

Study on the Applicability of Computational Models for RANS Simulation of Hydrogen-Xenon Mixture in a Channel

Authors: Wang Shunqi, Ji Yu, Sun Jun, Sun Yuliang, Sun Jun

Date: 2025-07-15T10:16:13+00:00

Abstract

Small gas-cooled nuclear reactor systems predominantly employ nitrogen-xenon mixtures as the working fluid and core coolant. At the recommended mixing ratio, the Prandtl number (Pr) can be as low as 0.2. The Reynolds-Averaged Navier-Stokes (RANS) method relies on turbulence models and turbulent Prandtl number (Pr_t) models. However, existing model development studies have focused primarily on the influence of Pr_t models on nitrogen-xenon heat transfer, yet have not thoroughly analyzed the role of turbulence models in heat transfer calculations, leading to a bias in understanding for subsequent Pr_t model development. Therefore, this study employs the RANS method to investigate flow and heat transfer of hydrogen-xenon gas in channels, comparing with Direct Numerical Simulation (DNS) results, sequentially conducting applicability studies of turbulence models and Pr_t models, obtaining preferred turbulence models suitable for channel flow, and elucidating the influence mechanism of turbulence models on heat transfer calculations. Results indicate that k -type models are the preferred turbulence models for channel flow; for nitrogen-xenon RANS calculations, current Pr_t models still have room for further improvement. Turbulence models are crucial for heat transfer calculations; it is recommended that for Pr_t model development for nitrogen-xenon flow and heat transfer, specific turbulence models adapted to these Pr_t models should be provided, and deviations between turbulence models and actual conditions should be integrated as coefficients to correct the Pr_t models.

Full Text

Computational Model Applicability Analysis of RANS Simulation for Helium-Xenon Mixture in a Parallel Channel

Shunqi Wang¹, Yu Ji¹, Jun Sun¹, Yuliang Sun¹

¹Institute of Nuclear and New Energy Technology, Key Laboratory of Advanced Reactor Engineering and Safety of Ministry of Education, Tsinghua University, Beijing 100084, China

Abstract

Small gas-cooled nuclear reactor systems predominantly utilize helium-xenon mixtures (He-Xe) as the cycle working fluid and reactor core coolant. At the recommended composition, the Prandtl number (Pr) of He-Xe can be as low as 0.2. The Reynolds-Averaged Navier-Stokes (RANS) method relies on turbulence models and turbulent Prandtl number (Prt) models for its simulations. However, existing model development studies have focused primarily on the influence of Prt models on He-Xe heat transfer, while inadequately analyzing the role of turbulence models in heat transfer calculations. This oversight introduces conceptual biases for subsequent Prt model development. Therefore, this paper employs the RANS method to investigate flow and heat transfer of He-Xe in a parallel channel, comparing results with Direct Numerical Simulation (DNS) data to systematically evaluate turbulence model and Prt model applicability. The study identifies preferred turbulence models for channel flow and elucidates the mechanisms by which turbulence models affect heat transfer calculations. The results demonstrate that k- class models are the optimal turbulence models for channel flows. For He-Xe RANS calculations, current Prt models still require further improvement. Turbulence model selection is crucial for heat transfer calculations, and we recommend that future Prt model development for He-Xe flow and heat transfer should specify the particular turbulence model to which the Prt model is adapted, incorporating corrections that account for deviations between the turbulence model and physical reality.

Keywords: Reynolds-Averaged Numerical Simulation; DNS Standard Data; RANS Models

Classification: TL333

Document Code: A

DOI:

1 Introduction

In nuclear engineering, helium-xenon mixtures (He-Xe) serve as the cycle working fluid and reactor core coolant for small gas-cooled nuclear reactor systems [1-3]. Research indicates that the Prandtl number of He-Xe depends solely on the mixing ratio: as the helium fraction decreases, the Pr of He-Xe first de-

creases then increases. In practical applications, the helium mole fraction is typically around 72% [4], yielding a Pr as low as 0.2—distinct from conventional working fluids. Different Pr fluids exhibit different heat transfer characteristics [5], making the investigation of He-Xe flow and heat transfer essential for thermal-hydraulic analysis of small gas-cooled reactor systems.

The Reynolds-Averaged Navier-Stokes (RANS) method is widely applied in scientific and engineering studies of working fluid flow and heat transfer due to its low computational cost and high efficiency. Previous studies [6,7] have shown that the turbulent Prandtl number (Prt) model in RANS methods significantly affects heat transfer calculation accuracy. For fluids with $Pr > 0.7$, such as water and air, a constant Prt model with $Prt = 0.85$ provides good accuracy. However, for low-Pr fluids like He-Xe and liquid metals, constant Prt models cannot effectively predict wall temperature and Nusselt number [6]. Consequently, researchers have developed variable Prt models for low-Pr fluids [6,8-11]. Yet these studies focused only on the influence of Prt models on heat transfer calculations, without deeply analyzing the role of turbulence models, creating conceptual biases for subsequent He-Xe Prt model development.

