse grid.

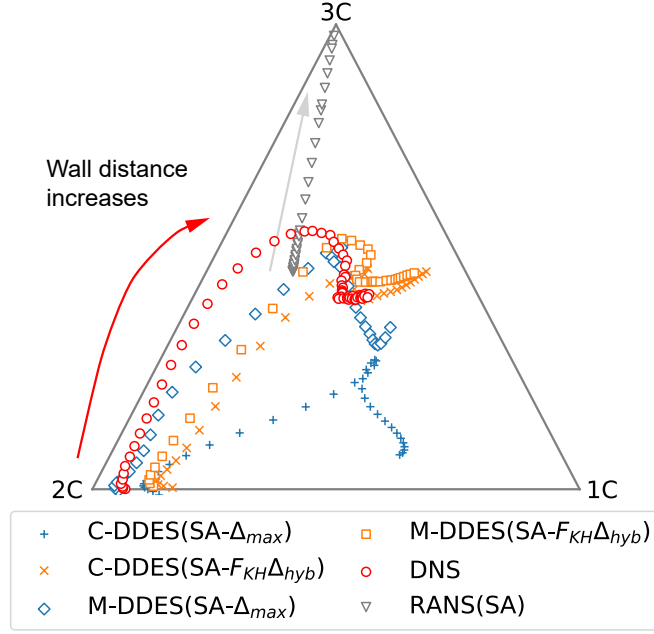


Figure 4.10: Turbulence anisotropy barycentric map of backward-facing step at $x/H = 4$ and $0 \leq y/H \leq 1$

4.4 Detached Eddy Simulation of BUAA Stage B Rotor

4.4.1 Case Description

The main case of interest in this chapter is the low-speed BUAA Stage B rotor from Du et al. [159]. This case is featured by tip leakage vortex (TLV), and it has been tested extensively by using five-hole probes at the rotor inlet and exit and stereoscopic particle image velocimetry (SPIV) inside the rotor passage. The available measured data are at the flow coefficient $\phi = u_x/U_m$ of 0.575 and 0.481. More details about the experimental data and the CFD setup are summarized in Sec. 3.4.3.

In this section, the five sets of grids introduced in Sec. 3.4.3 are used for DDES simulations, and the results of the medium, fine and ultrafine grids are analyzed in detail. The time step in local CFL number is $\Delta t \cdot U_t/\Delta_\theta \approx 1/3$, where U_t and Δ_θ denote the blade tip speed and the average grid spacing on the circumferential direction, respectively. This dimensionless time step is finer than the recommended value of unity [193] and hence achieves good time accuracy. Within each time step, 30 Newton iterations are performed so that the mean residual drops over 2 orders of magnitude. The converged steady RANS simulation results were used as the initial condition for the DDES simulations. After around 2 rotor revolutions, the DDES solutions reached a statistically steady state. The simulations were then performed for another 2 rotor revolutions in which all snapshots were collected for time-averaging.

4.4.2 DES Verification

To start with, verification of the DES methods is carried out in the BUAA Stage B rotor based on the medium grid. The time-averaged contours of the f_d and F_{KH} functions are shown in Fig. 4.11. The f_d function shields the boundary layer of the blade surfaces and the casing wall in RANS mode (i.e., $f_d \rightarrow 0$), while the tip gap between the casing and the blade tip surface is solved in LES mode (i.e., $f_d \rightarrow 1$). The F_{KH} contour is plotted on the iso-surface of Q-criterion [197] that envelopes the TLV. It shows that the F_{KH} function lowers the modeled viscosity in the vicinity of the TLV (i.e., $F_{KH} < 1.0$), which speeds up the RANS-to-LES transition of the turbulence field.

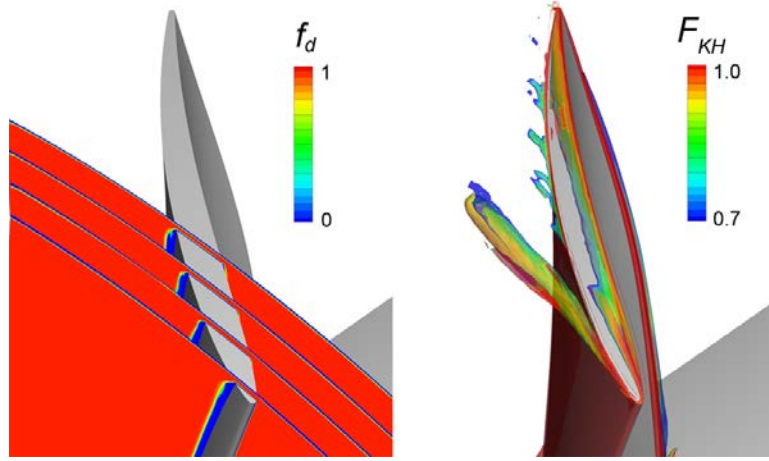


Figure 4.11: Contours of f_d on the cross sections and contours of F_{KH} on the iso-surface of $Q = (U_t/\tau)^2/50$ for the BUAA Stage B rotor at $\phi = 0.585$; time-averaged medium grid DDES(SA- $F_{KH}\Delta_{hyb}$) result.

To compare the DDES(SA- $F_{KH}\Delta_{hyb}$) method with the DDES(SA- Δ_{max}) method, the snapshot of iso-surfaces of Q-criterion colored by the IQ_ν index of Eq. (4.7) are presented in Fig. 4.12. It shows that DDES(SA- $F_{KH}\Delta_{hyb}$) resolves smaller turbulence structures and has a higher IQ_ν value compared to DDES(SA- Δ_{max}). Therefore, DDES(SA- $F_{KH}\Delta_{hyb}$) outperforms DDES(SA- Δ_{max}) in terms of prediction accuracy.

To compare the DDES(SA- $F_{KH}\Delta_{hyb}$) method with the DDES(SA- Δ_{max}) method further, the contours of TKE are shown in Fig. 4.13. Here, both DDES results are at the numerical near-stall condition at $\phi = 0.585$. The experimental near-stall condition is at a smaller flow coefficient of $\phi = 0.481$ due to the effect of the downstream stator, which is not considered in the current numerical model. Thus, the comparison between the experimental and the DDES results here are qualitative. The experimental results show that TKE is produced in the shear layer close to the leading edge (i.e., 30%-60% tip chord downstream of the leading edge). The TKE advects downstream and diffuses to the surrounding region, leading to the decay of the peak TKE value. DDES(SA- Δ_{max}) fails to capture the TKE production in the shear layer and predicts a turbulence transition further downstream. DDES(SA- $F_{KH}\Delta_{hyb}$) on the other hand predicts the production, advection and diffusion of TKE qualitatively well. These results again demonstrate the advantage of DDES(SA- $F_{KH}\Delta_{hyb}$) over DDES(SA- Δ_{max}).

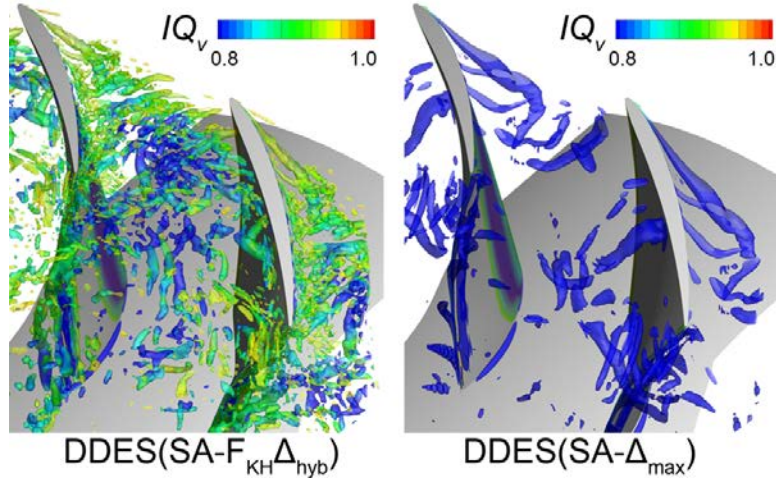


Figure 4.12: Contours of IQ_v on the iso-surface of $Q = (U_t/\tau)^2/50$ for the BUAA Stage B rotor at $\phi = 0.585$; snapshot medium grid result.

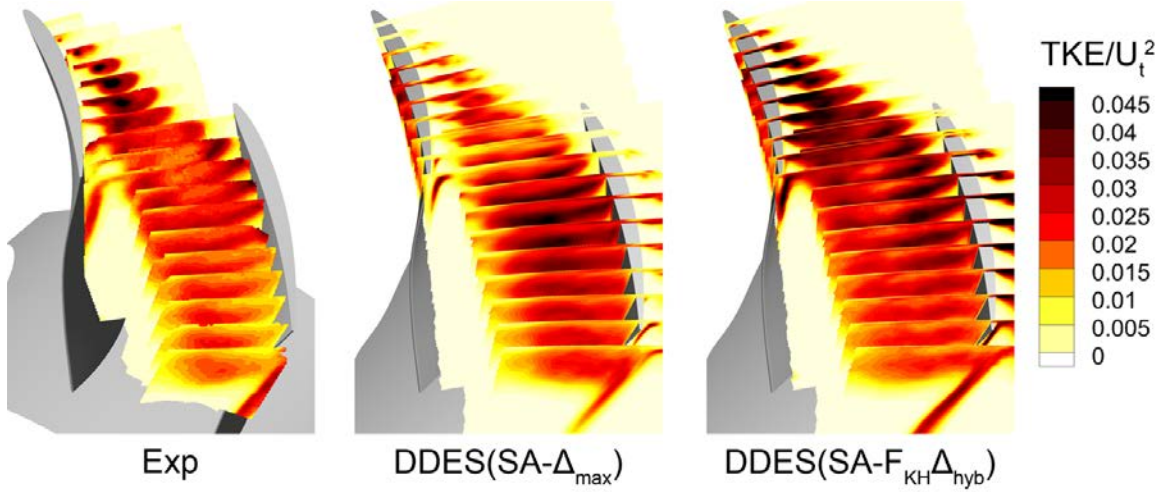


Figure 4.13: Turbulence kinetic energy contours of BUAA Stage B rotor near stall; Exp: $\phi = 0.481$; DDES: $\phi = 0.585$, medium grid results.

4.4.3 Grid Independence Study

The grid density has a significant effect on the accuracy of scale-resolving simulations. In Fig. 4.14, the static pressure rise characteristics $C_p = \Delta p / \frac{1}{2} \rho U_m^2$ predicted by different grids are presented. It shows that refining the grid to the fine and the ultrafine grid density reaches a grid-independent solution on the near-stall characteristics. Both the fine and the ultrafine results predict the C_p value comparable to that from the experiment near $\phi = 0.575$, but both simulation results predict an earlier stall onset than the experiment due to the absence of the downstream stator.

To check the grid independence further, the rotor exit radial profiles near $\phi = 0.575$ are shown in Fig. 4.15. Results again show that the fine grid result overlaps with the ultrafine grid result at most spans, indicating that grid independence has been reached. The fine and ultrafine results match the general trend of the measured data with only minor differences, which are attributed to the radial redistribution of flow by the downstream stator. It is envisaged that

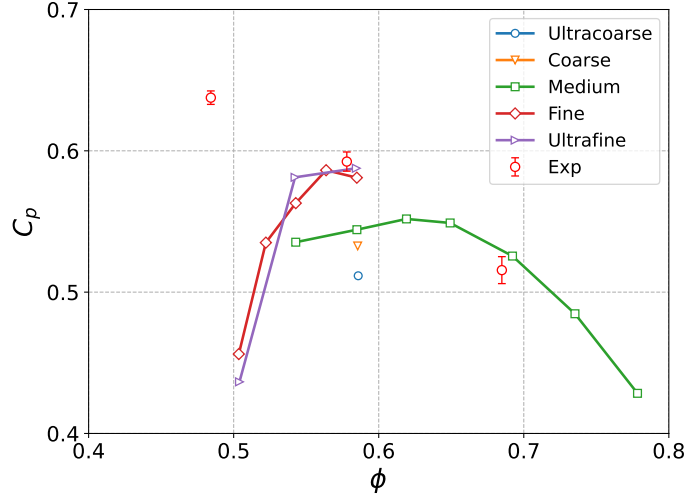


Figure 4.14: Static pressure rise characteristics of BUAA Stage B rotor; DDES(SA- $F_{KH}\Delta_{hyb}$) results.

including the stator in the numerical model can improve the prediction accuracy further, but this is out of the scope of this chapter.

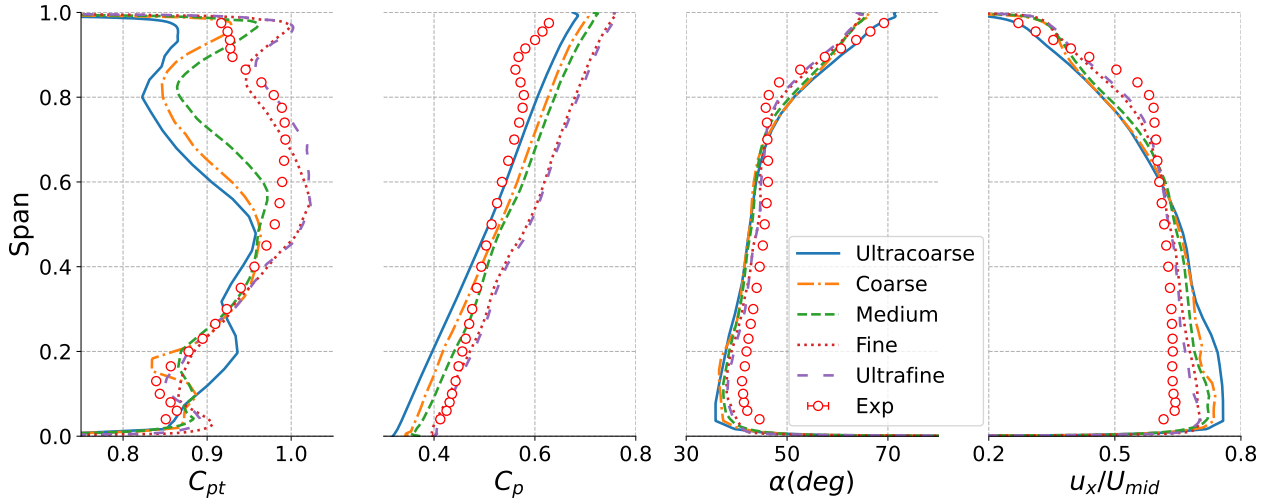


Figure 4.15: Rotor exit radial profiles of BUAA Stage B rotor; Exp: $\phi = 0.575$; DDES: $\phi = 0.585$, DDES(SA- $F_{KH}\Delta_{hyb}$) results.

In the following analysis, the fine and ultrafine grid results that have achieved grid independence will be analyzed in detail.

4.4.4 Transient Flow Fields

The transient flow field of the investigated rotor is illustrated in Fig. 4.16, where the vortical structures are identified by the iso-surfaces of the Q-criterion. The iso-surfaces are colored by the IQ_v index of Eq. (4.7), which measures the resolution of DDES.

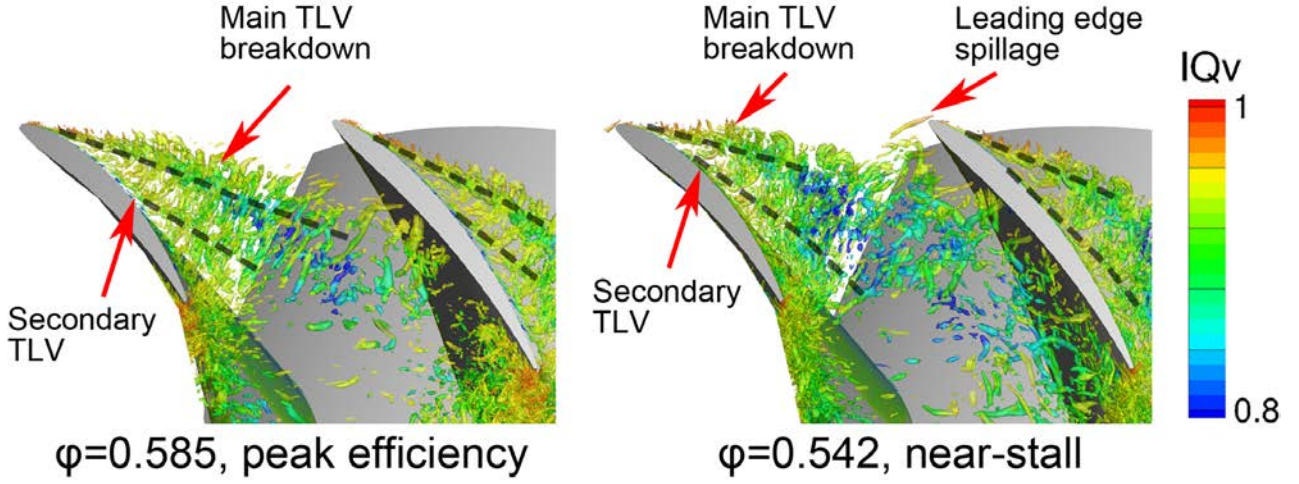


Figure 4.16: Contours of IQ_v on the iso-surface of $Q = (U_t/\tau)^2/20$ for the BUAA Stage B rotor; snapshot DDES(SA- $F_{KH}\Delta_{hyb}$) ultrafine grid result.

At the peak efficiency condition, a large-scale TLV is formed immediately after the leading edge due to the shear effect between the tip leakage flow and the incoming main flow. Afterward, the spiral-type vortex breakdown occurs on the main TLV near the mid-pitch, which generates smaller eddies that impinge on the pressure surface of the adjacent blade. Part of the main TLV flow passes through the tip gap of the adjacent blade and forms a secondary TLV, which detaches from the mid-chord suction surface and propagates toward the rotor exit. The impingement and the detachment of the TLVs exert unsteady forces on the blade.

At the near stall condition, a similar double-leakage structure can be observed. The difference is that the main TLV breakdown and therefore the formation of the secondary TLV move upstream. Part of the eddies originated from the main TLV breakdown spill over the leading edge of the adjacent blade, which can potentially initiate a spike-type rotating stall cell [198]. The evolution of the double-leakage structure found in this work is consistent with the previous research [72].

4.4.5 Mean Flow Quantities

The mean flow quantities of interest for compressor tip leakage flow include the TLV trajectory and the tip blockage size, which determine the stall margin and efficiency of a tip-loaded compressor. These quantities can be captured by streamwise relative vorticity and velocity respectively.

The contours of streamwise relative vorticity obtained from the SPIV measurement, the ultrafine grid DDES and the fine grid DDES are shown in Fig. 4.17. In these plots, the streamwise relative vorticity is non-dimensionalized by the blade rotational speed, where a negative value indicates the vorticity direction is opposite to the blade rotation. The trajectory of the TLV is captured by high negative values of vorticity, and the TLV breakdown is indicated by the rapid dissipation of the vorticity magnitude.

Comparing the measured data with both simulation results, it is observed that the measured TLV trajectory can be qualitatively predicted by DDES but at different flow coefficients,

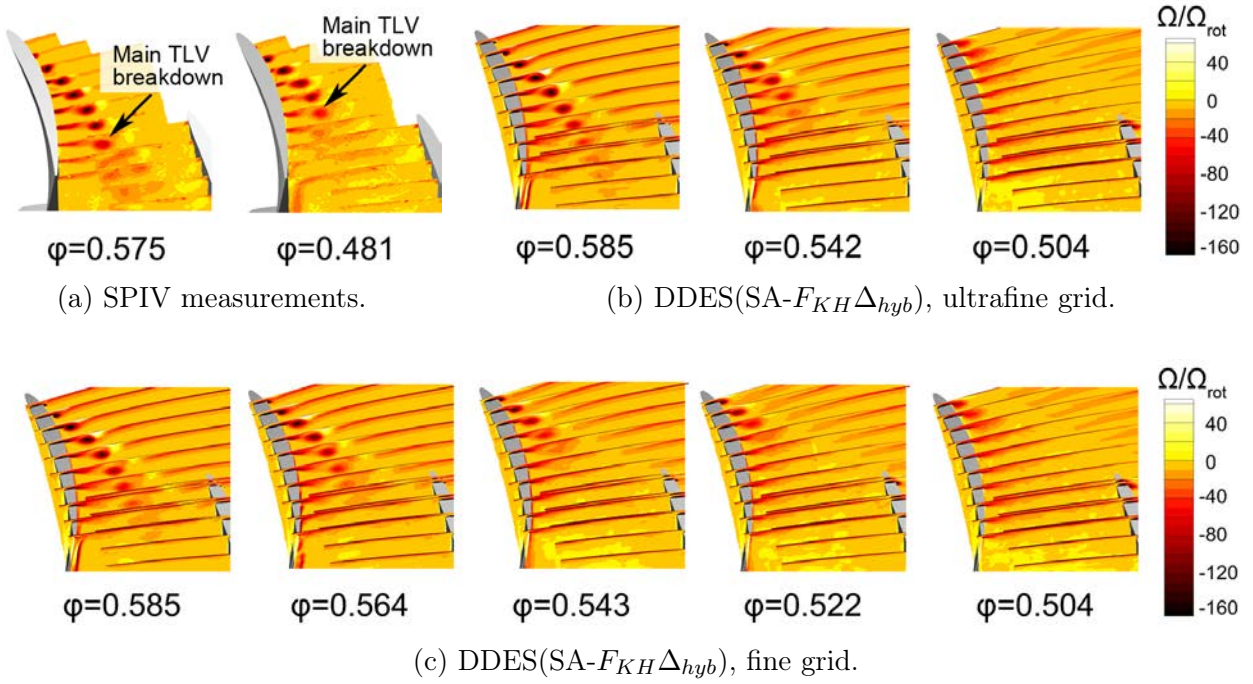


Figure 4.17: Streamwise relative vorticity contours of BUAA Stage B rotor.

i.e., measured data at $\phi = 0.575$ and $\phi = 0.481$ are qualitatively reproduced by ultrafine grid DDES at $\phi = 0.585$ and $\phi = 0.542$, respectively, as well as by fine grid DDES at $\phi = 0.585$ and $\phi = 0.564$, respectively. The flow coefficient mismatch between the measured results and the DDES results is caused by the downstream stator in the measurement. As observed in Fig. 4.15, the downstream stator radially redistributes the rotor blade loading. When the near-tip flow fields from DDES match with that of the experiment, the flow fields at the rest of the spans do not match. Hence, the axial velocity away from the tip is predicted differently by DDES, leading to the difference in the overall operating flow coefficient.

Comparing the results with different flow coefficients, the TLV breakdown occurs at a further upstream location when the flow coefficient is reduced (i.e., compressor throttling from choke to stall). When the vortex breakdown occurs before it enters the blade passage (e.g., $\phi \approx 0.54$ for DDES results), the small-scale vortices generated from the vortex breakdown can spill over the leading edge of the adjacent blade, which interacts with the TLV of the adjacent blade passage and potentially initiates a stall cell.

The contours of streamwise relative velocity obtained from the SPIV measurement, the ultrafine grid DDES and the fine grid DDES are presented in Fig. 4.18. In these plots, the streamwise relative velocity is non-dimensionalized by the blade tip speed, and the blockage cell is indicated by the low-momentum region. Together with the observations in Fig. 4.15, the tip blockage cell forms immediately after the main TLV breakdown in all the presented results.

Comparing the measured data with both simulation results, it again shows that the measured tip blockage size can be qualitatively captured by DDES at different flow coefficients, i.e., measured data at $\phi = 0.575$ and $\phi = 0.481$ are qualitatively reproduced by ultrafine grid DDES at $\phi = 0.585$ and $\phi = 0.542$, respectively, as well as by fine grid DDES at $\phi = 0.585$ and $\phi = 0.543$, respectively. This is likely caused by the downstream stator as discussed before.

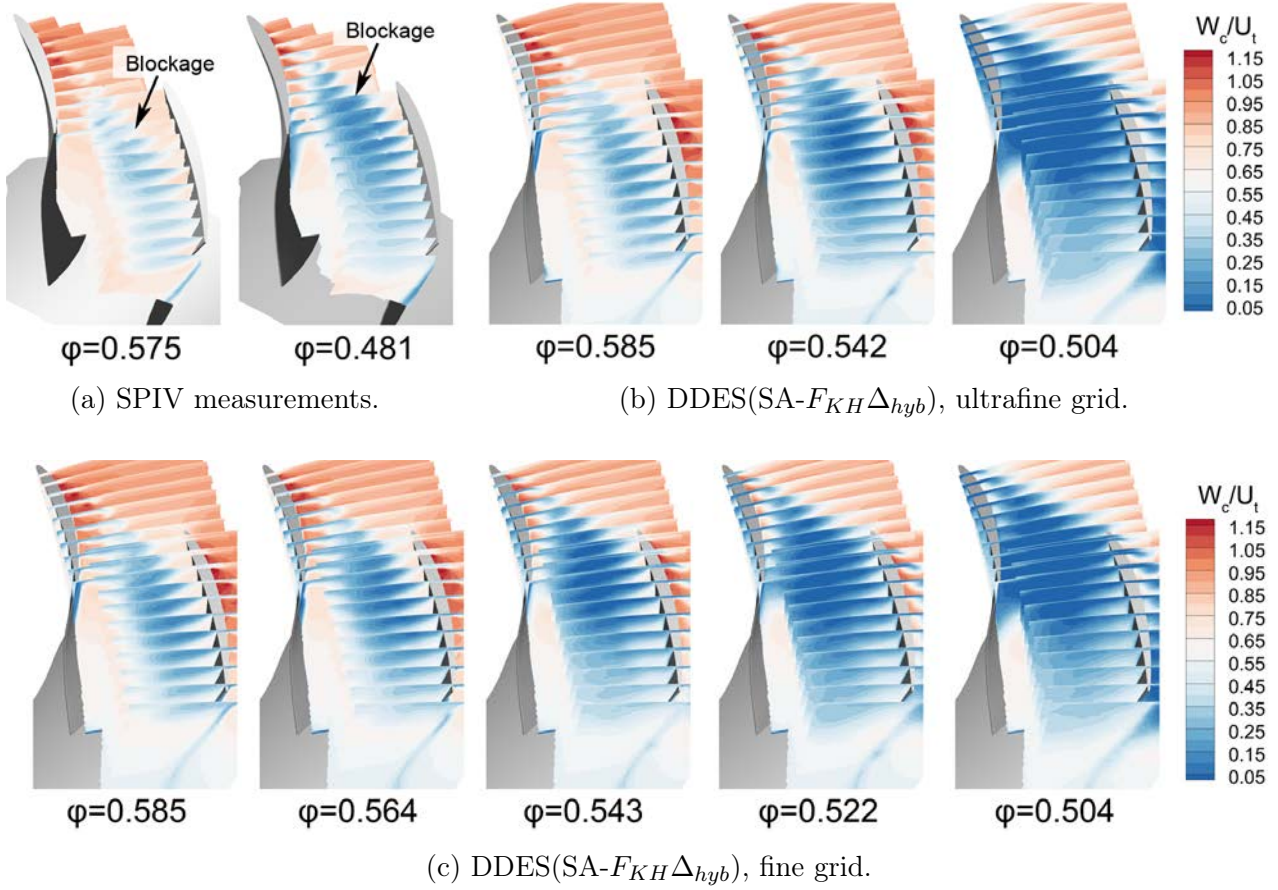


Figure 4.18: Streamwise relative velocity contours of BUAA Stage B rotor.

Comparing the results with different flow coefficients, the tip blockage cell enlarges with decreasing flow coefficient. Eventually (e.g., $\phi = 0.504$ for the DDES results), the tip blockage cell occupies the whole near-tip passage, and hence the compressor stalls.

The blockage area can be quantified by the area enveloped by the iso-surface of a threshold relative velocity. In Fig. 4.19, the blockage area normalized by the total section area is plotted against the streamwise coordinate at the measured two operating conditions. The threshold W_c/U_t in this plot is 0.4, and the error bars of the experimental results originate from the measurement uncertainty of 2.5% in velocity [160].

Comparing the experiment results with both DDES results, the DDES method predicts the blockage area well in the front part of the blade passage (streamwise coordinate between 0.4 and 1.1) but over-predicts it in the rear part (streamwise coordinate between 1.1 and 1.8), which can be caused by the downstream stator as discussed before. The difference between the two DDES results is in the same order of the measurement uncertainty, indicating the simulation results are grid independent.

Comparing the two operating conditions, the tip blockage cell grows in size and extends towards further upstream locations when reducing the flow coefficient, which eventually triggers compressor stall.

The entropy field is important for understanding the compressor loss of efficiency. Following the derivation of Denton [199], the entropy field can be non-dimensionalized by the compressor

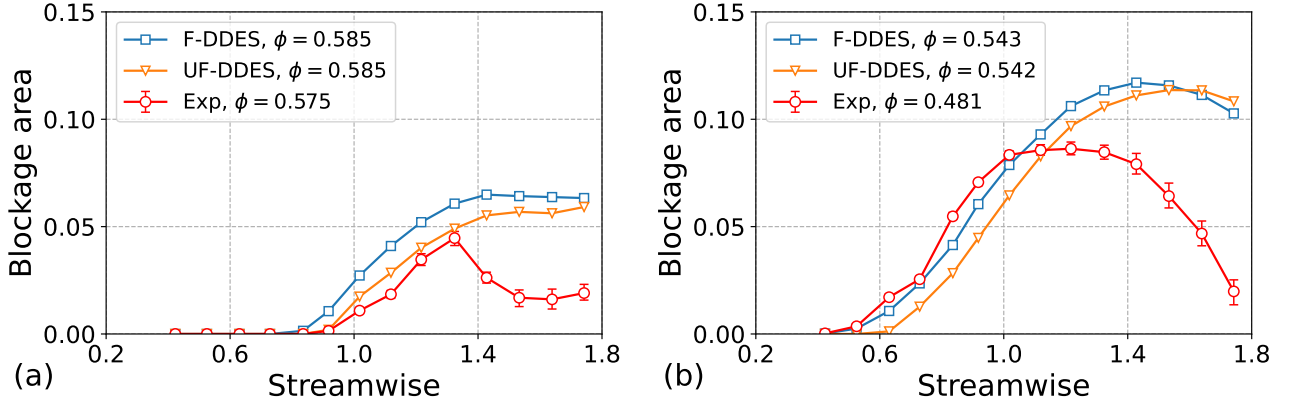


Figure 4.19: Streamwise development of dimensionless tip blockage area measured by $W_c/U_t \leq 0.4$: (a) peak efficiency; (b) near stall.

work input, yielding a form similar to the isentropic efficiency as denoted by Eq. (4.10):

$$\eta(\mathbf{x}) \approx 1 - \frac{T_{t2}\Delta s(\mathbf{x})}{c_p(T_{t2} - T_{t1})} \quad (4.10)$$

where $\mathbf{x}$ represents the spatial coordinates, and the approximation arises due to the assumption of small temperature changes of $T_{t2,isen} \approx T_{t2}$, which is reasonable especially for low-speed compressors.

The time-averaged non-dimensionalized entropy fields are compared in Fig. 4.20. For all operating conditions, entropy is generated mainly due to the formation of the main TLV (i.e., mixing between the main flow and the tip leakage flow); after the main TLV breakdown, the produced entropy propagates downstream and diffuses to lower spans. when the operating point moves towards stall (i.e., reducing flow coefficient), the tip blade loading increases, leading to a stronger mixing process near the TLV trajectory and hence a lower isentropic efficiency.

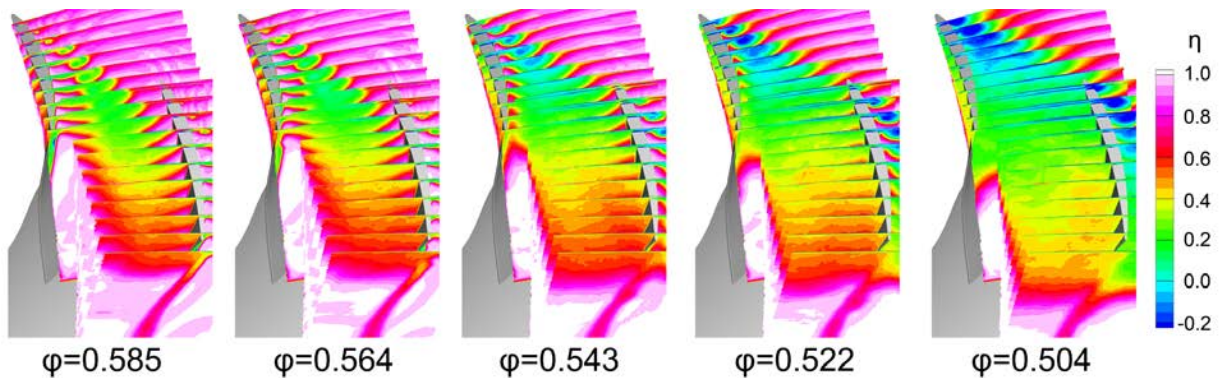


Figure 4.20: Non-dimensionalized entropy contours of BUAA Stage B rotor; DDES(SA- $F_{KH}\Delta_{hyb}$), fine grid results.

4.4.6 Turbulence Statistics

In this section, the TKE and the anisotropy of the Reynolds stress tensor of the compressor tip leakage flow are analyzed. This information is valuable for turbulence model developers.

The contours of TKE obtained from the SPIV measurement, the ultrafine grid DDES and the fine grid DDES are shown in Fig. 4.21, where the square of the blade tip speed is used to non-dimensionalize TKE. Together with the observations in Fig. 4.15, it is found that TKE is produced along the trajectory of the main TLV, where the local shear stress is large. After the main TLV breakdown, the TKE advects downstream and diffuses to the surrounding region, leading to the decay of the peak TKE value.

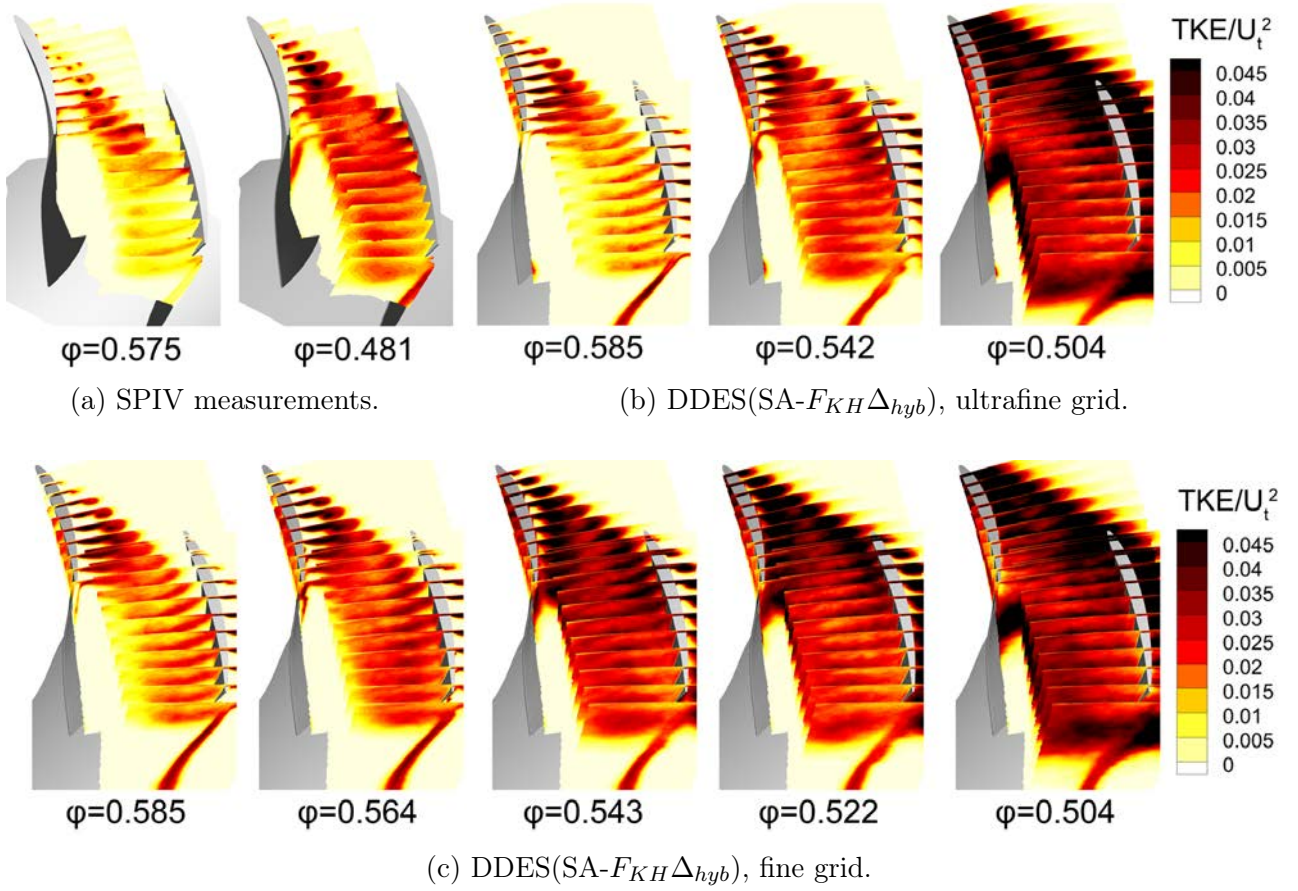


Figure 4.21: Turbulence kinetic energy contours of BUAA Stage B rotor.

Comparing the measured data with both simulation results, it again shows that DDES can qualitatively capture the measured TKE distributions, albeit with a flow coefficient offset. Such a resemblance validates the DDES method in predicting the turbulence statistics of compressor tip leakage flows.

Comparing the results with different flow coefficients, the turbulent fluctuation generally intensifies when the flow coefficient is reduced. This is expected because reducing the flow coefficient increases the compressor tip blade loading, enhances the tip leakage flow rate, and hence a more substantial shear effect between the main flow and the tip leakage flow that produces turbulence.

The turbulence anisotropy can be visualized in the barycentric map, whose coordinates are calculated via Eq. 4.9. However, this approach is inefficient for 3D flows. To help visualize the barycentric map further, the coordinate system in Eq. (4.9) can be coupled with the red-green-blue (RGB) coloring system shown in Eq. (4.11) [200]:

$$\begin{pmatrix} R \\ G \\ B \end{pmatrix} = C_{1c}^* \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + C_{2c}^* \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + C_{3c}^* \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad (4.11)$$

where $C_{ic}^* = (C_{ic} + C_{off})^{C_{exp}}$ and coefficients C_{off} and C_{exp} set up the color map. In this work, $C_{off} = 0.65$ and $C_{exp} = 5$ are used.

The turbulence anisotropy of compressor tip leakage flow is presented by the componentality contours in Fig. 4.22, where each turbulence state is represented by a color shown in the color triangle. At the first glance, none of the near-tip regions show an isotropic 3C state. Specifically, the turbulence anisotropy shows a 2C-3C compound state (color in blue) along the trajectory of the main TLV, which is surrounded by a 1C-3C compound state (color in purple). As the flow coefficient reduces, the regions with the 2C-3C compound state are gradually replaced by the 1C-3C compound state. A tentative explanation is that the 2C-3C compound state is associated with a strong rotation rate, and the 1C-3C compound state is associated with a strong strain rate. When the compressor is throttled to stall, the strain rate dominates over the rotation rate, and hence the change of anisotropy state. However, future work on turbulence modeling using this database is required to support this explanation.

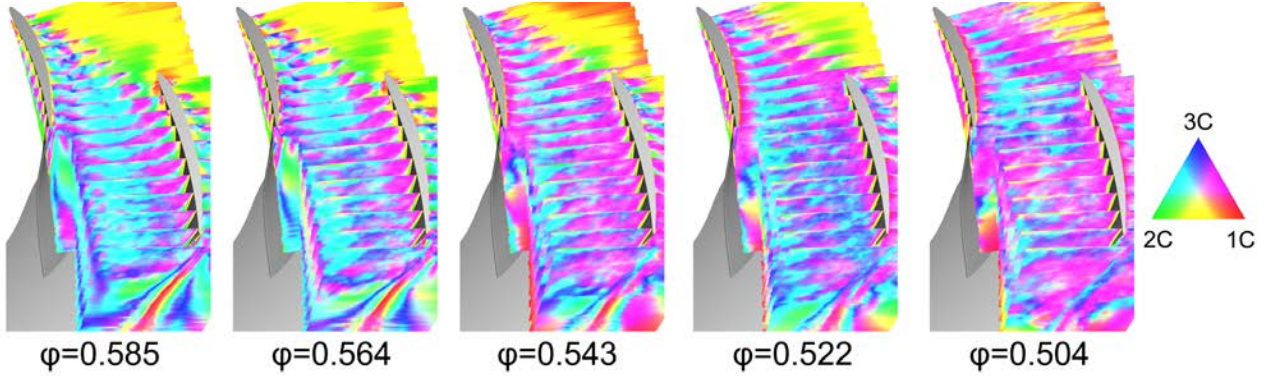


Figure 4.22: Turbulence anisotropy componentality contours of BUAA Stage B rotor; DDES(SA- $F_{KH}\Delta_{hyb}$), fine grid results.

4.5 Modal Analysis of BUAA Stage B Rotor

Following the generation of a DDES database of compressor tip leakage flow, this section unveils the modal component of compressor tip leakage flow by using spectral proper orthogonal decomposition (SPOD), which will be valuable for understandings of the aerodynamic/aeroelastic effects, turbulence modeling and reduced-order modeling of compressor tip leakage flow.

Based on the discussions in Sec. 4.4, the flow topology of the investigated compressor rotor is summarized in Fig. 4.23. The near-tip flow field can be roughly divided into four zones:

formation of main TLV (Zone I); main TLV breakdown (Zone II); formation of tip blockage cell (Zone III); formation of secondary TLV (Zone IV). In the following analysis, the modal component of each zone will be discussed in detail.

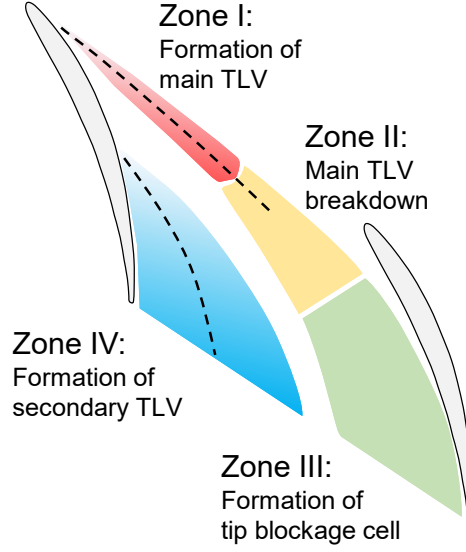


Figure 4.23: Flow topology of compressor tip leakage flow.

4.5.1 Spectral Proper Orthogonal Decomposition

SPOD is a frequency-domain variant of POD [201] that is designed for statistically stationary flows. It can capture the energy-ranked and mutually orthogonal modes at each frequency. Mathematically, the SPOD modes are eigenvectors of the cross-spectral density (CSD) matrix at each frequency, and the eigenvalues correspond to the energy of each mode at a distinct frequency. Detailed theory and derivation of the SPOD method can be found in [202, 203]. The PYTHON script of SPOD written for this work is open-accessed¹. Key procedures of SPOD are illustrated in Fig. 4.24. Each procedure is detailed as follows.

- (1) A matrix containing the spatio-temporal flow data is constructed first. Let the vector $\mathbf{q}_k \in \mathbb{R}^{N_q}$ represent the k_{th} time snapshot after subtracting the time-averaged data, and its length $N_q = N_g N_v$ where N_g and N_v are the number of grid points and investigated variables respectively. By assembling the snapshot flow field data in chronological order, the spatio-temporal data matrix is obtained:

$$\mathbf{Q} = [\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_{N_t}] \in \mathbb{R}^{N_q \times N_t} \quad (4.12)$$

where N_t is the total number of snapshots.

- (2) The data matrix $\mathbf{Q}$ is then segmented into N_b ($N_b \ll N_t$) blocks by applying the Welch periodogram method [204], with each block consisting of N_f snapshots. To improve the convergence of the mode decomposition, each block is overlapped with neighboring blocks

¹Package available from: https://github.com/HexFluid/spod_python. [Accessed in June 2021]

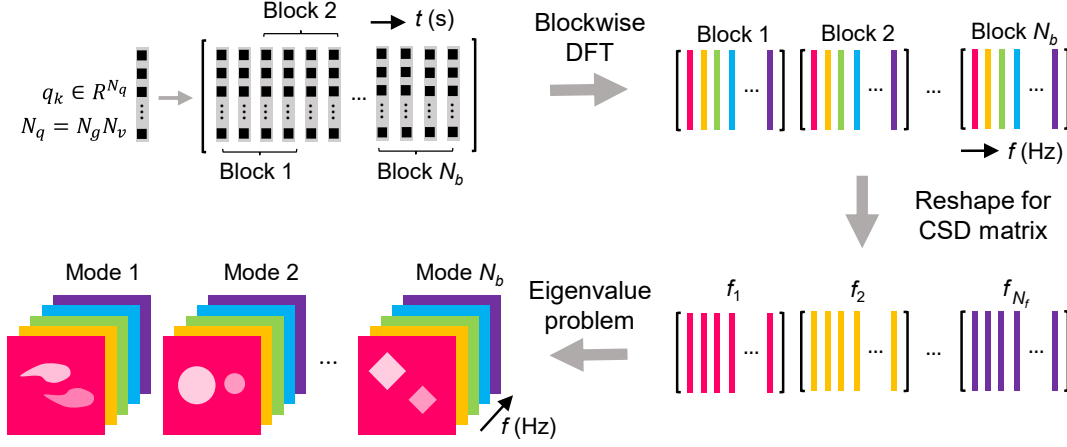


Figure 4.24: Schematic of the SPOD algorithm.

by N_o time snapshots. Each block is assumed to be a statistically independent realization under the ergodicity hypothesis. The discrete Fourier transform (DFT) is performed on each block to convert the problem to the frequency domain. To avoid spectral leakage, each block is windowed by the Hamming window function [205]. The resultant matrix for the j_{th} block is:

$$\hat{\mathbf{Q}}^{(j)} = [\hat{\mathbf{q}}_1^{(j)}, \hat{\mathbf{q}}_2^{(j)}, \dots, \hat{\mathbf{q}}_{N_f}^{(j)}] \in \mathbb{C}^{N_q \times N_f} \quad (4.13)$$

where N_f is equivalent to the number of resolved frequencies.

- (3) Next, the frequency-domain matrices of blocks are reshaped according to the frequency. For the k_{th} frequency, the corresponding matrix is:

$$\hat{\mathbf{Q}}_k = [\hat{\mathbf{q}}_k^{(1)}, \hat{\mathbf{q}}_k^{(2)}, \dots, \hat{\mathbf{q}}_k^{(N_b)}] \in \mathbb{C}^{N_q \times N_b} \quad (4.14)$$

The weighted CSD matrix for the k_{th} frequency is therefore obtained as:

$$\mathbf{S}_k = \frac{1}{N_b} \mathbf{W}^{\frac{1}{2}} \hat{\mathbf{Q}}_k^* \hat{\mathbf{Q}}_k \mathbf{W}^{*\frac{1}{2}} \in \mathbb{C}^{N_b \times N_b} \quad (4.15)$$

where $\mathbf{W}$ is the weight matrix for scaling of different flow variables. The definition of $\mathbf{W}$ determines the physical meaning of the SPOD mode energy. This work follows the derivation of total disturbance energy [206]:

$$\begin{aligned} E &= \frac{1}{2} \int_V \left\{ \frac{R\bar{T}}{\bar{\rho}} \rho'^2 + \frac{R\bar{\rho}}{(\gamma-1)\bar{T}} T'^2 + \bar{\rho} u_i'^2 \right\} dV \\ &= \frac{1}{2} \int_V \left\{ \frac{1}{\gamma\bar{p}} p'^2 + \frac{(\gamma-1)\bar{p}}{\gamma R^2} \Delta s'^2 + \bar{\rho} u_i'^2 \right\} dV \end{aligned} \quad (4.16)$$

where Δs is the entropy rise, V is the control volume of the grid cell, R is the gas constant, γ is the specific heat ratio, $(\cdot)'$ denotes the unsteady fluctuation of a quantity and $(\bar{\cdot})$ denotes the time-average of a quantity. For flows where the temperature fluctuation is of most interest (e.g., heat transfer in turbines), the quantities of interest $\mathbf{q} = [\rho, u_x, u_r, u_t, T]^T$ and the diagonal weight matrix $\mathbf{W}_q = \text{diag}[\frac{R\bar{T}}{\bar{\rho}}, \bar{\rho}, \bar{\rho}, \bar{\rho}, \frac{R\bar{\rho}}{\bar{T}(\gamma-1)}]$ are recommended; for flows where the pressure fluctuation is of most interest (e.g., compressor aeroelasticity), $\mathbf{q} = [p, u_x, u_r, u_t, \Delta s]^T$ and $\mathbf{W}_q = \text{diag}[\frac{1}{\gamma\bar{p}}, \bar{\rho}, \bar{\rho}, \bar{\rho}, \frac{(\gamma-1)\bar{p}}{\gamma R^2}]$ are preferred.

- (4) Finally, the eigenvalue decomposition is performed on the weighted CSD matrix $\mathbf{S}_k$ for each frequency:

$$\begin{aligned}
\mathbf{S}_k &= \mathbf{\Psi}_k \mathbf{\Lambda}_k \mathbf{\Psi}_k^* \\
\mathbf{\Phi}_k &= \hat{\mathbf{Q}}_k \mathbf{\Psi}_k \mathbf{\Lambda}_k^{-1/2} \\
\mathbf{\Phi}_k &= [\phi_k^{(1)}, \phi_k^{(2)}, \dots, \phi_k^{(N_b)}] \in \mathbb{C}^{N_q \times N_b} \\
\mathbf{\Lambda}_k &= \text{diag}(\lambda_k^{(1)}, \lambda_k^{(2)}, \dots, \lambda_k^{(N_b)}) \in \mathbb{C}^{N_b \times N_b}
\end{aligned} \tag{4.17}$$

The matrix $\mathbf{\Phi}_k$ calculated from the eigenvectors represents the SPOD mode shapes at the k_{th} frequency. These modes are ranked according to their corresponding eigenvalues $\mathbf{\Lambda}_k$, which can be physically interpreted as the total disturbance energy of the mode in the investigated flow domain.

In this section, the SPOD method is performed to extract and analyze the modal components of compressor tip leakage flow. The data comes from fine grid DDES at the peak efficiency ($\phi = 0.585$) and the near stall ($\phi = 0.543$) conditions. The flow quantities of interest are $\mathbf{q} = [p, u_x, u_r, u_t, \Delta s]^T$ in the upper 20% span of the blade passage. The sampling frequency of the snapshots is $f_s/\text{BPF} = 50$, which cuts off the high-frequency components of the sub-grid scales. Details of the snapshot data and the SPOD parameters for both cases are listed in Table 4.2.

Table 4.2: Parameters of databases and spectral estimation of the SPOD analysis.

