Bayesian uncertainty analysis of SA turbulence model for backward-facing step simulations

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Abstract. The Reynolds averaged Navier-Stokes models are still the workhorse in current engineering applications due to its high efficiency and robustness. However, the closure coefficients (also known as model parameters) of turbulence models are calibrated by model builders according to some fundamental flows, and the values suggested by the model builders may not be applicable to all flow types. In this work, the Bayesian method is applied to recalibrate the closure coefficients of SA turbulence model to improve its performance in backward-facing step problem. The results show that the four parameters $C_{b1}$, $C_w$, $C_{t1}$ and $\kappa$ are well informed by the experimental data of skin friction coefficient. The recalibrated model parameters show better performance than the nominal values in the prediction of skin friction coefficient.

1. Introduction
Backward-facing step flow is a classical fluid mechanics problem and often appears as a basic flow type in many complex engineering applications. With the development of computer technology, direct numerical simulation (DNS) and large eddy simulation (LES) are employed by many researchers to simulate the backward-facing step flow [1][2]. However, in many engineering applications, ones only focus on the mean flow, and the unsteady fluctuations are not of concern. Therefore, the Reynolds averaged Navier-Stokes (RANS) models are still the workhorse in current engineering applications due to its high efficiency and robustness [3]. The RANS method adopts some assumptions in the modeling process, which makes the numerical simulation results problem-dependent [3]. Moreover, the turbulence models often contain some closure coefficients (also called model parameters), which are calibrated by model builders according to some fundamental flows. The values of model parameters suggested by the model builders, often referred to as nominal values, may not be applicable to all flow types. Hence it is necessary to recalibrate the model parameters of turbulence models for a specific flow type. The Bayesian method is a good choice for parameter estimation. Cheung et al. [4] carried out the first application of Bayesian uncertainty quantification method to turbulence models. They calibrated the model parameters of Spalart-Allmaras (SA) turbulence model using incompressible boundary layer data. Subsequently, Edeling et al. [5] and Guillas et al. [6] applied the Bayesian method to different turbulence models and different flow types. In this work, the model parameters of SA turbulence model are recalibrated to improve its performance in backward-facing step problem, and the uncertainty of the quantities of interests (QoIs) is also quantified.
2. Numerical methods

All the simulations presented here are obtained by an in-house finite volume solver, and its reliability has been validated by various simulations [7]. The three-dimensional RANS equations are solved on structured meshes. The details of SA turbulence model can be found in Reference [8]. Referring to the previous works of Cheung et al. [4], 7 parameters of the SA turbulence model are considered in the calibration, namely $C_{b1}, C_{b2}, \sigma, C_w, C_v, C_{w3}$, and $\kappa$. In order to carry out Bayesian parameter estimation, the prior distributions of model parameters need to be given in advance. All parameters are assumed to have uniform prior distributions. The prior ranges of parameters are determined according to the work of Cheung et al. [4]. In order to ensure the stability of numerical solution, the prior range of parameter $\kappa$ is narrowed from $\pm 50\%$ of the nominal value to $\pm 30\%$ of the nominal value. The prior ranges and nominal values of all parameters are given in Table 1.

### Table 1. Prior ranges and nominal values of all parameters.

| Parameter | Normal | Lower   | Upper   |
|-----------|--------|---------|---------|
| $C_{b1}$  | 0.1355 | 0.101625| 0.169375|
| $C_{b2}$  | 0.622  | 0.4665  | 0.7775  |
| $\sigma$  | 0.667  | 0.6     | 1       |
| $C_w$     | 0.3    | 0.15    | 0.45    |
| $C_{w3}$  | 2      | 1       | 3       |
| $C_v$     | 7.1    | 3.55    | 10.65   |
| $\kappa$  | 0.41   | 0.287   | 0.533   |

