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UNCERTAINTY QUANTIFICATION FOR RANS SIMULATION OF DISPERSION OVER A WAVY WALL

Catherine Gorlé
Center for Turbulence Research, Stanford University, Stanford, CA 94305, USA
EMAT, University of Antwerp, Antwerp, Belgium
von Karman Institute for Fluid Dynamics, Sint-Genesius-Rode, Belgium
gorle.catherine@gmail.com

Gianluca Iaccarino
Center for Turbulence Research
Stanford University
Stanford, CA, 94305, USA
jops@stanford.edu

ABSTRACT

The goal of the present study is to establish a method that can capture the uncertainty in the Reynolds-averaged Navier-Stokes prediction for dispersion from a point source in the flow over a wavy wall. The methodology is based on 1. perturbing the modeled Reynolds stresses in the momentum equations, thereby establishing a method that is completely independent of the initial model form and 2. introducing uncertainty in the turbulent scalar flux vector in the transport equation for the scalar by using the perturbed Reynolds stresses in the generalized gradient diffusion model. The Reynolds stress perturbations are defined in terms of a decomposition of the Reynolds stress tensor, i.e. based on the tensor magnitude and the eigenvalues and eigenvectors of the normalized anisotropy tensor. Results of a previous study are further analyzed and show that a realistic representation of the uncertainty in the velocity field is obtained. In addition, an a priori analysis of the scalar flux model alignment indicates that, provided sufficient uncertainty is introduced in the Reynolds stresses, an adequate representation of the uncertainty in the scalar flux vector can be obtained. Based on these results, a UQ study will be formulated to quantify the uncertainty in the scalar dispersion.

INTRODUCTION

Reynolds-averaged Navier-Stokes (RANS) simulations remain the most affordable technique for simulating complex turbulent flow and scalar transport phenomena. For many engineering applications, the reliability of the results is limited by the assumptions introduced by turbulence models based on the linear eddy-viscosity hypothesis, and by turbulent scalar flux models based on the gradient diffusion hypothesis. Complex flow features such as flow separation and reattachment are not predicted with consistent accuracy and errors in the turbulent velocity field directly influence the solution for transported scalars. These errors can be amplified, or cancelled out, by the turbulent scalar flux model, which introduces further uncertainties in the solution for the scalar field.

In Gorlé & Iaccarino (2013) epistemic (model-form) uncertainty in the mixing of a jet in supersonic cross flow configuration was quantified by introducing perturbations in the Reynolds stress tensor and the turbulent scalar flux vector. The idea to quantify the uncertainty related to the turbulence model through the introduction of perturbations in the Reynolds stress tensor was first introduced in Emory *et al.* (2011). The method defines the perturbations in terms of the magnitude of the tensor, i.e. the turbulence kinetic energy, and the eigenvalues and eigenvectors of the normalized anisotropy tensor, thereby being completely independent of the initial turbulence model form. The approach can be extended to introduce perturbations in the turbulent scalar flux vector, by using the perturbed Reynolds stresses in the formulation for the diffusion coefficient tensor in a generalized gradient diffusion model.

The results presented in Gorlé & Iaccarino (2013) showed the promising capabilities of the approach, and also indicated a number of remaining questions for future research. In particular, the parametrization of the perturbation functions and a more efficient strategy to identify upper and lower bounds were identified as a major challenge. In (Gorlé *et al.* , 2012), these questions were further addressed, and the uncertainty in the location of the reattachment point for the flow over a wavy wall was successfully quantified.

In the present study we investigate the possibility of extending this result to include uncertainty quantification for the dispersion of a passive scalar over the wavy wall. We first present a further analysis of the results of Gorlé *et al.* (2012) to determine whether the representation of the uncertainty in the velocity field is sufficient to adequately represent the uncertainty in the advection of the scalar. Secondly we present the results of an a priori investigation of the scalar flux model alignment to investigate whether the method presented in Gorlé & Iaccarino (2013) is a suitable starting point for representing the uncertainty in the turbulent scalar flux models. A direct numerical simulation (DNS) database for the configuration is available from Rossi (2011) to perform this analysis.

The following section of this paper summarizes the configuration studied. Subsequently an overview of the epistemic uncertainty quantification (EUQ) methodology for quantifying uncertainty related to the turbulence model and the turbulent mixing model is presented. The results obtained in Gorlé *et al.* (2012) are summarized and complemented with additional post-processing to illustrate the uncertainty in the velocity field. Finally, the alignment of the turbulent scalar flux vector obtained from the DNS and from an a priori evaluation of the turbulent scalar flux models is presented. These results are the starting point for formulating a complete UQ approach to predict uncertainty in the scalar dispersion.

CONFIGURATION, DNS DATA AND RANS SIMULATIONS

The configuration considered is identical to the one used in the DNS simulations by Rossi (2011) and is shown in Figure 1. The geometry is defined as a two-dimensional channel, with the top wall a flat plate and the bottom wall a wavy surface with 4 wave crests. The DNS database includes results for the flow and for scalar dispersion at $Re = 6850$, based on the bulk velocity U_b at the wave crest and the average channel height H.