Therefore, this paper employs DNS data for He-Xe flow and heat transfer in a parallel channel [12] as the benchmark, with a Reynolds number of 13,700, to systematically evaluate turbulence model and Prt model applicability. The research approach involves first identifying optimal turbulence models for channel flow, then investigating Prt model applicability based on these models, and finally elucidating the influence mechanisms of both turbulence and Prt models on heat transfer calculations. Recommendations for He-Xe heat transfer Prt model development are provided.

2.1 Governing Equations

The governing equations for the RANS method are:

$$\begin{aligned}\frac{\partial \bar{u}_i}{\partial x_i} &= 0 \\ \frac{\partial \bar{u}_i}{\partial t} + \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} &= -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left[(\nu + \nu_t) \frac{\partial \bar{u}_i}{\partial x_j} \right] \\ \frac{\partial \bar{T}}{\partial t} + \bar{u}_j \frac{\partial \bar{T}}{\partial x_j} &= \frac{\partial}{\partial x_j} \left[(\alpha + \alpha_t) \frac{\partial \bar{T}}{\partial x_j} \right]\end{aligned}$$

where the overbar denotes time-averaged quantities, ν and α represent the kinematic viscosity and thermal diffusivity of the working fluid, respectively, while ν_t and α_t denote turbulent kinematic viscosity and turbulent thermal diffusivity—quantities with the same dimensions as ν and α but related to the turbulent flow field. The turbulence model and Prt model in the RANS method essentially solve for ν_t and α_t . The relationship between these three quantities is:

$$\alpha_t = \frac{\nu_t}{\text{Pr}_t}$$

where ν_t is obtained from the turbulence model, and Pr_t is specified by the user-defined Pr_t model, which together determine α_t .

2.2 Computational Domain and Boundary Conditions

The computational domain is a parallel channel, as shown in Figure 1 [Figure 1: see original paper]. The x, y, and z directions represent the streamwise, wall-normal, and spanwise directions, respectively. The domain dimensions are $6.4\delta \times 2.0\delta \times 3.2\delta$, where δ is the channel half-width, set to 5 mm in this study. The RANS calculations employ constant property assumptions, using the properties of He-Xe (40 g/mol) at 2 MPa and 1000 K. After sufficient development time, the flow and heat transfer become uniform in the streamwise and spanwise directions, enabling periodic boundary conditions. At the walls, no-slip velocity and constant heat flux boundary conditions are applied.

2.3 DNS Standard Data Introduction

Our research group performed DNS calculations for the domain shown in Figure 1 using the Nek5000 software [12]. Nek5000 employs the spectral element method to solve the governing equations with seventh-order numerical accuracy at Reynolds numbers of 5,600 and 13,700. For this computational domain, Kawamura et al. [5] conducted DNS calculations in 1998 and obtained dimensionless velocity and temperature fields for $\text{Pr} = 0.2$ at $\text{Re} = 5,600$. By comparing the low-Re Nek5000 results with Kawamura's data, the accuracy of the DNS results was validated [12], as shown in Figure 2 [Figure 2: see original paper]. This study selects DNS data from the high-Re case to evaluate RANS model applicability.

2.4 RANS Models for Comparison

RANS calculations were performed using Fluent software. For channel flow domains, two-equation turbulence models are typically applied. The turbulence models compared in this study include the standard k- ϵ , Realizable k- ϵ , RNG k- ϵ , standard k- ω , and SST k- ω models. The Pr_t models are listed in Table 1. In the table, Pet is the turbulent Peclet number, defined as:

$$\text{Pet} = \frac{\nu_t}{\nu} \text{Pr}$$

Table 1 Pr_t Models Selected for Comparison

Prt	Jischa et	Reynolds	Azer et	Weigand et	Zhou et
Model	Fluent al. [8]	et al. [9]	al. [10]	al. [11]	al. [6]
Dependencies	Re, Pr	Re, Pr,	Re, Pr,	Re, Pr,	-
	Pr	y/R	ν_t/ν	ν_t/ν	

2.5 Grid Independence Analysis

This study employs steady-state calculations requiring grid independence analysis. Structured grids were generated using ICEM software, with independence verified for streamwise, wall-normal, and spanwise directions, as well as first-layer grid thickness. Using streamwise pressure gradient and Nusselt number as criteria, the final grid parameters are: 22 layers in the streamwise direction, 100 layers in the wall-normal direction, and 11 layers in the spanwise direction, totaling 24,200 cells. The maximum y^+ of the first grid layer is 0.45. A schematic of the cross-sectional grid is shown in Figure 3 [Figure 3: see original paper].