3. Bayesian uncertainty quantification approach

The dataset $X = \{(x^{(i)}, y^{(i)})\}_{i=1}^L$ is assumed to be a set of calibration data. The scalar $y^{(i)}$ is the observed value of flow variable (such as pressure coefficient and friction coefficient) at a certain position $x^{(i)}$. The following relation can be obtained:

$$y^{(i)} = f(\lambda; x^{(i)}) + \delta(x^{(i)}) + \epsilon_i$$  \hspace{1cm} (1)

where $f(\lambda; x^{(i)})$ represents the approximate model (such as the turbulence model) obtained by applying some assumptions, $\lambda$ is the model parameters, $\delta(x^{(i)})$ is the model-inadequacy term and $\epsilon_i$ is the measurement error. The measurement errors are assumed to be independent identically distributed (i.i.d.) Gaussian errors with vanishing mean

$$\epsilon_i \sim N(0, \sigma^2)$$ \hspace{1cm} (2)

To embed the model error, the original model parameters are augmented by a multivariate normal random variable as

$$\lambda \rightarrow \lambda = \lambda + \mathcal{N}(0, \Sigma)$$ \hspace{1cm} (3)

where

$$A(\alpha) = \begin{bmatrix} \alpha_{11} & 0 & 0 & \cdots & 0 \\ \alpha_{21} & \alpha_{22} & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \alpha_{M1} & \alpha_{M2} & \alpha_{M3} & \cdots & \alpha_{MM} \\ 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 \end{bmatrix}_{D \times M}$$

and

$$\Sigma = \begin{bmatrix} \sigma_1^2 & \cdots & \sigma_M^2 \\ \vdots & \ddots & \vdots \\ \sigma_M^2 & \cdots & \sigma_1^2 \end{bmatrix}_{M \times M}$$ \hspace{1cm} (4)
Here \( \xi \) is a vector of i.i.d. standard normal variables. The random vector is described by the new parameters set \( \hat{\lambda} = (\xi, \alpha) \). The relation (1) can be rewritten as

\[
y^{(o)} = f_\xi(x^{(o)}, \xi) + \sigma^2_M \xi_{M,i}
\]

(5)

where \( f_\xi(x, \xi) \) is a random process, and its mean and variance are expressed as \( \mu_\xi(x) \) and \( \sigma^2_\xi(x) \). The parameter estimation of \( \lambda \) is now transformed into a parameter estimation of \( \hat{\lambda} = (\xi, \alpha) \). Bayes’ theorem is applied to solve the parameter estimation problem. It can be expressed as

\[
p(\hat{\lambda} | X) \propto p(X | \hat{\lambda}) p(\hat{\lambda})
\]

(6)

where \( p(\hat{\lambda}) \) represents the prior distribution of the parameters, \( p(X | \hat{\lambda}) \) is the likelihood function, and \( p(\hat{\lambda} | X) \) is the posterior distribution of the parameters. The likelihood function is given as

\[
\log p(\hat{\lambda} | X) = -\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{m} \left( y^{(i)}(x^{(i)}) - \mu_\xi(x^{(i)}) \right)^2 + \frac{1}{2} \sum_{i=1}^{n} \log 2\pi \sigma^2_\xi(x^{(i)}) + \sigma^2
\]

(7)

The adaptive Metropolis-Hastings MCMC algorithm [9] is employed to obtain posterior samples by sampling from the joint posterior probability distribution of the parameters. The non-intrusive polynomial chaos (NIPC) is used to map flow variables to model parameters to reduce the computational cost. The Latin Hypercube sampling method is employed to sample from the prior distributions. The training set contains 108 samples, which are obtained by Latin hypercube sampling from the prior distributions of model parameters. \( 5 \times 10^5 \) posterior samples are generated by MCMC sampling. More detail about the Bayesian method used here can be found in the work of Sargsyan et al. [10].

4. Results and discussion

The backward-facing step case simulated here is based on the experiment of Driver et al. [11]. The flow geometry is presented in Figure 1. The Mach number is 0.128, step height is 0.0127m and the Reynolds number based on the step height is 37500. The case of \( \alpha = 0^\circ \) is investigated here. The computational grid is from NASA turbulence modeling Resource, and is given in Figure 2. To reduce the computational cost, the inlet boundary conditions are imposed at \( x/h = -4 \), and the inlet flow information is determined by an initial channel computation. The Roe flux-difference scheme and the implicit LUSGS scheme are applied in the simulation.