Database				
Case	Variable	N_g	N_t	f_s/BPF
Near-tip flow field	$p, u_x, u_r, u_t, \Delta s$	481493	4250	50

SPOD				
Case	N_f	N_o	N_b	Norm
Near-tip flow field	256	128	32	Total disturbance energy

4.5.2 Mode Energy Spectrum

For the multi-variable SPOD analysis performed in this case, the SPOD mode energy represents the total disturbance energy that can be subdivided to pressure potential energy, entropy potential energy and TKE, as shown in Eq. (4.16). The fraction of each component of the total disturbance energy is presented in Fig. 4.25. In this plot, the fractions of energy components are calculated at each snapshot; the time variations of the fractions are presented by probability density functions (PDF), which are obtained by using the kernel density estimation [207] with Gaussian kernels. Results show that the fraction of $\text{TKE} = E_{ux} + E_{ur} + E_{ut}$ is roughly three orders of magnitude stronger than the entropy potential $E_{\Delta s}$ and the pressure potential E_p at both the peak efficiency and near stall conditions. Therefore, the TDE of the investigated compressor tip leakage flow mostly represents the TKE.

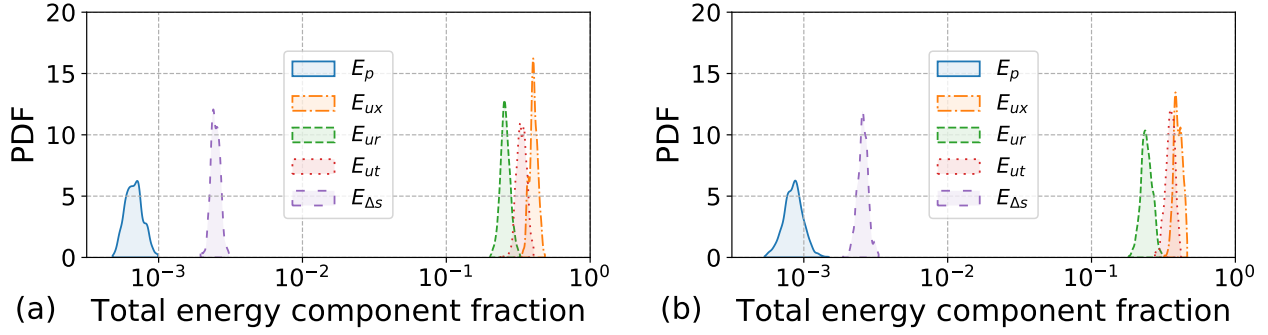


Figure 4.25: Total disturbance energy component fraction of near-tip flow: (a) peak efficiency and (b) near stall.

The SPOD modal energy spectrums of the near-tip flow field for the peak efficiency and near stall conditions are shown in Fig. 4.26(a) and (b) respectively. In general, the near-tip flow exhibits a broadband characteristic without any spikes in the spectrum; the majority of the flow energy is contained in the large-scale low-frequency components of the flow, and the energy is transferred successively to the smaller scales in the inertial subrange. A low-rank behavior is observed between 0.4 and 3.0 BPF at the peak efficiency condition and between 0.2 and 3.0 BPF at the near stall condition, where Mode 1 contains a significantly large portion of the energy and thus plays a dominant role. This low-rank behavior indicates that a physically dominant mechanism is present in the flow field, which will be seen later in the mode shapes. To illustrate these low-rank behaviors further, the premultiplied energy spectrums are presented in Fig. 4.26(c) and (d), where the energy contained in each mode equals the area beneath the curve of the mode. For the total energy spectrum, the near stall condition contains a larger amount of energy than the peak efficiency condition especially at low frequencies below 1.0 BPF. For the Mode 1 spectrum, an energy hump is formed near 1.6 BPF at the peak efficiency condition, and two energy humps are formed near 0.4 and 1.0 BPF at the near-stall condition. The energy contained in these humps of Mode 1 is significantly larger than the rest of the modes, and thus the low-rank behavior.

To quantify the contribution of each mode at each frequency to the total energy, the accumulated mode energy fraction is calculated, i.e., $\sum_{k=1}^n \sum_{j=1}^m \lambda_k^{(j)} / \sum_{k=1}^{N_f} \sum_{j=1}^{N_b} \lambda_k^{(j)}$ for the n_{th} frequency and m_{th} mode. The accumulated mode energy fractions of both the peak efficiency and near stall conditions are plotted as isolines in Fig. 4.27, where the horizontal axis is the non-dimensionalized frequency and the vertical axis is the number of modes. When using a large number of modes ($m \geq 20$), the near-stall condition requires fewer frequencies than the peak efficiency condition to restore the same fraction of total energy. It indicates that the low-frequency components of the near stall condition are more energetic than the peak efficiency condition, which is consistent with the observation in Fig. 4.26. When using a large number of frequencies ($f_n \geq 10$ BPF), the near stall condition requires more modes than the peak efficiency condition to restore the same fraction of total energy, indicating the modal component is more complex (i.e., non-low-rank) in the near stall condition than the peak efficiency condition. To restore 90% of the total energy, it requires at least $f_n > 4$ BPF and $m > 21$, which is equivalent to using $mn/N_b N_f > 10.5\%$ of the total modes.

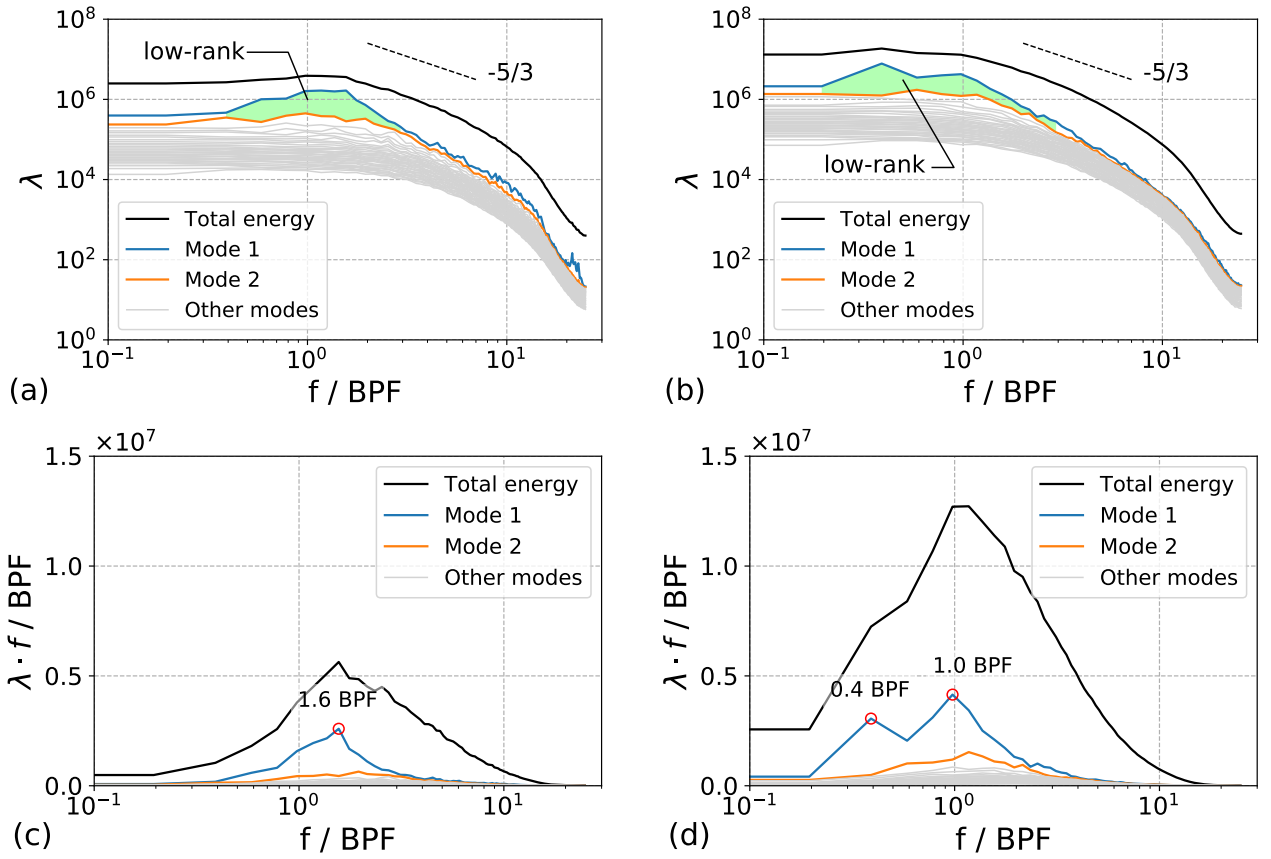


Figure 4.26: SPOD mode energy of near-tip flow: energy spectrum at the (a) peak efficiency condition and (b) near stall condition; premultiplied energy spectrum at the (c) peak efficiency condition and (d) near stall condition.

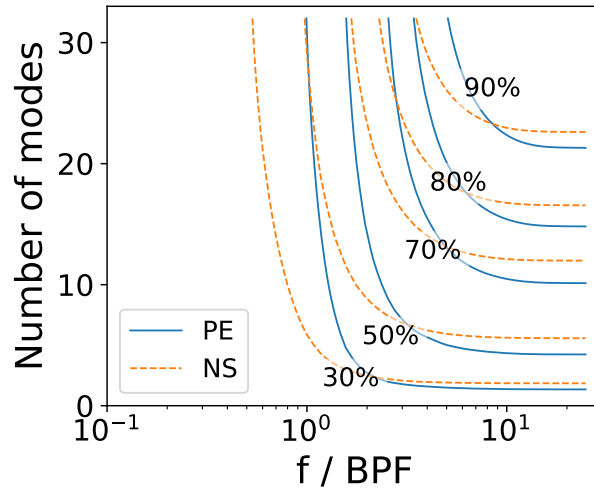


Figure 4.27: SPOD accumulated mode energy fraction of near-tip flow.

4.5.3 Mode Shape

To unveil the physical relevance of the above SPOD modes, the Mode 1 shapes at 1.0, 1.6 and 5.1 BPF for the peak efficiency condition and at 0.4, 1.0 and 5.1 BPF for the near stall condition are plotted in Fig. 4.28. In this figure, the wavepackets are represented by the

iso-surfaces of mode shapes at 50%, 67% and 100% of the minimum/maximum values of the color range. The frequencies of 1.0 and 1.6 BPF of the peak efficiency condition and 0.4 and 1.0 BPF of the near stall condition correspond to the low-rank behavior (i.e., energy humps); the frequency of 5.1 BPF at both the peak efficiency and near stall conditions represents the high-frequency non-low-rank region. For brevity, high-order modes are not presented since the energy contained in these modes is significantly smaller than the leading mode; only the mode shapes of u_x and p are analyzed since they are of most interest for compressor aerodynamics and aeroelasticity.

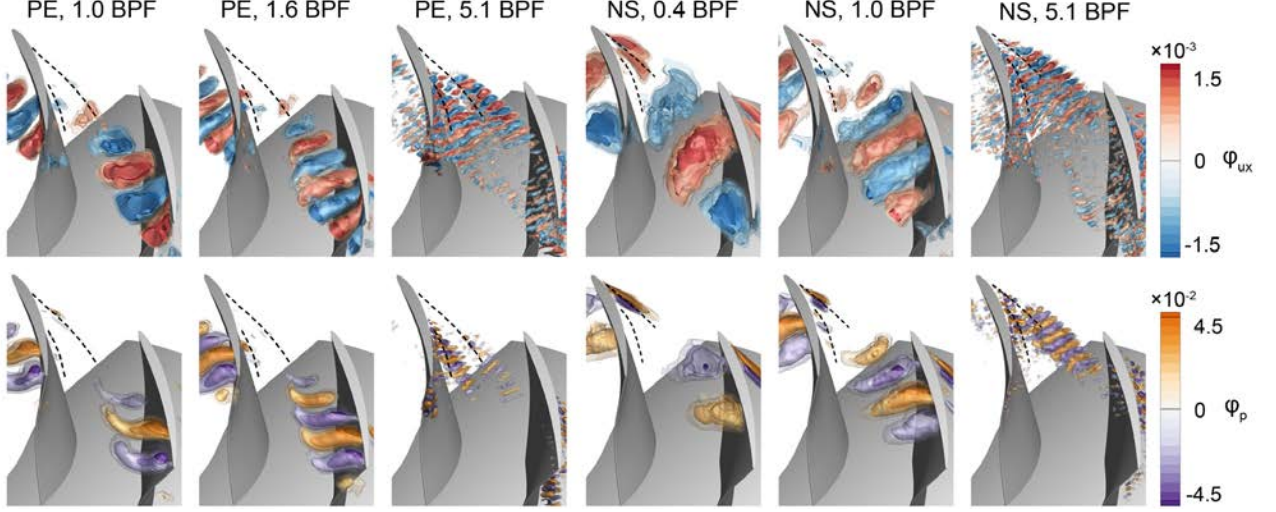


Figure 4.28: SPOD Mode 1 shape (real part) of near-tip flow at selected frequencies; dashed lines indicate the trajectory of the TLVs according to the time-averaged vorticity contours.

For the peak efficiency condition, the mode shapes of u_x and p at both 1.0 and 1.6 BPF show two coherent wavepackets: the dominant wavepackets is located in Zone III (Fig. 4.23, same reference for the following Zones), which corresponds to the vortex shedding downstream the main TLV breakdown; second wavepackets can be observed on the trajectory of the secondary TLV in Zone IV, but it is much weaker than the primary wavepackets. At 5.1 BPF, two small-scale wavepackets occur in Zone II and IV, which corresponds to the main TLV breakdown and the secondary TLV shedding respectively. These results indicate that the main TLV shedding in the tip blockage cell zone is most energetic in the flow domain, which creates the energy hump of Mode 1 near 1.6 BPF. For the near stall condition, a similar main TLV shedding mode in Zone III can be observed at 0.4 and 1.0 BPF; an oscillating mode of the main TLV around its time-averaged trajectory is also observed in Zone I at 0.4 BPF. These modes lead to the two energy humps of Mode 1 near 0.4 and 1.0 BPF. At 5.1 BPF, small-scale wavepackets occur in Zone II and IV, which is similar to the peak efficiency condition.

Given the physical phenomena behind the energy hump is the main TLV shedding, the next question is: what determines the frequency range of the energy hump? The shedded vortices create wave-like pulsations of flow quantities in blade passages: the wave speed is the propagation speed of the vortices, which equals to the local relative velocity W ; the wavelength is approximated by the distance l between two adjacent vortex cores, which can be measured by a pair of wavepacket shown in Fig. 4.23; thus, the wave frequency $f = W/l$. This relation can be non-dimensionalized by using the BPF, the blade tip speed U_t and the blade tip pitch

s (note $\text{BPF} = U_t/s$), as denoted in Eq. (4.18):

$$\frac{f}{\text{BPF}} = \frac{W}{U_t} \frac{l}{s} \quad (4.18)$$

It shows that the frequency range of the energy hump depends on two terms: W/U_t which depends purely on the operating condition of the compressor, and l/s which depends on both the operating condition and the design of the compressor. By substituting the values in Fig. 4.18 and Fig. 4.28 into Eq. (4.18), this relation is checked to be correct in principle.

The W/U_t term decreases when throttling the compressor from peak efficiency to near stall (from analysis of the inlet velocity triangle, or more intuitively from the observation in Fig. 4.18), leading to the shift of the energy hump towards the low-frequency direction shown in Fig. 4.26. When operating at the same operating condition, the wavelength decreases when increasing the frequency, which is captured in Fig. 4.28.

The minimum l/s value is determined by the Kolmogorov scale of the vortices, which scales with $\text{Re}^{-3/4}$. For large-scale high-speed industrial machines with high Re numbers, more high-frequency components are expected in the energy hump. The maximum l/s value depends on the trajectory of the main TLV, which changes with the operating condition and the design of the blade. Based on the 2D blade geometry of Fig. 4.29, the maximum possible l/s value is $\sqrt{\sigma^2 + 2\sigma \sin \xi + 1}$, where $\sigma = c/s$ is the solidity and ξ is the stagger angle. For compressor designs with high values of solidity and stagger angle, more low-frequency component is expected in the energy hump.

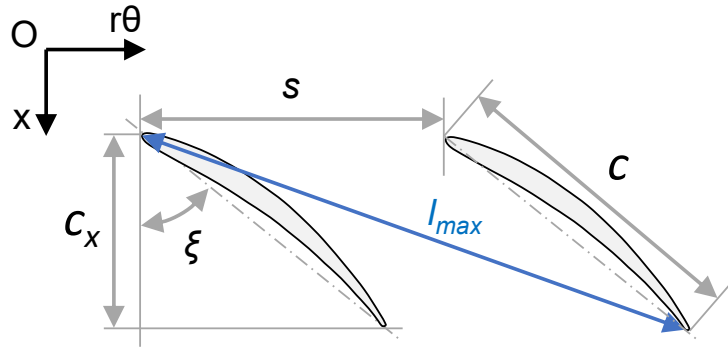


Figure 4.29: Illustration of 2D compressor blade section.

4.5.4 Implications for Turbulence Modeling of Tip Leakage Flow

From the SPOD mode energy spectrums and mode shapes of the near-tip flow field, it is indicated that the turbulent fluctuations in the main TLV formation region (Zone I) and the tip blockage cell formation region (Zone III) are conceptually easy to model because of the low-rank behavior at low frequencies (i.e., large scales). These fluctuations form a hump in the energy spectrum, which may not be captured by established RANS turbulence models developed from 2D canonical flows. In such cases, a modification to the production term of the established RANS models in the tip blockage cell is necessary.

On the contrary, modeling the turbulent fluctuations in the main TLV breakdown region (Zone II) and the secondary TLV formation region (Zone IV) is conceptually difficult due to the non-low-rank modal component at high frequencies. Zone II involves the laminar-to-turbulent transition process, which is related to the transition term in RANS turbulence models. The amplification mechanism during the turbulence transition process is not discussed in this work, which needs to be investigated in future research. Zone IV shows the interaction between the secondary TLV and the suction surface boundary layer flows, the latter of which is related to the destruction term in RANS turbulence models. Such an observation indicates the difficulty of modeling the destruction term in internal flows especially in the corner region.

4.6 Concluding Remarks

In this chapter, a review of the recent progress of DES-type methods is presented, and a combination of DES upgrades suitable for compressor tip leakage flow is demonstrated in the backward-facing step and the BUAA Stage B rotor. A turbulence database of compressor tip leakage flow is generated using the upgraded DES method, and the transient flow features, the mean flow quantities, the turbulence statistics and the modal components of the database are analyzed in detail. Several conclusions are drawn as follows.

The widely used default DES method, namely DDES(SA- Δ_{max}), fails to predict the RANS-to-LES transition in shear layers accurately, which leads to an inaccurate prediction of the mean flow fields when using a coarse grid. In the backward-facing step case with a coarse grid, DDES(SA- Δ_{max}) predicts the development of the Reynolds stress component further downstream than the measured data, leading to a worse prediction of velocity profiles and skin friction distribution than RANS(SA). Using a refined grid improves the prediction of the mean flow field quantities, but not the turbulence field. In the low-speed rotor case with a medium grid, DDES(SA- Δ_{max}) also predicts a delayed development of TKE. On the other hand, DDES(SA- $F_{KH}\Delta_{hyb}$) unlocks the physics of the shear-layer instability and maximizes the scale-resolving capability of the grid. In the step case and the rotor case studied in this chapter, DDES(SA- $F_{KH}\Delta_{hyb}$) predicts both the mean flow features and the turbulence statistics qualitatively well. Therefore, it is recommended as a suitable and accurate upgraded version of the default DDES(SA- Δ_{max}) for turbomachinery hybrid RANS/LES solvers.

The tip leakage flow in the investigated low-speed compressor rotor is governed by the double-leakage flow structure. The main TLV forms immediately after detaching from the leading edge (Zone I), breaks down into smaller eddies near the mid-pitch (Zone II), and then impinges on the pressure surface of the adjacent blade and forms a tip blockage cell (Zone III); part of the main TLV flow passes through the tip gap of the adjacent blade, leading to the formation of a secondary TLV (Zone IV). When throttling the compressor from the peak efficiency condition to the near stall condition, the trajectory of both TLVs moves upstream, the tip blockage cell grows in size and extends upstream, and the TKE in the near-tip flow field increases.

The SPOD modal analysis on the near-tip flow field revealed that a major part of the total disturbance energy originates from the fluctuations in Zone I and III, which are low-frequency (i.e., $0.2 < f/\text{BPF} < 3.0$ in this case), low-rank and thus conceptually easy to model by RANS turbulence models. These fluctuations correspond to the oscillating mode

of the main TLV in Zone I and the vortex shedding mode of the main TLV in Zone III. In particular, the frequency range of the shedding mode can be estimated based on the blade geometry and the operating condition. On the contrary, the fluctuations in Zone II and IV are broadband, non-low-rank, and thus conceptually difficult to model by RANS turbulence models. These fluctuations correspond to the laminar-to-turbulent transition in Zone II and the interaction between the secondary TLV and the suction surface boundary layer in Zone IV. When throttling the compressor from the peak efficiency condition to the near stall condition, the total disturbance energy increases, and the energy hump corresponding to the main TLV modes moves towards the low-frequency; however, the low-rank behavior of the main TLV modes becomes less pronounced.

5. Uncertainty Quantification of Turbulence Model Coefficients

“Much of our knowledge must always remain uncertain. The most we can know is in terms of probabilities.”

— Richard Feynman, *The Feynman Lectures on Physics*

5.1 Introduction

A turbulence database of compressor tip leakage flow has been generated in Chapter 4. Before feeding the data to train an ML model, it is crucial to determine at which level of the turbulence model should the ML model be implemented, i.e., the constitutive relation level (Level 2), the turbulence model transport equation level (Level 3) or the turbulence model coefficient level (Level 4). In this chapter, the potential of correcting the turbulence model coefficients for improving compressor stall prediction will be evaluated via a series of UQ studies.

This chapter is organized as follows. In the first place, the metamodel-based Monte Carlo UQ method will be introduced in Sec. 5.2. In Sec. 5.3, the UQ method will be applied to quantify the parametric uncertainty of the SA model on the 2D canonical flows, which represent part of the compressor tip leakage flow features. In Sec. 5.4 and Sec. 5.5, the parametric uncertainty of the SA model on predicting 2D airfoil stall and 3D compressor rotor stall will be investigated, respectively. Finally, conclusions will be drawn from all the UQ results.

5.2 An Efficient Uncertainty Quantification Method

Conventional UQ methods like Monte Carlo are computationally intensive to achieve high accuracy. In this work, the parametric uncertainty of the SA model coefficients is investigated through a metamodel-based Monte Carlo approach so that the required numerical resources can be alleviated. This UQ framework is illustrated in Fig. 5.1.

Firstly, the Latin Hypercube sampling (LHS) method [208] is applied to generate five independent databases of SA model coefficient sets within the intervals in Table 5.1. These coefficient intervals are suggested by the original model developer Spalart as reported in Schaefer et al. [92], which arose from the calibration process concerning free shear flows and simple wall-attached flows [44].

This Design of Experiment (DOE) method can generate random samples that are distributed as uniformly as possible in the investigated space. Five databases are generated including 16, 32, 64, 128 and 256 samples, respectively. These databases will be referred to as *db1*

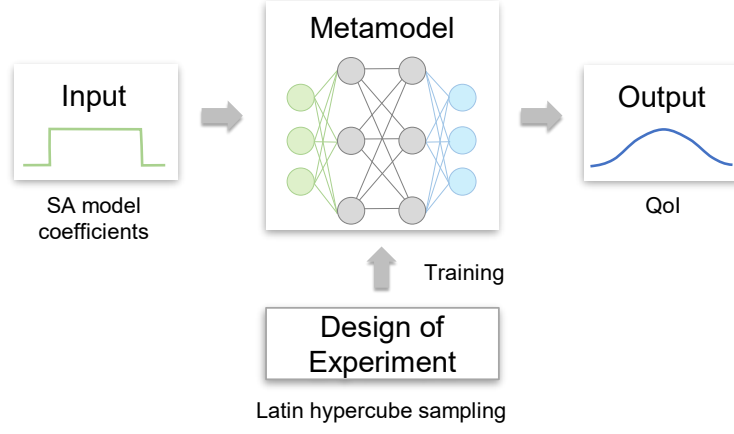


Figure 5.1: Illustration of the metamodel-based uncertainty quantification framework.

to *db5* in the following discussions. The sample distributions of representative databases are presented in Fig. 5.2. The minimum Euclidean distance between arbitrary two samples from different databases is longer than 7% of the longest distance in the domain (i.e., $\sqrt{7}$). Thus, all five databases are mutually independent.

Table 5.1: Intervals of Spalart-Allmaras turbulence model coefficients.

Coefficients	Physical relevance	Minimum	Default	Maximum
σ	diffusion coefficient	0.600	0.667	1.000
κ	log law slope	0.38	0.41	0.42
c_{v1}	log law intercept	6.9	7.1	7.3
c_{b1}	production coefficient	0.1280	0.1355	0.1370
c_{b2}	to conserve $\nu_t^{1+c_{b2}}$	0.609	0.622	0.688
c_{w2}	to calibrate skin friction	0.055	0.300	0.353
c_{w3}	to speed up destruction	1.75	2.00	2.50

The generated databases are then applied to train and test a metamodel of CFD. The metamodel is a reduced-order model that directly maps the input variables to the quantities of interest (QoIs) without solving RANS equations:

$$\hat{\mathbf{q}} \approx \mathbf{q} \equiv \mathbf{M}(\mathbf{x}) \quad (5.1)$$

where $\mathbf{x}$ is the vector of input variables, $\mathbf{M}(\cdot)$ denotes the metamodel, $\hat{\mathbf{q}}$ and $\mathbf{q}$ are the vector of QoIs from CFD and the metamodel, respectively. The fully connected neural network (FCNN) introduced in Sec. 3.3 is applied to construct a metamodel of the CFD solver.

Afterward, the probability density function (PDF) of the QoI can be obtained by feeding the PDF of the input variables into the metamodel, and the uncertainty of QoI can be quantified by the min-max values predicted by the metamodel. Concretely, a new database with n_{MC} samples (n_{MC} sufficiently large) will be generated for the Monte-Carlo experiment, and the samples follow the prior PDFs of the input variables. The physical relevance and the

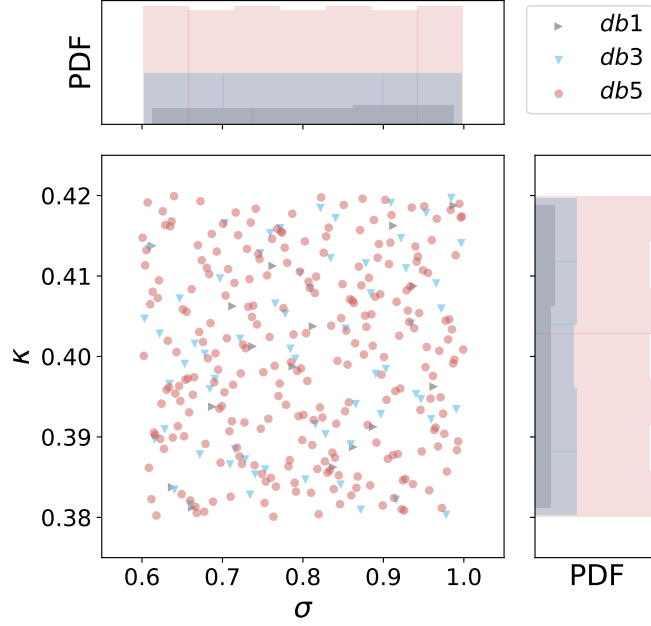


Figure 5.2: Sample distribution of representative databases.

investigated range of the SA model coefficients are shown in Table 5.1. These ranges were verified by Spalart [92], which arose from calibration for free shear flows and simple wall-attached flows [44]. The SA model with its default values of coefficients will be referred to as the original SA (OSA) model in the following discussions. The prior PDFs of SA model coefficients are assumed to follow the uniform distribution.

Finally, the local sensitivity of input variables on predicting the QoIs can be quantified by the gradient $\partial M_i / \partial \hat{x}_j$ calculated from the metamodel; the global sensitivity can be measured by the mean gradient defined in Eq. (5.2):

$$\frac{\overline{\partial M_i}}{\partial \hat{x}_j} = \underbrace{\int \cdots \int}_{nx} \frac{\partial M_i}{\partial \hat{x}_j} d\hat{x}_1 \cdots d\hat{x}_{nx} \quad (5.2)$$

where $\hat{x}_j$ is the input variable normalized to the range of $[0, 1]$, and n_x is the dimension of the input vector. To compare the sensitivity among different QoIs, the mean gradient will be normalized by the length of the mean gradient vector $|\nabla M_i|$. This term will be referred to as normalized gradient in the following discussion.

5.3 Uncertainty Quantification on Simplified Tip Leakage Flow Features

5.3.1 Case Description

In this section, the parametric uncertainty of the SA model is investigated in a backward-facing step and an axisymmetric transonic bump, which share similar flow physics to the tip

leakage flow of transonic compressors as justified in Sec. 3.4.1. The advantage of studying simplified 2D flows is two-fold. Firstly, it provides a better understanding of the capability of the SA model, as it decouples the tip leakage flow with the shock-boundary layer interaction. Secondly, the Hi-Fi data of Reynolds stress tensor, shock location and strength, and separation size are readily available in simplified 2D flows, but they are difficult to obtain in high-speed compressor rotors. However, it should be emphasized that the main physics of compressor near-tip flow is highly 3D, which cannot be fully represented by the 2D cases studied. These 2D cases represent the least challenging cases for the evaluation of turbulence models. An accurate prediction of the simplified 2D flows is necessary but may not be sufficient for the accurate prediction of the compressor near-tip flows.

In the following discussions, the UQ results will be compared with the experimental data of the step flow [143] and the bump flow [139, 140]. Results from Hi-Fi simulations are also employed for reference, including the IDDES for the step flow [144] and the WRLES for the bump flow [141]. For consistency and simplicity, both Hi-Fi simulations are referred to as the LES results.

The details of the experimental data and the CFD setups of the two cases have been summarized in Sec. 3.4.1. The QoIs include the velocity u_x , the shock front location x_{sf} , the shock front pressure coefficient $-C_{psf}$, the separation size L_s , and the Reynolds shear stress τ_{xy} . Here, the shock front is defined as the location with the lowest wall pressure; the separation size is defined as the distance between the separation and the reattachment points, both of which have zero skin friction. For each group of QoIs in each flow case, an individual FCNN metamodel is constructed with the details summarized in Table 5.2. The *db5* is applied as the training database, the *db4* serves as the testing database, and the union of *db1* to *db3* is used for cross-validation.

Table 5.2: Details of metamodels for different quantities of interest of the backward-facing step and the axisymmetric transonic bump.

QoI Group	n_q	Outputs	Figure
Velocity profile	8	$u_x(y_i)$	5.3, 5.4, 5.6
Shock	2	$x_{sf}, -C_{psf}$	5.3, 5.4, 5.7, 5.8, 5.10
Separation	1	L_s	5.3, 5.4, 5.9, 5.10, 5.11
Reynolds shear stress profile	8	$\tau_{xy}(y_i)$	5.3, 5.4, 5.12
Reynolds shear stress	1	$\tau_{xy}(x, y)$	5.13, 5.16

5.3.2 Cross-Validation, Training and Test of FCNN

5.3.2.1 Hyperparameter Study

In addition to the standard FCNN parameters (i.e., weight matrices and bias vectors) that can be learned from the training database, some hyperparameters need to be determined before the training process, namely the number of hidden layers L , the number of artificial neurons in each hidden layer n_L , the scale factor ω and the regularization factor λ .

A parametric study of n_1 , ω , and λ has been conducted by changing one hyperparameter at a time while keeping the others at the baseline setting, which is $L = 1$, $n_1 = 0.5(n_x + n_q)$, $\omega = 2$ and $\lambda = 10^{-4}$. To avoid the training process falling into a local optimum, 16 FCNNs with different initial conditions are trained parallelly, and the best FCNN is chosen. The prediction errors of FCNNs in various QoIs are plotted against each hyperparameter in Fig. 5.3. It is observed that using the FCNN model with the baseline hyperparameters achieves a mean error below 2% of the min-max range of each QoI (i.e., $\omega\epsilon < 2\%$), which is sufficiently small for the metamodel purpose. Therefore, a deep FCNN (i.e., $L > 1$) is not pursued, and the baseline setting is adopted throughout this section.

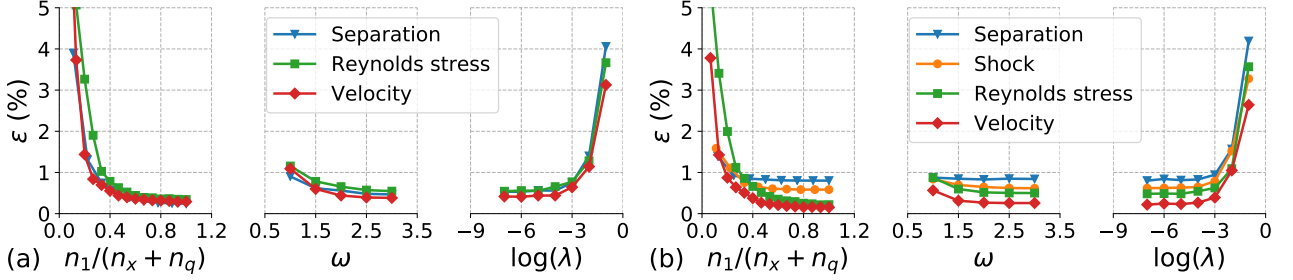


Figure 5.3: Hyperparametric study for the backward-facing step and the axisymmetric transonic bump: (a) backward-facing step and (b) axisymmetric transonic bump (training data: *db5*; cross-validation data: the union of *db1*, *db2* and *db3*).

5.3.2.2 Training Data Independence Study

The training database size has a crucial effect on the accuracy of a metamodel. A rule of thumb for the minimum training database size is $m_{min} = 10n_x$, which yields $m_{min} = 70$ in this study. However, this rule of thumb does not consider the complexity of the metamodel and thus may underestimate the value of m_{min} . Another approach to estimate m_{min} is to consider the number of equations (i.e., training data) should surpass the number of unknowns (i.e., FCNN parameters). For an FCNN with one hidden layer, this leads to $m_{min} = (n_x n_1 + n_1 n_q + n_1 + n_q)/n_q$, which yields $m_{min} = 37$ for all FCNNs listed in Table 5.2.

To analyze the effect of training database size further, a training data independence study has been performed by using different combinations of databases to train and test the FCNN. The training and test databases are $db\{i\}$ and $db\{i - 1\}$ so that the ratio of training-to-test database size can be kept the same as 2. When increasing the training database size, the difference between the test and training errors (i.e., ϵ_{te} and ϵ_{tr}) reduces to zero, and thus the accuracy of the FCNN model becomes independent of the training database size. It is confirmed in Fig. 5.4 that using the training database size of 256 achieves a data-independent result, where the differences between ϵ_{te} and ϵ_{tr} are below 0.3%. Hence, the *db5* with 256 samples has been chosen to train FCNNs in the following of this section.

5.3.2.3 Training and Test Results

By using the selected hyperparameters and the training/test databases from Sec. 5.3.2.1 and 5.3.2.2, an FCNN is trained and tested for each QoI. An example of the FCNN is provided

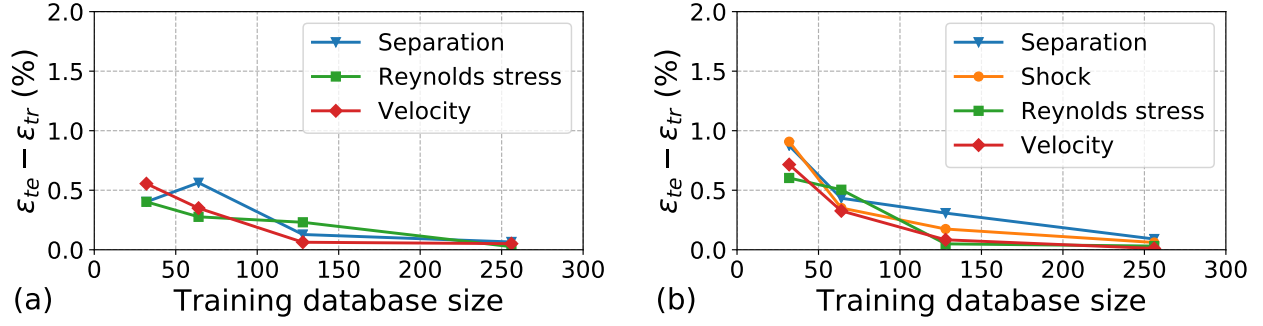


Figure 5.4: Training data independence study: (a) backward-facing step and (b) axisymmetric transonic bump (training data: *db5*; cross-validation data: the union of *db1*, *db2* and *db3*).

in Fig. 5.5, which maps the SA model coefficients with the separation size of the axisymmetric transonic bump. The training process is presented in Fig. 5.5(a), where the training and test cost functions are plotted against the optimization epochs. Convergence of the optimization algorithm can be achieved before reaching the set maximum iteration of 5000. The corresponding prediction accuracy is shown in Fig. 5.5(b), where the separation size obtained from FCNN and CFD are plotted on the vertical and horizontal axis, respectively. It shows that the maximum absolute error of FCNN on the test database is 0.005, and the mean relative error is 0.25%. This is sufficiently small for the metamodel purpose.

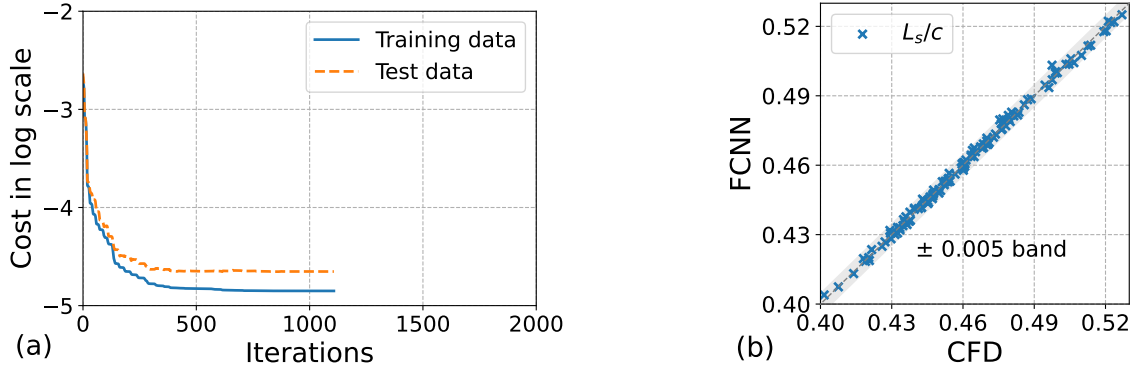


Figure 5.5: FCNN for predicting the separation size of the axisymmetric transonic bump: (a) training history and (b) prediction accuracy (training data: *db5*; testing data: *db4*).

5.3.3 Mean Flow Quantities

5.3.3.1 Velocity Profiles

The velocity profiles of the step case and the bump case are illustrated in Fig. 5.6. In these plots, the solid line represents the results of the SA model using the default coefficient values, the shaded area denotes the results of the SA model using different coefficient values, the dotted lines represent the LES simulations, the dashed lines denote the min-max bounds predicted by the FCNN, and the open circles represent the experimental data.

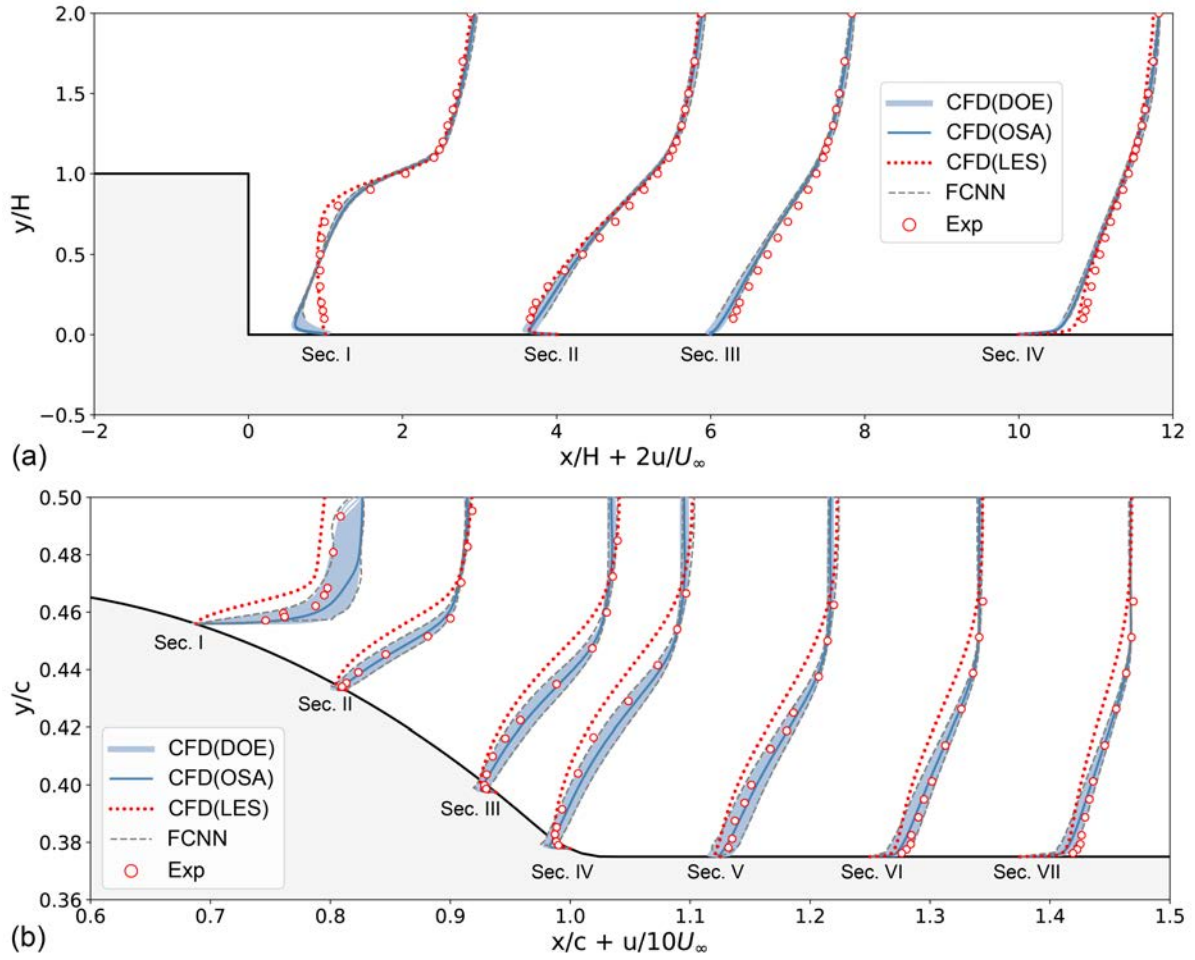


Figure 5.6: Uncertainty of predicted velocity profiles: (a) backward-facing step and (b) axisymmetric transonic bump.

For the step case shown in Fig. 5.6(a), a shear layer indicated by the high velocity gradient is generated right after the step at Sec. I. A separation bubble is also formed beneath the shear layer, which is captured by the change of velocity orientation in the lower parts of Sec. I and II. Comparing results from the SA model with the Hi-Fi data, the major deficiency is found at Sec. I where the flow just separates from the step wall. In other sections, the Hi-Fi data can be generally enveloped by the uncertainty bound of the velocity profile except for the near-wall region at Sec. IV, where the SA model under-predicts the velocity gradient and thus the local skin friction.

For the bump case presented in Fig. 5.6(b), the primary flow physics is the shock-induced flow separation. The shock front is located near Sec. I, which results in the wide uncertainty bound of the local velocity profile. When passing through the shock, a separation bubble is formed at the trailing edge corner of the bump, which is captured by the reverse flow in the lower parts of Sec. II to V. The uncertainty bounds are still evident in these sections inside the separation bubble. When the flow reattaches at Sec. VI and VII, the uncertainty in the velocity profile reduces. Compared to the results from the SA model, the measured data fall within the uncertainty bound, but the LES data does not. This is due to the early shock formation in LES, which will be presented in a later section.

5.3.3.2 Shock Location and Strength

The uncertainty in predicting the shock front location and pressure coefficient of the axisymmetric transonic bump is illustrated in Fig. 5.7. In the main plot, the shock front location is plotted against the negative of the shock front pressure coefficient. The scatters represent experimental or CFD results, and the contours illustrate the occurrence probability predicted by the FCNN. In the top and the right plots, the histogram represents the distribution of samples, and the curves are PDFs fitted by the kernel density estimation method [207] based on Gaussian kernels. It is observed that the SA model predicts a more downstream shock front location and a lower pressure coefficient at the shock front, indicating its deficiency in shock-capturing. Another observation is the apparent correlation between the shock front location and the pressure coefficient. This is because the pre-shock flow will experience an extended supersonic expansion and thus a reduced pressure if the shock is delayed.

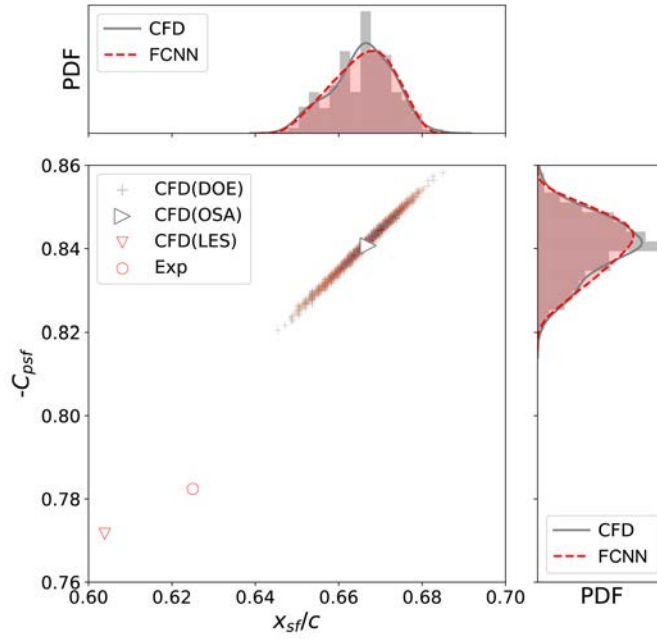


Figure 5.7: Uncertainty of predicted shock front location (x_{sf}/c) and shock front pressure coefficient ($-C_{psf}$) (scatters: samples from experiment and CFD; contours: occurrence probability by FCNN).

The sensitivity analysis on shock prediction is given in Fig. 5.8. The mean value and the standard deviation of the normalized gradient over the investigated coefficient intervals are denoted by the bars and the error bars, respectively. It is found that increasing coefficients σ , κ , c_{v1} , c_{b1} and c_{w2} leads to a delayed shock front, whereas c_{b2} and c_{w3} have negligible effects. Because the location and the pressure coefficient of the shock front are physically correlated, their sensitivity with respect to each SA model coefficient is similar to each other. The shock front location is physically determined by the pre-shock boundary layer: if the boundary layer thickness is increased by enhancing the Reynolds shear stress in the boundary layer, the main flow will experience a smaller streamline curvature and thus a delayed shock front and a reduced shock strength. It implies that the above sensitive coefficients are positively correlated with the Reynolds shear stress in the pre-shock boundary layer. This will be confirmed later in Sec. 5.3.4.

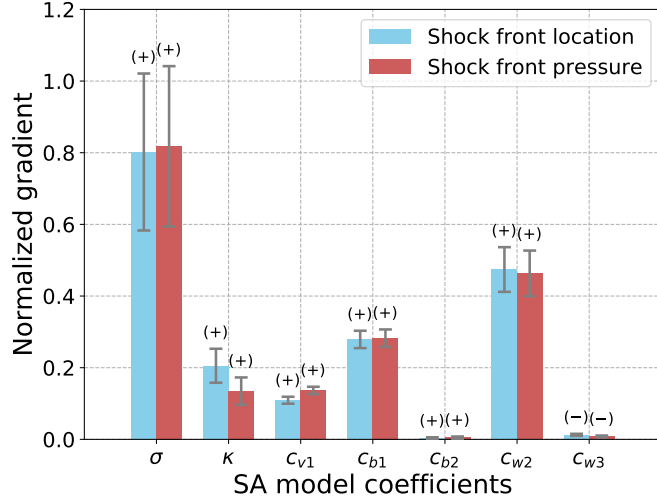


Figure 5.8: Sensitivity of predicted shock front location (x_{sf}/c) and shock front pressure coefficient ($-C_{psf}$).

5.3.3.3 Separation Size

The uncertainty in predicting the separation size of both cases is illustrated in Fig. 5.9. It is observed that the measured separation size of the step case is close to the prediction of the SA model, although the SA model cannot capture the velocity profile in the separated region accurately (i.e., Sec. I in Fig. 5.6(a)). However, the SA model predicts a smaller separation size in the bump case. Thus, the experiment dot falls out of the range of SA model results, and both separation sizes cannot be simultaneously captured accurately by tuning the SA model coefficients.

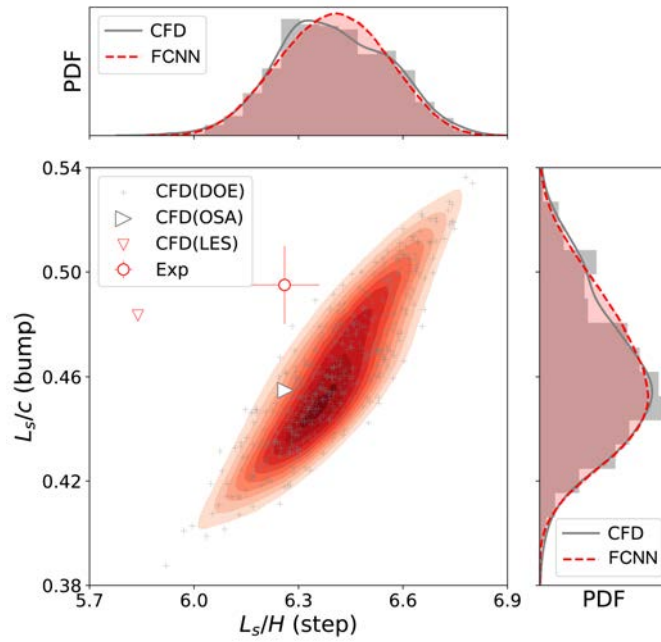


Figure 5.9: Uncertainty of predicted separation size in the step (L_s/c) and the bump (L_s/H) case (scatters: samples from experiment and CFD; contours: occurrence probability by FCNN).

It was shown in Sec. 5.3.3.2 that the SA model predicts a delayed shock front, which may be the cause of the under-predicted shock-induced separation size of the bump case. To elucidate this correlation, the shock front location is plotted against the separation size in Fig. 5.10. It can be observed that the separation size does increase with the upstream movement of the shock front. However, fixing the shock front prediction by changing the SA model coefficients would lead to an over-prediction of the separation size. Such a trade-off effect further indicates the deficiency of the SA model in predicting both the shock location/strength and the separation size accurately.