The RANS simulations were performed on a mesh of 256 x 96 x 128 cells, and the near wall resolution was sufficient ($y^+ \approx 1$) to avoid the use of wall functions. For the flow field periodic conditions are applied in the streamwise and spanwise directions. The flow is two-dimensional, but the point source dispersion problem is fully three-dimensional, and the boundary conditions for the scalar are zero-gradient conditions at the outlet and on the sides of the computational domain.

The governing equations are the incompressible Reynolds-averaged equations for conservation of mass and momentum. A two-equation linear eddy viscosity model based on the turbulent viscosity hypothesis was used:

$$\overline{u_i u_j} = \frac{2}{3} k \delta_{ij} - 2\nu_t S_{ij}, \tag{1}$$

where $\overline{u_i u_j}$ are the Reynolds stresses, k is the turbulence kinetic energy, ν_t is the turbulent viscosity and S_{ij} is the strain rate tensor. The results included in this paper were obtained by modeling the turbulent viscosity with the SST k-ω model. A similar analysis with the realizable k-ε model will be performed in the future.

The scalar dispersion is modeled by solving the Reynolds-averaged transport equation for a scalar quantity $\overline{\Phi}$. The turbulent scalar fluxes $\overline{u_i \phi}$ are represented with a generalized gradient diffusion model (Daly & Harlow, 1970):

$$\overline{u_i \phi} = -\alpha_\phi \tau_\phi \overline{u_i u_j} \frac{\partial \overline{\Phi}}{\partial x_j}, \tag{2}$$

where α_ϕ is a model coefficient and τ_ϕ a time scale. The tensorial diffusion coefficient formulation, which uses the Reynolds stresses for determining the different components, forms the basis of the UQ approach. The model will also be shown to provide a better prediction of the turbulent scalar flux vector than the standard gradient diffusion model (SGDH), which uses a scalar diffusion coefficient: $\overline{u_i \phi} = -\frac{\nu_t}{Sc_t} \frac{\partial \overline{\Phi}}{\partial x_i}$, where Sc_t is the turbulent Schmidt number.

EUQ METHODOLOGY

Turbulence Model EUQ

A standard approach for investigating the influence of the turbulence model is to compare different models, often belonging to the same class of two-equation turbulence models based on the turbulent viscosity hypothesis. Such traditional sensitivity studies can not capture the full model form uncertainty, because this uncertainty is largely determined by the fundamental model assumptions, i.e. those made in the turbulent viscosity hypothesis (Eq. 1).

The methodology proposed in Emory *et al.* (2011) is intended to overcome this limitation, by being completely independent of the initial model form. It consists in directly introducing perturbations in the Reynolds stress tensor computed by the model and used in the momentum equations. The definition of the perturbations is based on reformulating the Reynolds stress tensor R_{ij} in terms of the isotropic part and the eigenvalue decomposition of the normalized anisotropy tensor $a_{ij} = v_{ik}\Lambda_{kl}v_{jl}$:

$$R_{ij} = 2k\left(\frac{1}{3}\delta_{ij} + v_{ij}\Lambda_{kl}v_{jl}\right), \tag{3}$$

where k is the turbulent kinetic energy, δ_{ij} the Kronecker delta, v_{ij} the matrix of orthonormal eigenvectors and Λ_{kl} the diagonal matrix of eigenvalues λ_l. This formulation does not involve any modeling assumptions, thereby presenting a general way of introducing epistemic uncertainty in the Reynolds stress tensor, writing the perturbed Reynolds stresses as:

$$R^*_{ij} = 2k^*\left(\frac{1}{3}\delta_{ij} + v^*_{ik}\Lambda^*_{kl}v^*_{jl}\right). \tag{4}$$

The perturbations are thus specified in terms of a discrepancy in the turbulence kinetic energy $k^* = k + \Delta k$, the diagonal matrix Λ^*_{kl} of perturbed eigenvalues λ^*_l, and perturbed eigenvectors $v^*_{ij} = q_{ik}v_{kj}$, where q_{ik} is an orthonormal rotation matrix.

The main challenge in this approach is the definition of the perturbations, which should introduce sufficient uncertainty in the solution without being overly pessimistic about the performance of the turbulence model. In Gorlé *et al.* (2012) the definition of the perturbation functions is based on two basic concepts:

1. A marker, which identifies regions that deviate from parallel shear flow as regions where perturbations should be introduced.
2. Systematic perturbations introduced in the marked region by (1) moving the eigenvalue of the anisotropy tensor towards the one-, two- or three-component corners of the Barycentric map, shown in Figure 2 (Banerjee *et al.* , 2007); (2) rotating the eigenvectors with the Euler angle that preserves the two-dimensionality of the flow; and (3) using the turbulent production term computed with the modified anisotropy tensor to perturb the turbulence kinetic energy. It is important to note that this methodology only allows accessing realizable states of turbulence, since the updated eigenvalues are located inside the Barycentric triangle.