4.1. Prior samples and sensitivity analysis

The prior uncertainty of model parameters is propagated through the CFD solver, and 108 full RANS simulations are carried out. The wall pressure coefficient distributions and skin friction coefficient distributions of all prior samples are shown in Figure 3 and Figure 4. It can be found that the pressure coefficient distribution obtained by the nominal values of model parameters agree well with the experimental data, but the corresponding skin friction coefficient distribution deviates from the experimental data significantly. Therefore, the performance of SA turbulence model in the backward-
facing problem needs to be further improved. The skin friction coefficient variation of 108 prior samples can easily encompass the experimental data, which indicates the feasibility of improving the performance of SA turbulence model by adjusting parameters. Moreover, the prior uncertainty of the skin friction coefficient is obviously greater than that of the wall pressure coefficient.

Sobol index is utilized to rank the model parameters according to their contribution to the total variance of the QoIs. The definition of Sobol index can be found in Ref. [12]. The sobol indices for wall pressure coefficient and skin friction coefficient are presented in Figure 5 and Figure 6. For the wall pressure coefficient, the first four parameters that contribute greatly to the total variance are $\kappa, C_{b1}, \sigma$ and $C_{w1}$. For the skin friction coefficient, the first four parameters are $\kappa, C_{ti}, C_{b1}$ and $C_{w1}$.

![Figure 3. Wall pressure coefficient distributions of 108 prior samples.](image)

![Figure 4. Skin friction coefficient distributions of 108 prior samples.](image)

![Figure 5. Sobol indices for wall pressure coefficient.](image)

![Figure 6. Sobol indices for skin friction coefficient.](image)

4.2. Calibration results and uncertainty quantification

The experimental data of skin friction coefficient are served as calibration data due to the poor predictive performance of SA turbulence model for the skin friction in backward-facing step case. In Section 4.1, it can be found that the parameters $\kappa, C_{b1}, \sigma$ and $C_{w1}$ have great influence on the total variance of the skin friction coefficient. Thus, the model error is embedded in these four parameters.

The posterior distributions of parameters $\sigma, C_{b2}$ and $C_{w2}$ are not significantly different from the prior distributions, and thus only the posterior distributions of parameters $C_{b1}, C_{b2}, C_{w1}$ and $\kappa$ are exhibited in Figure 7. Only these four parameters are well informed by the experimental data of skin friction coefficient. For $C_{b1}$ and $C_{b2}$, the values at the peak of the probability density distributions are very close to the nominal values of the parameters. For $C_{w1}$, value less than the nominal value is preferred. For $\kappa$, there is a high probability for it to be greater than the normal value.
The posterior uncertainty of model parameters is propagated through the surrogate model (NIPC) to obtain the posterior uncertainty of the skin friction coefficient. The posterior mean of skin friction coefficient with estimated error (including model error, posterior uncertainty, and surrogate error) is displayed in Figure 8. Before the position of x/h=5, the posterior mean is no better than the predicted result of the nominal values of parameters. However, after the position of x/h=5, the posterior mean is closer to the experimental value than the nominal one, and the $\sigma_p$ error band can cover the experimental data at most positions.

The prediction using the maximum a posteriori (MAP) estimation of model parameters is presented in Figure 9. The MAP estimation of the parameters shows better predictive performance than the nominal values.

![Figure 7. Marginal posterior distributions of the model parameters (C_b1, C_w3, C_v1, $\kappa$).](image)

![Figure 8. Posterior mean of skin friction coefficient with estimated error.](image)

![Figure 9. Prediction using the maximum a posteriori (MAP) estimation of model parameters.](image)
5. Conclusions
In this work, the Bayesian method is applied to recalibrate the closure coefficients of SA turbulence model to improve its performance in backward-facing step problem. The results show that the four parameters $C_{\alpha_1}, C_{\alpha_3}, C_{\alpha_4}$ and $\kappa$ are well informed by the experimental data of skin friction coefficient. The recalibrated model parameters show better performance than the nominal values in the prediction of skin friction coefficient.

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