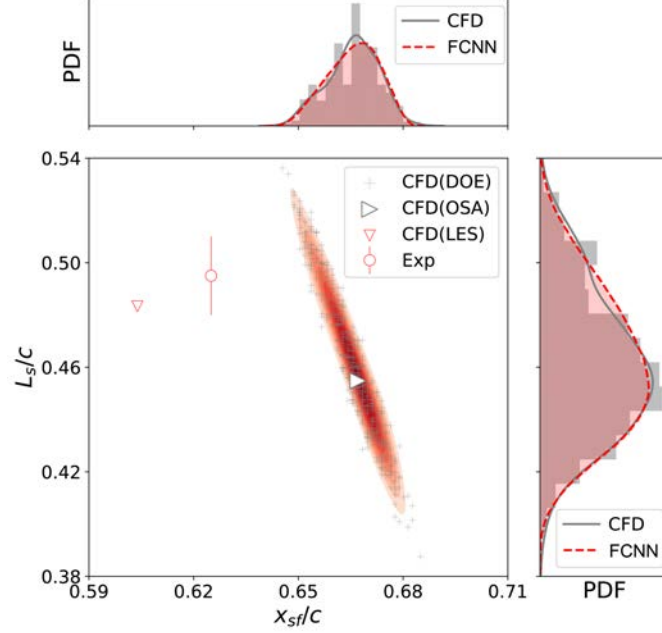


Figure 5.10: Correlation between the shock front location (x_{sf}/c) and the separation size (L_s/c) (scatters: samples from CFD; contours: occurrence probability by FCNN).

The sensitivity analysis of the separation prediction is presented in Fig. 5.11. Regardless of the cause of separation, the sensitivities in predicting the separation size of both cases are similar to each other: increasing σ , κ , c_{b1} and c_{w2} or decreasing c_{w3} will reduce the separation size, meanwhile c_{v1} and c_{b2} have negligible effects. A common mechanism that reduces the separation size of both cases is by enhancing the Reynolds shear stress in the separation region. It implies that the Reynolds shear stress in the separation region is positively correlated with σ , κ , c_{b1} and c_{w2} , whereas it is negatively correlated with c_{w3} . These correlations will be examined later in Sec. 5.3.4.

5.3.4 Turbulence Quantities

The Reynolds shear stress profiles of the step case are shown in Fig. 5.12(a). It is observed that the Hi-Fi data overlap with the uncertainty bound when the flow just detaches from the step at Sec. I. As the flow develops to Sec. II, the SA model under-predicts the downward advection of the peak of the Reynolds shear stress profile. Consequently, the Hi-Fi results cannot be fully enveloped by the uncertainty bound. At Sec. III, the uncertainty bound converges to the profile predicted by the SA model, but the deficiency persists. When the

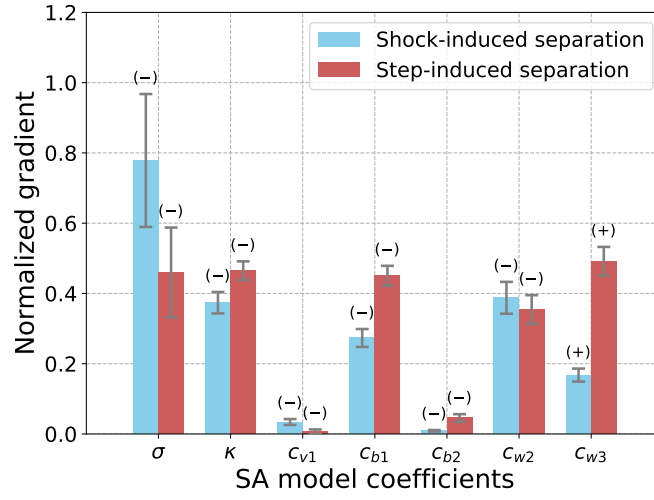


Figure 5.11: Sensitivity of predicted separation size.

flow is reattached at Sec. IV, the Hi-Fi data become closer to the results from the SA model again. These observations indicate that the uncertainty and deficiency of the SA model become evident in the separation region.

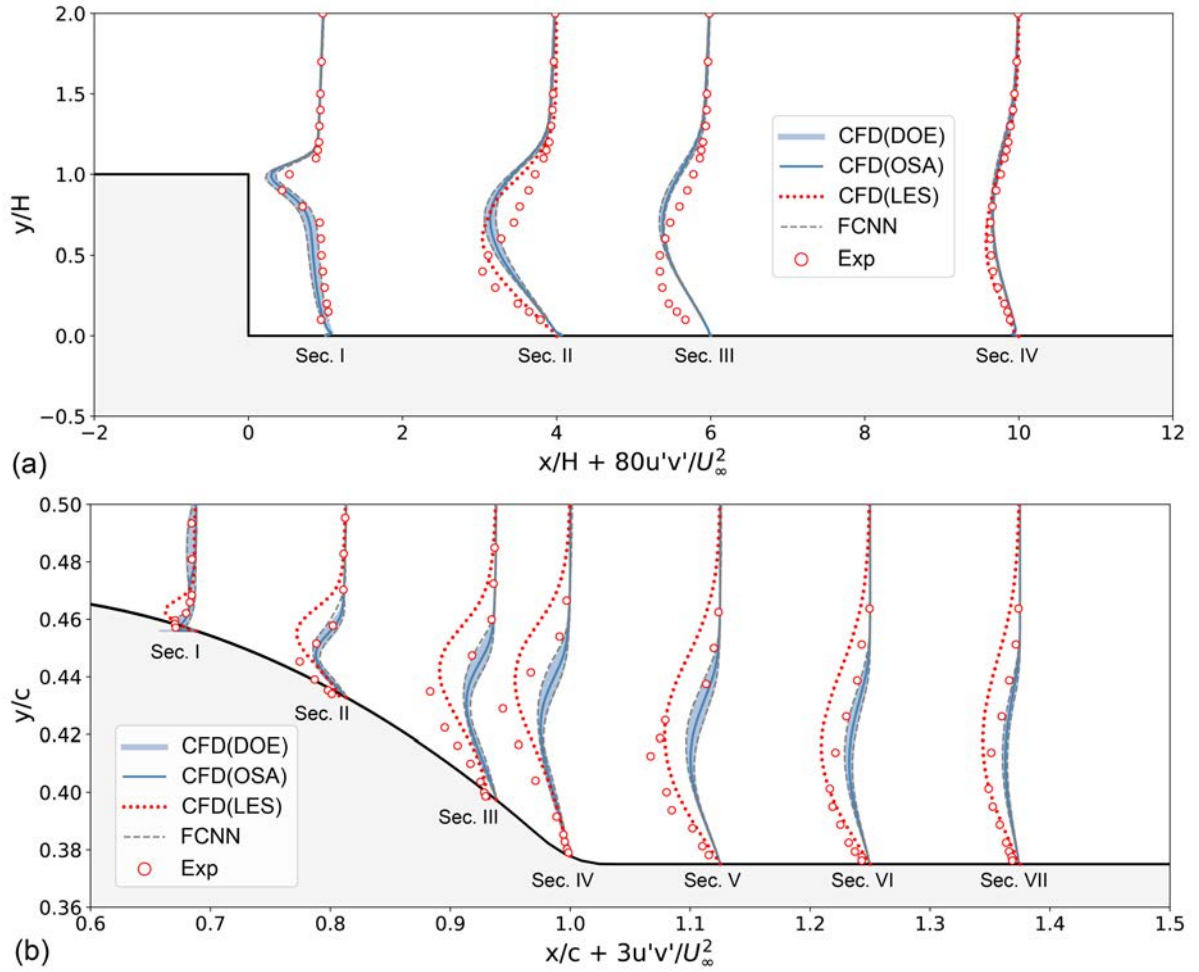


Figure 5.12: Uncertainty of predicted Reynolds shear stress profiles: (a) backward-facing step and (b) axisymmetric transonic bump.

The Reynolds shear stress profiles of the bump case are presented in Fig. 5.12(b). Results show that the uncertainty of the Reynolds shear stress and the discrepancy between the SA model results and the Hi-Fi results are much higher in the shock region near Sec. I and the separation region between Sec. II and Sec. VI than elsewhere. Moreover, the peak values of the Reynolds shear stress profiles are under-predicted by the SA model. It should be noted that the strain rate downstream of the bump mainly depends on the shock-induced separation strength. An accurate prediction of the shock front location and the separation size is a prerequisite for predicting the Reynolds shear stress field correctly.

The sensitivity analyses on predicting the Reynolds shear stress field of the step flow are performed in Fig. 5.13. The contour shown in these figures represents the mean gradient of Reynolds shear stress with respect to each SA model coefficient, which is non-dimensionalized by the square of the mainstream velocity U_∞^2 and the coefficient interval. This gradient at each mesh point is calculated by a separate FCNN model, and a total of about 4000 mesh points were investigated.

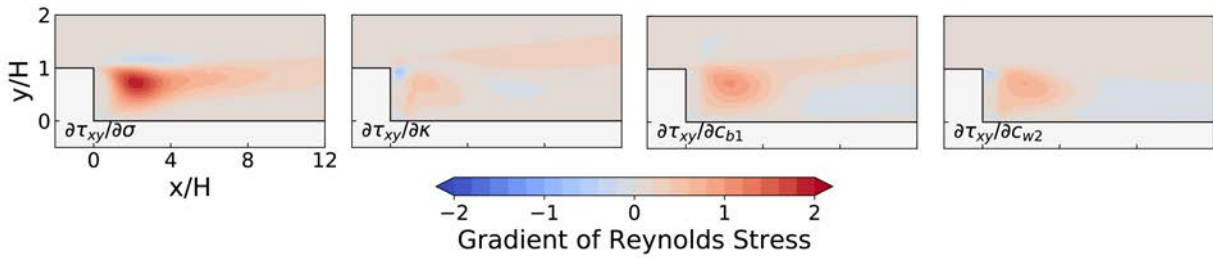


Figure 5.13: Sensitivity of predicted Reynolds shear stress for the backward-facing step.

In general, the SA model coefficients σ , κ , c_{b1} and c_{w2} have significant effects, whereas c_{v1} , c_{b2} and c_{w3} are negligible and thus are not shown here. The most sensitive region is the separation bubble.

The coefficient σ affects the Reynolds shear stress via both the diffusion term and the destruction term. Increasing σ reduces the diffusion of eddy viscosity from the separation bubble to the nearby region, thus the increase in Reynolds shear stress in the separation bubble. Also, an increase in σ will reduce c_{w1} and the near-wall turbulence destruction. As a result, the diffusion of eddy viscosity to the wall is reduced, which further increases the Reynolds shear stress in the separation bubble.

The coefficient κ exists in the modified strain rate term $\hat{S}$, which affects both the production and the destruction terms. The net source term related to κ is $(f_{v2} - f_w)c_{b1}\hat{\nu}^2/\kappa^2d^2$. To determine the sign of $f_{v2} - f_w$, the values of f_{v2} and f_w are plotted as functions of r and χ respectively in Fig. 5.14, and the corresponding contours of r and χ are shown in Fig. 5.15. In Fig. 5.14(a) and (b), it is observed that $f_w > 0$ in most region except for the region of $r = 0$, which corresponds to the farfield (see Fig. 5.15(a)). In Fig. 5.14(c), it shows that $f_{v2} \leq 0$ in most regions except for the near-wall boundary layer and the farfield where the viscosity ratio $\chi < 1$ (see Fig. 5.15(b)). Therefore, $f_{v2} - f_w < 0$ holds true for the separation region, and an increase in κ will enhance the Reynolds shear stress there.

The coefficient c_{b1} mainly determines the magnitude of the production term, but it also exists in the destruction term. The net source term related to c_{b1} is $c_{b1}\hat{\nu}(\Omega + (f_{v2} - f_w)\hat{\nu}/\kappa^2d^2)$, and the sign of the bracket term determines whether the source term increases or decreases

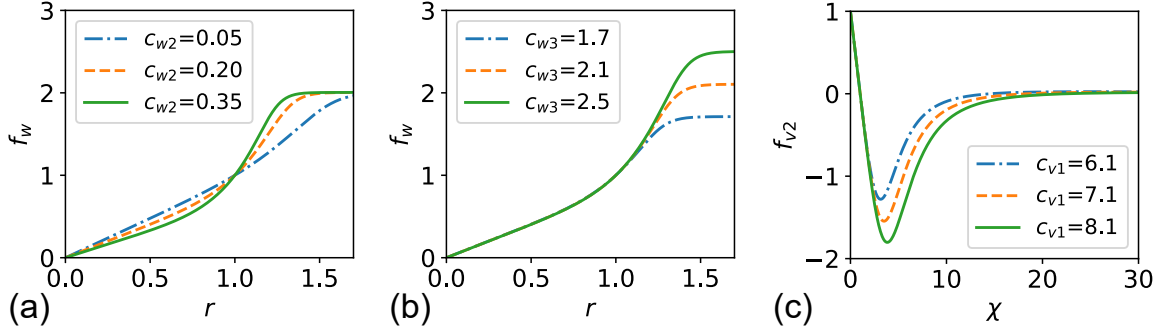


Figure 5.14: Empirical functions in the SA turbulence model: (a) f_w as a function of r and c_{w2} , (b) f_w as a function of r and c_{w3} , and (c) f_{v2} as a function of χ and c_{v1} .

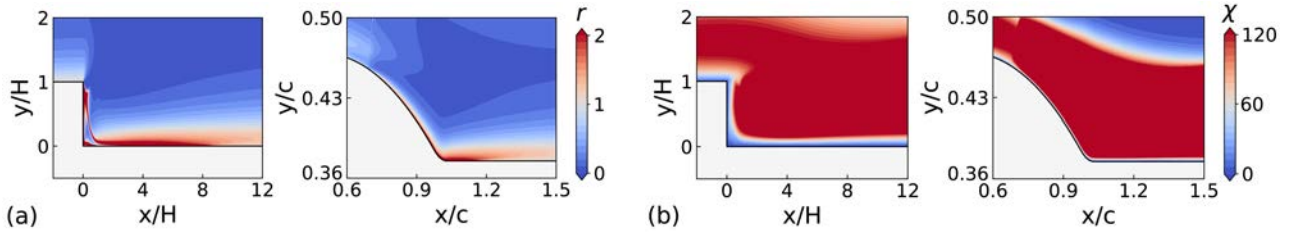


Figure 5.15: Contours of (a) r and (b) χ in the backward-facing step and the axisymmetric transonic bump.

with c_{b1} . In the separation region where both Ω and d are large, the bracket term is positive (i.e., net production of eddy viscosity), and thus an increase in c_{b1} will enhance the Reynolds shear stress. In the reattached boundary layer where both Ω and d are small, the bracket term is negative (i.e., net destruction of eddy viscosity), and thus an increase in c_{b1} will reduce the Reynolds shear stress.

The coefficient c_{w2} alters the f_w term in the destruction term, as illustrated in Fig. 5.14(a). In regions where $r < 1$ (e.g., farfield, outer part of boundary layer and near-wall boundary layer with favorable pressure gradient [44]), an increase in c_{w2} will reduce the f_w term, reduce the eddy viscosity destruction term and thus increase the Reynolds shear stress. This corresponds to the separation region in the step case (see Fig. 5.15(a)). In regions where $r > 1$ (e.g., near-wall boundary layer with adverse pressure gradient [44]), an increase in c_{w2} , however, will reduce the Reynolds shear stress, as observed in the reattached boundary layer of the step case (see Fig. 5.15(a)).

The coefficient c_{w3} is positively correlated with the destruction term in regions with $r > 1$, as illustrated in Fig. 5.14(b). However, its effect is not visible in the major part of the flow domain, because the affected region is limited to the near-wall region (see Fig. 5.15(a)). Thus, its gradient contours are not shown here.

The coefficient c_{v1} is negatively correlated with the production term in regions with $1 < \chi < 20$, as illustrated in Fig. 5.14(c). Since the affected region is close to the wall (see Fig. 5.15(b)), its gradient contours are not visible in the major part of the flow domain and thus are not shown either.

The sensitivity analyses on predicting the Reynolds shear stress field of the bump flow are presented in Fig. 5.16. Likewise, the mean gradient of Reynolds shear stress is non-

dimensionalized by U_∞^2 and the coefficient interval; the gradient at each mesh point is calculated by a separate FCNN model, and a total of about 5000 mesh points were investigated.

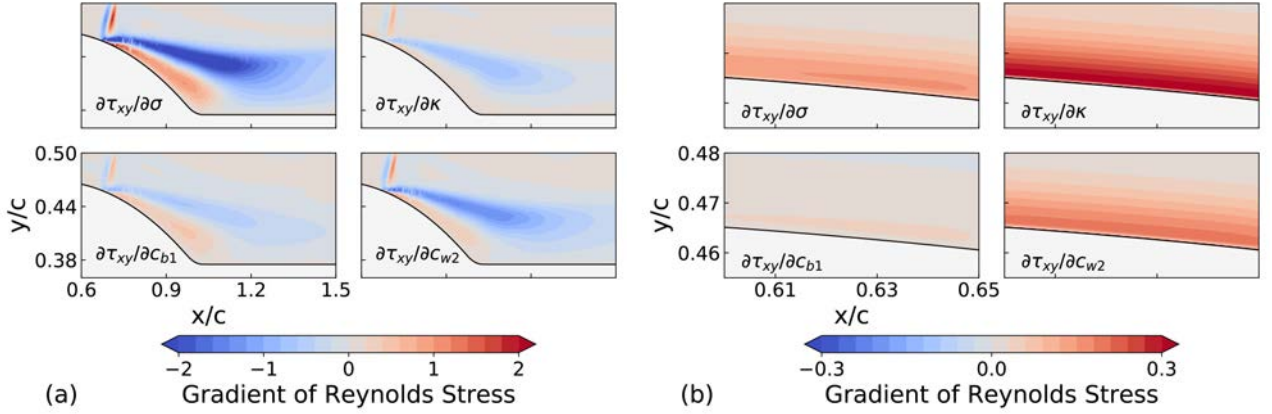


Figure 5.16: Sensitivity of predicted Reynolds shear stress for the axisymmetric transonic bump: (a) full view and (b) zoom-in view.

For the aft-shock region illustrated in Fig. 5.16(a), the change of the Reynolds shear stress field is mainly due to the change in the mean flow strain rate. Recall from Sec. 5.3.3.2, increasing either coefficient of σ , κ , c_{b1} and c_{w2} leads to a delayed shock front, which reduces the shock-induced separation size and hence the reduced Reynolds shear stress near the upper separation region. In the lower separation region, the same mechanism as that of the step case exists, and the coefficients σ , κ , c_{b1} and c_{w2} will increase the local Reynolds shear stress.

The delayed shock front is physically caused by a thickened pre-shock boundary layer. In the pre-shock region shown in Fig. 5.16(b), it is confirmed that the magnitude of Reynolds shear stress increases with σ , κ , c_{b1} and c_{w2} , which thickens the pre-shock boundary layer and eventually leads to the delay of the shock formation. The mechanisms that how these coefficients change the Reynolds shear stress are similar to that of the step case.

5.3.5 Role of the Diffusion Coefficient

From the analyses in Sec. 5.3.3 and Sec. 5.3.4, the diffusion coefficient σ is found overall the most sensitive to both the mean flow quantities and the turbulence quantities. Since σ occurs both in the diffusion term and the destruction term, it is worth investigating which term plays the dominant role. In this section, the coefficient σ has been split into σ_{des} in the destruction term and σ_{diff} in the diffusion term. A full factorial experiment with additional 25 samples is designed and tested in both cases by CFD. These samples differ in the values assigned to σ_{des} and σ_{diff} , whereas other coefficients are kept as the default values of the OSA model.

The quantities of interest obtained by different σ_{des} and σ_{diff} values are presented as contours in Fig. 5.17. For the prediction of the shock front location shown in Fig. 5.17(a), both σ_{des} and σ_{diff} have a similar effect as the isolines are largely diagonal. This is because either term can change the near-wall Reynolds shear stress magnitude and thus the pre-shock boundary layer thickness. For the prediction of the separation size presented in Fig. 5.17(b) and (c), however, the source-related σ_{des} term is more sensitive than the σ_{diff} term as the isolines

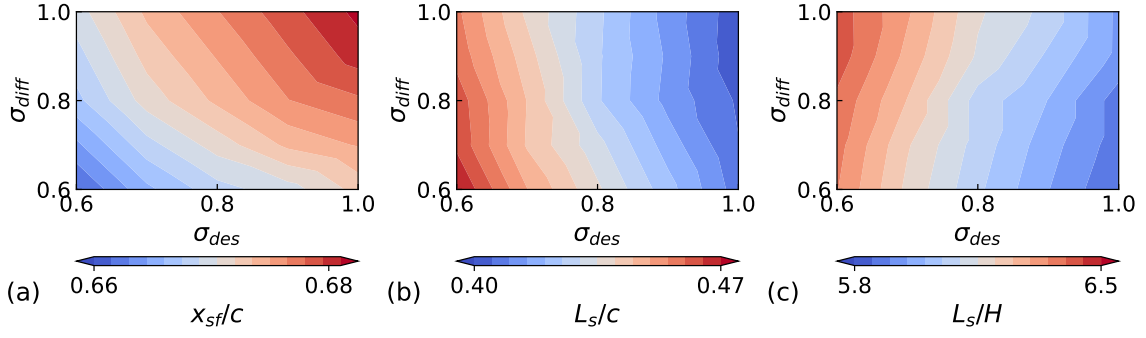


Figure 5.17: Effect of σ_{des} and σ_{diff} on predicting the (a) shock front location, (b) shock-induced separation size and (c) step-induced separation size.

of the separation size are almost vertical. It indicates that the total budget of Reynolds shear stress determines the separation size, rather than its spatial distribution.

5.3.6 Correlation between Model Coefficients and Flow Fields

Based on the analysis in Sec. 5.3.3 and Sec. 5.3.4, there are four common coefficients that are sensitive to both the mean flow quantities and the turbulence quantities, namely σ , κ , c_{b1} and c_{w2} . The causal links between the model coefficients, the turbulence quantities and the mean flow quantities are illustrated in Fig. 5.18.

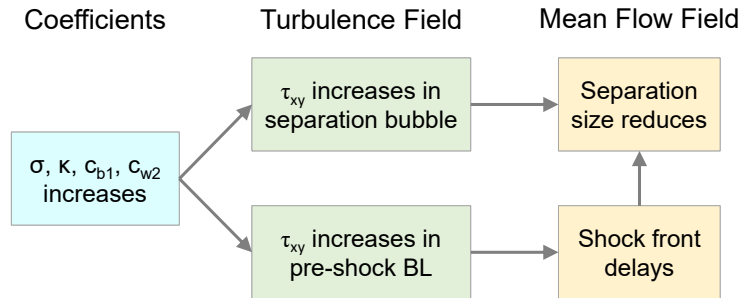


Figure 5.18: Illustration of causal links between the model coefficients, the turbulence quantities and the mean flow quantities for the backward-facing step and the axisymmetric transonic bump.

For the backward-facing step case, the separation size is determined by the reattachment location, which is physically correlated with the Reynolds shear stress magnitude. Since increasing coefficients σ , κ , c_{b1} and c_{w2} will increase the Reynolds shear stress magnitude in the separation region, it reduces the separation size due to a stronger turbulent mixing effect.

For the axisymmetric transonic bump case, the separation size is determined by both the separation location and the reattachment location. The mechanism of the backward-facing step still holds true in the bump case, which determines the reattachment location. In addition, increasing coefficients σ , κ , c_{b1} and c_{w2} will also increase the Reynolds shear stress in the pre-shock boundary layer, which postpones the shock front and the separation location further downstream and thus reduces the separation size.

5.4 Uncertainty Quantification on Stall Prediction of NACA 0012

5.4.1 Case Description

In this section, the uncertainty of the SA model coefficients is quantified in the subsonic airfoil NACA 0012, which is featured by the trailing edge stall. To help illustrate this stall phenomenon, the trailing edge separation and its size are shown in Fig. 5.19. In the contour plot of Mach number, the flow separation is captured by the low-Mach region, and the separation size L_s is quantified by the chordwise distance between the separation point (identified by zero skin friction) and the sharp trailing edge. In the line plot, the separation size L_s is plotted against the angle of attack (AoA). The line with dots is the result of the OSA model, and the smooth lines are results of the SA model with coefficients in all the DOE databases. Results show that the separation region expands towards the leading edge when increasing the AoA, leading to a gradual reduction in lift coefficient and thus the trailing edge stall.

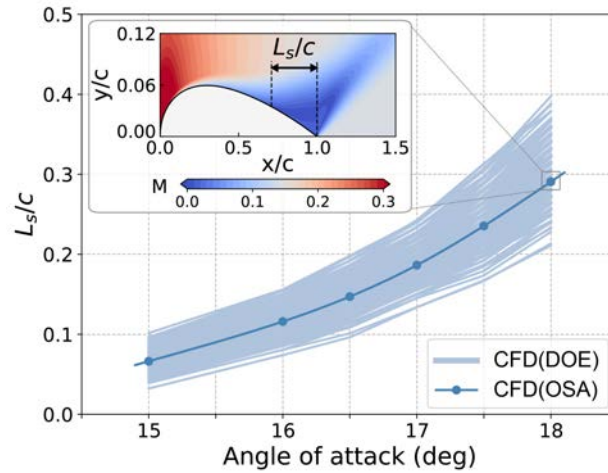


Figure 5.19: Separation size of NACA 0012 airfoil under different angles of attack.

The details of the experimental data [145] and the CFD setups of NACA 0012 have been introduced in Sec. 3.4.1. In the following UQ study, the main QoIs include the lift coefficient C_L , the drag coefficient C_D , the separation size L_s , the stall AoA and the Reynolds shear stress τ_{xy} . Here, the stall AoA is defined as the AoA that achieves the peak C_L . To find the peak C_L point, six near-stall operating points (i.e., AoA=15, 16, 16.5, 17, 17.5 and 18 deg) are simulated by CFD for each set of the SA model coefficients, and a cubic spline is fitted through these points to represent the characteristic curve. An independent FCNN metamodel is trained and tested for each group of QoIs, and the details are summarized in Table 5.3. The *db5* is applied as the training database, the *db4* serves as the testing database, and the union of *db1* to *db3* is used for cross-validation.

Table 5.3: Details of metamodels for different quantities of interest of the NACA 0012.

QoI Group	n_q	Outputs	Figure
Lift coefficient	6	$C_L(\text{AoA})$	5.20, 5.21, 5.23, 5.24
Drag coefficient	6	$C_D(\text{AoA})$	5.20, 5.21, 5.23, 5.24
Separation	1	L_s	5.20, 5.21, 5.25, 5.26
Stall	1	stall AoA	5.20, 5.21, 5.25, 5.26
Reynolds shear stress	1	$\tau_{xy}(x, y)$	5.27

5.4.2 Cross-Validation, Training and Test of FCNN

5.4.2.1 Hyperparameter Study

In this section, the FCNN hyperparameters, namely the number of hidden layers L , the number of artificial neurons in each hidden layer n_L , the scale factor ω and the regularization factor λ , are determined for the NACA 0012 airfoil case. A parametric study of n_1 , ω , and λ has been conducted by changing one hyperparameter at a time while keeping the others at the baseline setting, which is $L = 1$, $n_1 = 0.5(n_x + n_q)$, $\omega = 2$ and $\lambda = 10^{-4}$. To avoid the training process falling into a local optimum, 8 FCNNs with different initial conditions are trained parallelly, and the best FCNN is chosen.

The prediction errors of FCNNs in various QoIs are plotted against each hyperparameter in Fig. 5.20. Using the FCNN model with the baseline hyperparameters, the errors in predicting the separation size, the lift coefficient and the drag coefficient are within 3% of the min-max QoI range (i.e., $\omega\epsilon < 3\%$), which is comparable to that of the backward-facing step and the axisymmetric transonic bump in Sec. 5.3.2.1. The error in predicting the stall AoA is slightly higher, within 5% of the min-max QoI range. However, considering the min-max range of the stall AoA is only about 0.8 degrees, the mean relative error of the FCNN is only 0.14%, which is sufficiently small for the metamodel purpose. Therefore, a deep FCNN (i.e., $L > 1$) is not pursued, and the baseline setting is adopted throughout this section.

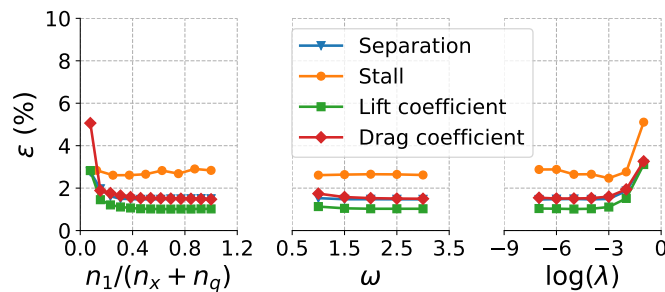


Figure 5.20: Hyperparametric study for the NACA 0012 airfoil (training data: *db5*; cross-validation data: the union of *db1*, *db2* and *db3*).

5.4.2.2 Training Data Independence Study

In this section, a training data independence study is performed using different database combinations to train and test the FCNN. The training and test databases are $db\{i\}$ and $db\{i - 1\}$ so that the ratio of training-to-test database size can be kept the same as 2. The difference between the test and training errors (i.e., ϵ_{te} and ϵ_{tr}) is plotted against the training database size in Fig. 5.21. It shows that using the training database size of 256 achieves an almost data-independent result, where the differences between ϵ_{te} and ϵ_{tr} are below 0.5%. Hence, the $db5$ with 256 samples has been chosen to train FCNNs in the following of this section.

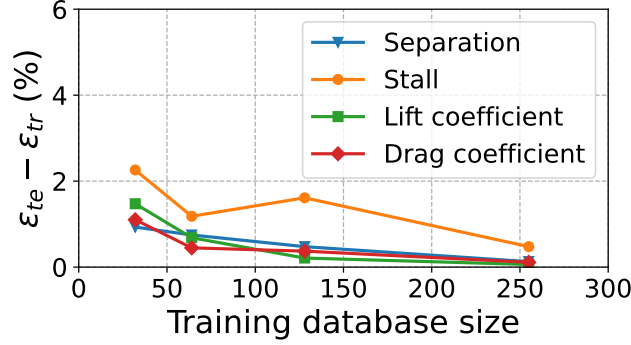


Figure 5.21: Training data independence study for the NACA 0012 airfoil (training data: $db5$; cross-validation data: the union of $db1$, $db2$ and $db3$).

5.4.2.3 Training and Test Results

Using the selected hyperparameters and the training/test databases from Sec. 5.4.2.1 and 5.4.2.2, an FCNN is trained and tested for each QoI. A representative example of the FCNN is provided in Fig. 5.22, which maps the SA model coefficients with the stall AoA of the NACA 0012 airfoil. The training process is presented in Fig. 5.22(a), where the convergence of the optimization algorithm is achieved after about 1000 iterations. The corresponding prediction accuracy is shown in Fig. 5.22(b), where the stall AoA obtained from FCNN and CFD is plotted on the vertical and horizontal axis, respectively. It shows that the maximum absolute error of FCNN on the test database is 0.1 degrees, and the mean relative error is 0.14%. This is sufficiently small for the metamodel purpose.

5.4.3 Mean Flow Quantities

5.4.3.1 Lift and Drag Characteristics

The uncertainty in the predicted characteristics of the NACA 0012 airfoil is illustrated in Fig. 5.23. In these plots, the open circles are measured data [145], the solid lines are CFD results, and the dashed lines are the min-max bounds predicted by the FCNN. The region enveloped by the dashed lines represents the parametric uncertainty.

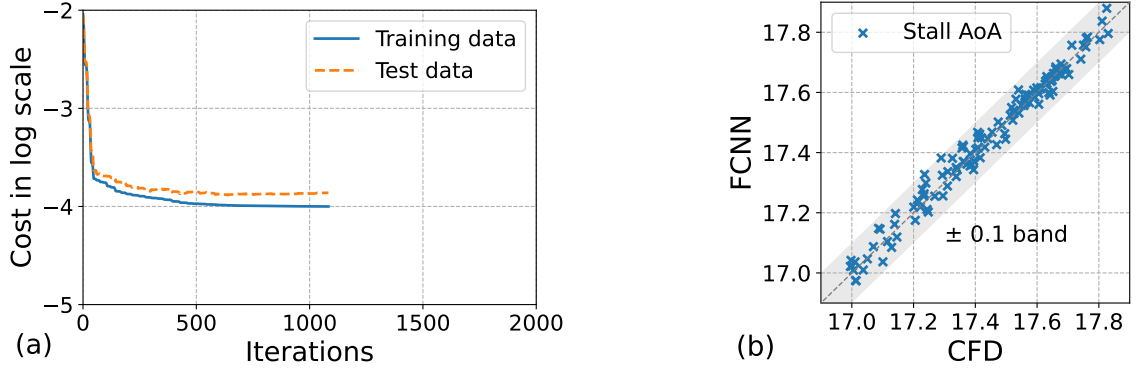


Figure 5.22: FCNN for predicting the stall angle of attack (in degree) of the NACA 0012 airfoil (training data: *db5*; testing data: *db4*).

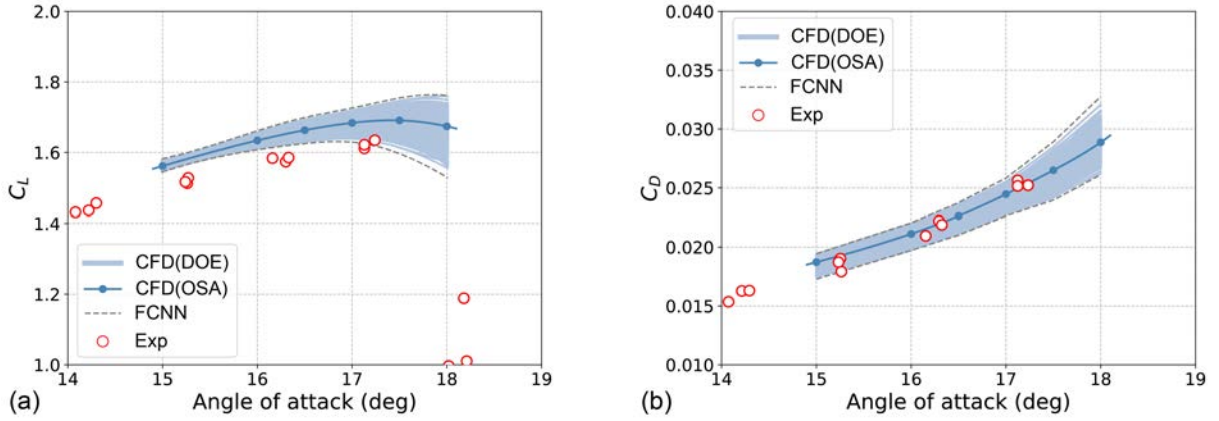


Figure 5.23: Uncertainty of predicted characteristics of NACA 0012 airfoil: (a) lift coefficient and (b) drag coefficient.

For the lift coefficient C_L presented in Fig. 5.23(a), the uncertainty is small when operating away from stall, where the separation size is relatively small. When stall is approached, the separation grows in size, resulting in a much larger uncertainty in C_L . Specifically, the uncertainty in C_L increases from 2.4% to 13.9% of the OSA prediction as the AoA increases from 15 to 18 degrees. It is also observed that the SA model over-predicts C_L when the AoA is higher than 15 degrees, which is not seen when using other forms of the turbulence model [54]. This indicates the limitation of the SA model form.

For the drag coefficient C_D shown in Fig. 5.23(b), the uncertainty is evident at all the AoAs, and the uncertainty range slightly increases when approaching stall. At low AoA, the drag is mainly composed of skin friction, which can be influenced by the SA model coefficients via tuning the boundary layer log-law. At high AoA, the form drag induced by the flow separation takes a more important role, which can be affected by the SA model coefficients via changing the separation size. Since the separation size increases with the AoA (see Fig. 5.19), the uncertainty in C_D also increases with the AoA. In this case, it increases from 11.8% to 23.1% of the OSA prediction when the AoA increases from 15 to 18 degrees.

The sensitivity analyses on predicting the lift and the drag coefficients are presented in Fig. 5.24. In this plot, each point represents the normalized gradient of a coefficient at a fixed AoA. The coordinates of each point are the mean values of the normalized gradient over the

investigated coefficient intervals, and the error bar represents the standard deviation. The farther away from the origin, the more sensitive the coefficient is.

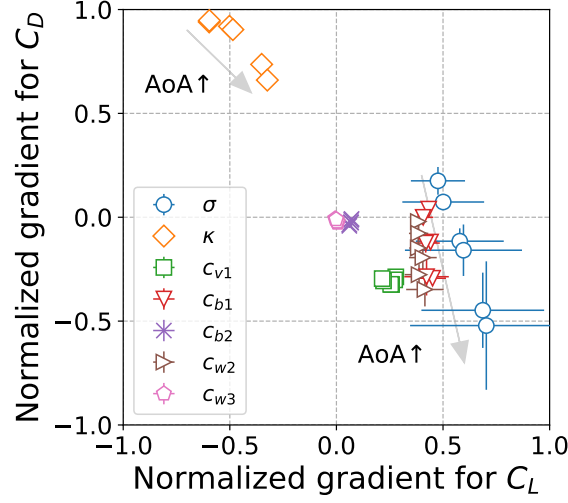


Figure 5.24: Sensitivity of predicted lift and drag coefficient for the NACA 0012 airfoil.

In general, it is found that increasing σ , c_{v1} , c_{b1} and c_{w2} or decreasing κ leads to higher C_L and lower C_D , whereas the coefficients c_{b2} and c_{w3} have negligible effects on the results. When increasing the AoA (indicated by the direction of the arrow), both C_L and C_D tend to be more sensitive to changes in σ , c_{b1} and c_{w2} and less for κ . Such a result implies that increasing σ , c_{b1} and c_{w2} can lead to a more positive slope of the lift coefficient curve and thus delay the onset of stall.

Coefficients σ , c_{b1} and c_{w2} modify the characteristics mainly through changing the separation size: when the separation size is reduced, the C_L will increase and C_D will decrease. As the flow separation becomes more evident at a higher AoA, the above coefficients become more sensitive when the AoA is increased. The separation of this case is caused by the boundary layer development under an adverse pressure gradient. By thickening the boundary layer (i.e., increasing τ_{xy}) upstream of the separation point, the onset of the separation will be postponed to a further downstream location and thus the reduction of separation size. The separation size will also be reduced if the turbulent mixing effect in the separation region is enhanced. In the previous studies on the bump case and the step case in Sec. 5.3.4, it has been demonstrated that increasing either σ , c_{b1} or c_{w2} will increase the Reynolds shear stress in both the boundary layer and the separation region. In the current NACA 0012 airfoil case, these changes of Reynolds shear stress will be confirmed later in Sec. 5.4.4.

Coefficients κ and c_{v1} influence the characteristics mainly by tuning the boundary layer log-law. Decreasing κ and increasing c_{v1} will result in a steeper log-law slope and a higher intercept respectively [44], both of which squeeze the buffer layer thickness, increase the near-wall τ_{xy} , delay the separation point, and eventually lead to a higher C_L and a lower C_D . Moreover, since κ is proportional to the skin friction [209], a lower value of κ also leads to a lower value of skin friction and thus a lower C_D .

5.4.3.2 Stall Angle of Attack

The uncertainty of the SA model coefficients in predicting the stall angle of attack and the separation size at 18 degrees of AoA is presented in Fig. 5.25. In the main plot, each scatter represents the result from one set of SA model coefficients, and the contour illustrates the occurrence probability predicted by the FCNN metamodel. In the top and the right plots, the distribution of samples is represented by the histogram, and the corresponding PDF is fitted using the kernel density estimation method [207] based on Gaussian kernels. It is seen that the predicted stall angle of attack ranges from 16.9 to 18.0 degrees, which successfully envelopes the measured result of 17.2 degrees [145] as presented earlier in Fig. 5.23(a). The OSA result is close to the maximum likelihood estimation, which shows the original set of the SA model coefficients is an effective representative of the investigated coefficient range. Another observation is the evident negative correlation between the stall angle of attack and the separation size, which is consistent with the physical understanding of the trailing edge stall.

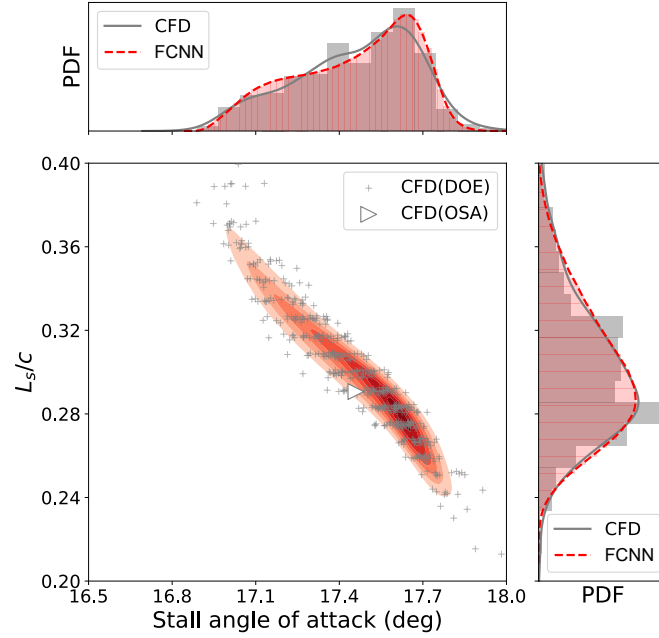


Figure 5.25: Uncertainty of predicted stall angle of attack and separation size at AoA=18 deg of NACA 0012 airfoil (scatters: samples from CFD; contours: occurrence probability of FCNN).

The sensitivity analyses on predicting the stall angle of attack and the separation size are illustrated in Fig. 5.26, where the mean value and the standard deviation of the normalized gradient with respect to each coefficient are represented by bars and error bars, respectively. It is illustrated that increasing coefficients σ , c_{b1} or c_{w2} reduces the separation size and thus delays the occurrence of stall, whereas other coefficients have a relatively negligible effect. This result highlights the significance of coefficients related to the source term on stall prediction, which is also consistent with the sensitivity analyses on predicting C_L as presented earlier in Fig. 5.24. The mechanisms that σ , c_{b1} and c_{w2} influence the separation size are by changing the boundary layer thickness before the separation point, which has been discussed earlier in Sec. 5.4.3.1.

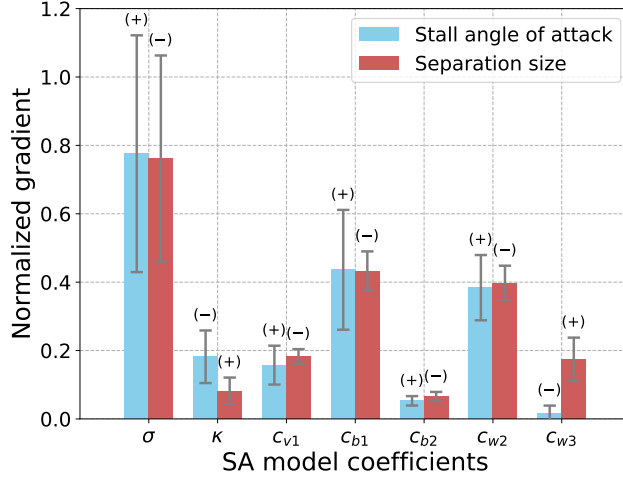


Figure 5.26: Sensitivity of predicted stall angle of attack and separation size at AoA=18 deg for the NACA 0012 airfoil.

5.4.4 Turbulence Quantities

To consolidate the above analysis, the contours of the Reynolds shear stress gradient with respect to the sensitive coefficients are plotted in Fig. 5.27. The gradient has been non-dimensionalized by the freestream velocity and the coefficient range. To construct the contour view in these figures, around 25000 independent FCNNs were trained at the mesh points to calculate the gradient value.

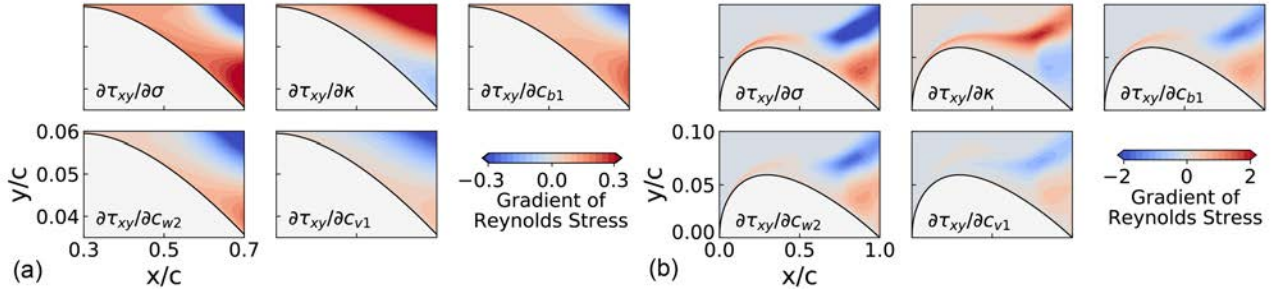


Figure 5.27: Sensitivity of predicted Reynolds shear stress near the suction surface at AoA=18 deg of NACA 0012 airfoil: (a) zoom-in view and (b) full view.

In the zoom-in plot in Fig. 5.27(a), it is confirmed that the near-wall Reynolds shear stress increases with higher σ , c_{b1} , c_{w2} and c_{v1} and lower κ , which thickens the boundary layer before the separation point, reduces the separation size, and thus increases C_L and decreases C_D .

In the full view in Fig. 5.27(b), it is confirmed that the Reynolds shear stress in the separation region near the trailing edge increases with higher σ , c_{b1} , c_{w2} and c_{v1} and lower κ , which reduces the separation size and thus increases C_L and decreases C_D . The change of the separation size by each coefficient is also captured by the change of local Reynolds shear stress: when the separation bubble is pushed rearwards, the strain rate near the mid-chord and the trailing edge will be decreased and increased accordingly, leading to the Reynolds shear stress reduction near the mid-chord and increment near the trailing edge.

5.4.5 Correlation between Model Coefficients and Flow Fields

Based on the analysis in Sec. 5.4.3 and Sec. 5.4.4, there are three common coefficients that are sensitive to both the mean flow quantities and the turbulence quantities, namely σ , c_{b1} and c_{w2} . The causal links between the model coefficients, the turbulence quantities and the mean flow quantities are summarized here in Fig. 5.28. Concretely, increasing either σ , c_{b1} or c_{w2} will increase the Reynolds shear stress in the separation region and the boundary layer, both of which reduces the separation size and hence an increased C_L , an increased stall AoA and a reduced C_D .

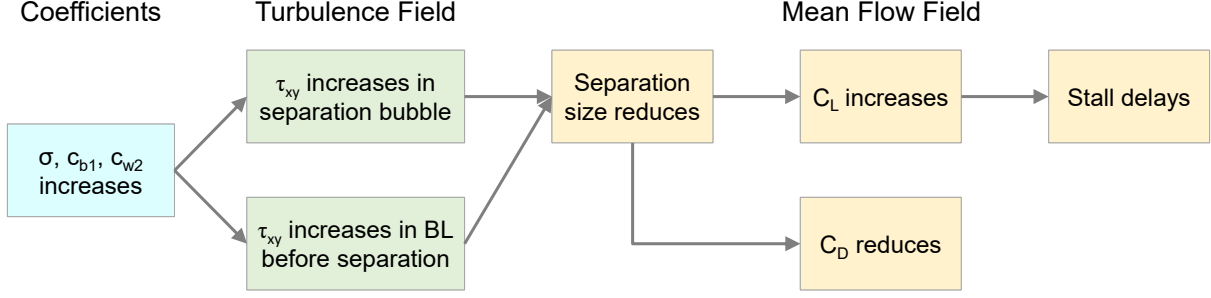


Figure 5.28: Illustration of causal links between the model coefficients, the turbulence quantities and the mean flow quantities for the NACA 0012 airfoil.

5.5 Uncertainty Quantification on Stall Prediction of NASA Rotor 67

5.5.1 Case Description

In this section, the uncertainty of the SA model coefficients is quantified in the NASA Rotor 67, which is featured by tip-driven spike-type rotating stall [210]. There are two conditions required for the formation of spike-type perturbations [198]: the spillage of the tip leakage flow at the leading edge and the reversal of the tip leakage flow at the trailing edge. These two conditions are equivalent to the formation of a tip blockage cell that extends from the leading edge to the trailing edge. To help illustrate the stall phenomena of NASA Rotor 67, the tip blockage cell and its size are plotted against the mass flow in Fig. 5.29. As shown in the contours of circumferentially-averaged axial velocity, the size of the tip blockage cell L_b can be estimated by the axial length of the isoline of $U_x = 0$, which envelops the blockage cell. In the line plot, L_b is plotted against the normalized mass flow. It is shown that the blockage size increases when decreasing the mass flow. At the last converged point, the blockage size surpasses the axial length of the tip chord $c_{x,tip}$, leading to the leading edge flow spillage and the trailing edge flow reversal, and thus the spike-type rotating stall.

The details of the experimental data [26, 165, 166] and the CFD setups of NASA Rotor 67 have been introduced in Sec. 3.4.3. In the following UQ study, the main QoIs include the total pressure ratio π_{1t-2t} , the isentropic efficiency η_{1t-2t} , the blockage size L_b , the stall mass flow m_s

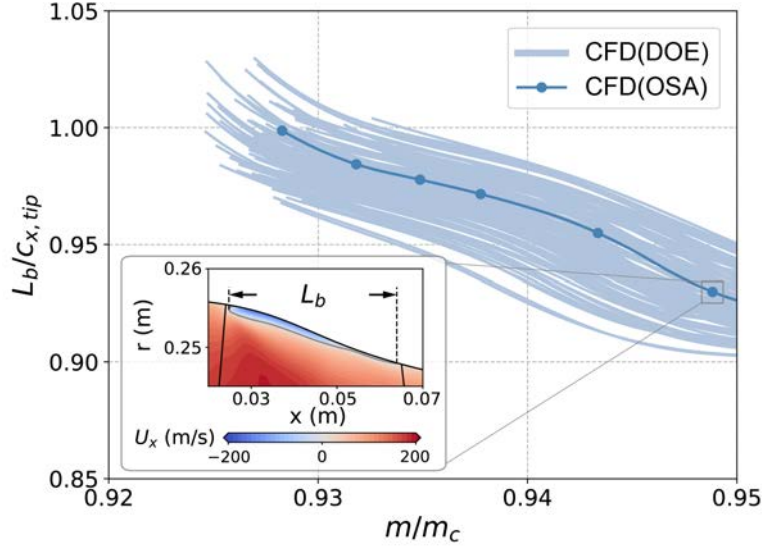


Figure 5.29: Blockage size of NASA Rotor 67 under different mass flow conditions.

and the eddy viscosity ν_t at the design operating speed. Here, m_s is defined as the mass flow that achieves the peak π_{1t-2t} . To find the peak π_{1t-2t} point, twelve operating points (including eight points near stall) are simulated by CFD for each set of the SA model coefficients, and a cubic spline is fitted through these points to represent the characteristic curve. An independent FCNN metamodel is trained and tested for each group of QoIs, and the details are summarized in Table 5.4. The *db3*, *db2* and *db1* are applied as the training, testing and cross-validation database, respectively.

Table 5.4: Details of metamodels for different quantities of interest of the NASA Rotor 67.

QoI Group	n_q	Outputs	Figure
Total pressure ratio	7	$\pi_{1t-2t}(m)$	5.30, 5.31, 5.33, 5.35
Isentropic efficiency	7	$\eta_{1t-2t}(m)$	5.30, 5.31, 5.33, 5.35
Blockage	1	L_b	5.30, 5.31, 5.36, 5.37
Stall	1	m_s/m_c	5.30, 5.31, 5.36, 5.37
Eddy viscosity	1	$\nu_t(x, y)$	5.38

5.5.2 Cross-Validation, Training and Test of FCNN

5.5.2.1 Hyperparameter Study

In this section, the effects of the FCNN hyperparameters on the prediction error of the NASA Rotor 67 case are studied. A parametric study of n_1 , ω , and λ has been conducted by changing one hyperparameter at a time while keeping the others at the baseline setting, which is $L = 1$, $n_1 = 0.5(n_x + n_q)$, $\omega = 2$ and $\lambda = 10^{-4}$. To avoid the training process falling into a local optimum, 8 FCNNs with different initial conditions are trained parallelly, and the best FCNN is chosen.

