Uncertainty Quantification of SST k-ω Turbulence Model Parameters for Flow in the Reactor Upper Plenum

Authors: Li Xiaobin, Guo Liqi, Xiaobin Li

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Abstract

The temperature oscillation phenomenon in the upper plenum of a lead-based reactor core constitutes one of the critical factors influencing the safe and stable operation of nuclear power plants, and its accurate depiction holds significant importance for analyzing thermal pulsation mechanisms. Numerical simulation studies of this phenomenon were conducted using the SST k-ω turbulence model, quantitatively analyzing the influence of three parameters—$ $1, $ $2, and β—*in the model on temperature results and their uncertainty intervals, and performing parameter sensitivity analysis. The findings reveal that the distribution characteristics of temperature uncertainty are intimately correlated with fluid flow and mixing processes. Regions in the immediate vicinity of the nozzle exhibit relatively low temperature uncertainty due to direct nozzle jet influence, whereas the intermediate zone between hot and cold nozzles displays comparatively higher uncertainty stemming from vigorous fluid mixing, with parameters $ $2 and P* particularly contributing substantially to temperature result uncertainty within the investigated scope. These discoveries offer scientific guidance for subsequent model refinement and engineering applications.

Full Text

Uncertainty Quantification of SST k-ω Turbulence Model Parameters in Upper Plenum Flow of Nuclear Reactors

Guo Liqi[1], Li Xiaobin[1]*, Zhang Hongna[1], Li Fengchen[1], Meng Shuqi[2]
[1]School of Mechanical Engineering, Tianjin University, Tianjin 300350, China
[2]China Nuclear Power Technology Research Institute Co., Ltd., Shenzhen 518000, China

Abstract

The temperature oscillation phenomenon in the upper plenum of lead-based reactor cores is one of the key factors affecting the safe and stable operation of nuclear power plants, and its accurate description is of great significance for analyzing thermal striping mechanisms. This study employs the SST k-ω turbulence model for numerical simulation of this phenomenon, quantitatively analyzing the impact of three parameters ($ $1, $ $2, and β) *on temperature results and their uncertainty intervals, along with parameter sensitivity analysis. The results demonstrate that the distribution characteristics of temperature uncertainty are closely related to fluid flow and mixing processes. Regions near the nozzles exhibit relatively low temperature uncertainty due to the direct influence of jet flow, while intermediate regions between cold and hot nozzles show relatively high uncertainty due to intense fluid mixing. In particular, the $ $2 and* β parameters contribute significantly to temperature result uncertainty within the studied range. These findings provide scientific guidance for subsequent model improvements and engineering applications.

Keywords: Turbulence Model; Temperature Oscillation; Uncertainty Quantification; Sensitivity Analysis

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The fuel assemblies in nuclear reactor cores consist primarily of rod bundles with different functions, such as fuel rods and control rods. Since the heat generation rates of these bundles vary, the coolant temperatures flowing through different channels differ. When coolants of different temperatures mix in the upper plenum of the reactor core, complex high-frequency temperature oscillations occur, known as thermal striping. This phenomenon generates cyclic thermal stresses in critical metallic components, leading to thermal fatigue over time, accelerating material aging, and reducing structural integrity and reliability. Additionally, temperature oscillations interfere with the measurement accuracy of core outlet temperatures, affecting normal operation and protective actions of nuclear power plants, posing a potential threat to safe operation [1]. Lead-based reactors, as an advanced reactor type, use liquid lead or lead-bismuth alloy coolants with unique flow and heat transfer characteristics and very low Prandtl numbers (Pr), making the temperature oscillation phenomenon particularly complex and challenging to study [2]. Therefore, in-depth research on thermal striping in lead-based reactors is crucial for optimizing nuclear reactor design and improving operational safety and reliability.

Computational Fluid Dynamics (CFD) is one of the primary methods for studying temperature oscillation phenomena. Related numerical simulation methods include Direct Numerical Simulation (DNS), Large Eddy Simulation (LES), and Reynolds-Averaged Navier-Stokes (RANS) simulation. Among these, the RANS method simplifies turbulence description through modeling, requiring fewer computational resources and offering higher efficiency, making it the preferred approach for engineering applications. The SST k-ω turbulence model, as a commonly used turbulence model in RANS methods, combines the advantages of k- and k-ω models and can accurately simulate many complex flow phenomena. It is frequently used for flow and heat transfer simulations in reactors. Li et al. [3] simulated the flow and heat transfer characteristics of liquid lead-bismuth in triangular rod bundles, finding that the SST k-ω turbulence model could accurately capture near-wall turbulent flow. He et al. [4] conducted numerical simulations of lead-bismuth flow in the CiADS subcritical reactor, discovering that the SST k-ω turbulence model had lower grid resolution requirements and could better predict fully developed flow. Jeong et al. [5] used the SST k-ω turbulence model to simulate three-dimensional flow phenomena in wire-wrapped fuel assemblies, investigating complex vortex flow patterns within wire-wrapped rod bundle channels. Liu et al. [6] studied fluid-structure coupling and stress distribution in T-junctions through numerical simulation, comparing results from different turbulence models and finding that the SST k-ω turbulence model could more accurately calculate flow field details, yielding results closer to experimental data.