3.1 Turbulence Model Applicability Analysis

The dimensionless velocity (U^+) is defined as:

$$U^+ = \frac{U}{u_\tau}$$

where U is the fluid velocity and u_τ is the friction velocity, characterizing wall friction properties, defined as $u_\tau = \sqrt{\tau_w/\rho}$, with τ_w being the wall shear stress. The U^+ profiles are shown in Figure 4 [Figure 4: see original paper], where the abscissa is the dimensionless wall distance $y^+ = yu_\tau/\nu$, with y being the perpendicular distance to the wall. Deviations between different turbulence model solutions and DNS data are relatively small. For more intuitive analysis of differences between RANS and DNS results, the relative deviation is defined as:

$$\text{deviation} = \frac{\phi_{\text{RANS}} - \phi_{\text{DNS}}}{\phi_{\text{DNS}}}$$

where ϕ represents any physical quantity. Results are shown in Figure 5 [Figure 5: see original paper]. When $y^+ < 50$, the three k- models show better agreement with DNS data. However, for $y^+ > 50$, the two k- models exhibit the highest accuracy, with relative deviations within 2%.

Under constant property assumptions, the velocity profile is only affected by ν_t . The ν_t values solved by different turbulence models are shown in Figure 6 [Figure 6: see original paper]. The three k- models show better agreement with DNS data in the region $y^+ < 75$, but display significant trend differences for

$y^+ > 75$. In contrast, the two k- models show better agreement with DNS data, with the standard k- model demonstrating the best match.

Shear stress in the flow field, determined by the product of velocity gradient and viscosity, governs pressure drop and thus pumping power requirements. The Reynolds decomposition approach in RANS methods divides shear stress into molecular shear stress (from molecular viscosity) and turbulent shear stress (from ν_t , also called Reynolds stress). Figures 7 [Figure 7: see original paper] through 9 show comparisons of molecular shear stress, turbulent shear stress, and total shear stress with DNS data.

In these RANS calculations, k- class turbulence models employ “Enhanced Wall Treatment” for near-wall flow, based on the “two-layer model” for boundary layer flows. This model assumes molecular shear stress dominates in the region $y^+ < 30$, while turbulent shear stress dominates for $y^+ > 30$. Figure 7 shows that in the $y^+ < 30$ region, the three k- models produce molecular shear stress closer to DNS data but poorer wall shear stress characterization than the two k- models—a value that directly determines pressure drop in the flow field.

In Figure 8 [Figure 8: see original paper], k- class models are slightly lower than k- class models in the $y^+ > 30$ region but closer to DNS results. However, because k- models produce larger turbulent shear stress in the $y^+ < 30$ region, enhancing turbulence effects in the inner boundary layer, their total shear stress characterization is inferior to k- class models.

Based on the shear stress data in Figures 7-9, the streamwise pressure gradient and its relative deviation from DNS data are obtained, as shown in Table 2. k- class models yield streamwise pressure gradients closest to DNS data, with relative deviations around 2.15%, outperforming other turbulence models.

Overall, although the five turbulence models exhibit varying strengths in flow field characterization, all deviations are within engineering acceptable ranges. In summary, k- class models are the preferred turbulence models for He-Xe flow and heat transfer calculations in parallel channels.

Table 2 Relative Deviation of Streamwise Pressure Gradient from DNS Data for Different Turbulence Models

Turbulence Model	Standard k-	RNG k-	Realizable k-	Standard k-	SST k-
Relative Deviation	4.92%	4.47%	4.84%	2.16%	2.15%

3.2 Prt Model Applicability Analysis

Based on the previous results, this section evaluates Prt model applicability using the SST k- turbulence model. Figure 10 [Figure 10: see original paper]

shows dimensionless temperature (T^+) profiles solved by different Prt models. T^+ is defined as:

$$T^+ = \frac{T_w - T}{T_\tau}$$

where T_w is the wall temperature, T is the fluid temperature in the domain, and T_τ is the friction temperature, defined as $T_\tau = q_w/(\rho c_p u_\tau)$, with q_w being the wall heat flux.

Figure 10 indicates that all models produce T^+ profiles similar in trend to DNS data but with significant numerical differences. In the channel flow, the constant Prt = 0.85, Reynolds et al., and Azer et al. models show smaller deviations from DNS data. However, this phenomenon contradicts previous research [6], possibly due to differences in geometry and Reynolds number. The Zhou et al. model [6], developed for higher-Re circular pipe RANS calculations, shows larger deviations from DNS data in this study. These observations suggest that existing Prt models require further improvement for He-Xe calculations.