The prediction errors of FCNNs in various QoIs are plotted against each hyperparameter in Fig. 5.30. Using the FCNN model with the baseline hyperparameters, the errors in predicting all the QoIs are within 4% of the min-max QoI range (i.e., $\omega\epsilon < 4\%$). The prediction in normalized stall mass flow is the highest among all the QoIs. However, considering the min-max range of the normalized stall mass flow m_s/m_c is only about 0.06, the mean relative error of the FCNN is only 0.03%, which is sufficiently small for the metamodel purpose. Therefore, a deep FCNN (i.e., $L > 1$) is not pursued, and the baseline setting is adopted throughout this section.

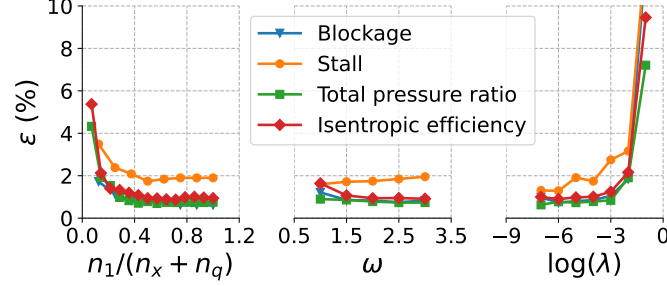


Figure 5.30: Hyperparametric study for the NASA Rotor 67 (training data: *db3*; cross-validation data: *db1*).

5.5.2.2 Training Data Independence Study

In this section, a training data independence study is performed using *db1*, *db2* and *db3* only; due to the high computation cost of the 3D compressor case, *db4* and *db5* are not available. The training and test databases are $db\{i\}$ and $db\{i - 1\}$ so that the ratio of training-to-test database size can be kept the same as 2. The difference between the test and training errors (i.e., ϵ_{te} and ϵ_{tr}) is plotted against the training database size in Fig. 5.31. Results show that the differences between ϵ_{te} and ϵ_{tr} are still decreasing with the training database size, indicating a training database larger than *db3* can improve the accuracy of the FCNN model further. However, the current FCNN model is already accurate enough for the metamodel purpose, which will be shown later in Sec. 5.5.2.3. Thus, a larger training database size is not pursued.

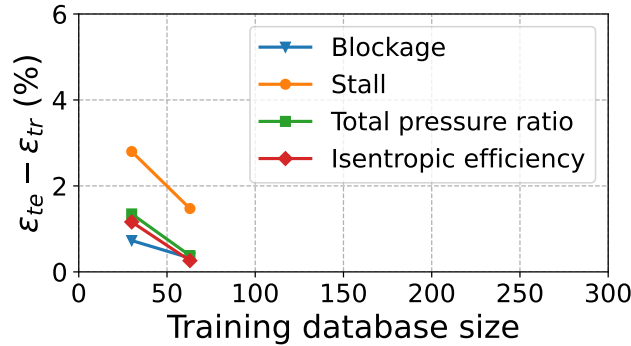


Figure 5.31: Training data independence study for the NASA Rotor 67 (training data: *db3*; cross-validation data: *db1*).

5.5.2.3 Training and Test Results

The training process and the test accuracy of the FCNN for predicting the normalized stall mass flow are presented in Fig. 5.32. In Fig. 5.32(a), the training and test cost functions are plotted against the optimization epochs, and convergence is achieved after around 1000 iterations. The corresponding prediction accuracy is shown in Fig. 5.32(b), where the normalized stall mass flow obtained from FCNN and CFD are plotted on the vertical and horizontal axis, respectively. The maximum absolute error of FCNN is 0.001, and the mean relative error is 0.03%. The error is sufficiently small and hence the metamodel is adequate for the purpose of UQ.

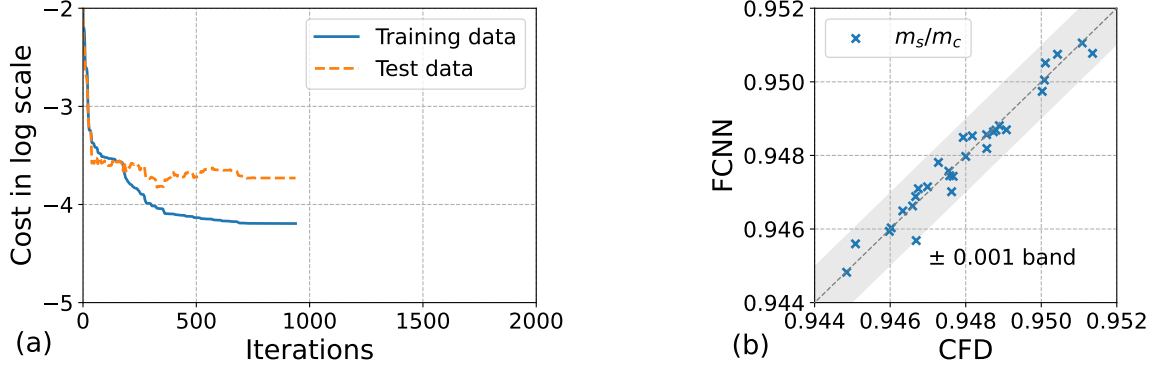


Figure 5.32: FCNN for predicting the normalized stall mass flow of the NASA Rotor 67 (training data: *db3*; testing data: *db2*).

5.5.3 Mean Flow Quantities

5.5.3.1 Performance Characteristics

The uncertainty in the characteristics of the NASA Rotor 67 is illustrated in Fig. 5.33. In these plots, all the CFD results are shown in solid lines, the min-max uncertainty bounds from the FCNN metamodel are represented by dashed lines, and the measured data [26, 165, 166] are presented by the open circles with error bars.

In Fig. 5.33(a), the uncertainty in the rotor total pressure ratio π_{1t-2t} is presented. It shows that the uncertainty bound of π_{1t-2t} slightly increases from 0.9% to 1.5% of its OSA value when throttling the compressor from the PE condition to the NS condition. This increased uncertainty originates from the enlarged tip blockage cell, as observed previously in Fig. 5.29. Another observation is that the measured data away from the stall condition can be enveloped by the uncertainty bound, but the measured π_{1t-2t} near stall is higher than all the CFD results. Consequently, the SA model with different model coefficients consistently under-predicts the stall margin.

In Fig. 5.33(b), the uncertainty in the rotor isentropic efficiency η_{1t-2t} is presented. It shows that the uncertainty bound of η_{1t-2t} increases slightly from 0.3% to 0.5% in absolute value when changing from the PE condition to the NS condition. The reason why the uncertainty in η_{1t-2t} has a similar value across the operating speed line is twofold. Firstly, a major part of the

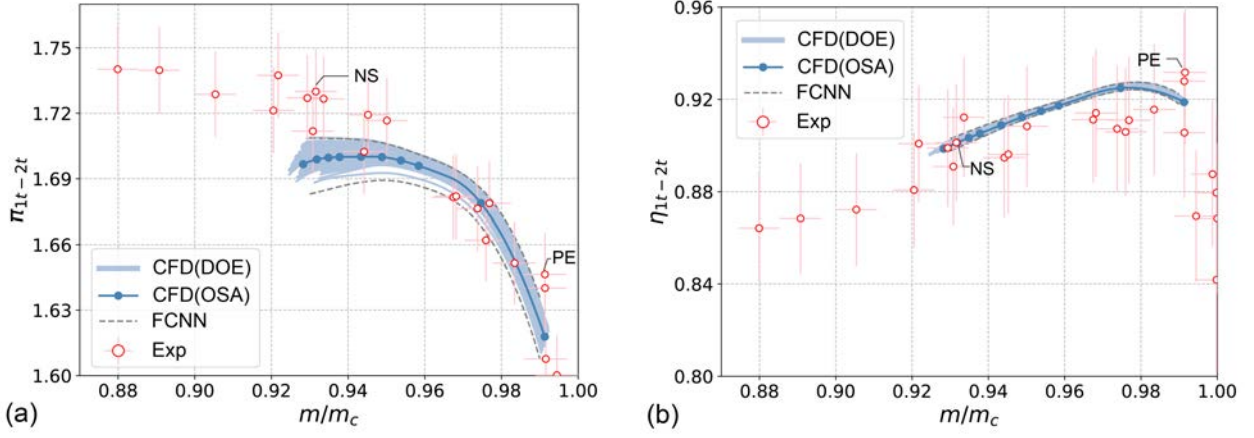


Figure 5.33: Uncertainty of predicted characteristics of NASA Rotor 67: (a) pressure ratio and (b) isentropic efficiency.

efficiency loss under all operating conditions comes from the skin friction on the blade surfaces and the endwalls. This loss is sensitive to the SA model coefficients that control the boundary layer log-law, as presented in the NACA 0012 airfoil case in Sec. 5.4.3.1. Secondly, there will always be mixing loss from 3D separated flows (e.g., tip leakage flow) inside a compressor blade passage regardless of the operating condition. This loss is also sensitive to the SA model coefficients, as demonstrated in the bump case and step cases in Sec. 5.3.3.3 and in the NACA 0012 airfoil case presented in Sec. 5.4.3.1.

To identify at which span the uncertainty is most pronounced, the rotor exit circumferentially-averaged radial profiles of the total pressure ratio, the total temperature ratio and the absolute flow angle are checked in Fig. 5.34. Here, the scatters represent the measured data [26], the solid curves denote the CFD results, and the colors in red and blue represent the PE and the NS conditions, respectively. At the PE condition, the uncertainty of the total pressure ratio mainly comes from the lower 10% span (i.e., the local minimum of total pressure), which corresponds to a hub corner separation. The uncertainty in the work input (i.e., total temperature ratio and flow angle) is almost uniform along the span. At the NS condition, a large uncertainty is observed near 90% span (i.e., the local minimum of total pressure), which corresponds to the tip blockage cell. The uncertainty in the work input is also higher near 90% span than elsewhere. Therefore, the increase in uncertainty when approaching stall is caused by the enlarged tip blockage cell.

The sensitivity analyses on predicting the total pressure ratio and the isentropic efficiency are presented in Fig. 5.35. In this plot, the normalized gradient of π_{1t-2t} is plotted against that of η_{1t-2t} for seven operating points, which are evenly spaced in the m/m_c range between 0.93 to 0.99. The coordinates of each point are the mean values of the normalized gradient over the investigated coefficient intervals, and the error bar represents the standard deviation. The farther away from the origin, the more sensitive the coefficient is.

In general, it is found that increasing σ , c_{v1} , c_{b1} , c_{w2} and c_{w3} or decreasing κ will lead to higher π_{1t-2t} and η_{1t-2t} , whereas the coefficient c_{b2} has negligible effects. Another observation is the U-shape of the gradient curves of some coefficients (indicated by the arrows¹). This is because the sensitivity is influenced by the severity of flow separation in the compressor blade

¹The two ends of the U-shape gradient curve of c_{b1} overlap with each other.

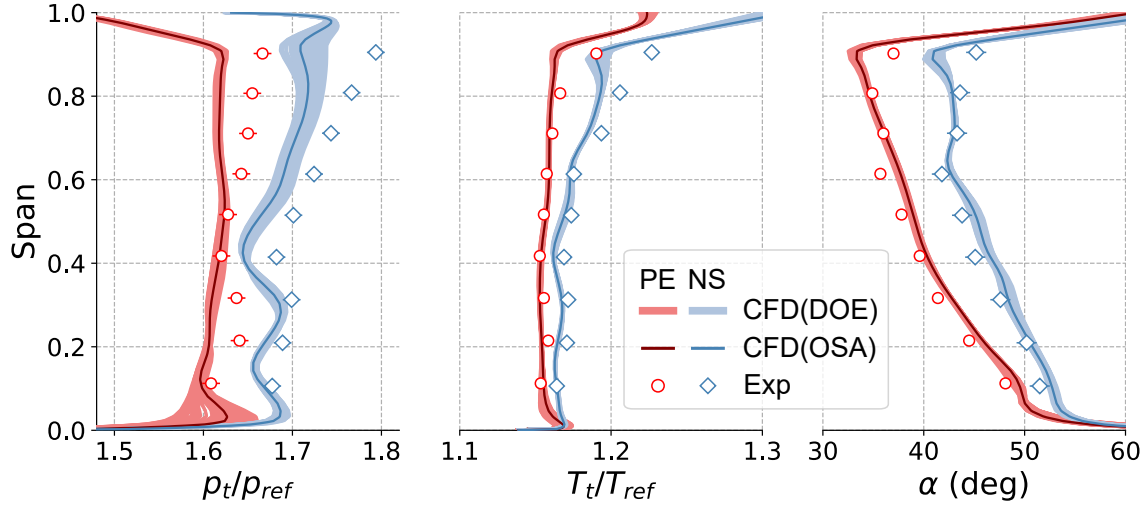


Figure 5.34: Uncertainty of predicted circumferentially averaged radial profiles at the exit of NASA Rotor 67 (peak efficiency: $m/m_c = 0.989 \pm 0.004$; near stall: $m/m_c = 0.924 \pm 0.004$).

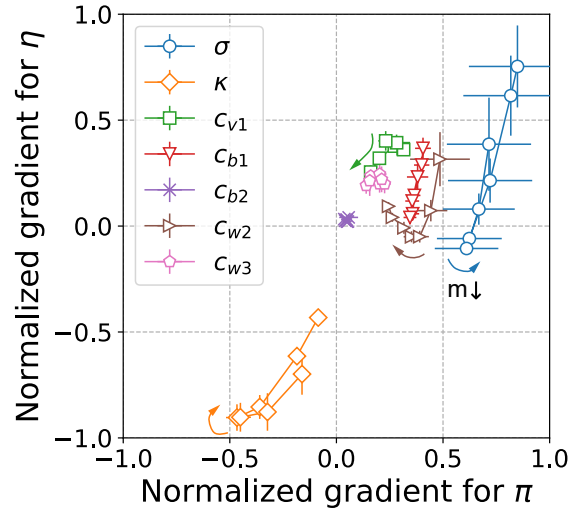


Figure 5.35: Sensitivity of predicted total pressure ratio and isentropic efficiency for the NASA Rotor 67.

passage. As the compressor is throttled from choke to stall, the incidence (i.e., AoA) decreases from a high negative value to zero first and then increases to a high positive value, leading to the reduction and then the increase of the separation size and hence the U-shape. Finally, when operating between the peak efficiency and stall condition, the gradient of π_{1t-2t} with respect to the coefficients σ and c_{b1} increases with the throttling process; for other coefficients, the gradient of π_{1t-2t} is nearly constant (e.g., c_{b2} and c_{w3}) or is decreased (e.g., c_{v1} and c_{w2}) or approaches zero (e.g., κ) during the throttling process. It implies that only coefficients σ and c_{b1} turn the slope of the pressure ratio characteristic curve more negatively near the stall condition and thus delay the stall inception.

Coefficients σ , c_{b1} and c_{w2} alter the characteristics mainly by changing the blockage size: increasing σ and c_{w2} reduces the turbulence destruction near the casing, and increasing c_{b1} enhances the turbulence production in the blockage zone, both of which increase the turbulence mixing in the blockage cell, reduces the blockage size and thus increases π_{1t-2t} and η_{1t-2t} . The

sensitivities of coefficients σ and c_{b1} increase during the throttling process from peak efficiency to stall, which is due to the increase of blockage size in the compressor blade passage. The sensitivity of coefficient c_{w2} , however, is reduced during this throttling process. This is because a higher value of c_{w2} will increase the turbulence destruction in the near-wall region with an adverse pressure gradient [44]; since the level of the adverse pressure gradient increases during the throttling process, this effect of c_{w2} becomes more prominent and thus the reduced sensitivity. Note the behavior of c_{w2} is different from the NACA 0012 airfoil in Sec. 5.4.3.1, where C_L is insensitive to c_{w2} . This is fundamentally caused by the different levels of pressure gradient in the flow field.

Coefficients κ and c_{v1} control the boundary layer log-law in attached flows: a lower κ or a higher c_{v1} delays the flow separation on the blade suction surface by increasing the turbulence intensity in the boundary layer, which should suppress the blockage size and increase both π_{1t-2t} and η_{1t-2t} as observed previously in the NACA 0012 airfoil in Sec. 5.4. However, this mechanism does not play a dominant role in compressor tip leakage flows where 3D flow separation always exists. In the separated flow regime, it is the turbulence intensity in the separation region that controls the blockage size and thus π_{1t-2t} and η_{1t-2t} . The net eddy viscosity source term related to κ and c_{v1} is $(f_{v2} - f_w)c_{b1}\hat{\nu}^2/\kappa^2d^2$. Recall from the discussions from Fig. 5.14 and Fig. 5.15: an increase in κ will increase the eddy viscosity since $f_{v2} - f_w < 0$ holds true for most of the flow region, which consequently leads to a reduced blockage size and an increased π_{1t-2t} and η_{1t-2t} ; c_{v1} is negatively correlated with f_{v2} and the eddy viscosity source term, and a reduction in c_{v1} will reduce the blockage size and increase π_{1t-2t} and η_{1t-2t} . The net effects of κ and c_{v1} are determined by the trade-off between the above two mechanisms. It is this trade-off effect that leads to the U-shape of its gradient curve.

5.5.3.2 Stall Mass Flow

The uncertainty of the SA model coefficients in predicting the stall mass flow is plotted against the uncertainty in the tip blockage size in Fig. 5.36. In the main plot, each scatter represents the result from one set of SA model coefficients, and the contour illustrates the occurrence probability predicted by the FCNN metamodel. In the top and the right plots, the distribution of samples is represented by the histogram, and the corresponding PDF is fitted using the kernel density estimation method [207] based on Gaussian kernels. It is found that the normalized stall mass flow ranges from 0.944 to 0.952, which is significantly higher than the measured data of 0.88. The OSA result is similar to the maximum likelihood estimation, indicating the original set of SA model coefficients well represents the coefficients within the investigated range. A positive correlation between the stall mass flow and the blockage size is also observed, which is consistent with the physical understanding of the spike-type stall inception.

The sensitivity analyses on predicting the stall mass flow and the tip blockage size are illustrated in Fig. 5.37, where the mean value and the standard deviation of the normalized gradient with respect to each coefficient are represented by bars and error bars, respectively. It is found that increasing coefficients σ , κ and c_{b1} can effectively reduce the blockage size, which is achieved by energizing the blockage cell as discussed in previous cases. However, since the enhanced skin friction due to the increased κ will cancel out its contribution to the reduced blockage size, the coefficient κ will have a neutral effect on the slope of the total pressure ratio characteristic curve. Thus, only the coefficients σ and c_{b1} have a significant effect on the

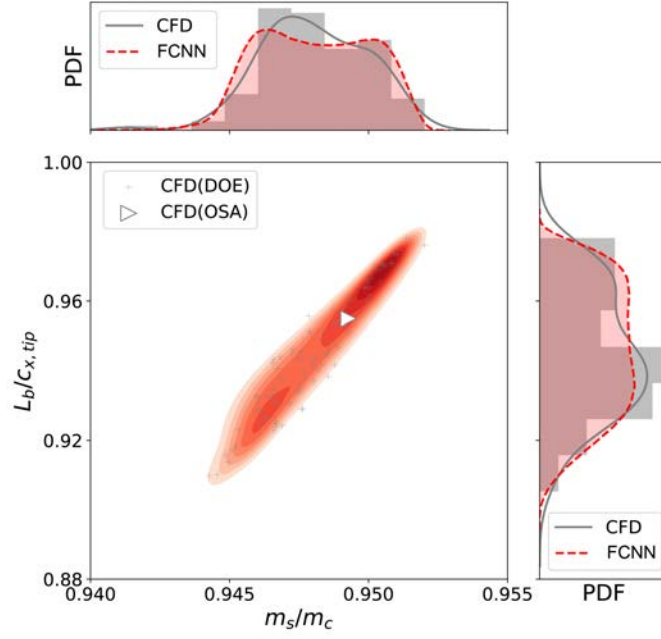


Figure 5.36: Uncertainty of predicted stall mass flow and tip blockage size at $m/m_c = 0.943$ of NASA Rotor 67 (scatters: samples from CFD; contours: occurrence probability of FCNN).

stall mass flow, which is consistent with the uncertainty analysis in the total pressure ratio characteristics in Sec. 5.5.3.1.

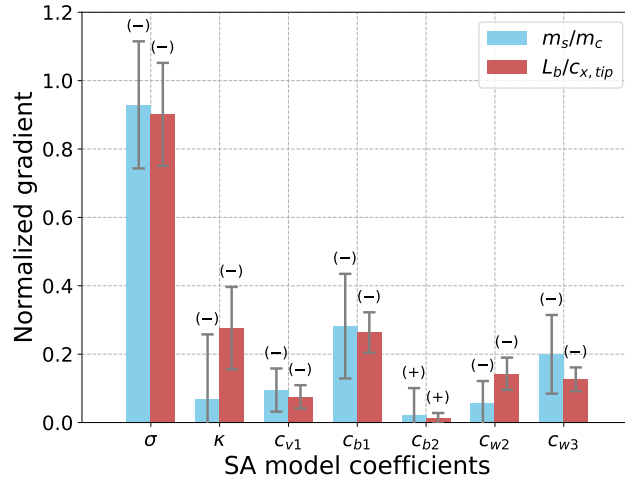


Figure 5.37: Sensitivity of predicted stall mass flow and tip blockage size at $m/m_c = 0.943$ for the NASA Rotor 67.

5.5.4 Turbulence Quantities

To check the effect of the SA model coefficients on predicting the eddy viscosity field, the gradient of the circumferentially-averaged eddy viscosity with respect to each coefficient is plotted as contours in Fig. 5.38. These contours are represented by around 13000 mesh points, and the gradient value at each mesh point is calculated by an independent FCNN model.

It is confirmed that either increasing one of the coefficients σ , κ , c_{b1} and c_{w2} or reducing the coefficient c_{v1} will increase the eddy viscosity in the separation region, which leads to a stronger turbulent mixing effect and thus a reduced blockage size.

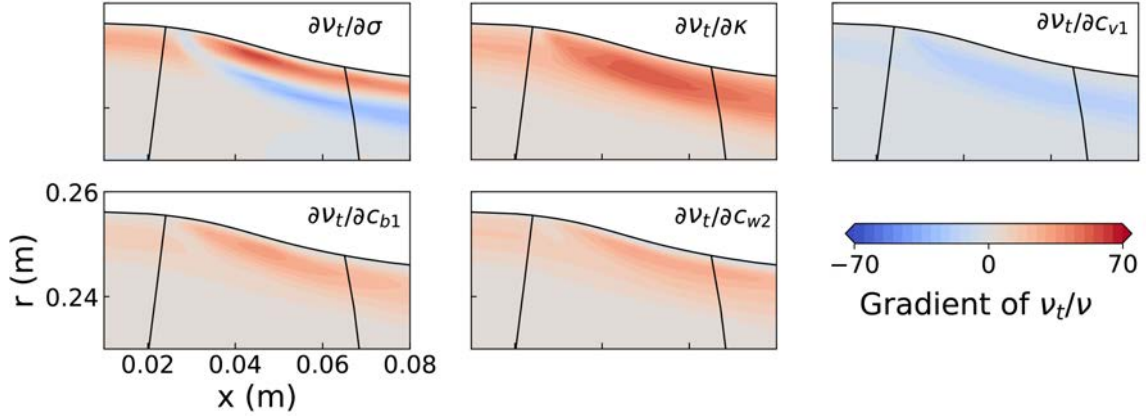


Figure 5.38: Sensitivity of predicted circumferentially-averaged eddy viscosity at $m/m_c = 0.943$ of NASA Rotor 67.

5.5.5 Correlation between Model Coefficients and Flow Fields

Based on the analysis in Sec. 5.5.3 and Sec. 5.5.4, there are two common coefficients that are sensitive to both the mean flow quantities and the turbulence quantities, namely σ and c_{b1} . The causal links between the model coefficients, the turbulence quantities and the mean flow quantities are summarized here in Fig. 5.39. Concretely, increasing σ or c_{b1} will increase the eddy viscosity in the blockage cell, which unblocks the compressor passage via a stronger turbulent mixing effect, increases both π_{1t-2t} and η_{1t-2t} , and eventually delays the stall onset.

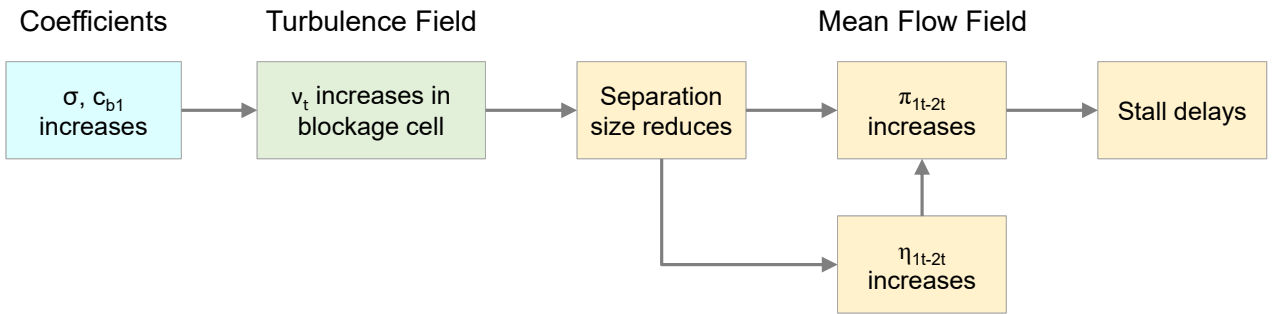


Figure 5.39: Illustration of causal links between the model coefficients, the turbulence quantities and the mean flow quantities for the NASA Rotor 67.

5.6 Concluding Remarks

In this chapter, a metamodel-based uncertainty quantification framework is presented. Using the established framework, the parametric uncertainty of the SA model coefficients is

quantified in the backward-facing step, the axisymmetric transonic bump, the NACA 0012 airfoil and the NASA Rotor 67 in ascending order of flow complexity.

In general, the SA model with different model coefficients can predict the attached flows (e.g., reattached boundary layer of the backward-facing step) and the mild separated flows (e.g., NACA 0012 and NASA Rotor 67 away from stall) with adequate accuracy, where the Hi-Fi data are enveloped by the uncertainty bounds. In flow regimes with shock or strong separation, however, the velocity profiles, the Reynolds shear stress profiles, the shock front, the separation size and the stall onset cannot be accurately predicted by the SA model, where the Hi-Fi data are often beyond the uncertainty bounds. Such results indicate the limitation of the SA model in predicting transonic and separated flows.

Among the SA model coefficients, σ and c_{b1} were found overall most influential in predicting all the cases studied. Specifically, increasing either σ or c_{b1} will increase the eddy viscosity/Reynolds shear stress, postpone the shock front, reduce the separation size, increase the lift coefficient/total pressure ratio and delay the onset of stall. Considering σ and c_{b1} are related to the turbulence destruction term and the turbulence production term, respectively, the significance of the source term is highlighted. For reference, the full sensitivity study results for the prediction of separation and stall are summarized in Table 5.5.

Table 5.5: Summary of Spalart-Allmaras turbulence model coefficients sensitivity for prediction of separation and stall.

Case	σ	κ	c_{v1}	c_{b1}	c_{b2}	c_{w2}	c_{w3}
Backward-facing step, separation	-0.46	-0.46	-0.01	-0.45	-0.05	-0.35	+0.50
Transonic bump, separation	-0.78	-0.37	-0.03	-0.27	-0.01	-0.39	+0.17
NACA 0012, NS, separation	-0.77	+0.07	-0.18	-0.43	-0.07	-0.40	+0.17
NASA Rotor 67, NS, blockage	-0.90	-0.28	-0.08	-0.26	+0.01	-0.14	-0.13
NACA 0012, stall margin	+0.78	-0.18	+0.16	+0.44	+0.05	+0.38	-0.01
NASA Rotor 67, stall margin	+0.93	+0.08	+0.10	+0.29	-0.00	+0.06	+0.20

Recalibration of the influential SA model coefficients is not helpful for compressor stall prediction. The reasons are twofold: firstly, when considering multiple QoIs across flow regimes, recalibration of the model coefficients leads to contradictory results (e.g., the shock front and the separation size of the axisymmetric transonic bump cannot be simultaneously predicted accurately by tuning the model coefficient); secondly, the uncertainty bounds of the stall onset of a compressor may not envelop the Hi-Fi data (e.g., the stall onset of NASA Rotor 67), and tuning the model coefficients alone cannot match with the Hi-Fi data. Such results suggest that the SA model formulation (i.e., either the constitutive relation, or the transport equation, or both) needs data-driven corrections, which will be pursued in the following chapters.

6. Evaluation of Turbulence Model Forms

“Absorb what is useful, reject what is useless, add what is essentially your own.”

— Bruce Lee, *Tao of Jeet Kune Do*

6.1 Introduction

In the parametric uncertainty quantification studies in Chapter 5, it was found that correcting the turbulence model coefficients alone is not sufficient for accurate compressor stall prediction, and modifications to the model formulations are required. In this chapter, established modified turbulence model forms at the constitutive relation level (Level 2) and the turbulence model transport equation level (Level 3) are evaluated for compressor stall prediction first. The outcome will unveil (1) whether corrections at Level 2 or Level 3 will be more promising; (2) what compressor flow features should be incorporated into the ML model.

This chapter is organized as follows. To begin with, the rationale and the formulation of established modified turbulence models will be introduced, followed by the evaluation of the modified models in predicting the blockage of canonical flows and the stall onset of NASA Rotor 67. Afterward, two novel modified turbulence models will be proposed, which improve the prediction in transonic flows and 3D separated flows by using a baroclinicity correction and a vortical pressure gradient correction, respectively. Lastly, conclusions will be drawn from all the evaluation and validation results.

6.2 Established Modifications of Spalart-Allmaras Turbulence Model

6.2.1 Modifications at Constitutive Relation Level

The SA model is based on the linear correlation of the Boussinesq assumption of Eq. (2.9), which is well established to be deficient in 3D and separated flows [49]. A more general constitutive relation can be formulated by a linear combination of ten basis tensors, whose coefficients are functions of five tensor invariants [101]. By using the leading two basis tensors, the quadratic constitutive relation (QCR) [50] is obtained in Eq. (6.1):

$$\tau_{QCR,ij} = \tau_{ij} - 2c_{cr1}\mu_t[O_{ik}S_{jk} + O_{jk}S_{ik}] \quad (6.1)$$

where the coefficient $c_{cr1} = 0.3$ was calibrated in the outer region of a simple boundary layer [50], and the additional terms are calculated as Eq. (6.2):

$$O_{ij} = 2W_{ij}/\sqrt{\frac{\partial u_m}{\partial x_n} \frac{\partial u_m}{\partial x_n}} \quad W_{ij} = \frac{1}{2}(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i}) \quad S_{ij} = \frac{1}{2}(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}) \quad (6.2)$$

Note that the trace of the additional Reynolds stress tensor is zero. Thus, the quadratic term does not change the turbulent kinetic energy budget but only redistributes it in space. When applied to the SA model, the SA-QCR model has demonstrated improved prediction accuracy in supersonic square duct [50], NASA junction [130] and LMFA NACA65 compressor cascade [211].

A more recent version of the QCR [212] takes into account the $-2/3\rho k\delta_{ij}$ term of the Boussinesq assumption, which is generally ignored when using with the SA model. This is achieved by modeling the turbulence kinetic energy k with Eq. (6.3):

$$k = \frac{3}{2}c_{cr2}\nu_t\sqrt{2W_{ij}W_{ij}} \quad (6.3)$$

where the coefficient $c_{cr2} = 2.5$. Although this version evidently improves the prediction of the Reynolds normal stress, its effects on the mean flow quantities are limited [130]. Thus, it is not used in this chapter.

6.2.2 Modifications at Transport Equation Level

The transport equation of the SA model is based on the assumption of equilibrium turbulence (i.e., production balances destruction), which holds true for zero pressure gradient flat plate flows but not for flows with a strong pressure gradient, a large curvature or separation. To tackle the deficiencies of the SA model in such flows, some modifications to the SA model transport equation have been proposed in previous research, including the rotation and curvature correction (i.e., SA-RC) [213], the helicity correction (i.e., SA-H) [214] and the pressure gradient correction (i.e., SA-PG) [215]. Among these modifications, the SA-RC model was inspired by first principles, where the rotation term is explicitly shown in the Reynolds shear stress transport equation; the SA-H and the SA-PG models were inspired by engineering experience, which is suitable for 3D swirling flows and adverse pressure gradient flows, respectively. Before evaluating these modifications for compressor stall prediction, their formulations are first introduced in the following. Unless stated elsewhere, all the flow variables are calculated in the reference frame attached to the blade (i.e., relative frame).

The SA-RC model considers that a strong shear enhances turbulence intensity whereas a strong rotation reduces it [216]. In addition, the effect of streamline curvature leads to an effective rotation rate, which can be treated in a similar fashion to the rotation effect. To incorporate the above features in the SA model, its production term is replaced by $c_{b1}(f_{r1} - f_{t2})\hat{S}$ where the f_{r1} function is defined in Eq. (6.4):

$$f_{r1}(r^*, \hat{r}) = (1 + c_{r1})\frac{2r^*}{1 + r^*}[1 - c_{r3}\tan^{-1}(c_{r2}\hat{r})] - c_{r1} \quad (6.4)$$

where the coefficient $c_{r1} = 1.0$ was calibrated in wingtip flows, and the coefficients $c_{r2} = 12$ and $c_{r3} = 1.0$ were calibrated in curved and rotating boundary layers [216]. Additional terms are

calculated as Eq. (6.5):

$$\begin{aligned}\hat{r} &= \frac{8\omega_{ik}S_{jk}}{(S^2 + \omega^2)^2} \left(\frac{DS_{ij}}{Dt} + (\epsilon_{imn}S_{jn} + \epsilon_{jmn}S_{in})\Omega'_m \right) \\ r^* &= S/\omega \\ \omega_{ij} &= W_{ij} + \epsilon_{mji}\Omega'_m\end{aligned}\tag{6.5}$$

with Ω'_m the rotating rate of the reference frame and ϵ_{mji} the Levi-Civita symbol. Note the original definition of r^* has a singularity at $\omega = 0$. To avoid this, a reference strain rate $\epsilon = u_{ref}/l_{ref}$ is usually added to both the denominator and the numerator of r^* , where u_{ref} and l_{ref} are characteristic velocity and length scale of the case¹. For pure shear flows, the production of eddy viscosity is enhanced since $r^* \rightarrow +\infty$, $\hat{r} = 0$ and thus $f_{r1} = 2 + c_{r1} > 1$. For pure rotation flows, the production of eddy viscosity is reduced because $r^* = 1/2$, $\hat{r} = 0$ and hence $f_{r1} = (2 - c_{r1})/3 < 1$.

The SA-RC model has demonstrated improved prediction accuracy in a range of 2D/3D rotating/curved channel flows [213], wake-type flows [217] and centrifugal compressor flows [218]. However, the f_{r1} term of the SA-RC has an abnormal behavior in a turbomachinery blade passage, which may deteriorate the prediction. A thought experiment to illustrate this deficiency can be performed on an inviscid round duct flow without swirl: by solving the problem in an axially rotating reference frame, $\omega = 0$ but $S \neq 0$, leading to $r^* \rightarrow +\infty$, $\hat{r} = 0$ and eventually $f_{r1} = 2 + c_{r1} > 1$. Such a behavior of the f_{r1} term will over-predict the eddy viscosity production.

The SA-H model tries to account for the transient effect of turbulence energy backscatter in helical flow region [219]. It multiplies the vorticity Ω in the modified strain rate term $\hat{S}$ by an empirical function $\beta_h(h)$:

$$\begin{aligned}\beta_h(h) &= 1 + c_{h1} \tanh(c_{h2}h^{c_{h3}}) \\ h &= \frac{|\Omega_i u_i|}{\Omega U}\end{aligned}\tag{6.6}$$

In Eq. (6.6), the form $c_{h1} \tanh(c_{h2}h^{c_{h3}})$ is used instead of the original proposal $c_{h1}h^{c_{h2}}$ so that an additional degree of freedom is available for calibration. For consistency with the original $\beta_h(h)$ function, the coefficients are calibrated as $c_{h1} = 0.71$, $c_{h2} = 2.0$ and $c_{h3} = 1.0$. An increase in helicity leads to a higher modified strain rate and thus increases the eddy viscosity source term. Since helicity in 2D flows is always zero², the modification has no effect on those flow cases.

The SA-PG model accounts for the observation that an adverse pressure gradient enhances turbulence whereas a favorable pressure gradient diminishes it [220]. Similar to the SA-H model, the vorticity Ω in the modified strain rate $\hat{S}$ is multiplied by an empirical function $\beta_p(\hat{p})$:

$$\begin{aligned}\beta_p(\hat{p}) &= \begin{cases} 1 + c_{p1} \tanh(c_{p2}\hat{p}^{c_{p3}}), & \text{if } \frac{\partial p}{\partial x_i} u_i \geq 0 \\ 1, & \text{otherwise} \end{cases} \\ \hat{p} &= \sqrt{\frac{\partial p}{\partial x_i} \frac{\partial p}{\partial x_i}} / \frac{\rho^2 U^3}{\mu Re_{ref}}\end{aligned}\tag{6.7}$$

¹ $u_{ref} = 100m/s$ and $l_{ref} = 1m$ are used for all cases studied in this work.

²In 2D flows, the vorticity vector is always perpendicular to the 2D plane and thus $|\Omega_i u_i| = 0$.

with $Re_{ref} = 10^6$ for better scaling. To avoid singularity at $U = 0$, U in the denominator is limited to be greater than $10^{-3}u_{ref}$. Compared to the original proposal of $\beta_p(\hat{p}) = c_{p1}\hat{p}^{c_{p3}}/(c_{p2} + \hat{p}^{c_{p3}})$ [215], the form $c_{p1} \tanh(c_{p2}\hat{p}^{c_{p3}})$ is adopted instead for better interpretations of the model coefficients. For consistency with the original $\beta_p(\hat{p})$ function, the coefficients are calibrated as $c_{p1} = 0.80$, $c_{p2} = 0.05$, $c_{p3} = 3.0$. Another difference is that the current β_p term only switches on when an adverse pressure gradient is detected, which is more physically justified.

Despite the engineering success of the SA-H model, SA-PG model and their combinations in predicting the stall margins of several aeroengine fans [221–223], they suffer from two drawbacks from the general perspective of turbulence modeling [224]:

- **Non-universality.** Both h and $\hat{p}$ do not enter the incompressible vorticity equation, indicating the turbulence production term should not respond to h and $\hat{p}$ in incompressible flows³. Therefore, these terms may only help specific types of flows but are non-universal. Specifically, h only measures the alignment between the velocity vector and the vorticity vector but not their magnitude. Thus, it is sufficiently large in a wide range of flows, but only a few of them need a boost in turbulence production. Likewise, $\hat{p}$ is also pronounced in a wide range of flows, but only a few need a correction accordingly.
- **Non-Galilean invariance.** The calculation of both h and $\hat{p}$ is dependent on the reference frame, which violates the Galilean invariance that the laws of motion are the same in all inertial frames. From a practical perspective, the lack of Galilean invariance should not confuse a turbomachinery flow solver because the reference frame is by convention set attached to the blade. However, at the rotor-stator interface, discontinuity of h , $\hat{p}$ and hence eddy viscosity will arise. Although the SA diffusion term can smooth out such a discontinuity, it should generally be avoided.

Lastly, there are two less-known variants of the SA model that reduces the destruction term. The first variant ignores the rotor casing wall in the wall distance calculation, and hence the turbulence destruction in the vicinity of the casing is reduced [223]. This variant allows aerodynamic/aeroelastic instability analysis at near-stall operating conditions, which are otherwise unachievable using the original SA model. However, it should be deprecated due to a lack of physical explanations. The second variant replaces the wall distance with an integral turbulence length scale [225], which is solved from a Hamilton-Jacobi differential equation with user-specified boundary conditions for tuning the desired length scale. This variant has shown some improvements in wake-type flows, but it needs post-hoc knowledge (e.g., separation location) to achieve good accuracy.

³Phenomenologically, turbulence is a range of vortices with different scales; the production of turbulence and vorticity are expected to resemble each other.

6.3 Evaluation of Established Modified Spalart-Allmaras Turbulence Models

6.3.1 Case Description

In this section, the established SA model forms are evaluated in selected canonical flows (i.e., the supersonic square duct, the axisymmetric transonic bump and the backward-facing step) and NASA Rotor 67.

The flow physics of the selected canonical flows resemble part of the compressor tip flow features, as justified in Sec. 3.4.1. Due to their simple configurations, there are abundant Hi-Fi experimental data [138–140, 143] and Lo-Fi RANS data [54] available for these cases, which are suitable for the validation and verification of the SA model forms. However, it should be emphasized that the selected canonical flows cannot fully represent the physics of compressor tip flow, which is featured by strong adverse pressure gradients and 3D swirls. Hence, an accurate prediction of these cases is necessary but may not be sufficient for the accurate prediction of compressor tip flow. Details of the CFD setups for all three cases have been summarized in Sec. 3.4.1.

The flow physics of NASA Rotor 67 is illustrated in Fig. 6.1, where the relative Mach number contours overlapped by the relative streamlines near the blade tip are shown. At the PE condition, a shock is formed at the suction surface near the trailing edge. Upstream of the shock, the pressure on the suction surface is reduced due to the supersonic expansion, which leads to an increased blade loading and thus an enhanced tip leakage flow. Downstream of the shock, the shock induces boundary layer separation. The interaction between the two flow structures downstream and upstream of the shock is limited. At the NS condition, the shock front moves further upstream, and the shock-enhanced tip leakage flow and the shock-induced separated flow interact with each other, which forms a tip leakage vortex that contributes to the blockage cell at the pressure surface-casing corner. It is the growth of this tip blockage cell that limits the compressor pressure rise capability and thus triggers stall. In the following evaluation, the main QoIs include the total pressure ratio π_{1t-2t} , the isentropic efficiency η_{1t-2t} , the blockage size L_b and the eddy viscosity ν_t . Details of the experimental data [26, 165, 166] and the CFD setups of NASA Rotor 67 have been introduced in Sec. 3.4.3.

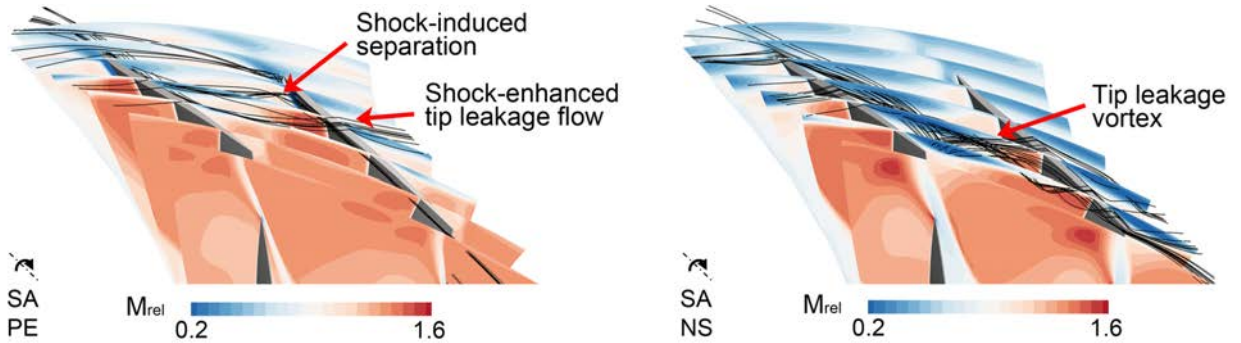


Figure 6.1: Contours of relative Mach number superimposed with relative streamlines near the tip region of the NASA Rotor 67 case.

6.3.2 Verification of Model Implementation

In the first place, the implementation of the SA-QCR model and the SA-RC model is verified against that in the established RANS flow solvers CFL3D and FUN3D [54]. In Fig.6.2(a), the predicted and measured skin friction distribution along the edge of the supersonic square duct are presented. It shows that the SA and SA-QCR predictions obtained from the in-house solver overlap with that from the established RANS solvers, which verifies the implementation of these SA models. It also shows that the SA-QCR model evidently outperforms the original SA model in this case. In Fig.6.2(b), the predicted and measured wall pressure coefficient of the axisymmetric bump are shown. Again, the SA model and the SA-RC model implemented in the in-house solver are verified against established solvers. Also, the SA-RC model predicts a more accurate shock front compared to that of the original SA model.

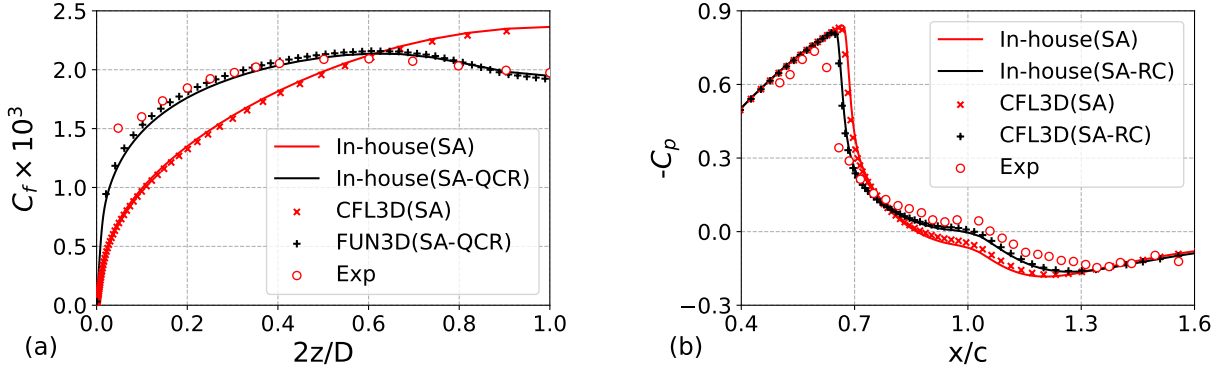


Figure 6.2: Validation and verification: (a) skin friction at $x/D = 50$ of the supersonic square duct; (b) wall pressure coefficient of the axisymmetric transonic bump.

6.3.3 Evaluation in Supersonic Square Duct

The flow feature of interest in the square duct flow is the endwall corner blockage. To compare the flow capacity predicted by different turbulence models, the axial velocity profiles are presented in Fig. 6.3(a). In this plot, the coordinates are normalized by the duct width D , and the axial velocity u is normalized by its value at the duct center line u_{CL} . For both velocity profiles along the wall-normal direction and the diagonal direction, the SA-QCR model matches reasonably well with the measured data. The other models all over-predict the endwall corner blockage since the predicted velocity near the corner is smaller than the measurements.

To quantify the endwall blockage, the blockage parameter B from Khalid et al. [226] is adopted, which is physically analogous to the momentum thickness of a boundary layer. In this context, B is calculated in Eq. (6.8):

$$B(x) = 1 - \int_0^D \int_0^D \frac{\rho(x)u(x)}{\rho_{CL}u_{CL}D^2} dydz \quad (6.8)$$

The streamwise distribution of B is shown in Fig. 6.3(b), where the experimental results are calculated from the averaged profile data of the wall-normal profile (lower bound) and the diagonal profile (upper bound) profile. It again shows that the SA-QCR model predicts a lower

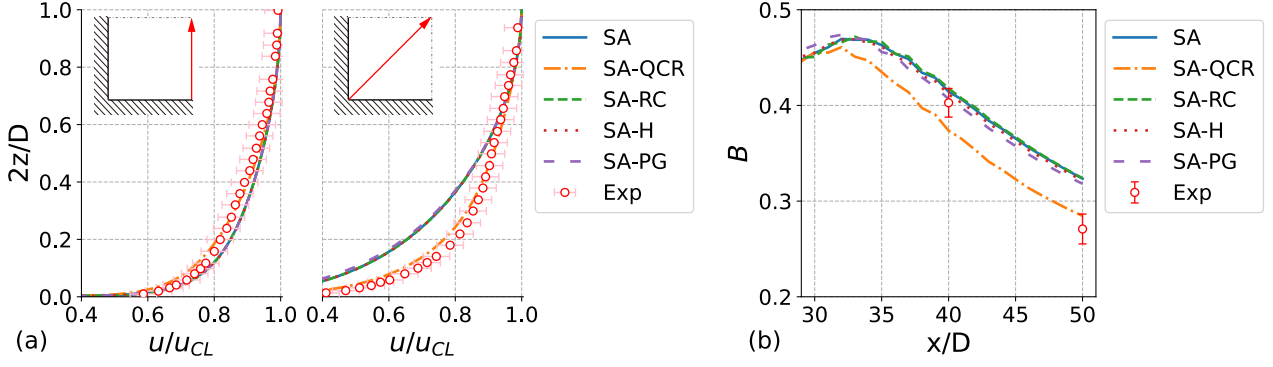


Figure 6.3: Profiles of supersonic square duct: (a) wall-normal and diagonal profiles of axial velocity at $x/D = 50$ and (b) streamwise distribution of blockage parameter.

blockage than the rest of the SA model modifications, which is closer to the measured data. Also, note in this case the blockage decreases with the streamwise flow development because of the supersonic inlet condition. For subsonic flow, the blockage should increase with the streamwise coordinates.

The endwall corner blockage is correlated with the strength of the secondary flow. Contours of velocity magnitude of secondary flow overlapped by the velocity vectors are presented in Fig. 6.4(a). It is observed that the secondary flow predicted by the original SA model is effectively zero, but a pair of secondary vortices is captured by the SA-QCR model. These vortices enhance the mixing between the endwall corner flow and the mainstream and thus reduce the local blockage. In Fig. 6.4(b), it is illustrated that the secondary flow is driven by the additional Reynolds shear stress (indicated by the arrows) generated by the quadratic term in Eq. (6.1). Hence, the non-linear component of the Reynolds shear stress is crucial for generating secondary flows in this case.

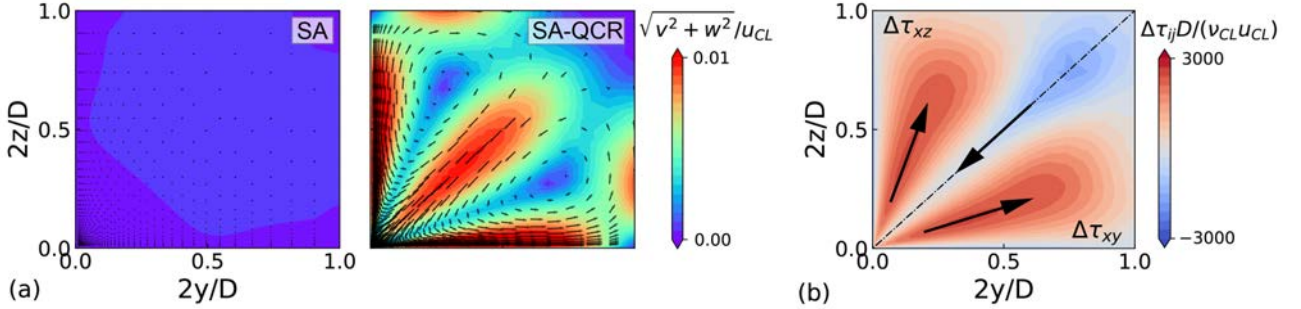


Figure 6.4: Contours of the supersonic square duct at $x/D = 50$: (a) secondary flow velocity magnitude and (b) additional Reynolds shear stress from the quadratic term.