However, the application of RANS methods introduces significant uncertainty due to inherent modeling and assumptions. The engineering field has not yet widely adopted quantitative evaluation of turbulence model parameter uncertainties and their impact on simulation results. NASA's vision for CFD development by 2030 specifically emphasizes that effective management of turbulence model parameter uncertainties and errors is a key requirement for future CFD technology development [8]. Therefore, in-depth investigation of uncertainty quantification for turbulence model parameters in RANS methods is crucial for improving CFD simulation accuracy and reliability.

Uncertainty quantification analysis methods based on probability theory can effectively quantify the impact of input uncertainties on output results. Initially widely applied in engineering design and reliability analysis, these methods have gradually been introduced to turbulence model uncertainty analysis, providing strong support for related research. In CFD, the Non-Intrusive Polynomial Chaos (NIPC) expansion method has become a commonly used and effective uncertainty quantification approach. This method constructs basis functions based on random input variables and describes output results through polynomial chaos expansion, establishing a surrogate model between output responses and random inputs. Based on this surrogate model, efficient uncertainty analysis can be conducted, providing a powerful tool for understanding uncertainty propagation mechanisms in turbulence models.

This paper employs the SST k-ω turbulence model for numerical simulation of temperature oscillation phenomena in nuclear reactor upper plenums, introducing uncertainty quantification analysis to quantitatively evaluate the impact of model parameter uncertainties on flow calculation results. Through sensitivity analysis, we investigate and precisely identify key parameters in the SST k-ω turbulence model that significantly affect results. This process not only provides a solid theoretical basis for subsequent model optimization and improvement but also establishes a scientific foundation for engineering applications, ensuring the reliability and applicability of the model in complex flow simulations such as reactor thermal hydraulics.

2.1 Model and Grid

In research on upper plenum temperature oscillations, the parallel triple-jet physical model is widely used for analysis and simulation [9,10]. Its geometric structure is relatively simple, facilitating numerical simulation and uncertainty analysis. However, it should be noted that the actual upper plenum geometry is more complex, with internal structures and boundary conditions differing from the simplified parallel triple-jet model. Nevertheless, this study focuses on establishing a systematic, scientific, and universal uncertainty quantification methodology for numerical simulation of upper plenum temperature oscillation problems, rather than pursuing high-precision simulation of the actual upper plenum. Therefore, differences in Reynolds numbers and geometric characteristics between the parallel triple-jet model and actual upper plenum do not pose issues for this study. The key lies in methodology establishment and validation.

The research object in this paper is the parallel triple-jet geometric model shown in [Figure 1: see original paper]. The fluid mixing region is a rectangular prism with dimensions of 0.3 m $\times$ 0.1 m $\times$ 0.6 m (length $\times$ width $\times$ height). The fluid pipes are 0.02 m long and 0.1 m high, with horizontal spacing of 0.05 m. All three inlet cross-sections measure 0.02 m $\times$ 0.1 m. To establish a turbulence model uncertainty quantification methodology, this study selects water as a substitute working fluid, which has precedent in upper plenum temperature oscillation research and provides abundant experimental data and numerical simulation experience.

Grid division details are shown in [Figure 2: see original paper]. The total grid count is 5.4 million, with the first boundary layer grid height of 5×10^{-5} m, a growth rate of 1.2, 18 layers, and grid quality exceeding 0.9. For boundary conditions, velocity inlets are set at the model bottom with a flow velocity of 0.5 m/s. The two side inlets are hot fluid inlets at 303.15 K, while the middle inlet is a cold fluid inlet at 298.15 K. The model top is a pressure outlet boundary with relative pressure of 0 Pa. All other surfaces have no-slip adiabatic wall boundary conditions. The solver uses the SIMPLE algorithm, with standard discretization for pressure terms, central differencing for momentum discretization, and second-order upwind scheme for energy terms.