Under constant property assumptions, temperature is a passive scalar determined by α_t . Figure 11 [Figure 11: see original paper] shows α_t profiles calculated by different Prt models. According to the Enhanced Wall Treatment model, the region $y^+ > 30$ is of primary interest. Near $y^+ = 100$, the constant Prt = 0.85 model provides the best α_t characterization, corresponding to the T^+ results. However, as the fluid approaches the mainstream region (larger y^+), wall-normal turbulent heat flux exhibits a linear decreasing trend [6], making temperature field predictions less sensitive to α_t deviations in this region.

Figure 12 [Figure 12: see original paper] shows Prt values calculated by different models. In the region near $y^+ = 100$, the constant Prt = 0.85 model shows the largest relative deviation from DNS data, contrary to the trends in Figures 10 and 11. This discrepancy arises because, according to Equation (4), α_t is determined by both ν_t and Prt. Since the selected turbulence model introduces deviations in ν_t (Figure 6), Prt models that accurately capture Prt (such as Weigand et al.'s model) produce larger α_t deviations, resulting in greater temperature field calculation errors.

This analysis demonstrates that turbulence models are equally important for heat transfer calculations. Deviations between ν_t solved by turbulence models and actual values propagate into α_t calculations, affecting heat transfer accuracy. As shown in Figure 6, different turbulence models yield significantly different ν_t values, indicating that the same Prt model combined with different turbulence models produces different heat transfer results. Previous Prt model development studies focused only on individual model performance without emphasizing turbulence model selection, leading to situations where Prt predictions match DNS data closely but α_t and temperature field accuracy are inferior to other models. Therefore, future He-Xe Prt model development must emphasize compatibility

with specific turbulence models. The recommended approach is: first identify optimal turbulence models through applicability studies, then incorporate corrections into the Prt model that account for deviations between the turbulence model's ν_t and actual values.

4 Conclusions

Based on DNS standard data for He-Xe, this study evaluates RANS computational model applicability, reaching the following conclusions:

1. Considering accuracy in solving stress fields and streamwise pressure gradients, k- class models are the preferred turbulence models for He-Xe channel RANS calculations. Regarding temperature field accuracy, existing Prt models require further improvement for effective He-Xe applications.
2. Turbulence and Prt models jointly determine α_t and thus temperature field calculation accuracy. For He-Xe Prt model development, final models must emphasize compatibility with turbulence models, incorporating corrections that account for deviations between turbulence model ν_t predictions and actual values.

References

- [1] LIU J Z, HU C B, PANG F C, et al. Chinese Science: Technology Science, 2020, 50(9): 1126-1139. (in Chinese)
- [2] YE X W, WANG D, QIN T, et al. Ship Engineering, 2023, 45(5): 159-167. (in Chinese)
- [3] LIU X Y, GUAN C R, DENG J L, et al. High Power Laser and Particle Beams, 2023, 35(11): 116002_1-9. (in Chinese)
- [4] EL-GENK M S, TOURNIER J M. Nucl Eng Des, 2008, 238: 1353-1372. doi: 10.1016/j.nucengdes.2007.10.021
- [5] KAWAMURA H, OHSAKA K, ABE H, et al. Int J Heat Fluid Fl, 1998, 19: 482-491. doi: 10.1016/S0142-727X(98)10026-7
- [6] ZHOU B. Study and application of flow and heat transfer characteristics of helium and xenon mixtures[D]. Beijing, China, 2022: 17-42. (in Chinese)
- [7] MENG T. Characteristic analysis and research of 700 kWe gas-cooled space reactor and System Transient Characteristics[D]. Haerbin, China, 2019: 73-105. (in Chinese)
- [8] JISCHA M, RIEKE H B. Int J Heat Mass Transfer, 1979, 22: 1547-1555. doi: 10.1016/0017-9310(79)90134-0
- [9] REYNOLDS A J. Int J Heat Mass Transfer, 1975, 18: 1055-1069. doi: 10.1016/0017-9310(75)90223-9

[10] KAYS W M. ASME J Heat Transfer, 1994, 116: 195-284. doi: 10.1115/1.2911398

[11] WEIGAND B, FERGUSON J R, CRAWFORD M E. Int J Heat Mass Transfer, 1997, 40(17): 4191-4196. doi: 10.1016/S0017-9310(97)00084-7

[12] WANG S Q, JI Y, SUN J, SUN Y L. Effect research of Reynolds number on distribution of Prt of helium-xenon mixtures[C]. Proceedings of the 4th Academic Annual Conference of the Nuclear Reactor Thermal Fluid Dynamics Branch of the Chinese Nuclear Society, Beijing, China, 2024. (in Chinese)

Note: Figure translations are in progress. See original paper for figures.

Source: ChinaXiv –Machine translation. Verify with original.