6.3.4 Evaluation in Axisymmetric Transonic Bump

The flow feature of interest in the axisymmetric transonic bump is the shock-induced flow separation. To check the prediction accuracy of this phenomenon, the wall pressure coefficient distribution is examined in Fig. 6.5(a) first. Results show that all the SA models predict a delayed shock front compared to the measured data. The SA-QCR model and the SA-RC

model slightly improve the prediction accuracy, but the performance of the SA-PG model is worse than the original SA model.

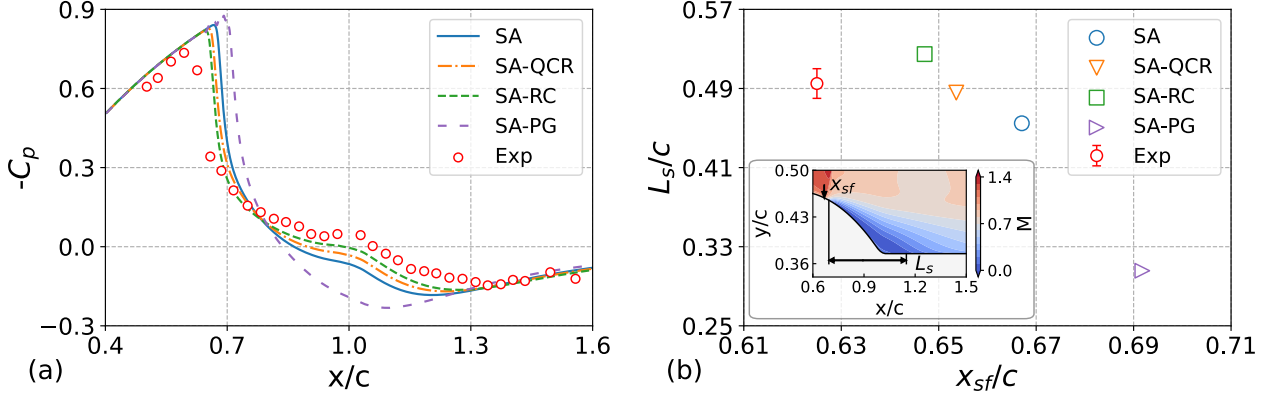


Figure 6.5: Shock in the axisymmetric bump: (a) wall pressure coefficient distribution and (b) shock front location versus separation size.

The shock-induced separation size L_s is plotted against the shock front location x_{sf} in Fig. 6.5(b). Here, the axial location of the peak wall pressure is defined as x_{sf} , and the axial distance between the separation and the reattachment points is defined as L_s , as illustrated in the Mach number contour plot obtained from the original SA model. Compared to the experimental result, the SA-RC model and the SA-QCR model predict the separation size reasonably well, but both of them predict a more downstream shock; meanwhile, the original SA model and the SA-PG model predict a further downstream shock front and thus a smaller separation size. The shock front location is physically related to the pre-shock boundary layer thickness: an enhanced near-wall turbulence intensity thickens the pre-shock boundary layer and thus delays the onset of the shock. Based on this flow mechanism, it is deduced that the SA-QCR model and the SA-RC model reduce the near-wall turbulent intensity, and the SA-PG model enhances it.

The additional Reynolds stress components from the quadratic term are presented in Fig. 6.6(a), which are calculated using the converged mean flow quantities from the SA-QCR model. It is confirmed that the SA-QCR model reduces the Reynolds normal stress τ_{xx} near the entire bump wall and the Reynolds shear stress τ_{xy} in the front half of the bump wall slightly. The net effect is a reduction in the streamwise Reynolds stress in the boundary layer. Thus, the SA-QCR model predicts an earlier shock front compared to the original SA model.

The eddy viscosity difference between the modified and the original SA model (i.e., $\Delta\nu_t = \nu_{t,mod} - \nu_t$) is illustrated in Fig. 6.6(b). Here, the eddy viscosity ν_t from the original SA model is obtained by only solving the transport equation of the turbulence model without updating the mean flow fields of velocity, pressure and temperature, which are frozen at the converged solution obtained by using the modified SA model. It is confirmed that the SA-RC model predicts lower near-wall eddy viscosity due to the convex curvature, whereas the SA-PG model predicts higher eddy viscosity due to the adverse pressure gradient. Thus, the SA-RC model predicts a more upstream shock, and the SA-PG model predicts a more downstream shock.

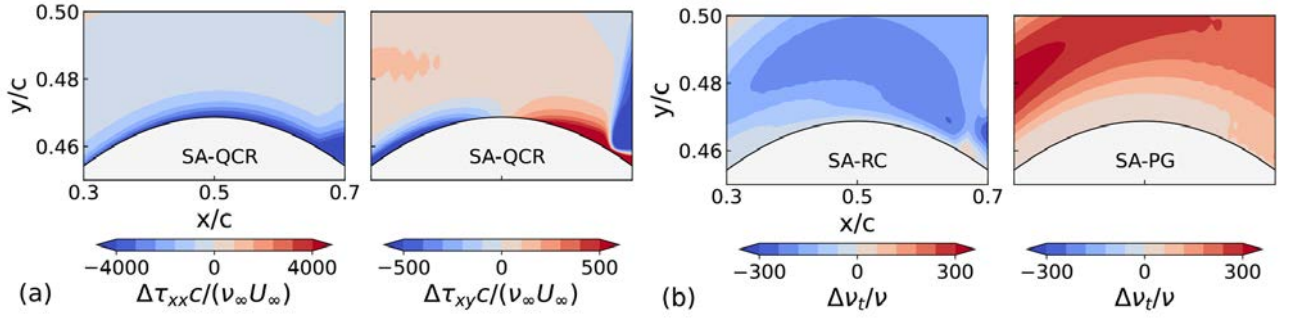


Figure 6.6: Contours of axisymmetric transonic bump: (a) additional Reynolds stress component from the quadratic term and (b) eddy viscosity difference.

6.3.5 Evaluation in Backward-Facing Step

The flow feature of interest in the backward-facing step is the geometry-induced separation. To help illustrate the flow physics, the contours of vorticity magnitude and the streamlines obtained from the original SA model are presented in the contour plot of Fig. 6.7. A strong shear layer indicated by high vorticity magnitude is formed immediately after the step, and a recirculation vortex is generated beneath the shear layer. Between the recirculation vortex and the endwall corner, a small corner vortex is also formed whose rotation direction is opposite to the recirculation vortex. To quantify the total blockage size L_s , the axial distance between the step location and the reattachment point of the recirculation vortex is used. This reattachment point can be found at the location where the skin friction equals zero.

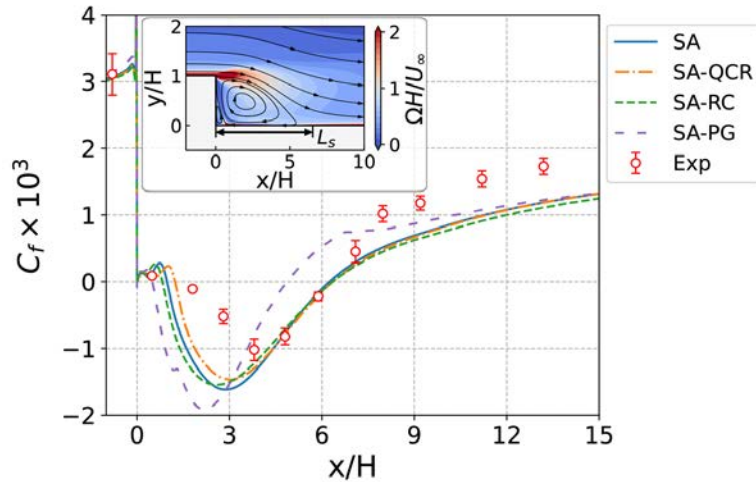


Figure 6.7: Skin friction coefficient distribution of the backward-facing step.

The skin friction coefficient distribution is shown in the line plot of Fig. 6.7. Regarding the blockage size, the SA-PG model predicts a smaller blockage size compared to the measured data, but all the other models predict the blockage size with reasonably good accuracy. The predicted locations of minimum skin friction by all the models are more upstream compared to the experimental data, and the skin friction after the reattachment point (i.e., $x/H > 7$) is under-predicted by all the models. A minor improvement in the distribution of skin friction in the recirculation zone is obtained by the SA-QCR model, whereas that is deteriorated by the SA-RC model and the SA-PG model.

The additional Reynolds stress components from the quadratic term are presented in Fig. 6.8(a), which are calculated using the converged mean flow quantities from the SA-QCR model. Results show that the SA-QCR model reduces the Reynolds normal stress τ_{xx} and increases the Reynolds shear stress τ_{xy} in the blockage region. The net effect is a reduced streamwise Reynolds stress (i.e., $\Delta\tau_{xx} + \Delta\tau_{xy} < 0$), which slightly squeezes the blockage cell in the axial direction as observed in Fig. 6.7.

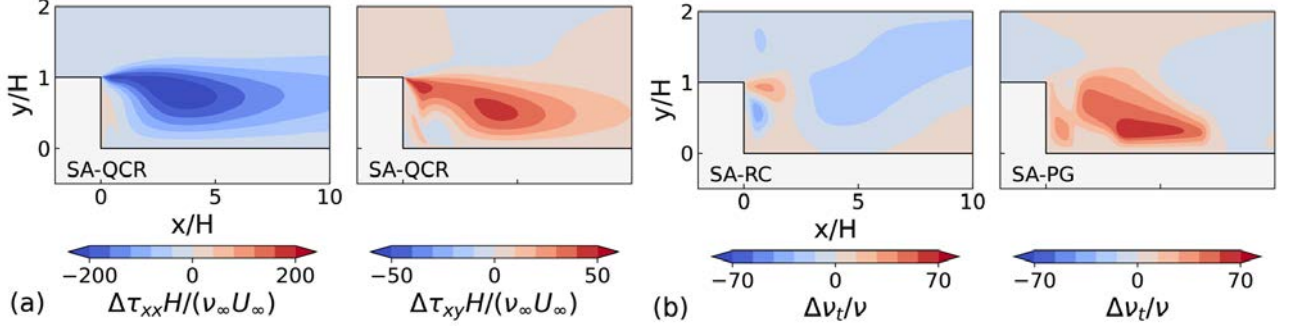


Figure 6.8: Contours of backward-facing step: (a) additional Reynolds stress component from the quadratic term and (b) eddy viscosity difference.

The eddy viscosity difference between the modified and the original SA model (i.e., $\Delta\nu_t = \nu_{t,mod} - \nu_t$) is illustrated in Fig. 6.8(b), where both $\nu_{t,mod}$ and ν_t are solved based on the mean flow field solutions from the modified SA model. Results show that the SA-RC model increases eddy viscosity in the shear layer and reduces it in the recirculation vortex featured by rotation and streamline curvature, which agrees with its design intention. However, the change of eddy viscosity by the RC correction is too small to affect the blockage size. The SA-PG model boosts eddy viscosity in regions with adverse pressure gradients, which enhances the turbulent mixing effect between the blockage cell and the main flow and thus reduces blockage size.

6.3.6 Evaluation in NASA Rotor 67

The performance characteristics of NASA Rotor 67 at the design speed are presented in Fig. 6.9. In these plots, the open circles with error bars are measured data [26, 165, 166], and the lines represent the results obtained by using different SA models.

For the pressure ratio characteristics presented in Fig. 6.9(a), the shape of the characteristic curves predicted by the SA, SA-QCR and SA-RC models are similar to each other, but they all predict stall prematurely compared to the measured data; the SA-H model predicts higher pressure ratio than all the other models at all mass flows, which matches well with the measured total pressure ratio at the NS condition but over-predicts it at the PE condition; the SA-PG model results show the best overall agreement with the measured data, although it still predicts an earlier stall onset than the experimental results. The variation range of the predicted total pressure ratio is about 3.0% and 2.4% of the measured data at the PE and the NS condition, respectively.

For the isentropic efficiency characteristics shown in Fig. 6.9(b), because of the large measurement uncertainty in the experiment, all the predicted characteristic curves fall within the measurement error bars and thus are considered reasonably accurate. Comparing the predicted

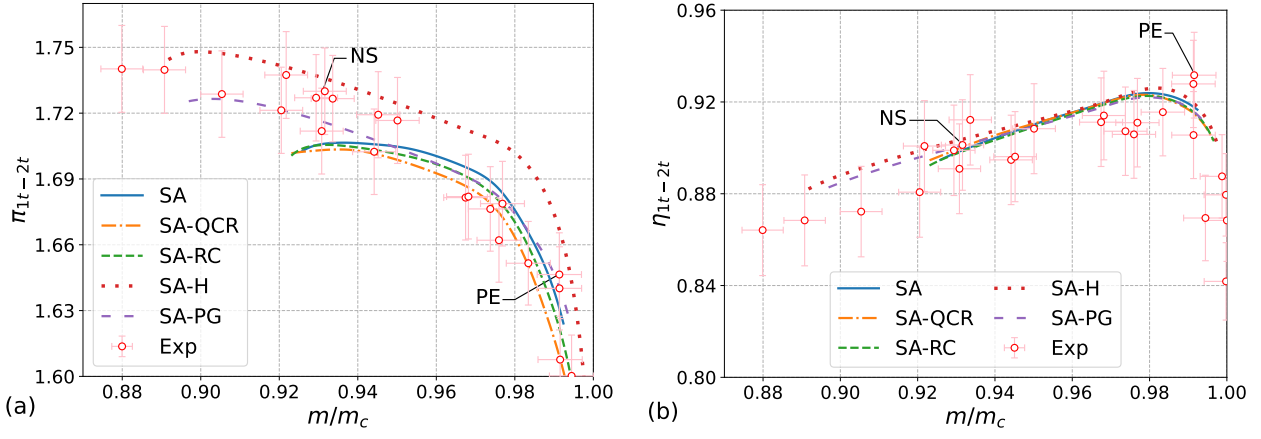


Figure 6.9: Performance characteristics of NASA Rotor 67 predicted by different SA model forms: (a) pressure ratio and (b) isentropic efficiency.

characteristic curves with each other, they are all similar in terms of the overall shape and the peak efficiency mass flow. The largest difference occurs near stall, where the variation range of efficiency is about 0.5% in absolute value at the NS condition of the experiment.

The circumferentially-averaged axial velocity contour is presented in Fig. 6.10(a). Here, the tip blockage cell is enveloped by the isoline of $u = 0$; the start and end locations of the tip blockage cell are denoted by $x_{b,s}$ and $x_{b,e}$, respectively; the size of tip blockage cell can be measured by its axial length $L_b = x_{b,e} - x_{b,s}$. At the last converged point predicted by the SA model (i.e., $m/m_c = 0.926$), the tip blockage cell extends from the LE to the TE, leading to the leading edge flow spillage and the trailing edge flow reversal and hence the onset of spike-type rotating stall [198]. At the last converged point predicted by the SA-H model (i.e., $m/m_c = 0.892$), the tip blockage cell only reaches the LE but not the TE. This scenario often occurs in cases where the chordwise distribution of leakage axial momentum is skewed towards the TE, and the casing corner separation is thus suppressed by the tip leakage flow [227]. The difference between the SA result and the SA-H result shows that the choice of the turbulence model can change the interpretation of the stalling mechanism.

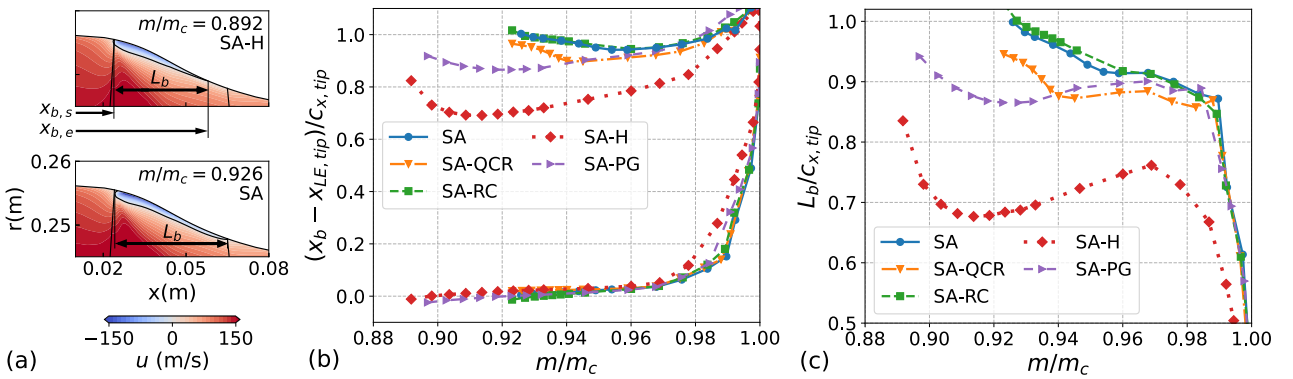


Figure 6.10: Blockage size of NASA Rotor 67 predicted by different SA model forms: (a) contours of circumferentially mass-weighted averaged axial velocity; (b) start and end locations of blockage versus mass flow rate; (c) blockage size versus mass flow rate.

In Fig. 6.10(b), $x_{b,s}$ and $x_{b,e}$ are plotted against the mass flow rate. When operating near

the choke condition, the tip blockage cell is partially outside the blade passage and its size is small. As the compressor is throttled towards stall, the tip blockage cell moves upstream in the blade passage and extends its size towards both the LE and the TE. The turbulence model has a more significant effect on $x_{b,e}$ than $x_{b,s}$, indicating the reversal of the tip leakage flow near TE is more susceptible than the spillage near LE.

In Fig. 6.10(c), L_b is plotted against the mass flow rate. It is illustrated that the SA-H model reduces the tip blockage size over the whole speed line, which explains its over-prediction in the pressure ratio near PE as shown in Fig. 6.9(a). In contrast, the SA-PG model and the SA-QCR model only reduce the tip blockage when approaching stall, which is favored for better prediction accuracy. No major difference in tip blockage prediction between the original SA model and the SA-RC model is found.

To check the effect of tip blockage on the downstream flow quantities, the circumferentially averaged radial profiles of total pressure, total temperature and absolute flow angle (measured from the axial direction) are presented in Fig. 6.11. Since both the total temperature and the absolute flow angle are positively correlated with the compressor work input, they are discussed together.

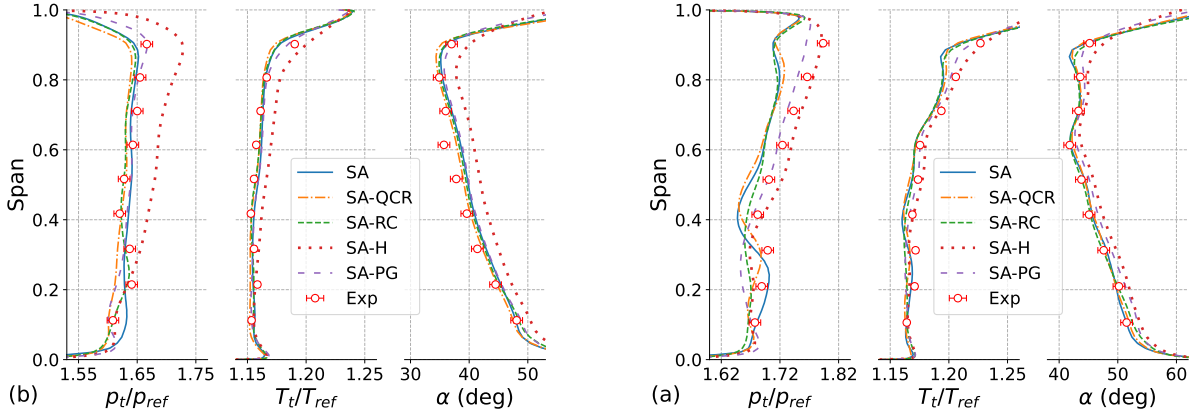


Figure 6.11: Circumferentially mass-weighted averaged radial profiles at the exit of NASA Rotor 67: (a) peak efficiency ($m/m_c = 0.989 \pm 0.004$); (b) near stall ($m/m_c = 0.924 \pm 0.004$).

For the measured PE condition shown in Fig. 6.11(a), the original SA model predicts slightly lower values of total pressure ratio and work input near the tip region, and the modified model SA-PG improves the overall prediction accuracy the most. The SA-H model predicts a higher pressure ratio and work input at almost the whole span. The SA-QCR and the SA-RC models predict a lower near-tip pressure ratio and work input.

For the measured NS condition shown in Fig. 6.11(b), pressure ratio and work input values from the SA, SA-QCR, and SA-RC models are significantly under-predicted near the tip region, indicating an over-predicted tip blockage size. In contrast, both the SA-H and the SA-PG models improve the prediction, and the SA-H model shows the closest agreement with measurements. These observations are consistent with the performance characteristics shown in Fig. 6.9(a).

To investigate the near-tip flow fields further, the circumferential profiles of relative Mach number and relative flow angle at 90% span of the rotor exit are presented in Fig. 6.12. In these

plots, the circumferential coordinates are normalized by the blade pitch, and the location at 100% pitch corresponds to the trailing edge of the blade. At the trailing edge location, a wake can be observed featured by a local minimum of relative Mach number and a local maximum of relative flow angle. As the measurement plane is immediately downstream of the blockage region, the change of streamline curvature around the blockage cell results in a local reduction in relative flow angle near the suction surface between 100% and 110% pitch.

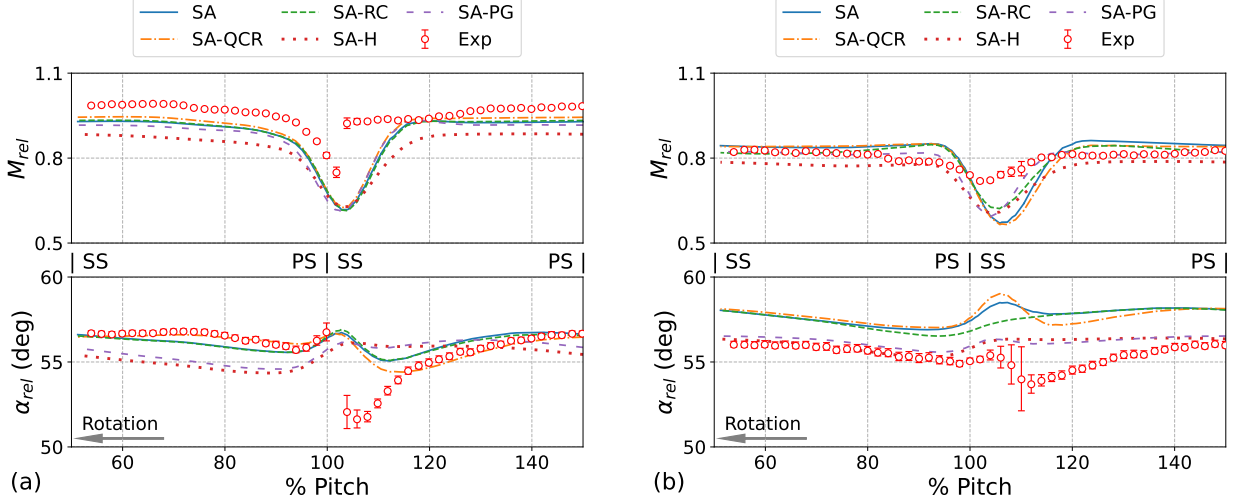


Figure 6.12: Circumferential profiles at 90% span and 24% chord downstream the trailing edge of NASA Rotor 67: (a) peak efficiency ($m/m_c = 0.989 \pm 0.004$); (b) near stall ($m/m_c = 0.924 \pm 0.004$).

For the measured PE condition shown in Fig. 6.12(a), the SA, SA-QCR, and SA-RC models predict qualitatively similar results to each other, and their predictions show adequate agreement with measurements. The SA-H and the SA-PG models predict a less steep change in the relative flow angle nearby the wake, which deviates from the measured data.

For the measured NS condition presented in Fig. 6.12(b), both the SA-H and the SA-PG models show adequate agreement with the measured relative flow angle, whereas the rest of the models overpredict the flow angle at the whole pitch. These results further demonstrate that the SA-H and SA-PG models help reduce the tip blockage size and thus reduce the overturning of the relative flow. The SA-QCR and SA-RC models, on the other hand, have negligible effects.

Finally, the eddy viscosity differences between the modified and the original SA model (i.e., $\Delta\nu_t = \nu_{t,mod} - \nu_t$) are examined in Fig. 6.13. The eddy viscosity field is determined by both the turbulence model and the mean flow fields of velocity, pressure and temperature. For a fair comparison between different turbulence models, the primary solutions are frozen at the converged solution from the modified SA model, and the eddy viscosity ν_t and $\nu_{t,mod}$ are obtained by only solving the transport equation of the turbulence model without updating the mean flow fields.

In general, the SA-H model has the largest influence on eddy viscosity, while the effects of the SA-PG model and the SA-RC model rank second and third.

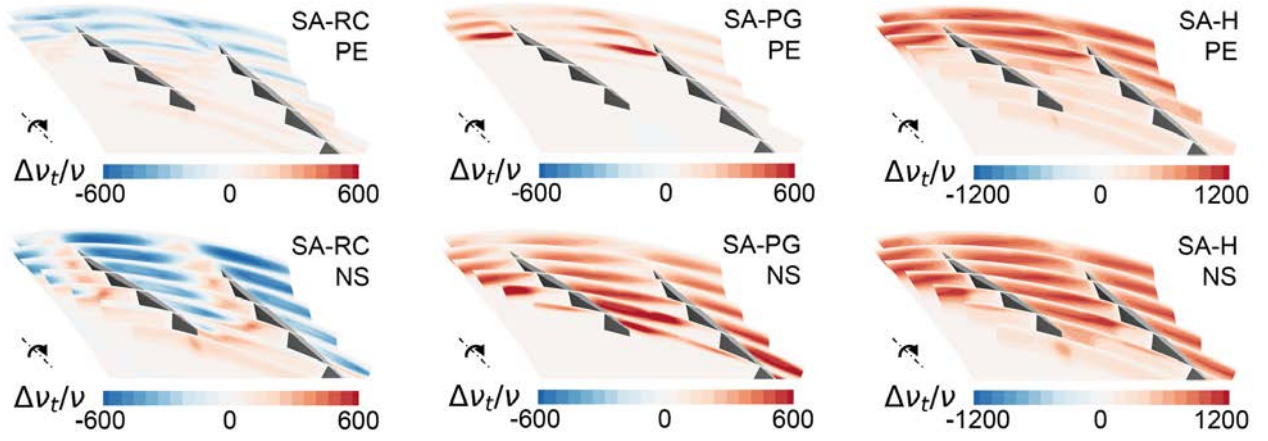


Figure 6.13: Contours of eddy viscosity difference between the modified SA models and the original SA model near the tip region of the NASA Rotor 67 case.

At the PE condition, the SA-RC model mainly reduces eddy viscosity in the wake region where the local rotation effect is strong, but little effect can be observed in the blade passage. The SA-PG model increases the eddy viscosity in the rear part of the blade passage corresponding to the location of the shock-induced separation. The SA-H model boosts eddy viscosity near the outer edge of the casing boundary layer. This region has a large relative helicity because the local vorticity generated by the relative motion of the casing wall is aligned with the local velocity vector. Besides, the eddy viscosity is further enhanced near the shock-enhanced tip leakage flow region where both the relative helicity and the vorticity magnitude are large.

At the NS condition, the SA-RC model reduces the eddy viscosity slightly in the trajectory of the tip leakage vortex but increases the eddy viscosity in the other parts of the tip region where the effect of shear between the main flow and the tip leakage flow is more significant than the effect of rotation. The SA-PG model still enhances the eddy viscosity in the vicinity of the passage shock, but its effect at the NS condition is larger than the PE condition due to the increased magnitude of the adverse pressure gradient. The results of the SA-H model show a similar level of increment in eddy viscosity to those at the PE condition, but the affected region moves more upstream with the trajectory of the shock-induced tip leakage vortex.

6.3.7 Summary of Model Form Evaluation

The effects of different SA model forms on the prediction accuracy of the investigated flows are summarized in Table 6.1. The original SA model predicts a larger blockage size in the supersonic square duct, a further downstream shock front in the axisymmetric transonic bump, a different shape of separation bubble in the backward-facing step and a larger tip blockage size in the NS flows of NASA Rotor 67. The SA-QCR and the SA-RC models generally improve the prediction accuracy in some canonical flows, but they have nearly neutral effects on the compressor flows. The SA-H and the SA-PG models improve the prediction accuracy on the NS flows of NASA Rotor 67, but they deteriorate the prediction on the PE flows of NASA Rotor 67 and some canonical flows, respectively.

The above results show a clear gap between the predictions of canonical flows and industrial flows—it is difficult to improve one end accurately without deteriorating another. Regarding applications to compressor flows, established turbulence model modifications at Level 3 (i.e.,

Table 6.1: Summary of evaluation of Spalart-Allmaras turbulence model forms.

Case	SA-QCR	SA-RC	SA-H	SA-PG
Supersonic Square Duct	Improved	Neutral	Neutral	Neutral
Axisymmetric Transonic Bump	Improved	Improved	Neutral	Deteriorated
Backward-Facing Step	Neutral	Neutral	Neutral	Deteriorated
NASA Rotor 67, PE	Neutral	Neutral	Deteriorated	Neutral
NASA Rotor 67, NS	Neutral	Neutral	Improved	Improved

transport equation level) are generally more effective than that at Level 2 (i.e., constitutive relation level). In the following sections, two novel modified SA model forms at Level 3 will be proposed to improve the prediction accuracy of the canonical flows and the compressor flows.

6.4 Proposal of Baroclinicity Modification

6.4.1 Model Formulation

The pressure gradient is a common flow feature in both canonical and industrial flows, but its usage in RANS turbulence modeling is generally disfavored because it does not enter the vorticity equation for incompressible flows [224]. In searching for a flow feature that incorporates the pressure gradient effect, the vorticity equations for incompressible and compressible flows [228] are examined in Eq. (6.9) and Eq. (6.10), respectively:

$$\frac{\partial \omega_i}{\partial t} + u_j \frac{\partial \omega_i}{\partial x_j} = \omega_j \frac{\partial u_i}{\partial x_j} + \epsilon_{ijk} \frac{\partial}{\partial x_j} \left(\frac{1}{\rho} \frac{\partial \tau_{kl}}{\partial x_l} \right) \quad (\text{incompressible}) \quad (6.9)$$

$$\frac{\partial \omega_i}{\partial t} + u_j \frac{\partial \omega_i}{\partial x_j} = \omega_j \frac{\partial u_i}{\partial x_j} + \epsilon_{ijk} \frac{\partial}{\partial x_j} \left(\frac{1}{\rho} \frac{\partial \tau_{kl}}{\partial x_l} \right) - \omega_i \frac{\partial u_j}{\partial x_j} + \epsilon_{ijk} \frac{1}{\rho^2} \frac{\partial \rho}{\partial x_j} \frac{\partial p}{\partial x_k} \quad (\text{compressible}) \quad (6.10)$$

In both equations, the vorticity source terms are written on the right-hand side. Specifically, the first term denotes the vortex stretching due to the velocity gradient, and the second term describes the vorticity diffusion due to the viscous effects. For the compressible vorticity equation, additional two terms arise: the third term denotes the vortex stretching due to flow compressibility, and the fourth term is the baroclinicity b_i , which comes from the interaction between the pressure gradient and the density gradient. The physics of the third term has been considered in previous modifications of the SA model (i.e., SA-comp) [229], but that of the fourth term, to the best knowledge of the author, has not yet been considered in eddy viscosity-based RANS turbulence models.

To help explain how the baroclinicity increases the vorticity production in the same direction, an illustrative diagram inspired by Thorne and Blandford [228] is presented in Fig. 6.14. In this example, a fluid particle is located in a flow field where the pressure gradient and the density gradient are orthogonal to each other, leading to a baroclinicity component pointing inward of the plane. The net pressure force acting on the fluid particle passes through its geometric center but not the center of mass. Therefore, a clockwise torque is generated, which produces a vorticity component also pointing inward of the plane.

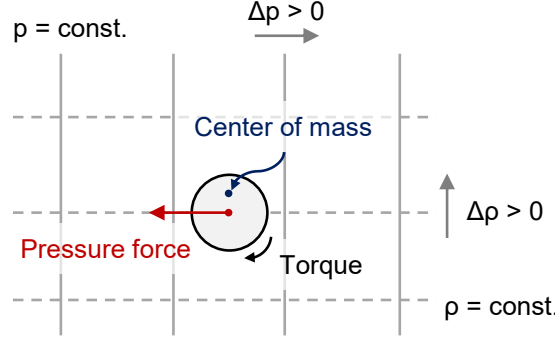


Figure 6.14: Mechanism of the baroclinicity term on changing the source of vorticity.

To examine the effects of baroclinicity on the Reynolds stress source terms, the transport equation of the Reynolds stress tensor for incompressible flows [49] and compressible flows [230] are presented symbolically (for simplicity) in Eq. (6.11) and Eq. (6.12), respectively:

$$\frac{\partial \tau_{ij}}{\partial t} + \frac{\partial(\tau_{ij} \bar{u}_k)}{\partial x_k} = \frac{\partial T_{ijk}}{\partial x_k} + P_{ij} - D_{ij} + \Pi_{ij} \quad (\text{incompressible}) \quad (6.11)$$

$$\frac{\partial \tau_{ij}}{\partial t} + \frac{\partial(\tau_{ij} \tilde{u}_k)}{\partial x_k} = \frac{\partial T_{ijk}}{\partial x_k} + P_{ij} - D_{ij} + \Pi_{ij} + M_{ij} \quad (\text{compressible}) \quad (6.12)$$

where $(\bar{\cdot})$ and $(\tilde{\cdot})$ denote the Reynolds-average and the Favré-average, respectively; T_{ijk} , P_{ij} , D_{ij} and Π_{ij} of both equations denote the diffusion term, the shear production term, the viscous dissipation term and the pressure-strain covariance term, respectively; the additional term M_{ij} of the compressible Reynolds stress transport equation describes the pressure acceleration, which writes in Eq. (6.13):

$$M_{ij} = -\overline{u_i''} \frac{\partial \bar{p}}{\partial x_j} - \overline{u_j''} \frac{\partial \bar{p}}{\partial x_i} \quad (6.13)$$

In this equation, the density fluctuation effect is reflected by the mass flux term $\overline{\rho u_i''} = -\overline{\rho' u_i'} \neq 0$ with $(\cdot)'$ and $(\cdot)''$ denoting the fluctuation part of Reynolds-average and the Favré-average, respectively. To close the M_{ij} term, previous research has proposed an algebraic model for the mass flux term $\overline{\rho u_i''}$ based on its transport equation, and the leading order terms were found proportional to the baroclinicity components [230].

From the rationales introduced above, the baroclinicity term b_i can affect the strength of Reynolds shear stress components differently, thereby changing the turbulence anisotropy. To fit into the established framework of eddy viscosity models, this research adopts the baroclinicity term to tune the source term of eddy viscosity only, and the constitutive relation that controls turbulence anisotropy is kept unchanged. This is achieved by projecting the baroclinicity to the vorticity direction, as written in Eq. (6.14):

$$b_\omega = \frac{b_i \omega_i}{\Omega}, \quad b_i = \epsilon_{ijk} \frac{1}{\rho^2} \frac{\partial \rho}{\partial x_j} \frac{\partial p}{\partial x_k} \quad (6.14)$$

The vortical baroclinicity b_ω measures the baroclinicity-induced vorticity production in the vorticity direction. Therefore, a positive b_ω will enhance the vorticity magnitude and potentially increase eddy viscosity, and vice versa.

The vortical baroclinicity b_ω has dimensions of $[T^{-2}]$, which needs to be non-dimensionalized

before entering the transport equation of eddy viscosity. Ideal terms for non-dimensionalization should be composed of mean flow quantities, be Galilean invariant and have dimensions of $[T^{-1}]$. This limits the choice to:

- (1) the Frobenius norm of the velocity gradient tensor $\sqrt{\partial_{x_j} u_i \partial_{x_j} u_i}$;
- (2) the magnitude of vorticity Ω ;
- (3) the magnitude of strain rate S ;
- (4) the combination of local speed of sound and laminar viscosity a^2/ν .

Among terms (1), (2) and (3) that carry similar information on velocity gradient, the magnitude of vorticity Ω is picked because b_ω/Ω has a physical meaning of relative vorticity production rate; term (4) incorporates additional flow physics of compressibility and viscosity than the other terms and thus is also picked. Therefore, the final dimensionless vortical baroclinicity $\hat{b}_\omega$ is written as Eq. (6.15):

$$\hat{b}_\omega = \frac{b_\omega}{\Omega} \frac{\nu}{a^2} C_{ref} \quad (6.15)$$

where $C_{ref} = 10^6$ is a constant for better scaling. To avoid division by zero, Ω in the denominator of Eq. (6.14) and Eq. (6.15) is limited to be greater than u_{ref}/l_{ref} .

Lastly, the dimensionless vortical baroclinicity is used to tune the eddy viscosity source terms of the original SA model. This is achieved by multiplying the modified strain rate $\hat{S}$ with the $\beta_{b\omega}$ function of Eq. (6.16):

$$\beta_{b\omega}(\hat{b}_\omega) = \begin{cases} 1 + c_{b\omega 1p} \tanh(c_{b\omega 2} |\hat{b}_\omega|^{c_{b\omega 3}}), & \text{if } \hat{b}_\omega \geq 0 \\ 1 + c_{b\omega 1n} \tanh(c_{b\omega 2} |\hat{b}_\omega|^{c_{b\omega 3}}), & \text{if } \hat{b}_\omega < 0 \end{cases} \quad (6.16)$$

where $c_{b\omega 1p}$, $c_{b\omega 1n}$, $c_{b\omega 2}$ and $c_{b\omega 3}$ are coefficients to be calibrated. Specifically, coefficients $c_{b\omega 1p}$ and $c_{b\omega 1n}$ determine the min-max values of the $\beta_{b\omega}$ function, which is expected to be $\beta_{b\omega} \geq 1$ (i.e., eddy viscosity boost) in the positive $\hat{b}_\omega$ branch and $0 < \beta_{b\omega} \leq 1$ (i.e., eddy viscosity reduction) in the negative $\hat{b}_\omega$ branch according to the rationale introduced before; coefficients $c_{b\omega 2}$ and $c_{b\omega 3}$ determine the transitional shape of the $\beta_{b\omega}$ function and are of secondary importance. Throughout this work, the new model is termed as SA-B.

6.4.2 Calibration of Model Coefficient by Global Optimization

The SA-B model coefficients are calibrated via a global optimization framework using wall pressure data of 2D transonic flows. Because the measurement uncertainty of such data is small, the calibration will be performed in a deterministic manner. In the following, details of the calibration framework and the calibration result will be introduced.

6.4.2.1 Calibration Framework

The calibration framework is a metamodel-based gradient-driven optimization framework, as illustrated in Fig. 6.15. It is essentially composed of two modules: a metamodel module and a gradient-driven optimizer module.

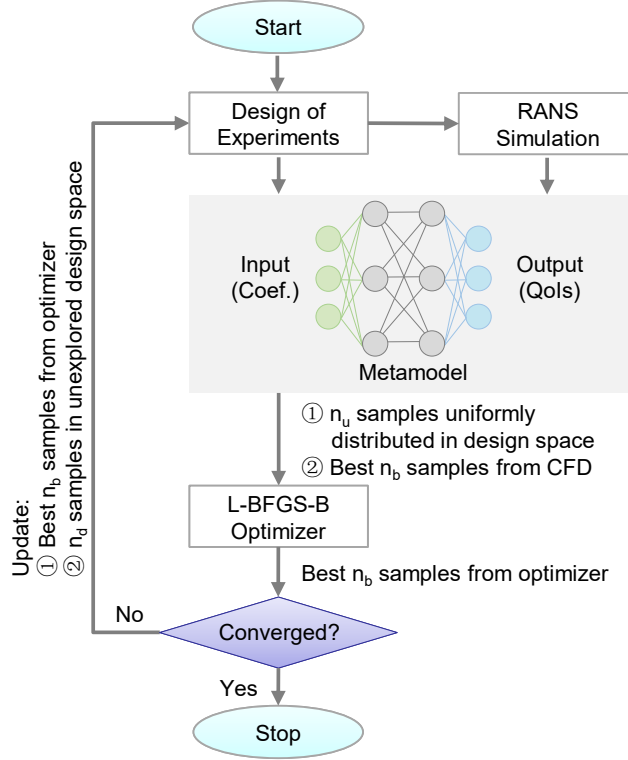


Figure 6.15: Framework of global optimization for SA-B coefficients calibration.

The metamodel module starts with the design of experiments (DOE) to generate a database of n_i samples of coefficients, whose prediction accuracy is evaluated by RANS simulations. The database is then used to train a metamodel of the RANS solver, which constructs an explicit functional mapping between the model coefficients and the prescribed objective function (i.e., a function that measures the prediction accuracy). The metamodel can then be used to calculate the gradient of the objective function with respect to each coefficient, which can be used by a gradient-driven optimizer to optimize the coefficients.

The gradient-driven optimizer module is based on the L-BFGS-B algorithm [135]. This algorithm will be performed $n_u + n_b$ times, with n_u times using the n_u samples of coefficients uniformly distributed in the design space as the initial conditions and n_b times using the best n_b samples of coefficients from the CFD database as the initial conditions. After the $n_u + n_b$ times of optimization runs, the best n_b samples will be chosen and verified by RANS simulations. The choice of n_u and n_b should consider the trade-off between efficacy and cost: higher values of n_u and n_b increase the chance of obtaining the global optimum, but they also require more numerical resources.

The efficacy of the optimization framework is highly dependent on the accuracy of the metamodel. A straightforward way to increase the metamodel accuracy is to increase n_i in the design of experiments, but this significantly increases the calculation cost since each sample of coefficients needs to be evaluated by RANS simulations. Alternatively, the training database size can be increased iteratively: at the end of each iteration, the best n_b samples found by the optimizer and an updated DOE database with n_d samples will be included for training the FCNN in the next iteration. The updated DOE database is initially generated using the same method as the first DOE database (i.e., including n_i samples). Samples in the updated database are then filtered by their objective function values lower than the 25% percentile of the existing

database and sorted by the shortest Euclidean distances between the current sample and any samples in the existing database. The leading n_d samples will thus be picked, representing high-potential but unexplored regions in the design space.

Finally, the optimization loop will terminate if the objective function (i.e., prediction accuracy) of the best coefficient set does not change with further iterations. The best coefficients verified by RANS simulations will be used as the final calibrated coefficients.

6.4.2.2 Application to SA-B Model Coefficients Calibration

The parameters of the optimization framework used for the SA-B model coefficients calibration are summarized in Table 6.2. Detailed explanations are as follows.

Table 6.2: Parameters of the optimization framework for SA-B model coefficients calibration.

Calibration data							
Case				Variable		n_q	
Transonic bump & RAE 2822				Integrated C_p error		2	

Coefficient range				Parameters			
$C_{b\omega 1p}$	$C_{b\omega 1n}$	$C_{b\omega 2}$	$C_{b\omega 3}$	n_i	n_u	n_b	n_d
[0.00, 0.50]	[-1.00, -0.50]	[10, 1000]	[0.1, 10.0]	1000	256	20	40

The data used for calibration are the wall pressure coefficient C_p of the axisymmetric transonic bump at $M_\infty = 0.875$ and $Re_c = 2.73 \times 10^6$ [139] and the RAE 2822 airfoil at $AoA = 2.80deg$, $M_\infty = 0.750$ and $Re_c = 6.2 \times 10^6$ (i.e., case 10 condition [147]). The measurement uncertainties of these quasi-2D configurations are usually small (e.g., $\Delta C_p = \pm 0.0026$ for the RAE 2822 airfoil) and thus are not considered in the calibration. More details of the test cases and their CFD setups have been introduced in Sec. 3.4.1 and Sec. 3.4.2. The baseline turbulence model during the calibration process is $SA - QCR - B$, where the QCR correction at Level 2 is also turned on since it has shown some improvements over the original SA model in predicting the bump flow (see Sec. 6.3.5).

To measure the prediction error, the absolute pressure coefficient error integrated over the suction surface is adopted, which writes as Eq. (6.17):

$$\epsilon = \int_{x_{min}}^{x_{max}} |C_{p,exp} - C_{p,CFD}| dx/c \quad (6.17)$$

where $x_{min}/c = 0.50$, $x_{max}/c = 1.50$ for the axisymmetric transonic bump and $x_{min}/c = 0.35$, $x_{max}/c = 0.95$ for the RAE 2822 airfoil. Based on the definition of ϵ , the objective function can thus be defined as Eq. (6.18):

$$J = \frac{1}{2}(\epsilon_{bump}^2 + \epsilon_{RAE}^2) \quad (6.18)$$

where the bump case and the RAE airfoil case are equally weighted. The goal of the calibration framework is to find a coefficient set that minimizes J .

To find the optimum set of coefficients $c_{b\omega 1p}$, $c_{b\omega 1n}$, $c_{b\omega 2}$ and $c_{b\omega 3}$, broad variation ranges of these coefficients are explored, i.e., $0.00 \leq c_{b\omega 1p} \leq 0.50$, $-1.00 \leq c_{b\omega 1n} \leq -0.50$, $10 \leq c_{b\omega 2} \leq 1000$ and $0.1 \leq c_{b\omega 3} \leq 10.0$. A database of model coefficients with $n_i = 1000$ samples is generated using the Latin hypercube sampling method [208], and the prediction accuracy of each sample of coefficients is evaluated by RANS simulations.

The fully connected neural network (FCNN) is used as the metamodel, which constructs a functional mapping between the SA-B model coefficients and the prediction accuracy on each calibration case. The FCNN used in this section consists of one input layer, two hidden layers (with the hyperbolic tangent activation function) and one output layer (with the sigmoid activation function). The rest hyperparameters of the FCNN are set as $n_1 = n_x + n_q$, $\omega = 2$ and $\lambda = 10^{-4}$. Such an FCNN setup achieves a relative error of about 0.8% when using 80% of the database samples for training and the rest 20% samples for testing. Details of the training history and the prediction accuracy of the FCNN are presented in Fig. 6.16.

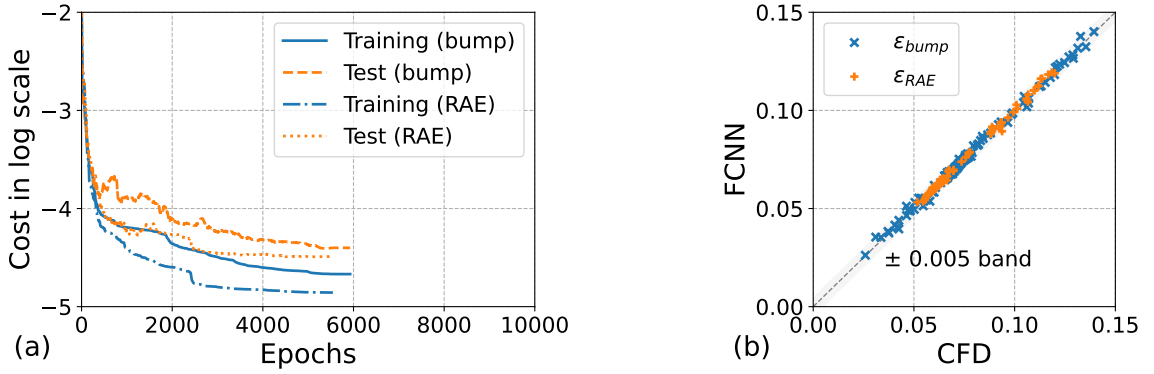


Figure 6.16: FCNN for predicting the integrated C_p error: (a) training history and (b) prediction accuracy (training/testing data: 80%/20% samples of the initial design of experiments database).

The rest parameters of the calibration framework are chosen as $n_u = 256$, $n_b = 20$ and $n_d = 40$. Higher values of these parameters can potentially improve the efficacy of the calibration framework further at the expense of a higher cost, but this is not pursued here since the current parameters are already capable of finding the optimum coefficients, as will be shown later in the next section.

6.4.2.3 Calibration Results

The convergence history of the calibration process is summarized in Fig. 6.17.

In Fig. 6.17(a), the minimum objective function J_{min} (i.e., the objective function of the optimum coefficients set) is plotted against the number of iterations. Here, the J_{min} values predicted by the FCNN are denoted by the solid line with open circles, and the mean relative errors of the FCNN are indicated by the shaded area; the J_{min} values obtained from CFD are indicated by the dashed line with open diamonds, and the value at zero iteration represents

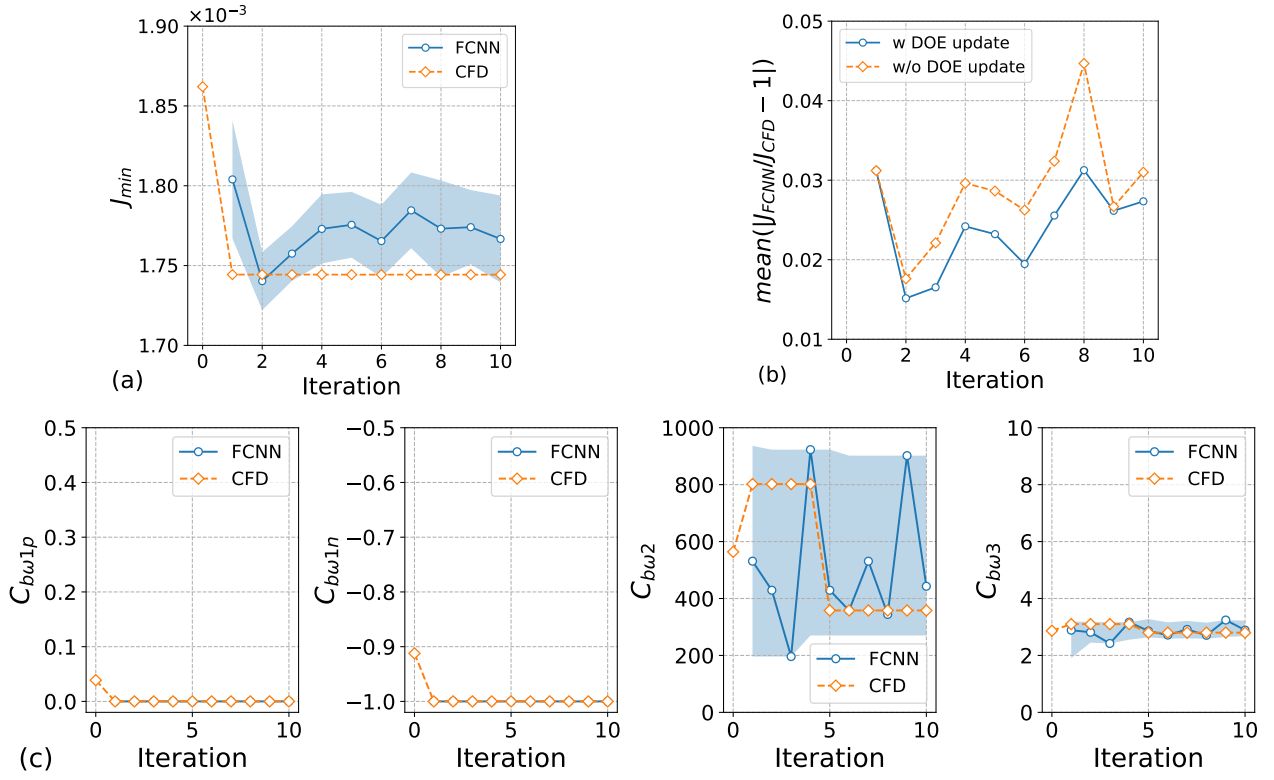


Figure 6.17: Convergence of the calibration framework: (a) minimum objective function versus iteration; (b) mean relative error of FCNN versus iteration; (c) optimum coefficient values versus iteration.

the J_{min} of the first DOE database. Results show that J_{min} drops quickly within the first two iterations, but in later iterations its variations are within the FCNN prediction error, indicating convergence of the optimization algorithm. The quick convergence of the optimization algorithm is owing to the large size of the first DOE database (i.e., $n_i = 1000$). When a smaller n_i is used, more iterations are required by the optimization algorithm to reach convergence.