2.2 Turbulence Model

The SST k-ω turbulence model was proposed by Menter [11]. This model combines k-ω and k- models through a blending function, effectively avoiding sensitivity to inlet conditions and reducing reliance on wall functions for near-wall flow calculations. The model solves transport equations for turbulent kinetic energy k and specific dissipation rate ω, combined with a specific turbulent viscosity model, to calculate Reynolds stresses.

In these equations, β is the dissipation term coefficient in the ω equation. In temperature fields, turbulent dissipation rate affects the conversion of turbulent energy to internal energy, thereby influencing temperature distribution. Here, $ $1 is the coefficient for near-wall region calculations, ensuring accurate simulation of boundary layer flow; $ $2 is the coefficient for regions far from walls; and β* is the coefficient related to cross-dissipation terms, affecting the interaction between turbulent energy k and specific dissipation rate ω. These parameters influence the simulation accuracy of boundary layer flow, free shear flow, and separation/reattachment phenomena, while also affecting turbulence model prediction precision for temperature fields. This study focuses on investigating the contribution of these three parameters to temperature simulation result uncertainties. The baseline values and uncertainty intervals of model parameters are shown in .

2.3 Grid Independence Verification

In the calculations, grid independence verification was performed using grids of different scales with 4 million, 5.4 million, and 7.3 million cells. Temperature results along the x-direction at different heights served as the benchmark, with results shown in [Figure 3: see original paper]. The simulation results are essentially similar between the 5.4 million and 7.3 million grid cases, so the 5.4 million grid was adopted for subsequent numerical simulations. [Figure 4: see original paper] shows temperature variation in the x-direction at height z=0.07 m, comparing our simulation results with experimental data from references [12], [13] and LES simulation results, demonstrating good agreement.

2.4 Uncertainty Quantification Methodology

The Non-Intrusive Polynomial Chaos (NIPC) method is commonly used for uncertainty analysis in CFD. This method constructs a surrogate model to replace direct CFD numerical simulation, significantly reducing computational complexity and resource consumption. The surrogate model effectively propagates turbulence model parameter uncertainties to calculation results [14,15]. The surrogate model is expressed as:

$$y(\xi) = \sum_{i=0}^{P} a_i \Psi_i(\xi)$$

where $y(\xi)$ is the system output (calculation result), ξ represents input variables (in this study, parameters in the SST k-ω turbulence model), $\Psi_i(\xi)$ is the polynomial chaos expansion based on input variables ξ, a_i are polynomial coefficients, and $\Psi_i(\xi)$ are orthogonal basis functions. Legendre polynomials are selected as the orthogonal basis functions [16].

The surrogate model construction process primarily involves building and solving the equation system. This requires sampling within the parameter uncertainty range, with sample size N_t determined by:

$$N_t = n_p \cdot \frac{(n+p)!}{n!p!}$$

where n_p is the oversampling rate ($n_p = 2$ in this study), n is the number of random variables ($n = 3$), and p is the polynomial order ($p = 2$). Latin Hypercube Sampling [17] is employed. Based on N_t sets of turbulence model parameter samples, CFD simulations calculate corresponding response results for each parameter set. Least squares fitting is used to solve for chaos polynomial expansion coefficients, constructing the surrogate model that efficiently approximates the complex relationship between turbulence model parameters and simulation results.

Based on the constructed surrogate model, Monte Carlo simulation is further applied to random input variables. With a simulation sample size of 1 million, the surrogate model rapidly calculates corresponding output values to compute uncertainty U_Q using:

$$U_Q = \frac{V_{\max} - V_{\min}}{\mu^*}$$

where $V_{\max}$ and $V_{\min}$ are the maximum and minimum output values, and μ^* is the mean output, completing the systematic quantification analysis of turbulence model parameter uncertainty impact on calculation results.

Sensitivity analysis employs the global sensitivity analysis method based on Sobol indices to evaluate the relative contribution of model parameters to uncertainty [18]. The Sobol index represents the ratio of random variable variance to total variance:

$$S_i = \frac{D_i}{D}$$

where S_i is the Sobol index for the i-th polynomial term, D_i is the variance of the i-th term, and D is the total variance. A larger calculated Sobol index for a parameter indicates greater sensitivity of the simulated physical quantity to that parameter, making the parameter more critical for predicting that quantity.