In Fig. 6.17(b), the mean relative error of FCNN is plotted against the number of iterations. At the i_{th} iteration, the FCNN is trained using all the CFD-verified samples from the previous i iterations and tested using the updated DOE database at the $(i+1)_{th}$ iteration. To demonstrate the advantage of using the updated DOE databases for training, the mean relative errors of the FCNN with or without using the updated DOE databases for training are represented by the solid line with open circles and the dashed line with open diamonds, respectively. Results show that including the updated DOE databases for training achieves a mean relative error between 1.5% and 3.0% during all the iterations, which is consistently lower than the case without the updated DOE databases. This is because the latter case increases the chance of overfitting in the FCNN: when excluding the updated DOE databases for training, the training database will be biased toward the region nearby the optimum coefficient sample as the number of iterations increases; as a result, the trained FCNN tends to overfit the optimum coefficient region but predict the unseen regions inaccurately.

In Fig. 6.17(c), the optimum model coefficients are plotted against the number of iterations. Here, the best model coefficients predicted by the FCNN are indicated by the solid line with open circles, with the shaded area representing the min-max coefficient range of the best n_b samples from the optimizer; the best model coefficients verified by CFD are presented by the

dashed line with open diamonds. Results show that $c_{b\omega 1p}$ and $c_{b\omega 1n}$ converge to $c_{b\omega 1p} = 0.00$ and $c_{b\omega 1n} = -1.00$ within the first two iterations, which is consistent with the observation in Fig. 6.17(a). However, $c_{b\omega 2}$ and $c_{b\omega 3}$ vary within the range of $196 \leq c_{b\omega 2} \leq 923$ and $2.4 \leq c_{b\omega 3} \leq 3.2$, despite their corresponding objective function values being similar to each other. Such results indicate that any values of $c_{b\omega 2}$ and $c_{b\omega 3}$ within these ranges can provide equally accurate results. Throughout this research, the CFD-verified best coefficients at the last iteration are adopted, which are $c_{b\omega 2} = 358$ and $c_{b\omega 3} = 2.8$.

To examine if the optimum coefficient ranges of $c_{b\omega 2}$ and $c_{b\omega 3}$ predicted by the FCNN are correct, a further database of 400 samples is created by the full factorial design within the range of $c_{b\omega 1p} = 0.00$, $c_{b\omega 1n} = -1.00$, $10 \leq c_{b\omega 2} \leq 1000$ and $0.1 \leq c_{b\omega 3} \leq 10.0$. The performances of all these samples are evaluated by CFD. The objective function values predicted by both the FCNN and the CFD are plotted as colored contours in Fig. 6.18. It is confirmed that the optimum ranges of $c_{b\omega 2}$ and $c_{b\omega 3}$ predicted by the FCNN are qualitatively the same as the CFD results. Another observation is that the FCNN results at the first and the last iteration are similar to each other, which again shows the quick convergence of the optimization algorithm.

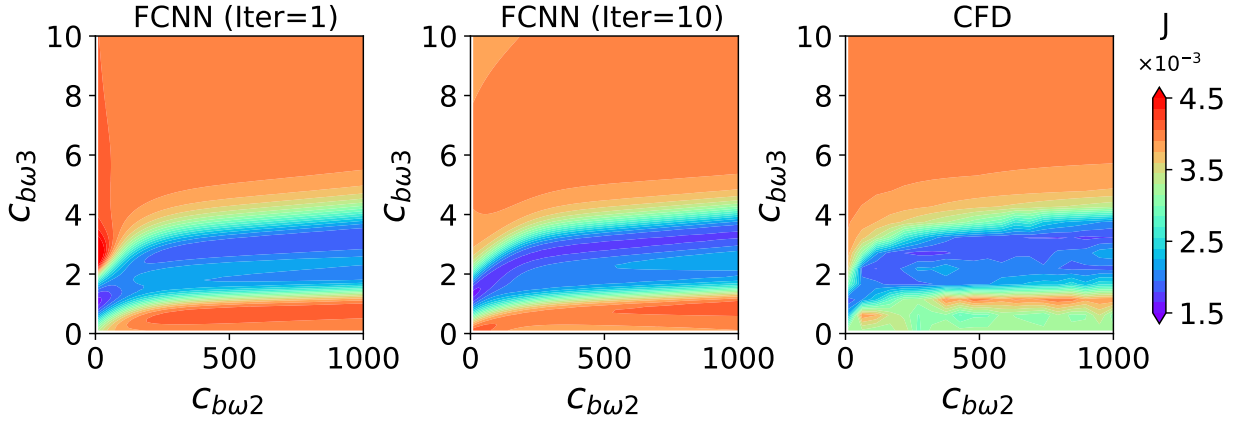


Figure 6.18: Objective function contours predicted by FCNN and CFD given $c_{b\omega 1p} = 0.00$ and $c_{b\omega 1n} = -1.00$.

To visualize all the samples obtained from the optimization algorithm, the integrated C_p error of the RAE 2822 airfoil case is plotted against that of the axisymmetric transonic bump case in Fig. 6.19. In this plot, the circles represent the initial DOE database, the squares represent the updated DOE databases, and the diamonds represent the optimum coefficients of each iteration. For reference, the errors of the SA and the SA-QCR models are also shown by the cross and the plus symbols, respectively. Results show that the calibrated SA-QCR-B model greatly reduces the error in the bump case and slightly reduces the error in the RAE 2822 case, compared to the SA and SA-QCR model. If other flow features (e.g., rotation and curvature) were considered in the turbulence model, the prediction errors can be reduced further.

6.4.3 Validation of Baroclinicity Modification

In this section, the calibrated SA-B model will be validated in the axisymmetric transonic bump and the RAE 2822 airfoil at both training and unseen conditions.

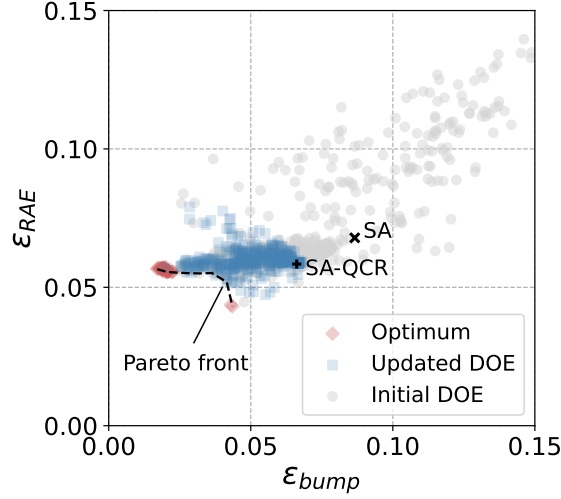


Figure 6.19: Integrated C_p errors of all the samples obtained from the optimization algorithm.

6.4.3.1 Axisymmetric Transonic Bump

The wall surface pressure coefficient distributions of the axisymmetric transonic bump at different operating Mach numbers are presented in Fig. 6.20. In these plots, only the $M_\infty = 0.875$ data has been used for calibration, and the rest conditions represent unseen data. At $M_\infty = 0.925$, 0.9 and 0.875, the SA-B and the SA-QCR-B model significantly improve the prediction accuracy of the original SA model, which predicts the shock front more downstream. At $M_\infty = 0.85$, the improvement is still visible but less pronounced. At $M_\infty = 0.80$ where the shock and shock-induced separation do not occur, all the models perform similarly to each other. These results indicate that the baroclinicity modification can improve prediction accuracy in unseen transonic flow cases.

6.4.3.2 RAE 2822 Airfoil

The surface pressure coefficient distributions of the RAE 2822 airfoil at different operating conditions are presented in Fig. 6.21. In these plots, three operating conditions are tested, namely Case 6, Case 9 and Case 10 following the naming convention of the experiment [147]. Details of the operating conditions are summarized in Table 3.3. In these cases, only Case 10 has been used for calibration, and the rest cases are unseen. Results show that the SA-B improves the prediction accuracy over the SA model in Case 10, but both models perform similarly in the other two cases. The SA-QCR model also shows improved prediction over the SA model in Case 10. However, combining both the baroclinicity modification and the QCR modification does not achieve further improvement in the prediction accuracy. Therefore, the baroclinicity modification improves the prediction accuracy in the training flow without deteriorating the prediction in unseen flows.

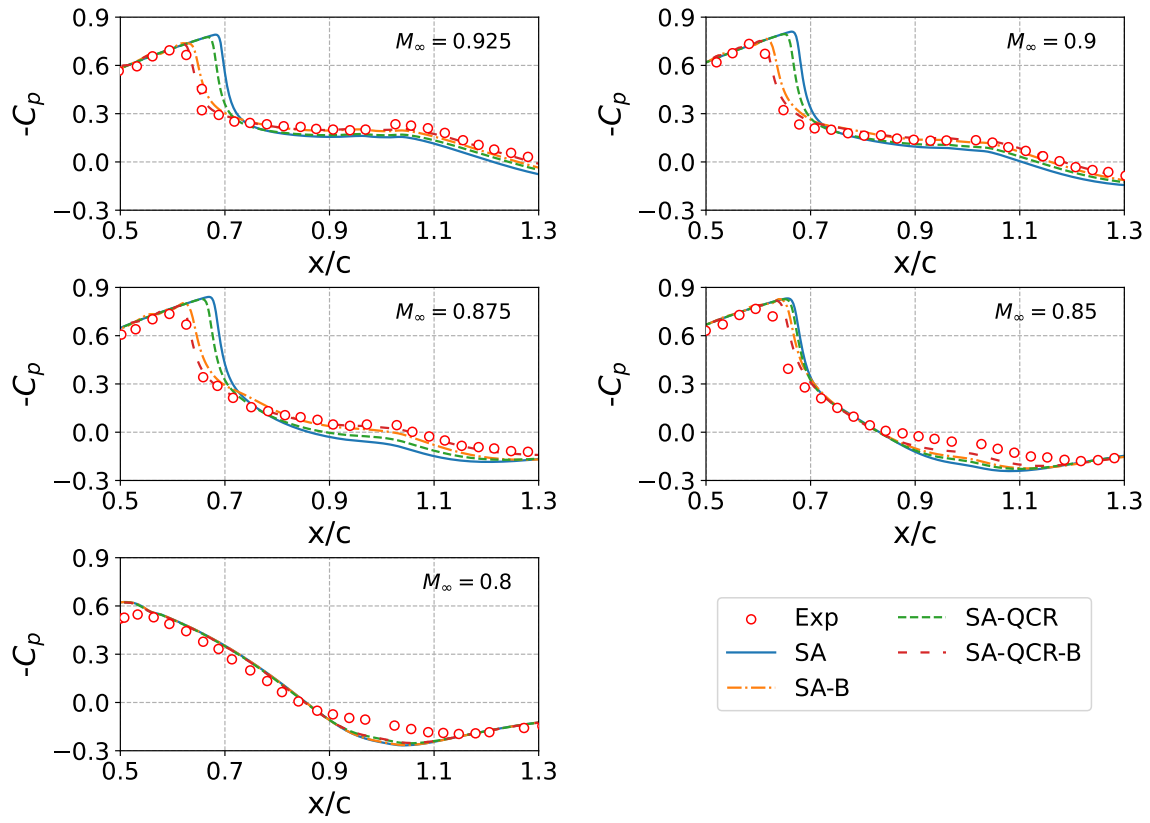


Figure 6.20: Validation of SA-B model on predicting the surface pressure coefficient of the axisymmetric transonic bump.

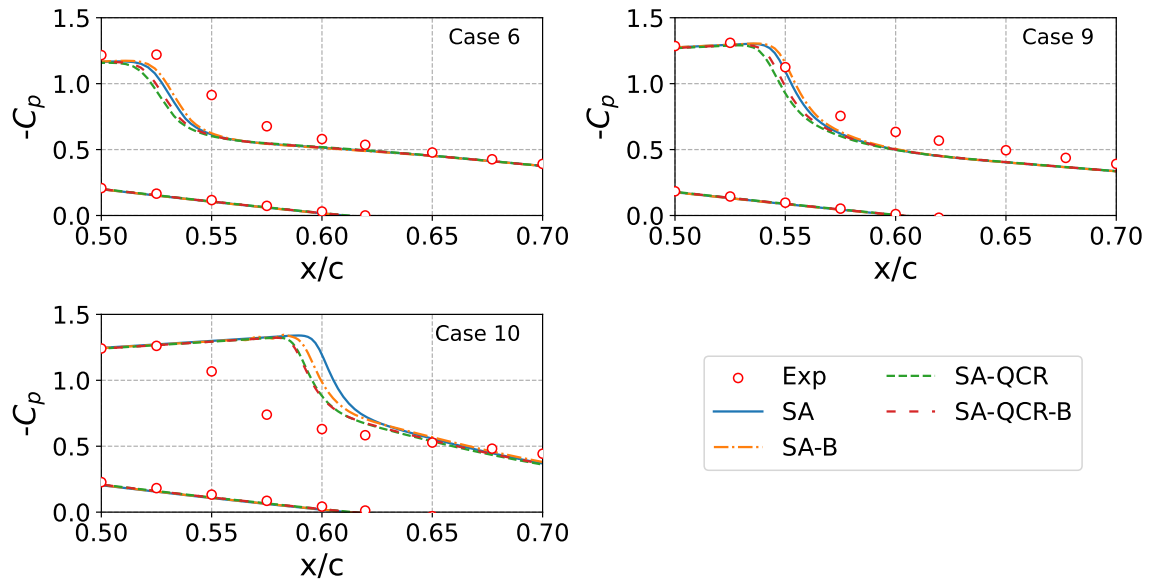


Figure 6.21: Validation of SA-B model on predicting the suction surface pressure coefficient of the RAE 2822 airfoil.

6.5 Proposal of Vortical Pressure Gradient Modification

6.5.1 Model Formulation

The flow topologies of compressor blockage cells are illustrated in Fig. 6.22. A compressor blockage cell is typically formed by the tip leakage vortex or the corner separation vortex, both of which are featured by 3D swirling motion, flow stagnation and adverse pressure gradient. In the blockage cells, the relative vorticity vector is almost aligned with the pressure gradient vector, which generally points from the upstream suction surface (SS) to the downstream pressure surface (PS). Based on these observations, an empirical compressor blockage identifier is proposed in Eq. (6.19):

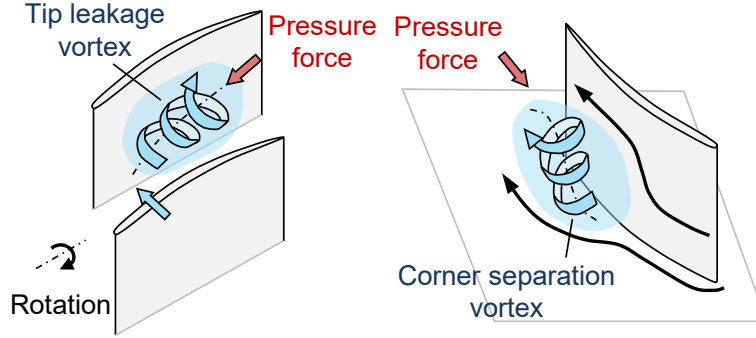


Figure 6.22: Illustration of compressor blockage cells.

$$\hat{p}_\omega = \left| \frac{\partial p}{\partial x_i} \frac{\omega_i}{\Omega} \right| / \frac{\rho^2 U^3}{\mu \text{Re}_{ref}} \quad (6.19)$$

Here, the vortical pressure gradient $\left| \frac{\partial p}{\partial x_i} \frac{\omega_i}{\Omega} \right|$ not only measures the alignment between the pressure gradient and the vorticity vector, but also the strength of the pressure gradient. Similar to the formulation of $\hat{p}$ in Eq. (6.7), the vortical pressure gradient is non-dimensionalized by the local kinetic energy and the local Reynolds number per unit length, both of which highlight regions of low-momentum flows. The same reference Reynolds number $\text{Re}_{ref} = 10^6$ applies for better scaling, and the same limiters of $10^{-3}u_{ref}$ and $10^{-3}u_{ref}/l_{ref}$ apply to Ω and U in the denominator, respectively.

Despite the similarity between the formulation of h , $\hat{p}$ and $\hat{p}_\omega$, the proposed $\hat{p}_\omega$ term has several advantages over h and $\hat{p}$:

- **Non-universality.** $\hat{p}_\omega$ has better compatibility with general fluid problems than h and $\hat{p}$. Compared to $\hat{p}$, $\hat{p}_\omega$ automatically switches off in 2D canonical flows⁴, which avoids deterioration of the prediction in such cases. Compared to h , the magnitude of $\hat{p}_\omega$ scales with the blockage in the compressor passage, which avoids deterioration of the prediction in stable operating conditions but improves it when approaching stall. Admittedly, $\hat{p}_\omega$ is still not included in the incompressible vorticity equation and may not be universal in incompressible flows. However, the proposed model is mainly intended for industrial

⁴In 2D flows, the vorticity vector is always perpendicular to the 2D plane and thus $|\omega_i \partial p / \partial x_i| = 0$.

compressors with a pronounced compressibility effect (i.e., $M > 0.3$), for which the application of $\hat{p}_\omega$ should not be hindered. For completeness, the proposed modified SA model based on the $\hat{p}_\omega$ term will be validated in low-speed cases later.

- **Non-Galilean invariance.** The calculation of $\hat{p}_\omega$ is still dependent on the reference frame. However, at the rotor-stator interface, the pressure gradient (mainly in the radial direction due to radial equilibrium) is almost perpendicular to the vorticity vector (mainly in the axial direction due to flow swirl), effectively leading to $\hat{p}_\omega = 0$ regardless of the reference frame. Hence, the discontinuity of $\hat{p}_\omega$ at the rotor-stator interface is minimal.

To demonstrate the advantages of $\hat{p}_\omega$ further, contours of h , $\hat{p}$ and $\hat{p}_\omega$ at typical compressor near-stall flow conditions are presented in Fig. 6.23.

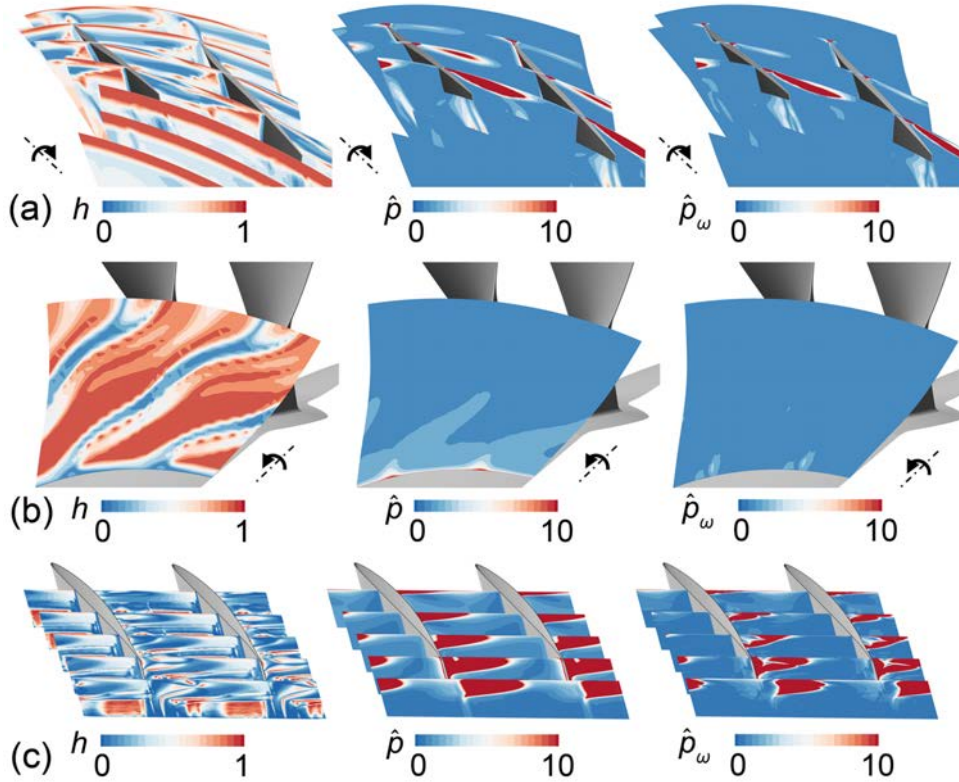


Figure 6.23: Contours of h , $\hat{p}$ and $\hat{p}_\omega$: (a) near-tip NASA Rotor 67 at the NS condition, looking from LE to TE; (b) near-hub NASA Rotor 67 at the NS condition, looking from TE to LE; (c) LMFA NACA65 cascade under 4 deg of incidence, looking from TE to LE. (steady RANS solution using the original SA model; variables calculated in the relative frame).

For the near-tip flows of NASA Rotor 67 in Fig. 6.23(a), both $\hat{p}$ and $\hat{p}_\omega$ identify the tip blockage region at the PS-casing corner. An increase in eddy viscosity in this region can effectively reduce the tip blockage size and thus extend the stall margin. In contrast, h identifies the casing boundary layer upstream of the blade leading edge (LE). An increase of eddy viscosity in this region will also reduce the tip blockage size, but such an effect applies to the whole characteristic curve of the compressor, and hence the overprediction of pressure ratio at operating conditions away from stall.

For the near-hub flows of NASA Rotor 67 in Fig. 6.23(b), h and $\hat{p}$ identify the wakes and the near-hub boundary layer, respectively. However, an increase in eddy viscosity in such regions is disfavored for three reasons: (1) it is not helpful for predicting the compressor blockage size and the stall boundary; (2) it over-predicts the wake mixing further [217]; (3) it creates discontinuity of eddy viscosity source term across the rotor-stator interface because the calculation of h and $\hat{p}$ changes with the reference frame. In contrast, $\hat{p}_\omega$ is effectively zero because the local pressure gradient is perpendicular to the vorticity vector.

For the LMFA NACA65 cascade flows shown in Fig. 6.23(c), both $\hat{p}$ and $\hat{p}_\omega$ identify the corner separation cell at the SS-hub corner. An increase in eddy viscosity in this region will help reduce the blockage size and hence extend the stall margin. In contrast, h identifies not only part of the corner separation cell but the PS-hub boundary layers, which may deteriorate prediction accuracy.

In summary, the proposed $\hat{p}_\omega$ term effectively recognizes both tip blockage cell and hub corner separation, but it remains neutral at the rotor-stator interface and in 2D canonical flows. It conceptually outperforms h and $\hat{p}$ because it is a targeted therapy for compressor stall prediction with minimum side effects.

Finally, the compressor blockage identifier $\hat{p}_\omega$ is applied to boost the eddy viscosity of the original SA model by multiplying the modified strain rate $\hat{S}$ with the $\beta_{p\omega}$ function:

$$\beta_{p\omega}(\hat{p}_\omega) = \begin{cases} 1 + c_{p\omega 1} \tanh(c_{p\omega 2} \hat{p}_\omega^{c_{p\omega 3}}), & \text{if } \frac{\partial p}{\partial x_i} w_i \geq 0 \\ 1, & \text{otherwise} \end{cases} \quad (6.20)$$

where the modification is only switched on in adverse pressure gradient flows (e.g., compressor flows), and $c_{p\omega 1}$, $c_{p\omega 2}$ and $c_{p\omega 3}$ are coefficients to be calibrated. Specifically, $c_{p\omega 1}$ determines the scaling of the $\beta_{p\omega}$ function and is most important, meanwhile, $c_{p\omega 2}$ and $c_{p\omega 3}$ only control the transitional shape of the $\beta_{p\omega}$ function and are of secondary importance. Throughout this work, the new model is termed as SA-PG $_\omega$.

6.5.2 Calibration of Model Coefficient by Bayesian Inference

Established turbulence models used high-fidelity flow field data of simple geometries for calibration, where the uncertainties in the measured quantities and the boundary conditions are small. Thus, the calibration was often conducted in a deterministic manner. For the calibration of SA-PG $_\omega$ model coefficients using turbomachinery data, however, a stochastic calibration approach is needed because the uncertainties in turbomachinery cases are large. In this work, the Bayesian inference calibration framework is applied, which was first practiced in turbulence modeling in Ref. [96]. Details of the calibration framework and the calibration results are as follows.

6.5.2.1 Calibration Framework

The core idea of the calibration framework is based on Bayes' theorem of Eq. (6.21):

$$P(\boldsymbol{\theta} \mid \epsilon \leq \epsilon_{cri}) = \frac{P(\epsilon \leq \epsilon_{cri} \mid \boldsymbol{\theta})P(\boldsymbol{\theta})}{P(\epsilon \leq \epsilon_{cri})} \quad (6.21)$$

where $P(\boldsymbol{\theta} \mid \epsilon \leq \epsilon_{cri})$ is the posterior probability of coefficients $\boldsymbol{\theta}$ given the condition of the prediction error $\epsilon \leq \epsilon_{cri}$; $P(\boldsymbol{\theta})$ is the prior probability of coefficients $\boldsymbol{\theta}$ before observing the data; $P(\epsilon \leq \epsilon_{cri} \mid \boldsymbol{\theta})$ represents the probability of obtaining a prediction error $\epsilon \leq \epsilon_{cri}$ when using the model coefficient $\boldsymbol{\theta}$; $P(\epsilon \leq \epsilon_{cri})$ represents the total probability of achieving the desired model accuracy. The goal of the calibration problem is to find $\boldsymbol{\theta}$ that maximizes $P(\boldsymbol{\theta} \mid \epsilon \leq \epsilon_{cri})$. It should be noted that $P(\epsilon \leq \epsilon_{cri})$ is independent of $\boldsymbol{\theta}$, and $P(\boldsymbol{\theta})$ is assumed to be a uniform distribution within the calibration range. Therefore, the calibration problem is equivalent to finding $\boldsymbol{\theta}$ that maximizes $P(\epsilon \leq \epsilon_{cri} \mid \boldsymbol{\theta})$. Once the formulation of the prediction error ϵ and the tolerance ϵ_{cri} are determined, $P(\epsilon \leq \epsilon_{cri} \mid \boldsymbol{\theta})$ can be obtained by performing a Monte Carlo experiment.

The prediction error ϵ is measured by the mean relative error defined by Eq. (6.22):

$$\epsilon = \frac{1}{n_q} \sum_{i=1}^{n_q} \epsilon_i = \frac{1}{n_q} \sum_{i=1}^{n_q} \left| \frac{q_{i,CFD} - q_{i,exp}}{\mu_{i,exp}} \right| \quad (6.22)$$

Here, $q_{i,CFD}$ and $q_{i,exp}$ are the i_{th} quantity of interest obtained by CFD and experiment, respectively. Both terms are random variables due to the uncertainties involved in CFD and the experiment. $\mu_{i,exp} = \mathbb{E}(q_{i,exp})$ is the mean measured value of the i_{th} quantity of interest.

The quantity obtained by the experiment is assumed to follow a normal distribution:

$$q_{i,exp} \sim N(\mu_{i,exp}, \sigma_{i,exp}^2) \quad (6.23)$$

where $\sigma_{i,exp}$ is set as half of the measurement uncertainty based on 2-sigma, leading to a 95% confidence level.

The quantity obtained by CFD is also assumed to follow a normal distribution:

$$q_{i,CFD} \sim N(\mu_{i,CFD}, \sigma_{i,CFD}^2) \quad (6.24)$$

where $\mu_{i,CFD}$ is post-processed from the converged solution and $\sigma_{i,CFD}$ is set as half of the prediction uncertainty. Such uncertainty mainly includes the estimated discretization error and the boundary condition uncertainty.

Obtaining $\mu_{i,CFD}$ by CFD requires a lot of numerical resources for a complete statistical experiment. To alleviate the numerical cost, $\mu_{i,CFD}$ can be estimated by a metamodel (MM):

$$\mu_{i,CFD} \sim N(\mu_{i,MM}, \sigma_{i,MM}^2) \quad (6.25)$$

where $\mu_{i,MM}$ is the predicted results from the MM, and $\sigma_{i,MM}$ is set half of the test error of the MM.

Combining Eq. (6.24) and Eq. (6.25), the quantity obtained by CFD obeys the following normal distribution:

$$q_{i,CFD} \sim N(\mu_{i,MM}, \sigma_{i,CFD}^2 + \sigma_{i,MM}^2) \quad (6.26)$$

Finally, the desired model accuracy ϵ_{cri} needs to be determined. A natural choice of ϵ_{cri} is:

$$\epsilon_{cri} = \frac{2k}{n_q} \sum_{i=1}^{n_q} \frac{\sqrt{\sigma_{i,CFD}^2 + \sigma_{i,MM}^2} + \sigma_{i,exp}}{\mu_{i,exp}} \quad (6.27)$$

where k is a user-specified parameter. When $k = 1$, the probability of observing $\epsilon \leq \epsilon_{cri}$ is about 95% given the condition $\mu_{i,exp} = \mu_{i,CFD}$. For cases where the difference between CFD and experimental results is large, a large k is required to obtain at least one set of plausible model coefficients; in contrast, a small k , i.e., a small tolerance of the prediction error ϵ_{cri} , is recommended for better accuracy.

6.5.2.2 Application to SA-PG $_{\omega}$ Model Coefficients Calibration

The Bayesian inference parameters used for the SA-PG $_{\omega}$ model coefficients calibration are summarized in Table 6.3. Detailed explanations are as follows.

Table 6.3: Parameters of Bayesian inference for SA-PG $_{\omega}$ model coefficients calibration.

Calibration data			Coefficient range		
Case	Variable	n_q	$c_{p\omega 1}$	$c_{p\omega 2}$	$c_{p\omega 3}$
NASA Rotor 67	p_{t2}, T_{t2}	36	[0.10, 2.00]	[0.10, 5.00]	[0.1, 10.0]

Parameters			
σ_{exp}/μ_{exp}	σ_{CFD}/μ_{CFD}	σ_{MM}/μ_{MM}	k
0.19% (avg.)	0.42%	0.01% (avg.)	0.55

The calibration data come from NASA Rotor 67, which is a tip-loaded high-speed fan rotor. More details of the experimental data and the CFD setups have been summarized in Sec. 3.4.3. In this work, the rotor exit radial profile data of total pressure and total temperature at the PE ($m/m_c = 0.989 \pm 0.004$) and NS ($m/m_c = 0.924 \pm 0.004$) conditions of the design speed are used for calibration. These profiles are measured at the plane 45.3% c_x downstream the TE at mid-span, and they consist of 9 probe locations uniformly distributed along the span, leading to a total number of 36 quantities of interest. The measurement uncertainties for the total pressure and the total temperature are 1 kPa and 0.6 K, respectively [26], which corresponds to $\sigma_{exp}/\mu_{exp} = 0.19\%$ on average.

In searching for an optimal set of coefficients $c_{p\omega 1}$, $c_{p\omega 2}$ and $c_{p\omega 3}$, broad variation ranges of these coefficients are explored, i.e., $0.10 \leq c_{p\omega 1} \leq 2.00$, $0.10 \leq c_{p\omega 2} \leq 5.00$ and $0.1 \leq c_{p\omega 3} \leq 10.0$. The prior distributions of these coefficients are assumed to be uniform. A database of model coefficients, including 585 samples uniformly distributed within these coefficient ranges, is generated and then simulated by CFD.

The fully connected neural network (FCNN) is used as the metamodel. The FCNN used in this work consists of one input layer, two hidden layers (with the hyperbolic tangent activation function) and one output layer (with the sigmoid activation function) with the rest hyperparameters inherited from the previous Chapter 5. Based on the aforementioned database, four FCNNs are trained, each predicting the profile of one quantity of interest (i.e., total pressure or total temperature) at one operating point (i.e., PE or NS). By using 80% of the database samples as the training set and the rest 20% as the test set, the FCNN shows a relative error

below 0.02%, i.e., $\sigma_{MM}/\mu_{MM} = 0.01\%$. Since the FCNN error is already sufficiently small, no further attempts to optimize the hyperparameters are made in this work.

The training history of one of the FCNNs is illustrated in Fig. 6.24(a), where the prediction error of the training and test sets are plotted against the training epochs. During the training process, the errors drop over an order of magnitude and converge near 10000 epochs. To avoid the gradient-based training process falling into a local optimum, 48 FCNNs with different initial parameter values are trained parallelly, and the FCNN with the highest accuracy is picked.

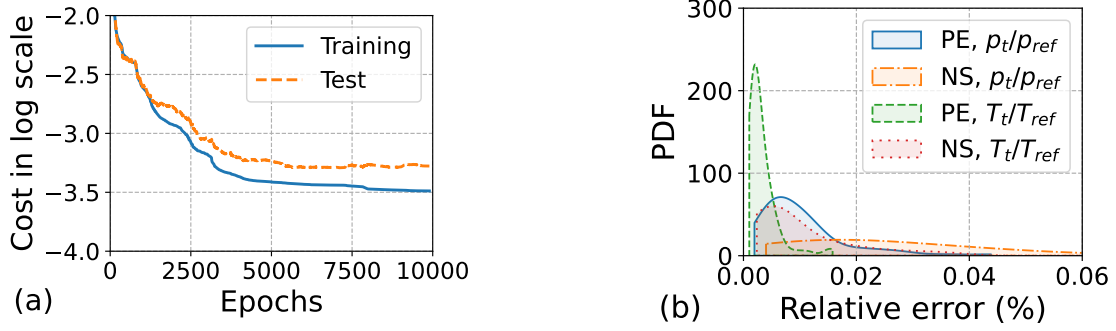


Figure 6.24: Fully connected neural network: (a) training history for total pressure ratio profile at the PE condition; (b) distribution of relative error on predicting the test set.

The distributions of the relative errors of the FCNNs are presented in Fig. 6.24(b). For all the test samples, the relative errors of all the FCNNs are within 0.06%. Comparing the two quantities of interest and two operating conditions, the FCNN shows a generally higher accuracy on predicting total temperature than total pressure (due to the difficulty of predicting isentropic efficiency) and on predicting PE than NS (due to the difficulty of predicting large separated flows).

Lastly, a parametric study of k is performed, and the result is presented in Fig. 6.25. It shows that the feasible range of k for this dataset is $0.40 < k < 0.70$. Beyond this range, the optimal coefficient set cannot be identified from the rest (i.e., $P(\epsilon \leq \epsilon_{cri} | \theta) = 1$ or 0 for most of θ). In this work, $k = 0.55$ is adopted to seek a balance between accuracy and feasibility.

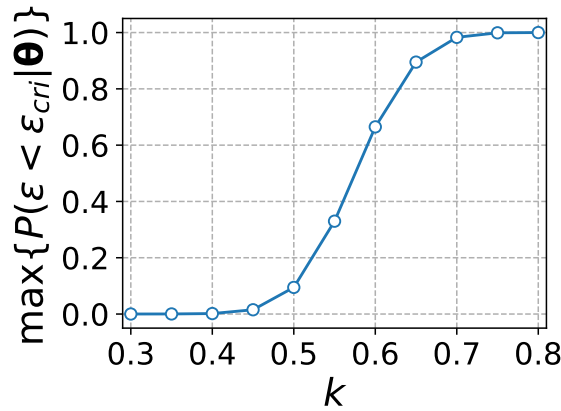


Figure 6.25: Effect of k parameter on the maximum probability of $P(\epsilon \leq \epsilon_{cri} | \theta)$.

6.5.2.3 Calibration Results

The calibration results are illustrated in Fig. 6.26. For better visualization, the posterior probability in Fig. 6.26(a) is plotted as a function of $c_{p\omega 2}$ and $c_{p\omega 3}$ only, i.e., $P(c_{p\omega 2}, c_{p\omega 3}) = \max_{c_{p\omega 1}} P(c_{p\omega 1}, c_{p\omega 2}, c_{p\omega 3})$; the corresponding optimal $c_{p\omega 1}$ is presented in Fig. 6.26(b). An optimal coefficient is found at $c_{p\omega 1} = 0.94$, $c_{p\omega 2} = 2.66$ and $c_{p\omega 3} = 4.8$, which will be used throughout this paper. However, results also suggest that any coefficients within the range of $0.75 \leq c_{p\omega 1} \leq 1.20$, $2.00 \leq c_{p\omega 2} \leq 4.00$ and $3.0 \leq c_{p\omega 3} \leq 7.0$ can provide an equivalently accurate prediction on the training quantities of interest (i.e., NASA Rotor 67 radial profile data). These coefficient ranges can be further narrowed when feeding in more data from other geometries for calibration in the future.

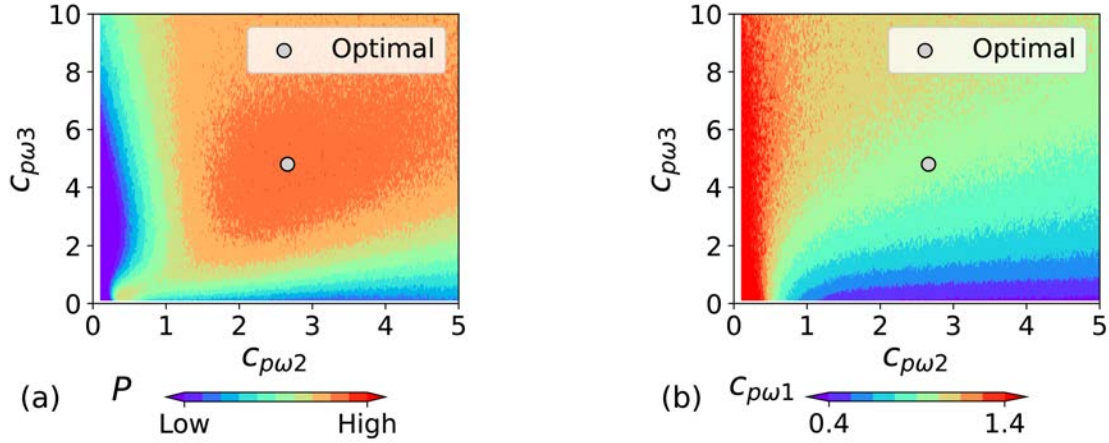


Figure 6.26: Calibration of coefficients: (a) posterior probability as a function of $c_{p\omega 2}$ and $c_{p\omega 3}$; (b) corresponding optimal $c_{p\omega 1}$.

6.5.3 Validation of Vortical Pressure Gradient Modification

In this section, the SA-PG $_{\omega}$ model with the optimal coefficient set is validated in four cases, namely NASA Rotor 67, TUDa-GLR-OpenStage, BUAA Stage B rotor and LMFA NACA65 cascade.

6.5.3.1 NASA Rotor 67

The details of the measured data and the CFD setup of NASA Rotor 67 have been introduced in Sec. 3.4.3. Firstly, the tip blockage sizes predicted by the SA and the SA-PG $_{\omega}$ model are compared in Fig. 6.27. In Fig. 6.27(a), contours of the circumferentially mass-averaged axial velocity normalized by the blade tip velocity are presented, and the tip blockage cell is enveloped by the isoline of $V_x/U_t = 0$. It shows that the SA model predicts a tip blockage cell extending from the LE to the TE, but the SA-PG $_{\omega}$ model predicts a smaller tip blockage cell and hence a more stable operating condition at the same normalized mass flow. To quantify the blockage size, the axial length of the blockage cell (L_b) is used, and it is plotted against the mass flow rate in Fig. 6.27(b). It shows that the SA-PG $_{\omega}$ model suppresses the tip blockage

size when approaching stall. Thus, it can predict a larger stall margin than the SA model does.

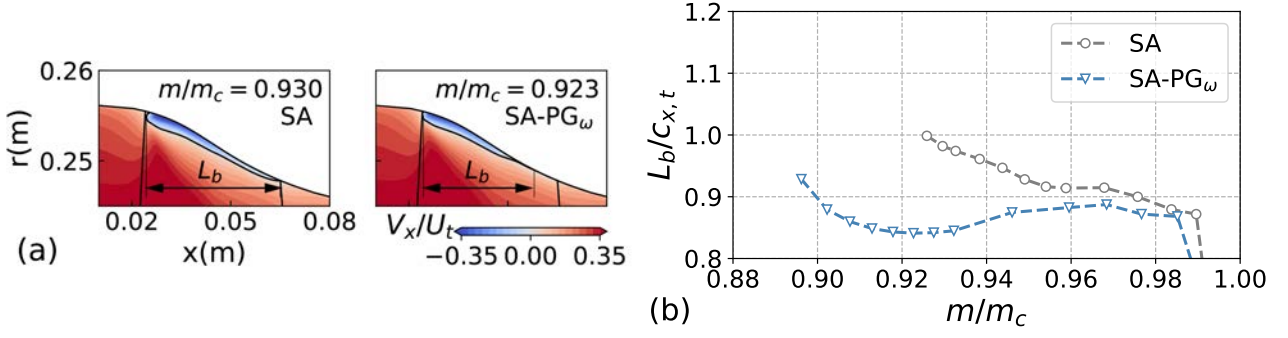


Figure 6.27: Evolution of blockage size of NASA Rotor 67 at the design speed: (a) contours of circumferentially mass-averaged axial velocity at the NS condition; (b) blockage size versus mass flow rate.

The rotor exit radial profiles of total pressure and total temperature are compared in Fig. 6.28. Note that the calibration is based on these measurement data (only), and hence the validation performed here is a posteriori. Results show that both the SA and the SA-PG $_{\omega}$ models predict the PE profiles with adequate accuracy. At the NS condition, the SA-PG $_{\omega}$ model outperforms the SA model between 60% and 100% span due to its unblocking effect near the tip. Minor deficiency of the SA-PG $_{\omega}$ prediction on the NS condition exists near 30% span, where a hub-SS corner separation bubble is formed. However, such a difference is likely caused by other factors (e.g., deficiency of Boussinesq assumption, transition modeling, etc.) that need further investigation in the future.

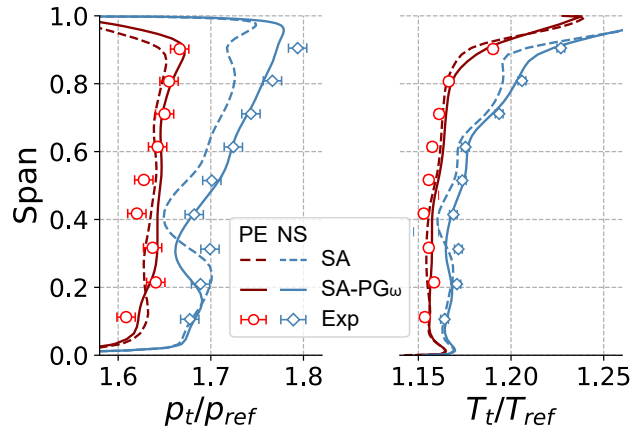


Figure 6.28: Validation of SA-PG $_{\omega}$ model on predicting the rotor exit radial profiles of NASA Rotor 67 at the PE and NS conditions of the design speed.

To validate the SA-PG $_{\omega}$ model on predicting the near-stall flow further, the circumferential profiles of relative Mach number (M_{rel}) and relative flow angle (α_{rel}) are presented in Fig. 6.29. The definition of α_{rel} is illustrated by the velocity triangle. Results show that the SA-PG $_{\omega}$ model predicts a generally smaller M_{rel} and α_{rel} than the SA model and thus improves the prediction accuracy. This is because the SA-PG $_{\omega}$ model unblocks the near-tip flow field, reduces the deviation and thus reduces M_{rel} and α_{rel} , as illustrated in the velocity triangle. Deficiency of

both the SA and SA-PG $_{\omega}$ model are observed near 105% pitch, where a slower wake mixing process is predicted. Such a deficiency is widely reported in linear eddy viscosity models and can be fixed by tuning the Boussinesq assumption [231], but this is outside the scope of the paper.

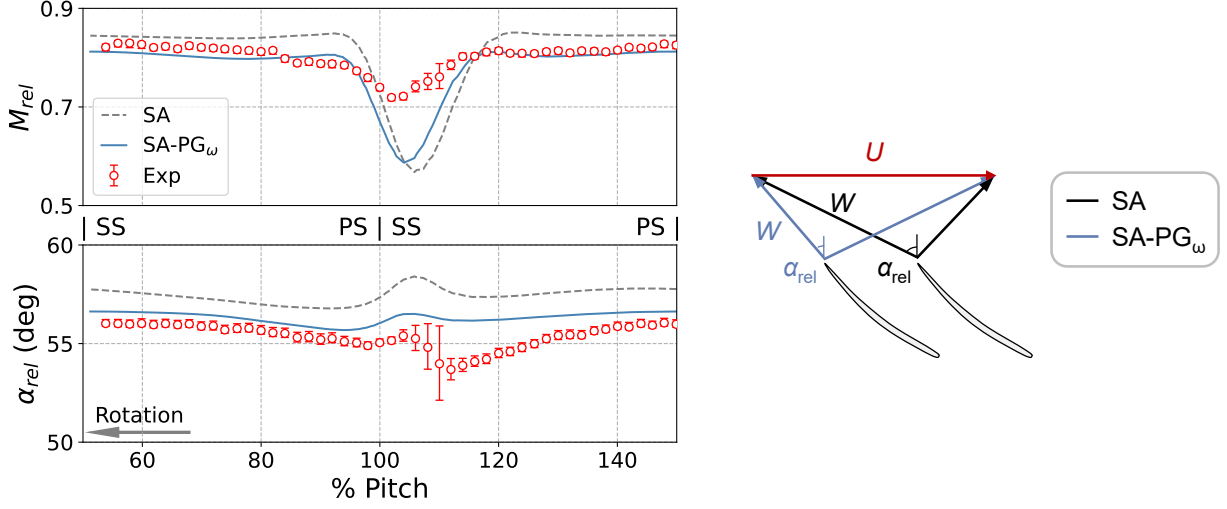


Figure 6.29: Validation of SA-PG $_{\omega}$ model on predicting the circumferential profiles at 90% span and 24% c_x downstream the TE of NASA Rotor 67 at the NS condition of the design speed.

Lastly, the total pressure ratio characteristics are presented in Fig. 6.30. It is illustrated that the SA-PG $_{\omega}$ model predicts the stall margins more accurately than the SA model at all operating speeds, although only data of the PE and NS points of the design speed are used for calibration. Thus, the capability of the SA-PG $_{\omega}$ model in predicting the compressor tip flow features and the tip-induced stall limit is validated.

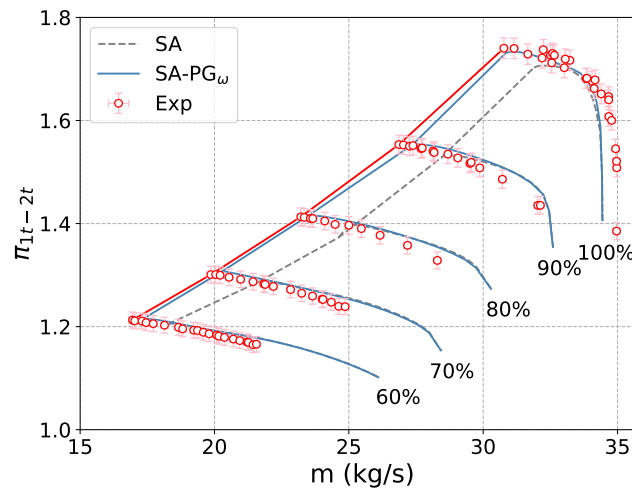


Figure 6.30: Validation of SA-PG $_{\omega}$ model on predicting the total pressure ratio characteristics map of NASA Rotor 67.

6.5.3.2 TUDa-GLR-OpenStage

The details of the measured data and the CFD setup of TUDa-GLR-OpenStage have been introduced in Sec. 3.4.3. Its total pressure ratio characteristics are examined in Fig. 6.31. Results show that the SA model slightly under-predicts the stall margins at all speeds; the SA-PG_ω model, however, predicts adequate agreement with the measured data. Besides, both CFD results slightly over-predict the near-stall total pressure ratio at the design speed. Such a deficiency is likely caused by geometric uncertainty (e.g., hot rotor geometry) and error (e.g., stator hub cavity flow), which are under investigation in concurrent research. In the following flow field analysis, only the 65% speed line is investigated where the geometric uncertainty and error are comparatively small.

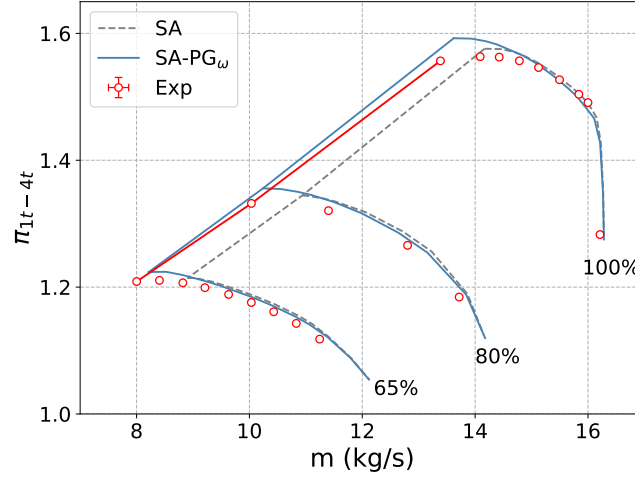


Figure 6.31: Validation of SA-PG_ω model on predicting the total pressure ratio characteristics of TUDa-GLR-OpenStage.

The stage exit radial profiles of the total pressure ratio are examined next. These profiles were available at all measured operating points. For better visualization, the profile data are interpolated and plotted as 2D contours in Fig. 6.32, where the horizontal axis represents the mass flow rate, the vertical axis represents the spanwise location and the colored contour represents the total pressure ratio. In this plot, the measured data present a tip-stall behavior: when throttling the compressor from choke to stall, the total pressure near 80% span reaches its maximum at 8.5 kg/s, which occurs earlier than the rest spans. Both CFD results present a similar tip-stall pattern, with the SA model result stalls at 9.0 kg/s and the SA-PG_ω model result at 8.6 kg/s. The reason why the SA-PG_ω model shows a delayed stall onset is that it increases the near-tip total pressure ratio by reducing the tip blockage size. Admittedly, there are still evident differences between the experimental results and the SA-PG_ω results especially near the 10% span. Such differences are likely caused by the stator hub cavity flow that is not considered in the computational model. However, the idea of how the SA-PG_ω model can extend the prediction of the stall margin is conveyed.

6.5.3.3 BUAA Stage B Rotor

The details of the measured data and the CFD setup of BUAA Stage B Rotor have been introduced in Sec. 3.4.3. The total-to-static pressure ratio characteristics are presented in

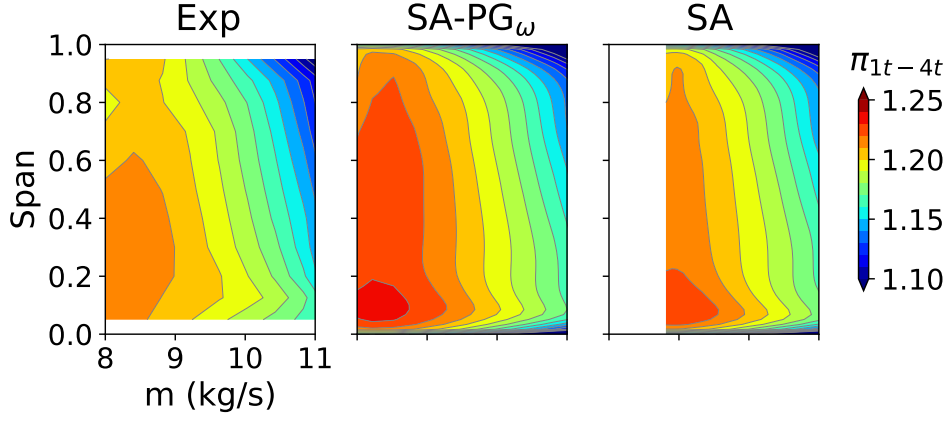


Figure 6.32: Validation of SA-PG $_{\omega}$ model on predicting the stage exit total pressure ratio radial profile contour of TUDa-GLR-OpenStage at 65% speed.

Fig. 6.33. Here, DDES results from the same RANS grid (11M) and a refined grid (23M) are also presented. Because the DDES and the RANS simulations used the same numerical setups except for the turbulence modeling approach, the DDES results serve better for the validation purpose than the measured results, the latter of which were obtained under the effect of a downstream stator. It shows again that the SA model under-predicts the stall margin; the SA-PG $_{\omega}$ model predicts a larger stall margin than the SA model, which is comparable to the one predicted by DDES with the same RANS grid.

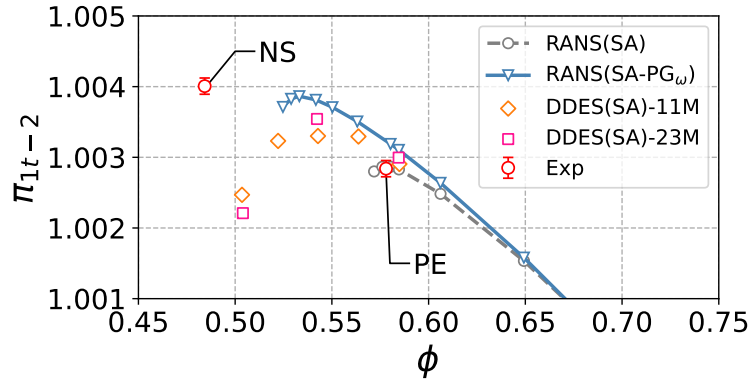


Figure 6.33: Validation of SA-PG $_{\omega}$ model on predicting the total-to-static pressure ratio characteristics of BUAA Stage B rotor.

The tip blockage cells at the PE condition are compared in Fig. 6.34. In Fig. 6.34(a), the chordwise component of relative velocity is plotted in contours, and the tip blockage cells can be visualized by the low-momentum region. Comparing the high-fidelity data with the RANS results, it shows that the SA model predicts a larger tip blockage cell, whereas the SA-PG $_{\omega}$ model shows qualitatively good agreement with the refined-mesh DDES and experiment data. To quantify the size of the tip blockage cell in each SPIV measurement section, the area enveloped by a threshold W_c/U_t value is calculated and normalized by the total section area. The streamwise development of such a blockage area is presented in Fig. 6.34(b), where the streamwise location is normalized by the chord length. It shows that the SA model over-predicts the tip blockage size, whereas the SA-PG $_{\omega}$ model shows a closer agreement with the DDES and the experimental results.

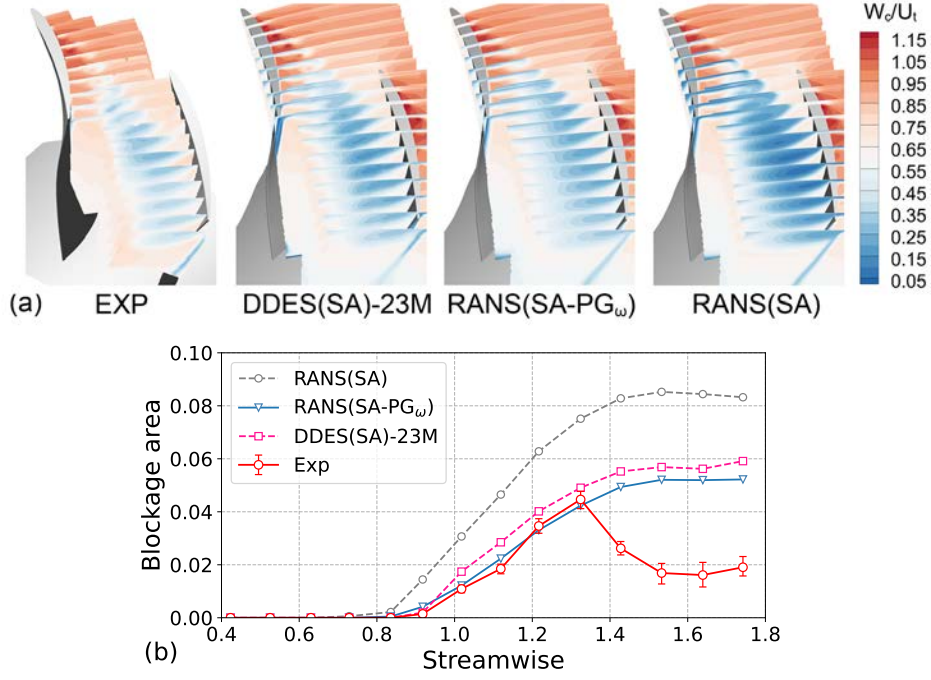


Figure 6.34: Validation of SA-PG $_{\omega}$ model on predicting the tip blockage cell of BUAA Stage B rotor at the PE condition: (a) contours of chordwise velocity in the relative frame and (b) streamwise development of dimensionless tip blockage area measured by $W_c/U_t \leq 0.4$.

6.5.3.4 LMFA NACA65 Cascade

The details of the measured data and the CFD setup of LMFA NACA65 cascade have been introduced in Sec. 3.4.3. The static pressure rise coefficient (C_p) characteristics are presented in Fig. 6.35. Results show that the SA model under-predicts the static pressure rise at a wide range of incidence; the SA-PG $_{\omega}$, SA-QCR and SA-QCR-PG $_{\omega}$ models predict higher pressure rise than the SA model, among which the SA-QCR-PG $_{\omega}$ model shows the closest agreement with the measured data. The deficiency of the SA model in predicting the static pressure rise originates from its over-prediction of the corner separation size, which is large even in the case of 0 degrees of incidence [153].

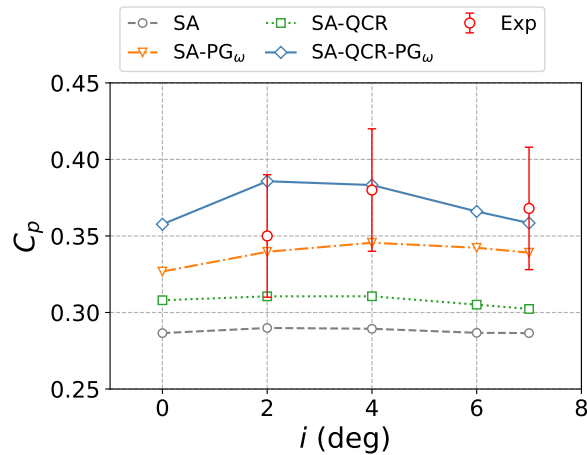


Figure 6.35: Static pressure rise coefficient characteristics of LMFA NACA65 cascade.

The spanwise profiles of static pressure rise coefficient (C_p), total pressure loss coefficient (ω_t) and flow angle (α) at the cascade exit are presented in Fig. 6.36. It shows that a corner separation bubble exists below 20% span, where the local ω_t and α are increased due to the mixing loss and the blockage effect of the corner separation, respectively. Amongst the simulation results, the SA model predicts the highest ω_t and α and the lowest C_p , indicating it over-predicts the corner separation size the most; the SA-PG $_{\omega}$, SA-QCR and SA-QCR-PG $_{\omega}$ models predict a smaller corner separation size and thus show better agreement with the experimental data than the SA model does. The SA-QCR-PG $_{\omega}$ model shows the closest agreement with the measured data, but it is still not perfect. Considering the current SA-PG $_{\omega}$ model coefficients are not calibrated using corner separation data, such a prediction accuracy is satisfactory.

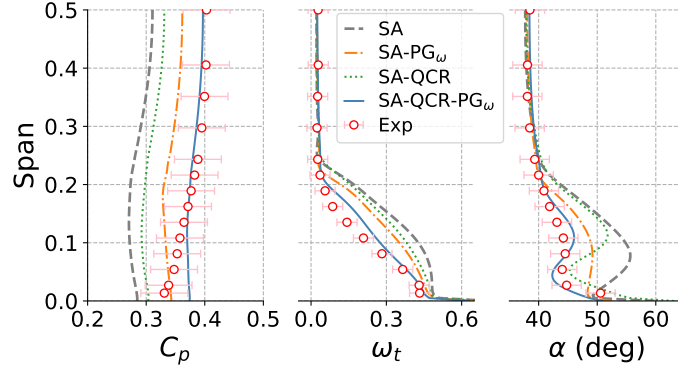


Figure 6.36: Validation of SA-PG $_{\omega}$ model on predicting the cascade exit spanwise profiles of LMFA NACA65 cascade under 4 degrees of incidence.

To investigate the corner separation effect further, the blade surface pressure profiles at 21.6% span are shown in Fig. 6.37. For the SA result, a pressure plateau is observed between 60% and 100% axial chord at the SS, which represents the corner separation region. For the SA-PG $_{\omega}$ and SA-QCR results, a similar pressure plateau is observed between 70% and 100% axial chord at the SS, indicating a smaller corner separation size compared to the SA result. The SA-QCR-PG $_{\omega}$ result and the measured data do not show such a pressure plateau, and they match with each other with adequate accuracy.

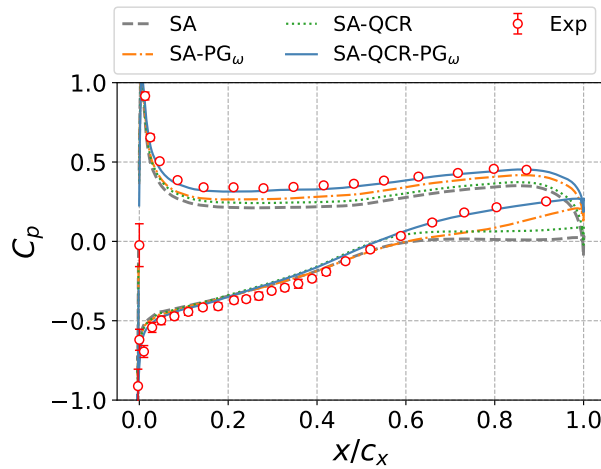


Figure 6.37: Blade surface pressure coefficient at 21.6% span of LMFA NACA65 cascade under 4 deg of incidence.

6.6 Concluding Remarks

In this chapter, the effect of modifying the turbulence model forms on the compressor near-stall flow prediction has been investigated.

Established modifications to the SA model have been evaluated in a range of canonical flows and the NASA Rotor 67. It was found that the SA-QCR and the SA-RC models slightly improve the prediction accuracy on transonic flows, but they have negligible effect in NASA Rotor 67 featured by 3D separated flows; the SA-PG model improves the prediction accuracy on 3D separated flows of NASA Rotor 67, but it deteriorates the prediction in transonic flows; the SA-H model improves the prediction of the near-stall compressor flows but deteriorates that of the peak-efficiency compressor flows. These results highlight the need for novel model modifications to improve the prediction in transonic flows and 3D-separated flows.

To improve the prediction accuracy in transonic flows, a novel modification to the SA model, i.e., SA-B, was proposed based on the dimensionless vortical baroclinicity. This modification reduces eddy viscosity in negative baroclinicity regions; whereas in incompressible flows, it is automatically switched off. The coefficients of the new model were calibrated by a global optimization framework using the surface pressure data of the axisymmetric transonic bump and the RAE 2822 airfoil. The calibrated SA-B model has been validated in the aforementioned test cases at unseen operating conditions, and improved prediction accuracy was achieved.

To improve the prediction accuracy in 3D separated flows, a novel modification to the SA model, i.e., SA-PG $_{\omega}$, was proposed based on the dimensionless vortical pressure gradient. This modification boosts eddy viscosity in the identified compressor blockage cells featured by 3D swirling, adverse pressure gradient and low-momentum flows; whereas in 2D canonical flows, the modification is automatically switched off. The coefficients of the new model were calibrated by Bayesian inference using the NASA Rotor 67 radial profile data at the PE and NS conditions of the design speed. The calibrated SA-PG $_{\omega}$ model has been validated extensively in four test cases, namely NASA Rotor 67, TUDa-GLR-OpenStage, BUAA Stage B rotor and LMFA NACA65 cascade. Results showed that the SA-PG $_{\omega}$ model predicts consistently adequate agreement with the experiment in terms of the tip/hub blockage size, the pressure rise capability of the compressor and the stall margin. Therefore, the SA-PG $_{\omega}$ model is recommended over the original SA model for compressor aerodynamic/aeroelastic instability analysis at near-stall operating conditions.

7. Explainability of Machine Learning Assisted Turbulence Model

“I propose to consider the question, ‘Can machines think?’ ”

— Alan Turing, *Computing Machinery and Intelligence*

7.1 Introduction

In Chapter 4, a cost-effective method to generate turbomachinery turbulence databases has been presented; in Chapter 5 and Chapter 6, corrections to the turbulence model transport equation (Level 3) have been found promising for better prediction of compressor near-stall flows, and several flow features have been proposed for turbulence modeling in transonic flows and 3D separated flows. Combining these elements, it is now ready to establish a machine learning (ML) assisted turbulence modeling framework. The focus of this chapter is on the explainability of the machine learning model, which is indispensable for industrial applications but has seldom been discussed in previous research.

This chapter is organized as follows. Firstly, the investigated ML-assisted turbulence modeling framework is introduced. Next, the intrinsic method and the post-hoc method that improve the explainability of an ML model will be introduced. Finally, the results of the intrinsic method and the post-hoc method will be presented, respectively.

7.2 Modeling Framework

7.2.1 Overview

The flowchart of the ML-assisted turbulence model is illustrated in Fig. 7.1, which generally follows the method of Ref. [115]. The idea is to introduce a data-driven correction term of eddy viscosity $\Delta\nu_t$, i.e., $\nu_t^{\text{ML}} = \nu_t + \Delta\nu_t$. This $\Delta\nu_t$ term can be interpreted as an additional source term calculated by ML, which reduces the deficiency of the established turbulence models in complex flows. The complete framework consists of two phases: (1) offline training and test; (2) online test and prediction. Here, the difference between online and offline lies in whether the ML model participates in the iterative process of the CFD solver.

During the offline phase, the first step is to select a range of learning flow cases considering the flow physics of interest and the availability of data. The selected cases are simulated by both high-fidelity (Hi-Fi) and low-fidelity (Lo-Fi) CFD to generate a database. This database

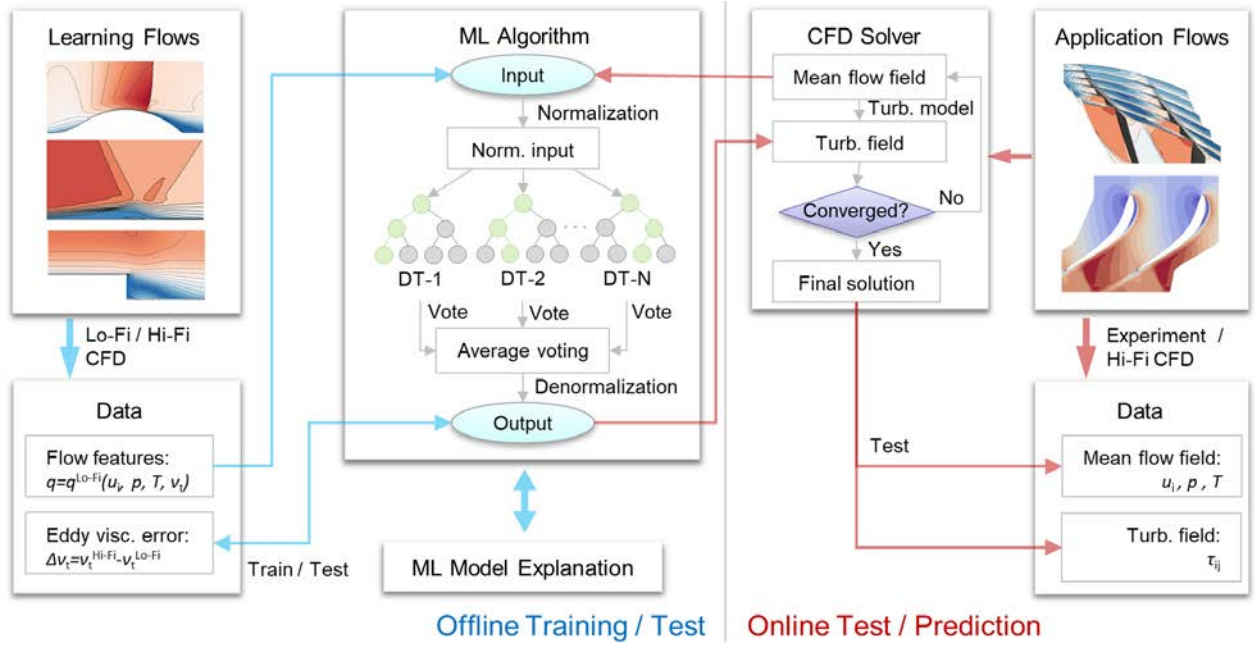


Figure 7.1: Illustration of machine-learning-assisted turbulence modeling framework.

will be divided into a training set and a test set, where the training set is seen by the ML model for training purposes, whereas the test set is unseen by the ML model in order to measure its prediction accuracy. The input of the ML model is the dimensionless flow features calculated from the Lo-Fi flow solutions, which inform the local flow physics to the model. The output of the ML model is the difference between the Hi-Fi and the Lo-Fi turbulence quantities, which can be either the Reynolds stress anisotropy tensor for L2 correction, or the eddy viscosity for L3 correction (adopted in this work), or the model coefficients for L4 correction. Finally, the developed ML model will be justified by explaining its behavior from a physics point of view.

For the online test and prediction phase, the trained ML algorithm will be implemented in the CFD solver to predict unseen flows. During each CFD iteration, the ML model will be called to correct the turbulence quantities predicted by an established turbulence model. The examined quantities of the online test include not only the turbulence quantities but the mean flow quantities. Because this chapter focuses on the model explanation, only results from the offline training/test phase are discussed.

In this framework, the numerical schemes of the CFD solver have been introduced in Sec. 3.2; the baseline turbulence model is the Spalart-Allmaras (SA) model with the quadratic constitutive relation (QCR), i.e., SA-QCR; the random forest (RF) algorithm is used to create the functional mapping, which has been introduced in Sec. 3.3. In the following sections, the learning flow cases, training and testing data, input formulation and output formulation will be introduced in detail.

7.2.2 Learning Flow Case

The learning flow case used in this chapter is the axisymmetric transonic bump, which is featured by shock-BL interaction and shock-induced separation. Details of this case and their CFD setups have been introduced in Sec. 3.4.1. In this chapter, two groups of grids are used,

as summarized in Table 7.1. The first group of grids (ID 1) is designed by NASA TMR [54] for RANS simulations. This grid will be used for demonstration of the intrinsic method to improve ML model explainability. The second group of grids (ID 2 and 3) is obtained from a previous LES study [141]. The refined grid (ID 2) was used to generate a turbulence database, but it is too dense for RANS simulations. Therefore, by picking every few grid nodes in each dimension of the original grid, a simplified grid (ID 3) is generated, which has a grid density comparable to RANS(medium). The simplified grid will be used for demonstration of the post-hoc method to improve ML model explainability.

Table 7.1: Summary of grid details of the axisymmetric transonic bump.

Grids				Domain size (in chord length)				Node number	
ID	Name	Source	Usage	x_{min}	x_{max}	r_{min}	r_{max}	n_x	n_r
1	RANS(medium)	[54]	Sec. 7.4	-3.2	4.4	0.375	4.0	181	81
2	LES(original)	[141]	-	-1.5	1.7	0.375	10.0	5921	489
3	LES(simplify)	[141]	Sec. 7.5	-1.0	1.7	0.375	4.4	320	120

7.2.3 Training and Testing Data

The open-accessed Hi-Fi data for transonic separated flows are currently limited to LES [141] and Laser Doppler velocimetry measurements [140] of the bump case at $M_\infty = 0.875$. Meanwhile, it was shown in previous research that the SST model [47] predicts the wall pressure distribution well at $M_\infty = 0.875$ [54]. Therefore, using the SST-QCR results to train the SA-QCR model in the bump case seems plausible. In the following, the fidelity of the SST-QCR result and its potential usage for the ML-assisted turbulence model are discussed in detail.

The accuracy of the SST-QCR model in predicting the mean flow field is compared against the SA-QCR model in Fig. 7.2. In Fig. 7.2(a), the pressure coefficient distributions at different M_∞ conditions are presented. It shows that the SST-QCR model predicts the pressure distribution well at all Mach number conditions, especially at $M_\infty \geq 0.85$ where the shock front location and the downstream pressure plateau in the separation region are well-captured; the SA-QCR model predicts the pressure distribution well at low Mach numbers without shocks, but it predicts a delayed shock front at $M_\infty \geq 0.85$. In Fig. 7.2(b), the velocity profiles at $M_\infty = 0.875$ are shown. The SST-QCR results show close agreement with the LES results especially in the pre-shock BL ($x/c < 0.6$) and the flow reversal region ($0.7 < x/c < 1.2$); the SA-QCR model predicts a delayed shock-induced separation and deviates from the LES data the most.

The accuracy of the SST-QCR model in predicting the turbulence quantity field is examined in Fig. 7.3. In Fig. 7.3(a), the Reynolds shear stress profiles at $M_\infty = 0.875$ are presented. Results show that both the SA-QCR and SST-QCR models under-predict the eddy viscosity downstream of the shock, and the SST-QCR model outperforms the SA-QCR model slightly. In Fig. 7.3(b), the viscosity ratio contours at $M_\infty = 0.875$ are presented in log-scale. Here, the eddy viscosity ν_t of LES is calculated from the turbulence statistics and the QCR, which will be introduced in detail later in Sec. 7.2.5. The SST-QCR model qualitatively captures the near-wall high eddy viscosity regions. Still, the details such as the contour shape and the eddy viscosity magnitude in these regions are different from the LES result.

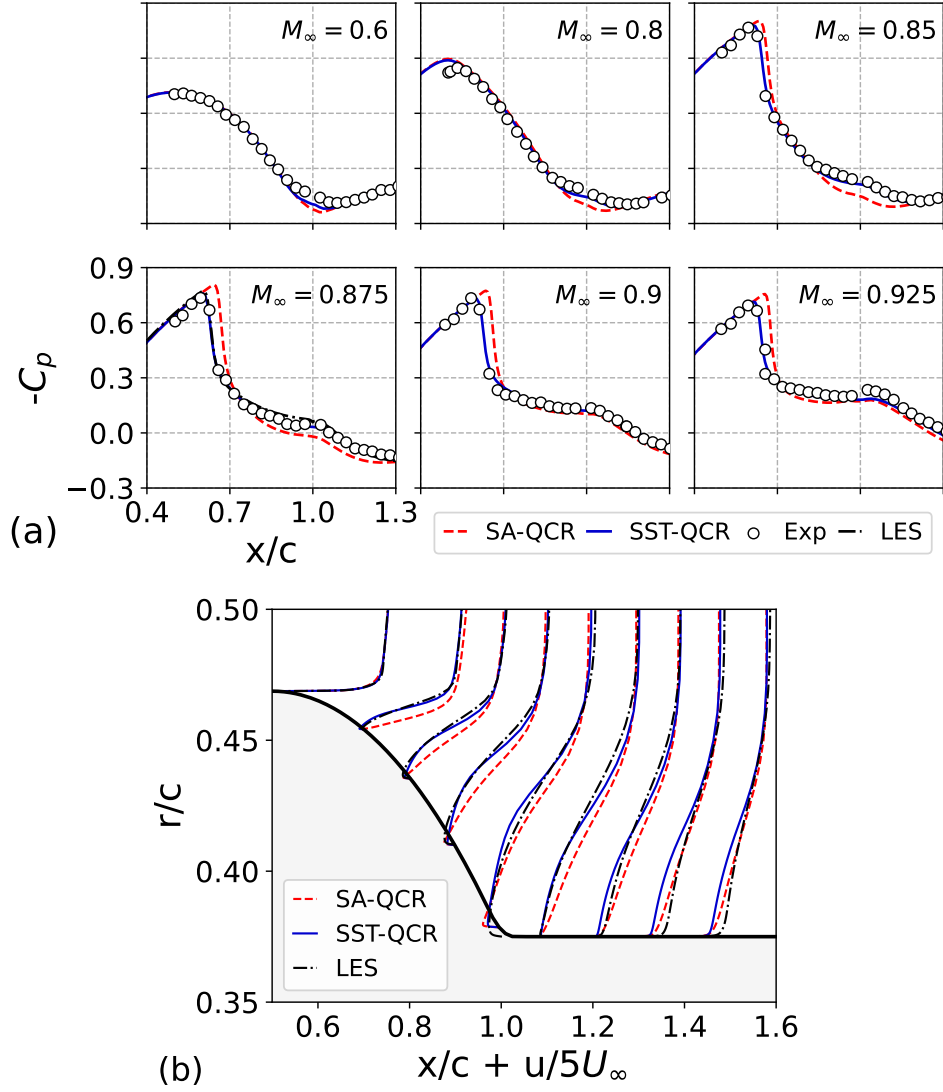


Figure 7.2: Comparison between the SA-QCR and SST-QCR model on predicting the mean flow field: (a) wall pressure coefficient distribution at all M_∞ numbers (LES is only available at $M_\infty = 0.875$ and is overlapping with SST-QCR); (b) velocity profiles at $M_\infty = 0.875$.

Considering the limited availability of LES data and the accuracy of the SST-QCR data, the SST-QCR data will be used for tuning the structural parameters of the ML model (Sec. 7.4), and the LES data will be used for the final training (Sec. 7.5). Flow physics hidden beneath the LES data is expected to be unveiled by the ML model explanation.

7.2.4 Input Formulation

The input formulation for the ML model is crucial because it incorporates physical domain knowledge into the model and hence enables the model to extrapolate beyond training flows. In this work, an abundant set of input features are formulated in Table 7.2, partly following the work of Ling and Templeton [232]. In total, nine input features ($q_i, 1 \leq i \leq 9$) from five physics groups (group A, B, C, D and E) are investigated. The physical relevance of each feature is discussed in the following.

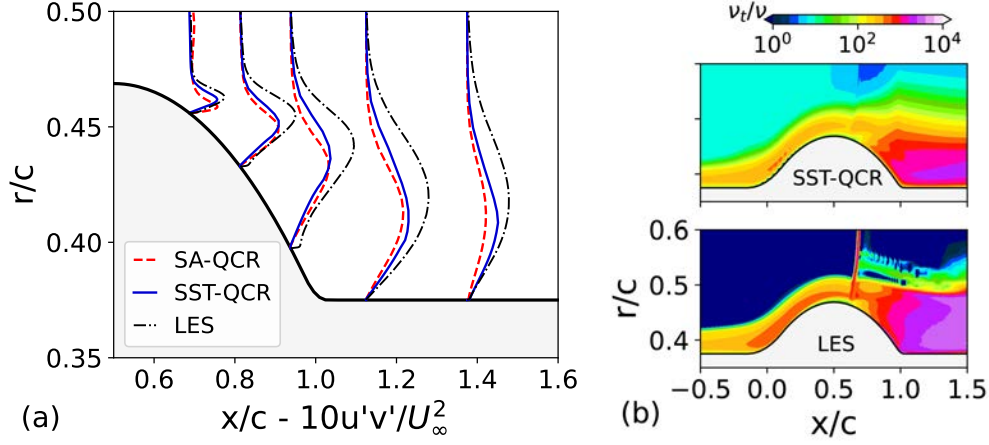


Figure 7.3: Comparison between the SA-QCR and SST-QCR model on predicting the turbulence quantity field: (a) Reynolds shear stress profiles at $M_\infty = 0.875$; (b) viscosity ratio contours at $M_\infty = 0.875$.

The group (A) pressure gradient features account for the observation that an adverse pressure gradient (APG) enhances turbulence while a favorable pressure gradient (FPG) diminishes it [220]. In particular:

- q_1 measures the alignment between the pressure gradient vector and the velocity vector. An APG is indicated by $q_1 > 0$ while an FPG is represented by $q_1 < 0$. q_1 is bounded within $[-0.5, 0.5]$.
- q_2 measures the streamwise pressure gradient magnitude, which is non-dimensionalized by the local kinetic energy and the local Reynolds number per unit length following the K parameter [220]. Its sign indicates APG/FPG as q_1 does, and its absolute value represents the streamwise pressure gradient magnitude. q_2 is bounded within $[-1.0, 1.0]$.
- q_3 measures the ratio of pressure normal stress to normal shear stress. q_3 is bounded within $[0.0, 1.0]$. $q_3 < 0.5$ indicates the normal shear stress dominates over the pressure normal stress, and vice versa.

In addition to the features discussed above, another possible candidate is the vortical pressure gradient $\omega_i \frac{\partial p}{\partial x_i}$ (Sec. 6.5). This feature is pronounced in industrial flows with a 3D swirl motion and a strong pressure gradient, but it remains zero in 2D flows and is thus not considered here. In previous BL flow research [233], the pressure gradient term was non-dimensionalized by using the wall shear stress τ_w and the BL thickness δ . However, when the investigated flow has separations or the geometry contains multiple walls, the physical relevance of using these wall quantities for non-dimensionalization becomes vague. Hence, they are not adopted for new feature development.

The group (B) strain versus rotation features address the fact that a strong shear enhances turbulence intensity whereas a strong rotation reduces it [216]. Specifically:

- q_4 represents the dimensionless Q-criterion [197] that measures the rotation-rate magnitude in excess of the strain-rate magnitude. It is bounded within $[-1.0, 1.0]$. When $q_4 > 0$, the rotation effect dominates over the shear effect, and vice versa.

Table 7.2: Input features of the ML-assisted turbulence model. $\|\cdot\|$ and $|\cdot|$ represent matrix norm and vector norm, respectively. All flow features are calculated in the reference frame attached to the bump.

Group	ID	Raw feature	Normalized feature
(A) pressure gradient	q_1	$U_k \frac{\partial p}{\partial x_k}$	$\frac{U_k \frac{\partial p}{\partial x_k}}{\sqrt{\frac{\partial p}{\partial x_j} \frac{\partial p}{\partial x_j} U_i U_i + U_k \frac{\partial p}{\partial x_k} }}$
(A) pressure gradient	q_2	$U_k \frac{\partial p}{\partial x_k}$	$\frac{U_k \frac{\partial p}{\partial x_k}}{10^{-5} \frac{\rho^2 U_i ^3}{\mu} + U_k \frac{\partial p}{\partial x_k} }$
(A) pressure gradient	q_3	$\sqrt{\frac{\partial p}{\partial x_k} \frac{\partial p}{\partial x_k}}$	$\frac{\sqrt{\frac{\partial p}{\partial x_k} \frac{\partial p}{\partial x_k}}}{\sqrt{\frac{\partial p}{\partial x_k} \frac{\partial p}{\partial x_k} + \frac{1}{2} \rho \frac{\partial U_k^2}{\partial x_k} }}$
(B) strain versus rotation	q_4	$\frac{1}{2} (\ W_{ij}\ ^2 - \ S_{ij}\ ^2)$	$\frac{\ W_{ij}\ ^2 - \ S_{ij}\ ^2}{\ W_{ij}\ ^2 + \ S_{ij}\ ^2}$
(B) strain versus rotation	q_5	$\frac{\ S_{ij}\ }{\ W_{ij}\ }$	$\tanh\left(\frac{\ S_{ij}\ }{\ W_{ij}\ }\right)$
(B) strain versus rotation	q_6	$\frac{\ W_{ij}\ }{\ S_{ij}\ ^2} (\ W_{ij}\ - \ S_{ij}\)$	$\tanh\left(\frac{\ W_{ij}\ }{\ S_{ij}\ ^2} (\ W_{ij}\ - \ S_{ij}\)\right)$
(C) flow misalignment	q_7	$ U_i U_j \frac{\partial U_i}{\partial x_j} $	$\frac{ U_i U_j \frac{\partial U_i}{\partial x_j} }{\sqrt{U_l U_l U_i \frac{\partial U_i}{\partial x_j} U_k \frac{\partial U_k}{\partial x_j} + U_i U_j \frac{\partial U_i}{\partial x_j} }}$
(D) wall proximity	q_8	$r = \frac{\hat{\nu}}{\hat{S} \kappa^2 d^2}$	$f_w = g(r) \left[\frac{1 + c_{w3}^6}{g(r)^6 + c_{w3}^6} \right]^{1/6}$
(E) viscosity ratio	q_9	ν_t / ν	$\frac{\nu_t / \nu}{500 + \nu_t / \nu }$

- q_5 measures the ratio of strain-rate magnitude over rotation-rate magnitude. For better scaling, it is limited to the interval of $[0.0, 1.0]$ by a hyperbolic tangent function. In previous research, modification to the SA model based on q_5 (i.e., SA-R) showed improved predictions on the wingtip vortex [234].
- q_6 is the Richardson number [235] that measures the rotation-rate magnitude over strain-rate magnitude (i.e., opposite to q_5). It is also limited to the interval of $[\tanh(-0.25), 1.0]$ by a hyperbolic tangent function. In previous research, implementation of q_6 in the SA model achieved certain improvements in predicting some flows with rotation and curvature [236].

To avoid division by zero, a reference strain rate u_{ref}/l_{ref} is added to both the $\|W_{ij}\|$ and $\|S_{ij}\|$ terms, where u_{ref} and l_{ref} are characteristic velocity and length scale of the investigated case.

The group (C) flow misalignment feature considers the fact that RANS models are tuned accurately in 2D parallel shear flows but often fail in flows deviating from them [237]. In

particular, q_7 measures the non-orthogonality between the velocity vector and the gradient of the streamline-aligned velocity. It is bounded within $[0.0, 0.5]$. When $q_7 = 0$, it indicates either a perfectly parallel flow or the shear vanishes; in the case of any deviation from a parallel shear flow, $q_7 > 0$. Another candidate of this group is the vortex tilting measure (VTM) [180], which identifies quasi-2D flow regions from developed 3D vortical regions. However, this feature remains zero in 2D flows and thus is not considered here.

The group (D) wall proximity feature considers that the turbulence length scale (i.e., mixing length) is proportional to the wall distance d in a classic log-law region of a BL. In the SA model, the destruction term scales with d^{-2} based on dimensional analysis [44]. Here, q_8 is based on the r parameter in the SA model, which represents the squared length scale ratio between the mixing length and the wall distance. It is bounded within $[0.0, 2.0]$ via the f_w function in the SA model, which is originally used to speed up turbulence destruction for better prediction of skin friction. The f_w function values and the corresponding identified flow regions are summarized in Table 7.3. Another option to normalize r is via the shielding function f_d of DDES [66]. This form of wall proximity is mostly binary and has low resolution inside the BL. Thus, it is not considered here.

Table 7.3: Identification of flow regions by the f_w function

f_w values	Flow region
$0.0 \leq f_w < 0.4$	free shear flow; viscous sublayer
$0.4 \leq f_w < 0.8$	outer part of BL
$0.8 \leq f_w < 1.0$	near-wall BL under FPG
$f_w = 1.0$	log layer of BL
$1.0 < f_w \leq 2.0$	near-wall BL under APG

The group (E) viscosity ratio feature measures the ratio between the turbulent viscosity ν_t and the laminar viscosity ν , which is high in the near-wall region and the separation region. From dimensional analysis, the production term and the destruction term of the SA model scale with ν_t and ν_t^2 , respectively [44]. Here, q_9 is a bounded version of the viscosity ratio, whose value falls within $[0.0, 1.0]$. A scaling factor of 500 applies to reflect the magnitude variation in this case.

7.2.5 Output Formulation

The output of the ML model is the normalized eddy viscosity difference (i.e., normalized $\Delta\nu_t = \nu_t^{\text{Hi-Fi}} - \nu_t^{\text{Lo-Fi}}$) with the same normalization scheme of q_9 shown in Table 7.2. Here, $\nu_t^{\text{Lo-Fi}}$ is calculated by solving the turbulence model transport equation(s) iteratively while keeping the mean flow field the same as the Hi-Fi results; $\nu_t^{\text{Hi-Fi}}$ is readily available for the SST-QCR data, but it needs to be approximated from the turbulence statistics of LES/DNS results.

The optimal approximation of $\nu_t^{\text{Hi-Fi}}$ minimizes $J = \|\overline{-\rho u'_i u'_j} - \tau_{ij}^{\text{RANS}}\|_F$. Therefore, the approximate ν_t value will be the root of $\partial J / \partial \nu_t = 0$. If τ_{ij}^{RANS} is calculated from the Boussinesq constitutive relation of Eq. (2.9), ν_t can be obtained from the following:

$$\nu_t = -\frac{\overline{u'_i u'_j} S_{ij} - \frac{1}{3} \overline{u'_k u'_k} S_{kk}}{2[S_{ij} S_{ij} - \frac{1}{3} (S_{kk})^2]} \quad (7.1)$$

which was derived in Spalart et al. [142]. If τ_{ij}^{RANS} is calculated from the QCR of Eq. (6.1) and the approximated turbulence kinetic energy of Eq. (6.3), ν_t can be obtained from the following:

$$\nu_t = -\frac{\overline{u'_i u'_j} X_{ij}}{2X_{ij}X_{ij}} \quad (7.2)$$

$$X_{ij} = S_{ij}^* - c_{cr1}(O_{ik}S_{jk}^* + O_{jk}S_{ik}^*) - c_{cr2}\sqrt{2W_{mn}W_{mn}}\delta_{ij} \quad (7.3)$$

Note that Eq. (7.2) becomes identical to Eq. (7.1) if $c_{cr1} = c_{cr2} = 0$.

When solving ν_t using Eq. (7.1) and (7.2) numerically, additional limiters may apply:

- Due to the deficiency of the linear/quadratic constitutive relation in predicting the transportation of each Reynolds stress component, a negative ν_t value can be obtained. This not only violates the non-negative assumption used by the notion of eddy viscosity but also is disfavored from the perspective of numerical stability. Thus, the calculated ν_t value is truncated as $\max\{\nu_t, 0\}$.
- The denominator may be effectively small, resulting in an unrealistic high value of ν_t . This can be solved by limiting the absolute value of the denominator to be no less than a threshold S_{ref}^2 .

The Boussinesq-based approach and the QCR-based approach with different S_{ref} values are compared in Fig. 7.4. In these plots, the contours of eddy viscosity ratio ν_t/ν and limiter indicator f_{lim} obtained from different methods are presented. The ν_t/ν contours are plotted in log-scale. The f_{lim} values of 0, 1, 2 and 3 correspond to regions without any limiter effect, with the S_{ref} limiter effect, with the $\nu_t \geq 0$ limiter effect and with both limiter effect, respectively.

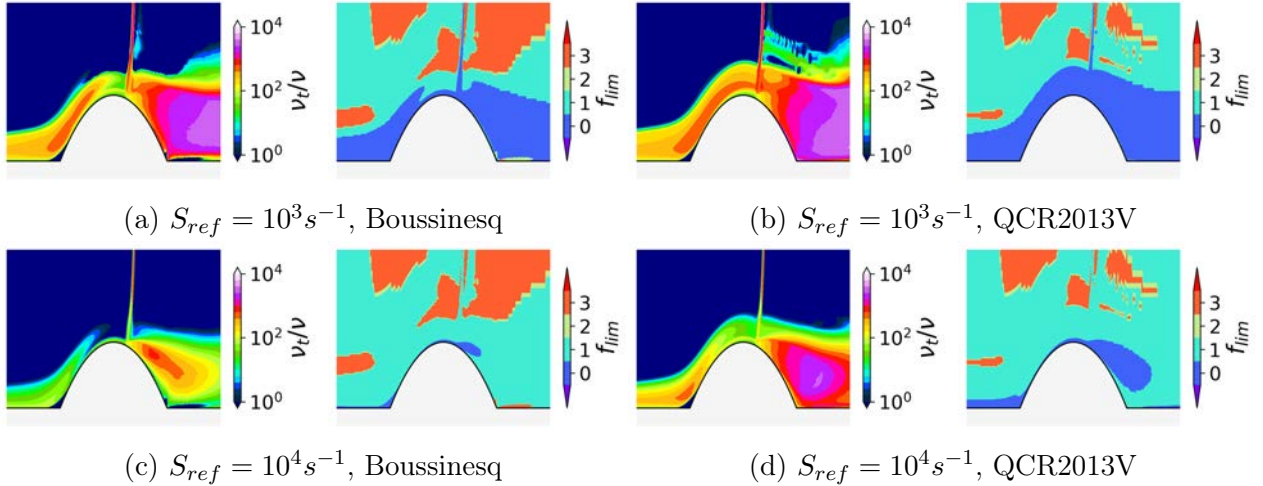


Figure 7.4: Contours of eddy viscosity ratio ν_t/ν and limiter indicator f_{lim} .

When comparing the constitutive relation effect at the same S_{ref} value, the QCR-based method identifies a larger area free of the limiter effect than the Boussinesq-based method. It indicates that the QCR-based method is less prone to fringe solutions and thus more reliable than the Boussinesq-based method. When comparing the S_{ref} limiter effect at the same constitutive relation, a low S_{ref} leads to a non-physical high ν_t/ν value above the shear layer,

meanwhile a high S_{ref} contaminates the ν_t/ν value in the shear layer, the separation bubble and the reattached BL. By trial-and-error, it is found that the QCR-based approach with $S_{ref} = 10^3 s^{-1}$ keeps the near-wall regions of interest uncontaminated from the limiters whilst reducing the non-physically high ν_t/ν value above the shear layer. Thus, this combination of settings is adopted in this work. To improve the quality of training data further, samples that are affected by the above limiters (i.e., $f_{lim} > 0$) are excluded from the training database.

Based on the above method, the normalized eddy viscosity difference between the LES and SA-QCR results at $M_\infty = 0.875$ are obtained, and they are presented as contours in Fig. 7.5(a). To help correlate the eddy viscosity difference with the flow field, the contours of the local Mach number are also shown in Fig. 7.5(b). It shows that the SA-QCR model over-predicts eddy viscosity in the separation bubble but under-predicts it in the pre-shock BL, the shear layer, the reattached BL and the shock front. Among these regions, the eddy viscosity in the pre-shock BL determines the location of the shock-induced separation point; the eddy viscosity in the separation bubble and the shear layer determines the location of the reattachment point; the eddy viscosity near the shock front, however, is generated due to the shock buffet, which is not an effect of turbulence and thus is conceptually impossible to be modeled by steady RANS simulations.

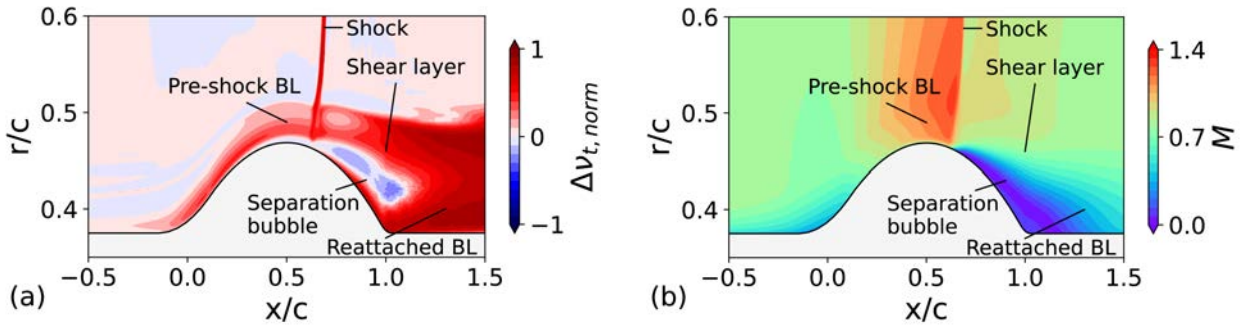


Figure 7.5: Contours of (a) normalized eddy viscosity difference (LES minus SA-QCR) and (b) Mach number (LES result) at $M_\infty = 0.875$.

To quantitatively measure the global accuracy of the ML model, the coefficient of determination R^2 , the $L1$ -type error ϵ_{L1} and the $L2$ -type error ϵ_{L2} are used, as defined in the following:

$$R^2 = 1 - \frac{\|y_t - y_p\|_F}{\|y_t - \bar{y}_t\|_F} \quad (7.4)$$

$$\epsilon_{L1} = \frac{|y_t - y_p|}{|y_t|} \quad (7.5)$$

$$\epsilon_{L2} = \frac{\|y_t - y_p\|_F}{\|y_t\|_F} \quad (7.6)$$

where y_t and y_p are the target value and the ML predicted value of the output, $(\bar{\cdot})$ is the average of a quantity, $\|\cdot\|_F$ is the Frobenius norm and $|\cdot|$ is the $L1$ norm. A good accuracy is indicated by a high R^2 value and low ϵ_{L1} and ϵ_{L2} values.

7.3 Methods to Improve Explainability of Machine Learning Model

The methods to improve the explainability of an ML model can be classified into two types: intrinsic methods and post-hoc methods [238]. The intrinsic methods improve the model’s explainability by restricting the complexity of the ML model. The rationale is that a simpler model is easier to understand for human users, and thus a higher level of explainability. An extreme example is to downgrade a random forest to a decision tree, which is self-explained. However, a trade-off between accuracy and complexity often exists—a predictive ML model can be simplified by the intrinsic method to some extent, but it does not necessarily become self-explanatory. Thus, a post-hoc method is needed for further explanations. The post-hoc methods use model-agnostic tools to analyze the ML model behavior. They can help identify the causal link between the inputs and the outputs and the interaction among different inputs.

7.3.1 Intrinsic Method

The time complexity to construct an RF model is estimated in Eq. (7.7) [239]:

$$\mathcal{O}(TNP \log_2 P) \quad (7.7)$$

where T is the number of trees, N is the maximum number of input features considered by each decision tree, and P are the number of samples. By reducing the time complexity, a simpler and thus more explainable RF model can be achieved. The $P \log_2 P$ term only depends on data and thus cannot be tuned. The rest term can be further divided into the TN/M term and the M term, where M is the total number of input features and N/M denotes the fraction of input features fed into each decision tree. Reducing T and N/M can be achieved by a hyperparameter study, which is a problem of ML and is independent of flow physics. Reducing M requires an input feature selection study, which involves knowledge of fluid mechanics. In this work, the hyperparameter study and the input feature study will be performed later in Sec. 7.4.1 and Sec. 7.4.2, respectively.

7.3.2 Post-Hoc Method

The model-agnostic explanation method named Shapley additive explanations (SHAP) [240] is used to explain the trained RF model in this work. SHAP is based on the Shapley value [241] from game theory, which assigns payouts to players depending on their contributions to a game. In the context of this work, the “game” is the prediction on $\Delta\nu_{t,norm}$; the “players” are the input features discussed in Sec. 7.2.4; the “payouts” are the contributions of each input feature to the predicted $\Delta\nu_{t,norm}$. Thus, the predicted $\Delta\nu_{t,norm}$ can be written as the sum of contributions from each feature, as denoted by Eq. (7.8):

$$\Delta\nu_{t,norm}(\mathbf{x}) = R(q_i(\mathbf{x})) = \phi_0 + \sum_{i=1}^M \phi_i(\mathbf{x}) \quad (7.8)$$

where $\mathbf{x}$ is the spatial coordinates, ϕ_i is the contribution term from q_i and is referred to as the SHAP value, and $\phi_0 = E(R(q_i))$ is the expectation of the RF prediction over ranges of all input features.

To calculate the SHAP value ϕ_i , contributions from q_i itself and all the possible coalitions between q_i and other features need to be considered. This is achieved by Eq. (7.9):

$$\phi_i = \sum_{S \subseteq Q \setminus \{q_i\}} \frac{|S|!(|Q| - |S| - 1)!}{|Q|!} \delta_i(S) \quad (7.9)$$

$$\delta_i(S) = R_x(S \cup \{q_i\}) - R_x(S) \quad (7.10)$$

$$R_x(S) = E(R(q_k)|S) \quad (7.11)$$

where the sum extends over all subsets S of the full set of input features Q excluding $\{q_i\}$; the factorial term is the weight based on probability, in which $|\cdot|$ denotes the number of elements in a set, e.g., $|Q| = M$; $\delta_i(S)$ represents the marginal contribution of $\{q_i\}$ when added to the subset S ; $E(R(q_k)|S)$ is the conditional expectation of the RF prediction, which can be efficiently calculated from the TreeSHAP algorithm [242].

The SHAP value ϕ_i provides global and local sensitivities for the RF model. The global significance of each input feature is ranked by the mean SHAP value $|\phi_i|$. By visualizing the ϕ_i field in the flow domain, it can be identified whether q_i will increase or reduce the eddy viscosity (i.e., $\phi_i > 0$ or < 0) in a specific region of interest.

Following the concept of the SHAP value, the interaction between q_i and q_j ($i \neq j$) can be quantified by the SHAP interaction value $\phi_{i,j}$ [243] defined by Eq. (7.12):

$$\phi_{i,j} = \sum_{S \subseteq Q \setminus \{q_i, q_j\}} \frac{1}{2} \frac{|S|!(|Q| - |S| - 2)!}{(|Q| - 1)!} \delta_{i,j}(S) \quad (7.12)$$

$$\delta_{i,j}(S) = R_x(S \cup \{q_i, q_j\}) - R_x(S \cup \{q_i\}) - R_x(S \cup \{q_j\}) + R_x(S)$$

where the factorial term is the weight based on probability; $\delta_{i,j}(S)$ represents the marginal contribution of $\{q_i, q_j\}$ when added to the subset S ; the total interaction effect is split equally to each feature, i.e., $\phi_{i,j} = \phi_{j,i}$, and thus the weight of 1/2. By subtracting all the interaction effects from the SHAP value, the pure effect of q_i can be defined by Eq. (7.13):

$$\phi_{i,i} = \phi_i - \sum_{j \neq i}^M \phi_{i,j} \quad (7.13)$$

The SHAP interaction value $\phi_{i,j}$ provides global and local explanations for the interaction effects between different input features. The mean SHAP interaction value $|\phi_{i,j}|$ quantifies the global significance of the interaction effect. Local interaction effects can be visualized by plotting the $\phi_{i,j}$ field in the flow domain. Interactions among three (or more) input feature $\phi_{i,j,k}$ can be derived in a similar fashion to Eq. (7.9) and Eq. (7.12), but this is not pursued in this work.

In this work, the SHAP analysis and the SHAP interaction analysis will be performed later in Sec. 7.5.1 and Sec. 7.5.2, respectively. These analyses are conducted using the open-source

7.4 Improving Explainability by Intrinsic Method

In this section, the intrinsic methods including the hyperparameter study and the input feature selection are demonstrated. The Hi-Fi data used in this section are obtained by the SST-QCR model, as justified in Sec. 7.2.3. Data at $M_\infty = 0.6, 0.8, 0.85, 0.875$ conditions form the cross-validation (CV) set, which is used for tuning the hyperparameters and selection of the input features. Afterward, two test scenarios are performed: the interpolation scenario takes data at $M_\infty = 0.9$ as the test set, bounded by the remaining conditions as the training set; the extrapolation scenario takes data at $M_\infty = 0.925$ as the test set, which is outside the remaining conditions used for training.