3.1 Flow Field Results

[Figure 5: see original paper] presents velocity and temperature field contours in the y=0.05 m plane after steady-state convergence using default turbulence model parameters (baseline values). Cold fluid flows vertically out from the middle, while hot fluids on both sides tilt toward the central region, achieving fluid mixing. In the region between cold and hot nozzles, temperature and velocity gradients are large, indicating intense fluid mixing and rapid temperature changes.

Further analysis shows temperature distributions at measurement points along the x-direction at heights z=0.07 m, 0.3 m, and 0.6 m in [Figure 6: see original paper]. Temperature is lowest near the middle nozzle and highest near the side nozzles. In the transition region between cold and hot nozzles, large temperature gradients occur, causing temperature oscillation phenomena.

3.2 Uncertainty Quantification Analysis

[Figure 7: see original paper] shows residual values between fitted curves and simulation results for temperature distributions at different heights (z=0.07 m, 0.3 m, 0.6 m). By comparing residual variation trends at different heights, the precision performance of the fitting model in each region can be visually assessed. Residuals for 95% of sample points are controlled within $±$0.2 K, indicating high reliability of the established surrogate model. [Figure 8: see original paper] presents uncertainty quantification results for temperature parameters along the x-direction at different heights (z=0.07 m, 0.3 m, 0.6 m). These results are based on training samples from Latin Hypercube Sampling and Monte Carlo simulation via the surrogate model to obtain mean temperature and uncertainty interval boundaries. specifically provides temperature uncertainty distributions at measurement points on the y=0.05 m plane.

The results show that model parameter uncertainties affect predicted temperatures. Temperature uncertainty is smaller near nozzle positions because these regions are primarily directly influenced by jet temperatures, making temperature values relatively stable. In the x-direction, intermediate regions between cold and hot nozzles experience mixing effects from both temperature fluids, resulting in higher temperature uncertainty in numerical simulations.

As flow develops along the positive z-direction, temperature uncertainty directly facing the nozzles gradually increases because jet mixing with surrounding fluid becomes more complex, increasing temperature distribution uncertainty. In regions between cold and hot nozzles, fluid mixing becomes more uniform, reducing uncertainty. Near side walls, flow velocity is slower and velocity/temperature distributions are relatively stable, resulting in smaller temperature uncertainty that remains essentially constant in the z-direction.

3.3 Parameter Sensitivity Analysis

[Figure 9: see original paper] shows Sobol index distributions for temperature parameters along the x-direction at different heights (z=0.07 m, 0.3 m, 0.6 m), where bar charts represent variance and curves show variations in Sobol indices for turbulence model parameters $ $1, $ $2, and β*. presents average Sobol index proportions for the three turbulence model parameters at different cross-sections. Larger Sobol index values indicate greater parameter influence on temperature results at that location.

The results demonstrate that the $ $2 parameter contributes significantly to temperature result uncertainty within the studied range. Parameter $ $2 is the calculation coefficient in regions far from walls, related to turbulence generation in the ω equation, affecting turbulence energy generation rates and consequently flow turbulence characteristics. In temperature fields, this influences fluid mixing and heat exchange processes, creating substantial impact on temperature distribution. β^* is the coefficient related to cross-dissipation terms, affecting interaction between turbulent energy and specific dissipation rate. In temperature fields, k and ω distributions directly influence turbulent mixing characteristics, and β^* indirectly affects temperature field mixing and distribution by regulating interactions between k and ω.

4 Conclusions and Outlook

This paper investigates temperature oscillation phenomena in the upper plenum of lead-based reactor cores using the SST k-ω turbulence model, establishes a parametric uncertainty calculation method, and quantitatively analyzes the impact of three parameters ($ $1, $ $2, and β^*) on temperature uncertainty. The main conclusions are:

1. Temperature uncertainty distribution characteristics are closely related to fluid flow and mixing processes. Regions near nozzles exhibit relatively low temperature uncertainty due to direct jet influence, while intermediate regions between cold and hot nozzles show relatively high uncertainty due to intense fluid mixing.
2. The $ $2 parameter in the turbulence model contributes significantly to temperature result uncertainty within the studied range, with Sobol index proportions exceeding 40%.

Given the complexity of temperature oscillation phenomena in lead-based reactor upper plenums and the numerous involved variables, future research will extend to higher-dimensional and multi-parameter numerical simulation uncertainty quantification analyses to more comprehensively understand and predict temperature oscillation behavior in reactor upper plenums, thereby providing more complete theoretical support for lead-based reactor design, safety analysis, and operation.

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Corresponding author: LI Xiaobin, E-mail: lixiaobin@tju.edu.cn.

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