7.4.1 Hyperparameter Study

The hyperparameters of interest in the RF model include the number of trees T and the fraction of the input features fed to each tree N/M . In searching for an optimal set of T and N/M , a grid search is conducted in the range of $0 < T \leq 300$ and $1/9 \leq N/M \leq 9/9$. During the hyperparameter study, the RF model uses all input features listed in Table 7.2 (i.e., $M = 9$) and all data in the CV set. The performance with each set of hyperparameters is quantified by the mean R_{CV}^2 score, which is calculated from the k-fold cross-validation with $k = 5$ considering the bias-variance trade-off [244].

In Fig. 7.6(a), contours of the R_{CV}^2 score in variation of T and N/M are presented. In general, it shows that a complex RF model with large values of T and N/M is not necessarily predictive. Regarding T , the R_{CV}^2 score increases rapidly with T when $T \leq 20$; however, increasing T further shows a relatively small increment in the R_{CV}^2 score. Regarding N/M , the R_{CV}^2 score increases rapidly with N/M when $N/M \leq 4/9$; when $5/9 \leq N/M \leq 7/9$, a high R_{CV}^2 score can be achieved given a sufficiently large value of T ; increasing N/M beyond $8/9$ reduces the R_{CV}^2 score. The best accuracy is found at $T = 130$ and $N/M = 6/9$, as represented by the diamond. However, hyperparameter values in the ranges of $5/9 \leq N/M \leq 7/9$ and $T \geq 20$ can also lead to an RF model with good accuracy. A cost-effect hyperparameter set within this range is identified at $T = 20$ and $N/M = 5/9$, as represented by the triangle shape.

In Fig. 7.6(b), the R_{CV}^2 score is plotted against the inverse of the RF model complexity $(T \cdot N/M)^{-1}$, where the top-right corner represents an RF model with high accuracy and explainability. The data obtained in the grid search are represented by circles enveloped by a shaded area, and the top-right boundary of the shaded area represents the Pareto front. Any hyperparameter set on the Pareto front can be taken as the optimal set, depending on whether accuracy or explainability is of priority. In particular, the best-accuracy hyperparameter set represented by the diamond shape has $R_{CV}^2 = 0.91011$ and $T \cdot N/M = 86.67$; the cost-effective hyperparameter set represented by the triangle shape has $R_{CV}^2 = 0.90682$ and $T \cdot N/M = 11.11$. The complexity of the cost-effective set is about $1/8$ of the best accuracy set, but the reduction in the R_{CV}^2 score is only 0.004.

¹Package retrieved from: <https://github.com/slundberg/shap>. [Accessed in May 2021]

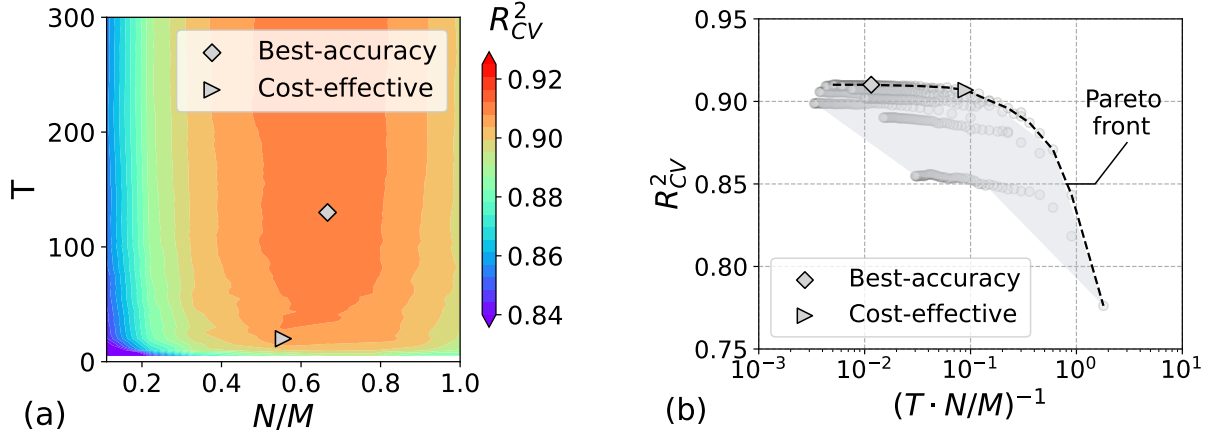


Figure 7.6: Hyperparameter study: (a) contours of mean R^2 scores; (b) mean R^2 scores versus RF model complexity.

7.4.2 Input Feature Selection

Within the input feature group (A) and (B) in Table 7.2, there is more than one feature sharing similar flow physics. To help find out the most informative feature(s) within the same group, a feature selection study is performed by using an additive method and a subtractive method. The additive method measures the performance improvement of the RF model by adding a feature to the input; here, the input refers to a subset of all the input features excluding the investigated feature group of interest. The subtractive method measures the performance deterioration of the RF model by removing a feature from the input; here, the input is the full set of input features. During the input feature selection, all data of the CV set and the best-accuracy hyperparameters are used by the RF model, and the mean R^2_{CV} score of the k -fold cross-validation procedure ($k = 5$) [244] is used to measure the RF performance.

The feature selection results of the group (A) are presented in Fig. 7.7(a). It shows that q_2 and q_3 are the most significant features, as adding either feature substantially increases the accuracy meanwhile subtracting either feature reduces the accuracy. On the contrary, q_1 seems redundant as subtracting q_1 does not reduce the RF accuracy but rather increases it. To visualize the flow regions identified by each feature, contours of q_1 , q_2 and q_3 at two representative conditions $M_\infty = 0.6$ and 0.9 are shown in Fig. 7.7(b). It is observed that q_1 and q_2 identify similar flow regions: the APG and the FPG regions in the attached flow of $M_\infty = 0.6$; the shear layer and the separation bubble in the shock-induced separation flow of $M_\infty = 0.9$. However, q_2 is more informative, because it not only informs the direction of the pressure gradient (as q_1 does) but also the pressure gradient magnitude. Thus, q_2 is selected but q_1 is dropped. On the other hand, q_3 identifies flow regions different from q_1 and q_2 because the flow physics behind these features are different: the former measures the pressure gradient magnitude, but the latter measures the streamwise component of the pressure gradient. Therefore, q_3 is also selected.

The feature selection results of the group (B) are presented in Fig. 7.8(a). It illustrates that q_4 , q_5 and q_6 have almost the same level of significance: including either one of the features to the subset of the input feature, or removing either one of the features from the full set of input features, has almost the same RF accuracy. From the contour plots of q_4 , q_5 and q_6 shown in Fig. 7.8(b), all three features identify similar flow regions including the pre-shock BL

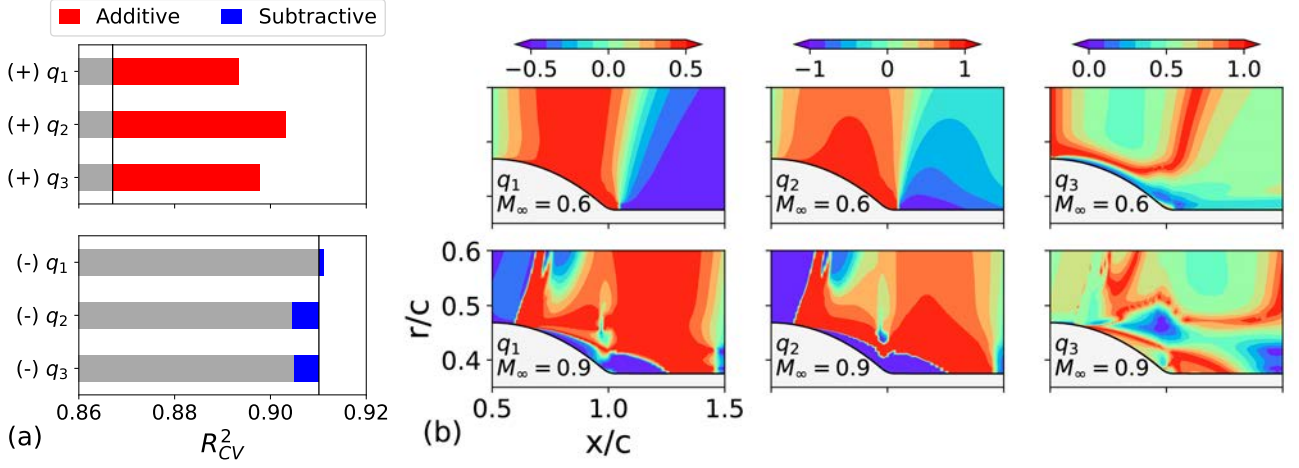


Figure 7.7: Feature selection within the group (A) pressure gradient: (a) mean R^2_{CV} scores obtained with different feature subsets (the black vertical line represents the performance without q_1, q_2 , and q_3 for the additive test and the performance with q_1, q_2 , and q_3 for the subtractive test); (b) contours of normalized input features.

near the curved surface and the shear layer downstream of the shock. Therefore, the group (B) features carry the same flow physics, although they were originally proposed for turbulence modeling by different authors. Either one of the group (B) features can be selected and the rest features can be dropped. In this work, only q_4 based on the Q-criterion is selected because its dimensionless form is free of the empirical hyperbolic tangent function.

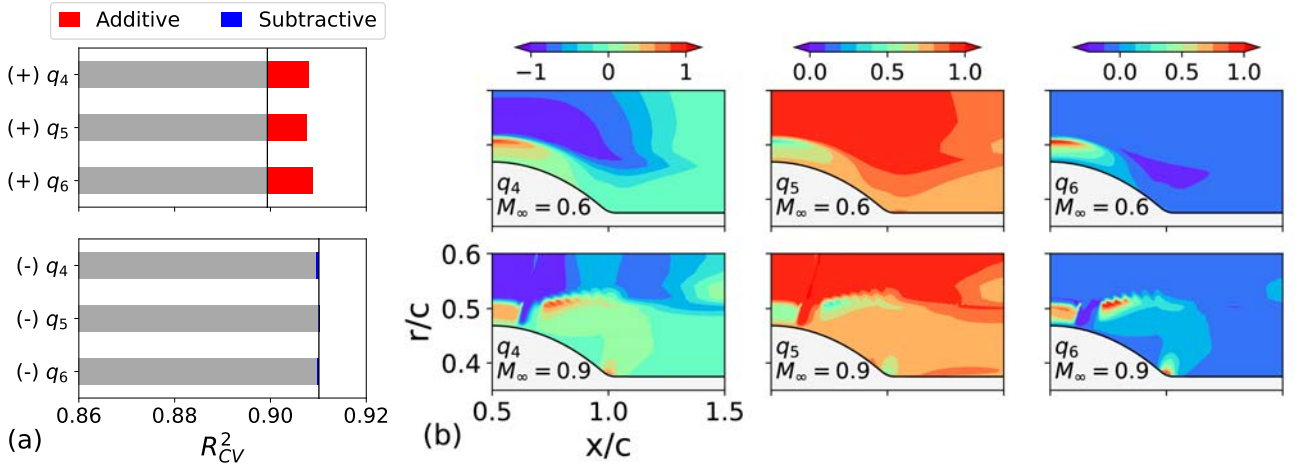


Figure 7.8: Feature selection within the group (B) strain versus rotation: (a) mean R^2_{CV} scores obtained with different feature subsets (the black vertical line represents the performance without q_4, q_5 , and q_6 for the additive test and the performance with q_4, q_5 , and q_6 for the subtractive test); (b) contours of normalized input features.

7.4.3 Comparison of Prediction Accuracy

To quantify the effect of different hyperparameter sets and input features on the RF model accuracy, the RF model is tested in an interpolation and an extrapolation scenario where the test

M_∞ is 0.9 and 0.925 respectively. Table 7.4 summarizes the prediction errors for different cases. In general, ϵ_{L2} for the extrapolation scenario is 3%-4% higher than that of the interpolation scenario, which is similar to that reported in subsonic separated flows [245]. Regarding the hyperparameters, ϵ_{L2} of the cost-effective hyperparameter set is only 0.3-1.4% higher than the best-accuracy set. Considering the cost-effective set reduces the RF model complexity to 1/8 of the best-accuracy set, this loss of accuracy is acceptable. Regarding the input features, using the selected features instead of the full features increases ϵ_{L2} by 0.2-1.1% but reduces the RF model complexity further to 2/3.

Table 7.4: Effect of input features of the random forest model on the prediction accuracy.

Random forest model					
Hyperparameter	Input feature	M	N	T	
Best-accuracy	Full features	9	6	130	
Best-accuracy	Selected features	6	4	130	
Cost-effective	Full features	9	5	20	
Cost-effective	Selected features	6	3	20	

Interpolation			Extrapolation		
R^2	ϵ_{L1}	ϵ_{L2}	R^2	ϵ_{L1}	ϵ_{L2}
0.98682	7.0%	11.0%	0.97632	10.8%	14.7%
0.98601	7.2%	11.3%	0.97551	10.9%	14.9%
0.98610	7.4%	11.3%	0.97393	11.6%	15.4%
0.98325	7.9%	12.4%	0.97057	11.9%	16.3%

For a direct comparison between the SA-QCR-ML results with the target SST-QCR results, the viscosity ratio profiles are presented in Fig. 7.9. In these figures, results from the SA-QCR-ML model using the best-accuracy hyperparameter set and the selected input features are represented by the circles; results obtained from all the four settings in Table 7.4 are enveloped by the error bars. For the interpolation scenario in Fig. 7.9(a), the SA-QCR model predicts the peak of the viscosity ratio profile at a higher radius than the SST-QCR model. The SA-QCR-ML model effectively reduces such differences and matches well with the SST-QCR model in all sections. For the extrapolation scenario in Fig. 7.9(b), a similar deficiency of the SA-QCR model is observed, and it is alleviated from the SA-QCR-ML results. In addition, it is found that using different RF settings in Table 7.4 predicts effectively the same viscosity ratio. A simple and thus more explainable ML model is sufficient to reduce the turbulence model deficiency in the current case.

7.5 Improving Explainability by Post-hoc Method

In this section, the post-hoc method SHAP [240] is demonstrated. The LES data at $M_\infty = 0.875$ from Uzun and Malik [141] is adopted to train the RF model with the best-accuracy hyperparameter set and the selected input features. The task of the SHAP method

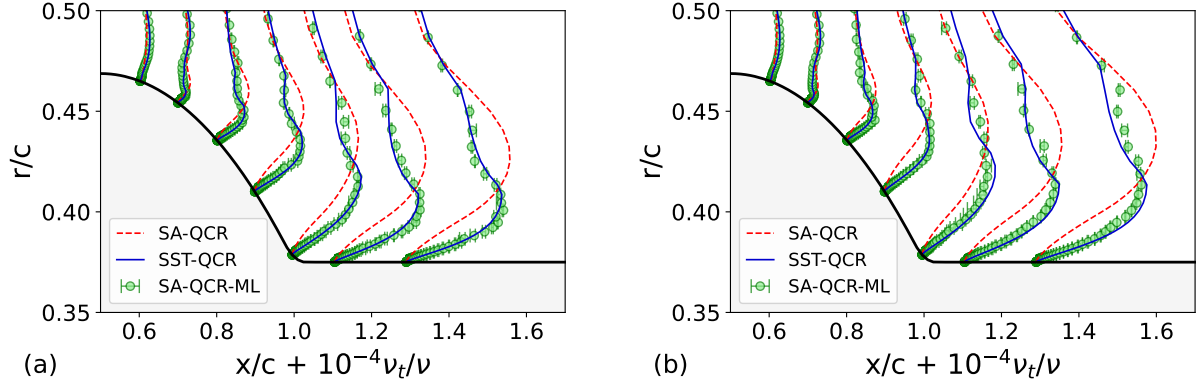


Figure 7.9: Viscosity ratio profiles: (a) $M_\infty = 0.9$ (interpolation) and (b) $M_\infty = 0.925$ (extrapolation).

is to unveil the causal link between the input features and the output eddy viscosity difference of the trained RF model.

7.5.1 SHAP Analysis

The SHAP value ϕ_i , as introduced in Sec. 7.3.2, quantifies the contribution of input feature q_i to the RF output, i.e., $R(q_i(\mathbf{x})) = \sum_{i=0}^M \phi_i(\mathbf{x})$. The SHAP values of the trained RF model for turbulence modeling are calculated, and the results are summarized in Fig. 7.10.

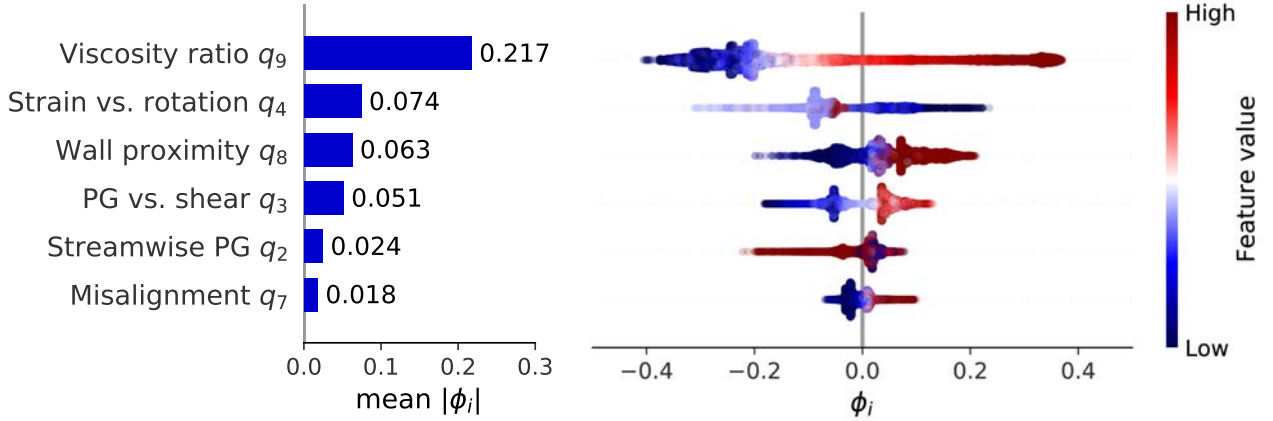


Figure 7.10: Summary of SHAP analysis. Left: bar chart of the mean absolute SHAP value. Right: bee swarm plots of SHAP values.

In the bar chart on the left of Fig. 7.10, the input features are ranked by their mean absolute SHAP values, which represent the global significance of each input feature to the output eddy viscosity difference. It shows that the contribution of viscosity ratio q_9 is significantly higher than the rest features, which was also observed in a previous research [114]. This is because the RF output is essentially an extra production or destruction term in the transport equation of the SA model, which scales with ν_t or ν_t^2 as introduced earlier in Sec. 7.2.4. The rest of the features in descending order of significance are Q-criterion-based strain versus rotation q_4 , wall

proximity q_8 , pressure normal stress versus normal shear stress q_3 , streamwise pressure gradient magnitude q_2 and flow misalignment q_7 .

In the bee swarm plot on the right of Fig. 7.10, each dot corresponds to a CFD grid point, with the horizontal location representing the SHAP value ϕ_i (impact of feature q_i on the RF prediction) and the color representing the feature value q_i at that grid point. When multiple points locate at the same horizontal position, they pile up in the vertical direction to show the occurrence probability density. From this plot, a general proportional relation between the SHAP value ϕ_i and the feature values q_i is found for the following features:

- $\phi_9 \propto q_9$, i.e., the eddy viscosity increases with the viscosity ratio. The rationale of q_9 is the scaling between $\Delta\nu_t$ and ν_t from dimensional analysis, as discussed in Sec. 7.2.4.
- $\phi_4 \propto -q_4$, i.e., the eddy viscosity is increased when the shear effect dominates over the rotation effect, and vice versa. Such an effect of q_4 has long been identified in the source term of Reynolds-stress models, as discussed in Sec. 7.2.4.
- $\phi_8 \propto q_8$, i.e., the eddy viscosity is increased near the identified BL log-law region and generally decreased in other regions. Such an observation indicates that the equilibrium turbulence assumption used by the original SA model fails in the transonic bump flow, which is featured by streamline curvature and strong pressure gradient.
- $\phi_3 \propto q_3$, i.e., the eddy viscosity is increased when the pressure normal stress dominates over the shear stress, and vice versa. The rationale of q_3 has not yet been reported and needs to be verified for future research.
- $\phi_7 \propto q_7$, i.e., the eddy viscosity is increased when the flow deviates from parallel shear flows. Note however this proportional relation is not as pronounced as the others because $|\phi_7|$ is very small.

The only exception is the streamwise pressure gradient magnitude q_2 , which has a non-monotonic relationship with the SHAP value ϕ_2 . It indicates that q_2 alone is incapable of determining the eddy viscosity difference, and interaction effects with other features may exist.

To correlate the SHAP values with the input feature values, the contours of the SHAP values and the input feature values are presented in Fig. 7.11. In this figure, the top row and the bottom row represent the SHAP value and the input feature value, respectively; each column corresponds to an input feature, and it is arranged in descending order of feature significance from left to right.

Based on the observations of the input feature values and the SHAP values, the causal link between the input and the output is interpreted as follows:

- The viscosity ratio q_9 highlights regions with high eddy viscosity (e.g., the shear layer and the reattached BL) and increases the local eddy viscosity further ($\phi_9 > 0$). The change of eddy viscosity ϕ_9 is qualitatively proportional to the feature value q_9 , which again shows the scaling between $\Delta\nu_t$ and ν_t .
- The dimensionless Q-criterion q_4 identifies the pre-shock BL and the shear layer by $q_4 > 0$, where the local rotation rate surpasses the strain rate. The eddy viscosity in these regions is decreased ($\phi_4 < 0$). On the other end, q_4 also identifies the reattached BL and the separation bubble by $q_4 < 0$, where the eddy viscosity in these regions is increased

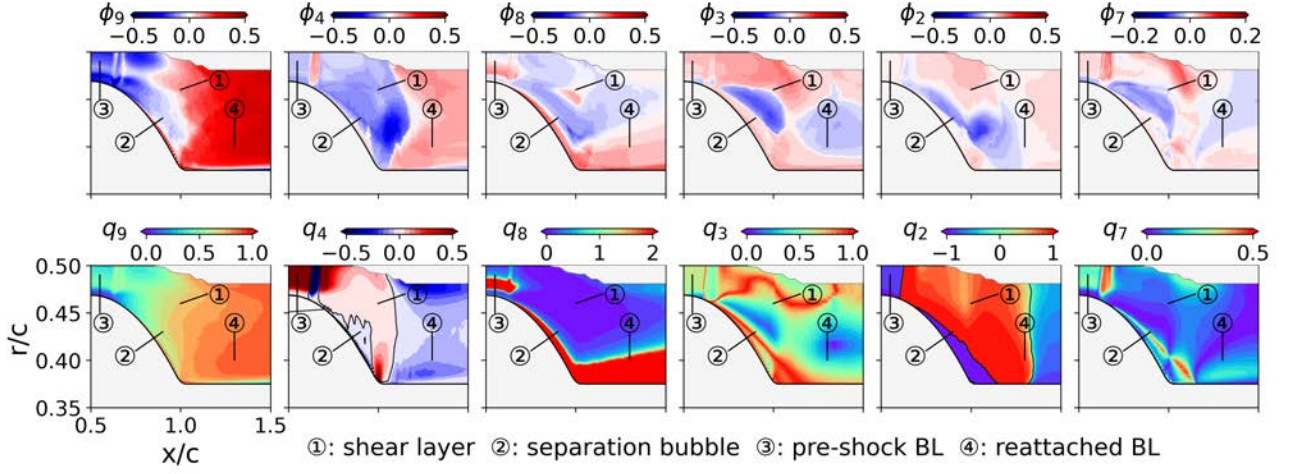


Figure 7.11: Contours of SHAP values (top row) and input feature values (bottom row). Notations of flow regions are consistent with Fig. 7.5. The isoline of $q_i = 0$ is represented by a solid curve.

($\phi_4 > 0$). It again shows the correlation that a strong shear enhances turbulence intensity whereas a strong rotation reduces it. Note however the shear layer and the separation bubble are almost indistinguishable by q_4 . Additional features are needed to distinguish these regions.

- The wall proximity q_8 identifies the near-wall log-law region (e.g., pre-shock BL and reattached BL) by a large q_8 value, and the eddy viscosity in these regions is increased ($\phi_8 > 0$). For far-wall regions with small q_8 (e.g., shear layer and separation bubble), the eddy viscosity can either be increased or decreased, indicating an interaction effect between q_8 and other features.
- The pressure normal stress versus the normal shear stress q_3 identifies the shear layer by large q_3 , where the local pressure normal stress dominates over the normal shear stress. The eddy viscosity in this region is increased ($\phi_3 > 0$). The separation bubble and the reattached BL are identified by small q_3 , indicating the local normal shear stress dominates over the pressure normal stress. The eddy viscosity in these regions is decreased ($\phi_3 < 0$).
- The streamwise pressure gradient magnitude q_2 identifies the shear layer, the upper half of the separation bubble (with forwarding flow) and the front part of the reattached BL as regions experiencing an APG ($q_2 > 0$), whereas the lower half of the separation bubble (reverse flow) and the rear part of the reattached BL are experiencing an FPG ($q_2 < 0$). However, the relation between q_2 and ϕ_2 is non-monotonic, which is consistent with the observation in Fig. 7.10.
- The flow misalignment q_7 identifies the pre-shock BL, the lower half of the separation bubble and the reattached BL by $q_7 > 0$, where the local flow deviates from the parallel flow; the upper half of the separation bubble and the shear layer are identified by $q_7 \rightarrow 0$, where the shear vanishes or the local flow is parallel. Although the effect of q_7 on the eddy viscosity field is comparatively small, a positive correlation between q_7 and ϕ_7 is still visible, which agrees with the observation in Fig. 7.10.

To sum up the SHAP analysis, it provides a ranked list of input features according to their contribution to the output eddy viscosity difference. Correlations between q_i and ϕ_i are

obtained qualitatively, but the pure effect of q_i and the interaction between q_i and other features remain unclear. These further details need to be obtained via SHAP interaction analysis.

7.5.2 SHAP Interaction Analysis

The SHAP value ϕ_i of input feature q_i can be further divided into a pure effect term $\phi_{i,i}$ and interaction terms $\phi_{i,j}$, i.e., $\phi_i(\mathbf{x}) = \sum_{j=1}^M \phi_{i,j}(\mathbf{x})$, as introduced in Sec. 7.3.2. The SHAP interaction values of the trained RF model for turbulence modeling are summarized in Fig. 7.12.

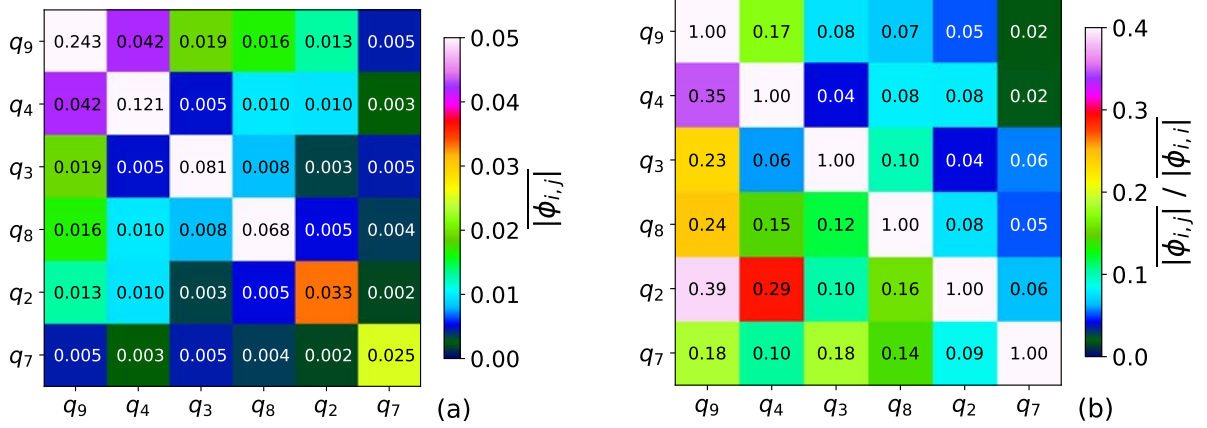


Figure 7.12: Heatmap of (a) mean absolute SHAP interaction values and (b) normalized mean absolute SHAP interaction values.

In Fig. 7.12(a), the mean absolute SHAP interaction values $|\phi_{i,j}|$ are presented in a symmetric square matrix (note $\phi_{i,j} = \phi_{j,i}$), with the diagonal elements denoting the pure effect terms and the off-diagonal elements denoting the interaction effect terms; the rows and columns are ranked in descending order of the pure effect terms $|\phi_{i,i}|$; the color and the number in each matrix element represent the corresponding value of $|\phi_{i,j}|$, which measures the global significance of the pure/interaction effects. Results show that the pure effect of each feature is generally stronger than its interaction effects with other features. The ranked list of input features by $|\phi_{i,i}|$ is almost the same as that by $|\phi_i|$. The only exception is the wall proximity q_8 which has dropped one place. It implies that q_8 relies more on the interaction effects than other features, which is expected because q_8 serves better as a flow region classifier rather than a regressor.

In Fig. 7.12(b), the mean absolute SHAP interaction values are normalized by the corresponding pure effect term, i.e., $|\phi_{i,j}| / |\phi_{i,i}|$, which shows the relative importance of the interaction effect better. Among the interaction effects, the interaction terms $\phi_{9,4}$, $\phi_{8,4}$, $\phi_{9,3}$ and $\phi_{8,3}$ are pronounced and need further examination. Interaction terms of q_2 are also significant as expected since the correlation between q_2 and ϕ_2 is non-monotonic. However, they are not examined in detail due to the low global significance of q_2 .

To help identify the correlation between the feature value q_i and its pure effect on the eddy viscosity difference $\phi_{i,i}$, $\phi_{i,i}$ are plotted against q_i in Fig. 7.13. In these plots, each scatter corresponds to a CFD grid point, whose horizontal and vertical coordinates represent the feature value q_i and the SHAP interaction value $\phi_{i,i}$ respectively; a solid curve is fitted through all the

scatter points to indicate the general relation between q_i and $\phi_{i,i}$. These plots clearly show the monotonic relations between some of the q_i and $\phi_{i,i}$, i.e., $\phi_{9,9} \propto q_9$, $\phi_{4,4} \propto -q_4$, $\phi_{3,3} \propto q_3$ and $\phi_{8,8} \propto q_8$ when ($q_8 > 0.1$), which are consistent with the observations in Fig. 7.10. In particular:

- The viscosity ratio q_9 scales with its pure effect on the eddy viscosity difference $\phi_{9,9}$.
- The dimensionless Q-criterion q_4 reduces the eddy viscosity ($\phi_{4,4} < 0$) when the rotation rate surpasses the strain rate ($q_4 > 0$), and vice versa.
- The pressure normal stress versus normal shear stress q_3 increases the eddy viscosity ($\phi_{3,3} < 0$) when the pressure normal stress surpasses the normal shear stress ($q_3 > 0.5$), and vice versa.
- The wall proximity q_8 reduces the eddy viscosity ($\phi_{8,8} < 0$) in free shear flow and the viscous sublayer ($0 < q_8 < 0.3$), but increases it ($\phi_{8,8} > 0$) in the log-law region ($0.3 < q_8 < 0.7$) and the outer part of the BL ($0.7 < q_8 < 2.0$).

Regarding the rest features, the streamwise pressure gradient magnitude q_2 is sensitive only at strong pressure gradients ($|q_2| \rightarrow 1$), and the flow misalignment q_7 is sensitive only when the flow is close to a perfectly parallel flow ($|q_7| \rightarrow 0$). Their mean effects $|\phi_{i,i}|$ are also relatively small. Thus, they are less informative than the other features in this case.

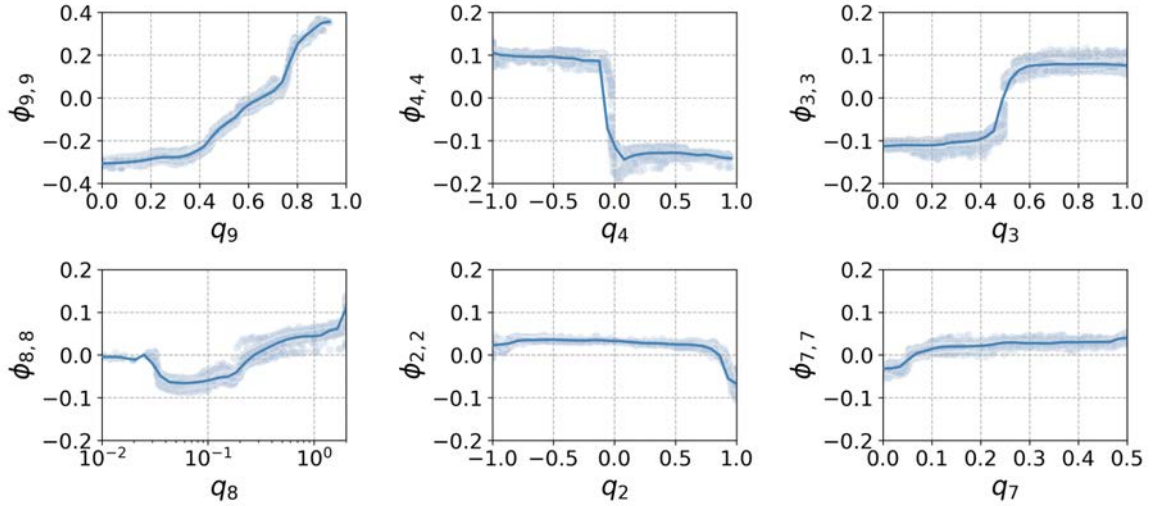


Figure 7.13: Dependency plot of feature values versus diagonal SHAP interaction values.

To help identify the interaction effect between two input features, the interaction effect terms $\phi_{i,j}$ in variation with the feature values q_i and q_j are presented in Fig. 7.14. In these plots, each scatter corresponds to a CFD grid point, whose horizontal coordinate, vertical coordinate and color represent the feature value q_i , the SHAP interaction value $\phi_{i,j}$ and the feature value q_j respectively; a solid curve is fitted through the scatters where $q_j > q_{j,mean}$, and a dashed curve is fitted through the rest scatters with $q_j < q_{j,mean}$. Observations of the interaction effects are listed as follows:

- For the viscosity ratio q_9 and the dimensionless Q-criterion q_4 , their interaction effect $\phi_{9,4}$ counteracts the pure effect $\phi_{4,4}$ when $q_9 < 0.8$ (i.e., $\nu_t/\nu < 2000$) whereas enhances it in the rest range of q_9 .

- For the viscosity ratio q_9 and the pressure normal stress versus normal shear stress q_3 , their interaction effect $\phi_{9,3}$ counteracts the pure effect $\phi_{3,3}$ when $q_9 < 0.5$ (i.e., $\nu_t/\nu < 500$) or $q_9 > 0.8$ (i.e., $\nu_t/\nu > 2000$) whereas enhances it when $0.5 < q_9 < 0.8$ (i.e., $500 < \nu_t/\nu < 2000$).
- For the wall proximity q_8 and the dimensionless Q-criterion q_4 , their interaction effect $\phi_{8,4}$ counteracts the pure effect $\phi_{4,4}$ when $q_8 < 0.1$ (i.e., free shear flow or viscous sublayer) or $q_8 > 1.6$ (i.e., near-wall BL under APG) whereas enhances it when $0.1 < q_8 < 1.6$.
- For the wall proximity q_8 and the pressure normal stress versus normal shear stress q_3 , their interaction effect $\phi_{8,3}$ counteracts the pure effect $\phi_{3,3}$ in most range of q_8 except the range of $0.04 < q_8 < 0.1$.

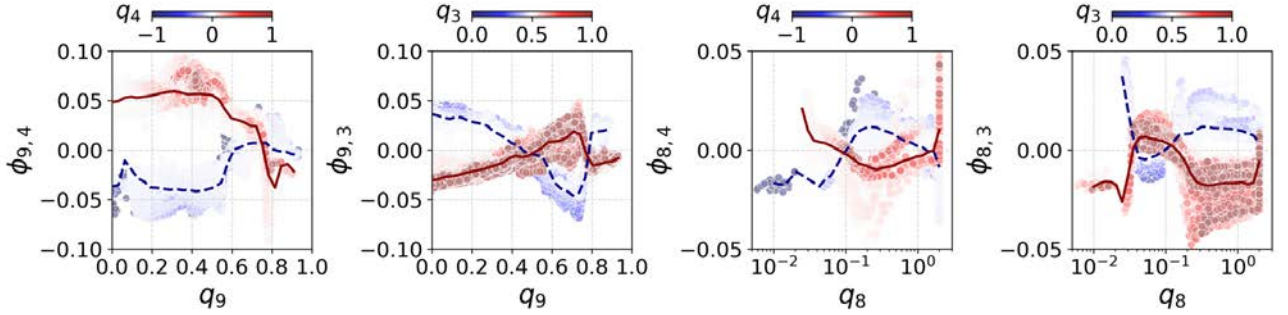


Figure 7.14: Dependency plot of feature values versus off-diagonal SHAP interaction values.

7.5.3 ML Model Explained

After the SHAP analysis and the SHAP interaction analysis, the black-box ML model that assists the SA turbulence model becomes partially transparent, as illustrated in Fig. 7.15. Here, the input features attached to the transparent box are ranked according to their global significance to the output; the arrowed lines in red or blue correspond to large or small values of the input feature. The major findings from the SHAP explanation are summarized as follows:

- The ML model has re-discovered the scaling between the eddy viscosity ν_t and its source term, which has already been found by human turbulence modelers via dimensional analysis.
- The ML model has re-discovered the shear versus rotation effect on the eddy viscosity source term (i.e., shear enhances turbulent fluctuation whereas rotation reduces it), which has already been found in Reynolds stress transport equations.
- The ML model suggests a possible correlation between the eddy viscosity source term and the ratio between the pressure normal stress and the normal shear stress (i.e., turbulent fluctuation is enhanced when the pressure normal stress dominates over the shear stress, and vice versa). Further studies in more flow cases are needed to verify this finding.

Despite the success of SHAP demonstrated above, limitations of the SHAP method do exist. Firstly, it should be reminded that the SHAP analysis is data-dependent. When training the ML model with a larger database, the input-output causal link identified by SHAP may

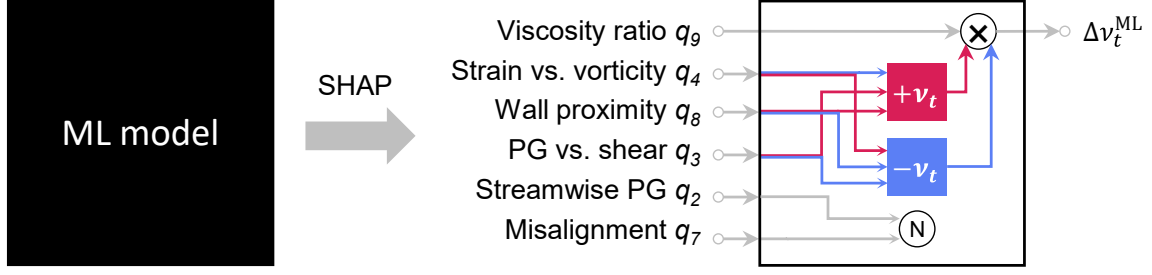


Figure 7.15: Illustration of the explained random forest model.

become more complex than that demonstrated in this work. Secondly, SHAP only describes how the model responds to the input features without offering why. A physical domain explanation still needs to be conducted by human researchers based on the SHAP results. Lastly, since the current ML-assisted turbulence model is based on a physics-informed framework, any physics beyond the range prescribed by the input features cannot be discovered by SHAP. Searching for suitable input features for RANS turbulence modeling should be regarded as the focus of future research.

7.6 Conclusions

In this chapter, two types of methods, i.e., the intrinsic methods and the post-hoc methods, were presented to improve the explainability of an ML-assisted turbulence model. The intrinsic methods improve the explainability by restricting the ML model complexity, which includes a physics-free hyperparameter study and a physics-based input feature selection. The post-hoc methods help identify the causal link between the inputs and the outputs of the ML model, among which the state-of-the-art post-hoc method SHAP was applied. The investigated ML-assisted turbulence modeling framework aims to improve the SA model accuracy in transonic bump flows. A random forest model was trained, cross-validated and tested to correct the eddy viscosity predicted by the SA model. Several conclusions can be drawn as follows.

In the hyperparameter study, a Pareto front of model complexity and model accuracy was identified, indicating the trade-off between the accuracy and complexity of the ML model. The ML model accuracy does not necessarily increase with the model complexity, and the best-accuracy hyperparameter set does exist. A cost-effective hyperparameter set was also identified, whose $L2$ -type error is 1.4% higher and model complexity is 87.5% lower than the best-accuracy set. Such a cost-effective hyperparameter set is advantageous when the model explainability or numerical efficiency is of equal concern as the model accuracy.

In the input feature selection study, it was found that dropping redundant input features can reduce the complexity and thus improve the explainability of the ML model with limited sacrifice in accuracy (e.g., 1.1% higher $L2$ -type error and 33.3% lower model complexity in this case). Among the feature group of the pressure gradient, the streamwise pressure gradient magnitude (q_2) and the pressure normal stress versus normal shear stress (q_3) were found most informative, whereas the feature regarding the alignment between the velocity and the pressure gradient (q_1) can be dropped. Among the feature group of strain versus rotation, using either one of the Q-criterion (q_4), the strain-to-vorticity ratio (q_5) or the Richardson number (q_6)

achieved the same level of accuracy. These understandings provide guidance for input feature selection for the future development of turbulence models.

By using the SHAP method, the ML model became partially explainable rather than a complete black-box system. The SHAP values provided a global significance rank of the input features, which in descending order reads viscosity ratio (q_9), Q-criterion (q_4), wall proximity (q_8), pressure normal stress versus shear stress (q_3), streamwise pressure gradient magnitude (q_2) and flow misalignment (q_7). In addition, the SHAP values also offered a local explanation of each input feature, e.g., q_4 reduced the eddy viscosity in the pre-shock BL but increases it in the reattached BL, etc. The SHAP interaction values not only showed the pure effects of input features, e.g., $\Delta\nu_t \propto q_9, -q_4, q_8, q_3$, but also unveiled the interaction effects between input features, especially the interaction with q_9 and q_8 . These results together showed that the trained SA-QCR-ML model discovered: (1) the scaling between the eddy viscosity and its source term; (2) the effect of shear and rotation on the eddy viscosity source term; (3) the effect of pressure-to-shear normal stress ratio on the eddy viscosity source term.

The methods presented in this work are transferable to a general ML turbulence model and are recommended for future ML turbulence model developments.

8. Conclusions and Future Work

8.1 Conclusions

The design of safe, efficient and reliable aero-engine compressors is hindered by the deficiency of conventional RANS turbulence models, which rely heavily on empiricism without observing turbomachinery data. This thesis pursues a data-driven turbulence modeling approach to improve the prediction of the compressor stall margin. To formulate the data-driven modeling problem, the thesis has proposed a package of tools and ideas to generate a turbomachinery turbulence database, analyze the pathology of the Spalart-Allmaras turbulence model, extract the flow features of turbomachinery, and establish an explainable machine learning framework for turbulence modeling. The major contributions are summarized as follows.

(1) DDES(SA- $F_{KH}\Delta_{hyb}$) for simulating compressor tip leakage flows.

The widely used default DES method, i.e., DDES(SA- Δ_{max}), fails to predict the RANS-to-LES transition in the shear layer of compressor tip leakage flow. The thesis has identified some recent upgrades of the DES-type method, i.e., DDES(SA- $F_{KH}\Delta_{hyb}$), to improve the prediction accuracy. The upgraded DDES method unlocks the physics of the shear-layer instability and maximizes the scale-resolving capability of the grid. In the backward-facing step case and the BUAA Stage B rotor case studied in this work, the upgraded DDES predicts both the mean flow features and the turbulence statistics qualitatively well. To the best knowledge of the author, this is the first evidence that a DES-type method can capture the turbulence kinetic energy distributions of compressor tip leakage flows. Future opportunities for the upgraded DDES method include the large-scale full-annulus compressor stall prediction and the generation of a turbomachinery turbulence database.

(2) Enhanced understandings of compressor tip leakage flows.

Based on the compressor tip leakage flow database generated by the upgraded DDES method, the steady and unsteady flow physics of compressor tip leakage flow have been analyzed.

The tip leakage flow in the investigated BUAA Stage B rotor is governed by the double-leakage flow structure. The main TLV forms immediately after detaching from the leading edge, breaks down into smaller eddies near the mid-pitch, and then forms a tip blockage cell at the casing-pressure surface corner; part of the main TLV flow passes through the tip gap of the adjacent blade, leading to the formation of a secondary TLV. When throttling the compressor towards the near stall condition, the trajectory of both TLVs moves upstream, the tip blockage cell grows in size, and the turbulent fluctuations in the near-tip spans intensify.

Further insights into compressor tip leakage flow are obtained by the modal analysis via SPOD. Results show that a major part of the total disturbance energy originates from the formation of the main TLV and the tip blockage cell, which are low-frequency and low-rank. These fluctuations correspond to the oscillating mode of the main TLV and the vortex shedding mode, respectively. When throttling the compressor towards the near stall condition, the

main TLV oscillating mode and the vortex shedding mode occupy a larger amount of total disturbance energy and show a lower frequency. These results indicate that the challenge of RANS turbulence models is to capture the increase in eddy viscosity in the tip blockage cell when approaching stall.

(3) Pathology of the Spalart-Allmaras model for compressor stall prediction.

The limitations of the SA model coefficients and the SA model formulations for compressor stall prediction have been analyzed via a comprehensive parametric UQ study and a model form evaluation study.

The UQ results show that the original SA model with different coefficient values within the calibration range can predict the attached flows and the mildly separated flows with adequate accuracy, but it cannot handle transonic flows with shock and strong separations. These results suggest that recalibration of the SA model coefficients alone is not enough for an accurate prediction of compressor stall.

The evaluation study reveals that established modifications at the transport equation level are more effective in improving the prediction accuracy compared to that at the constitutive relation level. In particular, a reduction in eddy viscosity in the pre-shock boundary layer and an increase in eddy viscosity in the compressor blockage cell can improve the prediction in transonic flows and compressor near-stall flows, respectively. These results highlight the opportunity of using a data-driven correction term at the transport equation level for better prediction of compressor stall.

(4) Novel models for transonic flows and separated compressor flows.

To improve the prediction accuracy in transonic flows, a novel modification to the SA model, i.e., SA-B, is proposed based on the dimensionless vortical baroclinicity. This modification reduces eddy viscosity in negative baroclinicity regions; while in incompressible flows, it is automatically switched off. The calibrated SA-B model achieves improved prediction on the axisymmetric transonic bump and the RAE 2822 airfoil under unseen working conditions.

To improve the prediction accuracy in separated compressor flows, a novel modification to the SA model, i.e., SA-PG $_{\omega}$, is proposed based on the dimensionless vortical pressure gradient. This modification boosts eddy viscosity in the identified compressor blockage cells featured by 3D swirling, adverse pressure gradient, and low-momentum flows; whereas in 2D canonical flows, the modification is automatically switched off. The calibrated SA-PG $_{\omega}$ model has been validated extensively in four test cases under unseen working conditions, namely NASA Rotor 67, TUDa-GLR-OpenStage, BUAA Stage B rotor, and LMFA NACA65 cascade. The SA-PG $_{\omega}$ model predicts consistently good agreement with the experimental data in terms of the tip/hub blockage size, the pressure rise capability of the compressor, and the stall margin.

(5) An explainable data-driven turbulence modeling framework.

An ML-assisted turbulence modeling framework is proposed and demonstrated in axisymmetric transonic bump flows, where a random forest model is trained, cross-validated, and tested to correct the eddy viscosity predicted by the SA model. The explainability of the model is improved by using both the intrinsic methods (e.g., hyperparameter study and input feature selection study) and the post-hoc SHAP method. Results show that the hyperparameter study and the input feature selection study can reduce the model complexity and thus improve the

model explainability with limited sacrifice in prediction accuracy. By using the SHAP method, the trained ML-assisted turbulence model is found to discover: (1) the scaling between the eddy viscosity and its source term; (2) the effect of shear and rotation on the eddy viscosity source term; (3) the effect of pressure-to-shear normal stress ratio on the eddy viscosity source term.

8.2 Future Work

Although this thesis has produced promising data-driven tools to improve compressor stall prediction, future work is still needed for a more universal turbulence model that is predictive in both academic flows and industrial flows. Proposals for future work are described below.

(1) Generation of larger turbomachinery turbulence databases.

The efficacy of a data-driven model is largely dependent on the size and quality of the training database. Based on the upgraded DDES method proposed in this thesis, a turbulence database of compressor tip leakage flow at the subsonic flow regime has been generated. However, this database does not include all flow physics of compressor near-stall flows. For future research, more databases for the following flow cases need to be generated:

- Compressor tip leakage flow at the transonic flow regime.
- Compressor corner separation flow.

Regarding the tip leakage flow at the transonic flow regime, the same upgraded DDES method can be applied to the NASA Rotor 67 or the TUDA-GLR-OpenStage rotor to generate such a database. The required number of grid points per blade passage is estimated (via the scaling with Re [33]) between 10^7 and 10^8 , which is within the capacity of many high-performance computing systems. A potential challenge lies in the convective scheme for shock capturing [246]. To obtain a stable and accurate solution for these cases, further investigations on high-order shock-capturing schemes are needed.

Regarding the corner separation flow, the upgraded DDES method can be applied to the LMFA NACA65 cascade or the TUDA-GLR-OpenStage stator to generate such a database. However, further upgrades on the baseline RANS model [184], the DDES shielding function, and the inlet turbulence boundary condition can improve prediction accuracy, which needs further investigation.

(2) A complete data-driven turbulence modeling framework for online tests.

The thesis has proved the concept of a data-driven correction to the eddy viscosity field, which can potentially improve the prediction accuracy in both academic flows and industrial flows. However, the framework was only demonstrated using 2D transonic flow data in an offline environment (i.e., the data-driven model does not interact with the CFD solver). Immediate actions following this research should be implementing the data-driven model in the CFD solver, training the model using both 2D academic flow data and 3D compressor flow data, and testing its efficacy in predicting both the eddy viscosity field and the mean flow fields. Considering the risk that a good prediction in the eddy viscosity field may not guarantee a good prediction in

the mean flow fields [3], the training of the data-driven model may need to be constrained by using high-fidelity mean flow data. This can be achieved by using the adjoint method [104, 122].

(3) Modeling of deterministic unsteadiness.

The thesis only focuses on the modeling of stochastic unsteadiness (i.e., turbulence) featured by broadband chaotic fluctuations. In real-world flow problems, there is also deterministic unsteadiness fluctuating at a constant frequency, such as rotor blade passing in turbomachinery, shock buffeting and vortex shedding [247]. Such deterministic unsteadiness can also affect the mean flow fields, but its characteristics are less well understood. For future research, the characteristics of deterministic unsteadiness and its effects on the mean flow need to be investigated. If the effect is significant in the flows of interest, a modeling framework for deterministic unsteadiness, based on either first principles or data-driven methods, needs to be established in the future.

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