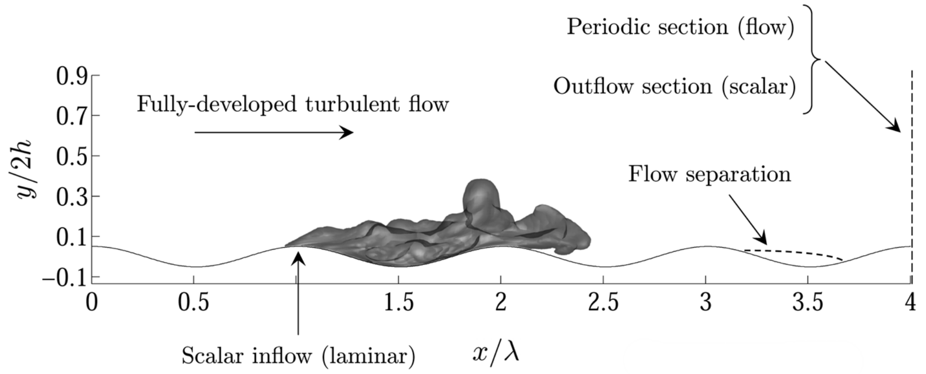

Figure 1. Flow configuration (Rossi, 2011).

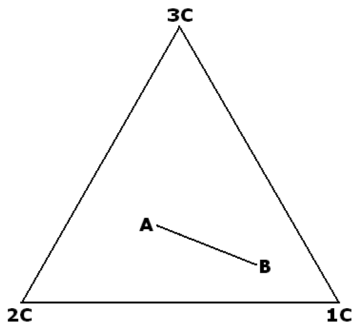

Figure 2. Barycentric map (Banerjee *et al.* , 2007).

The exact formulation of the marker can be found in Gorlé *et al.* (2012), where validation with the DNS database showed that the regions where the turbulence model fails to produce an accurate prediction are correctly identified. Subsequently, the perturbations introduced in these regions were selected by identifying which eigenvalue and eigenvector perturbations result in the maximum and minimum turbulence kinetic energy production term integrated over the marked region. These perturbation are then expected to show the smallest and largest separation bubble respectively.

The reasoning for perturbing the turbulence kinetic energy indirectly through the production term stems from an initial analysis where the influence of the turbulence kinetic energy production term on the solution in the turbulence model was investigated, by performing three different sets of simulations. First, both the RANS flow and turbulence equations were solved. Secondly, the effect of the coupling to the mean flow was eliminated by freezing the flow to the time-averaged DNS flow field and only solving the transport equations for the turbulence quantities. Finally, also the production term in the turbulence transport equations was frozen to the production term calculated from the DNS. Figure 3 presents the comparison for the turbulence kinetic energy for the last two solutions obtained, i.e. when using the DNS flow field and the DNS flow field in combination with the exact production term, $P_k = -u_i u_j \frac{\partial U_i}{\partial x_j}$. The difference between both sets of simulations is that when only freezing the DNS flow field, P_k is still determined from the inexact Reynolds stresses as computed using the turbulent viscosity hypothesis, while in the second case the exact Reynolds stresses are used. The result shows an underprediction of up to 100% with the SST $k-\omega$ model. However, when using the correct production term for k the model predicts k with much higher accuracy.

In Gorlé *et al.* (2012), it was found that the maximum and minimum integrated production terms are found when moving the eigenvalues to the one- and three-component corners of the map, respectively, without a rotation of the eigenvectors. It was shown that these two simulations capture the uncertainty in the size of the separated region and give a very realistic representation of the uncertainty in the streamwise wall shear stress for both models.

Mixing Model EUQ

The standard approach for quantifying the influence of the mixing model is to vary the coefficient in the formulation for the diffusion coefficient, i.e. the turbulent Schmidt number when using the standard gradient diffusion hypothesis. As for the turbulence model, this does not allow adequate characterization of the uncertainty, since the solution is still governed by the basic assumption that the turbulent scalar fluxes and mean scalar gradients are aligned, and that the proportionality coefficient is isotropic.

In Gorlé & Iaccarino (2013) it was shown that these limitations can be overcome by using the perturbed Reynolds stresses from Eq. 4 in the generalized gradient diffusion hypothesis (GGDH) given in Eq. 2. While the GGDH model is not the most general or accurate model available, it is the simplest model that uses the Reynolds stresses. This allows to induce a scaling and rotation of the vector by defining perturbations in the GGDH model formulation based on the perturbations introduced in the Reynolds stresses as follows:

$$\overline{u_i\phi}^* = \alpha_\phi^* \tau_\phi \overline{u_i u_j}^* \frac{\partial \overline{\Phi}}{\partial x_j}. \qquad (5)$$

The perturbed scalar fluxes $\overline{u_i\phi}^*$ are then defined in terms of a perturbed model constant α_ϕ^*, which scales the original vector and the perturbed Reynolds stress tensor $\overline{u_i u_j}^*$, which will induce a rotation of the vector.

For the simulation of a jet in a supersonic cross flow, the approach was capable of quantifying the uncertainty in a quantity of interest (QoI) representative of the downstream mixing, when defining the perturbations based on a comparison of the Reynolds stresses obtained from RANS with

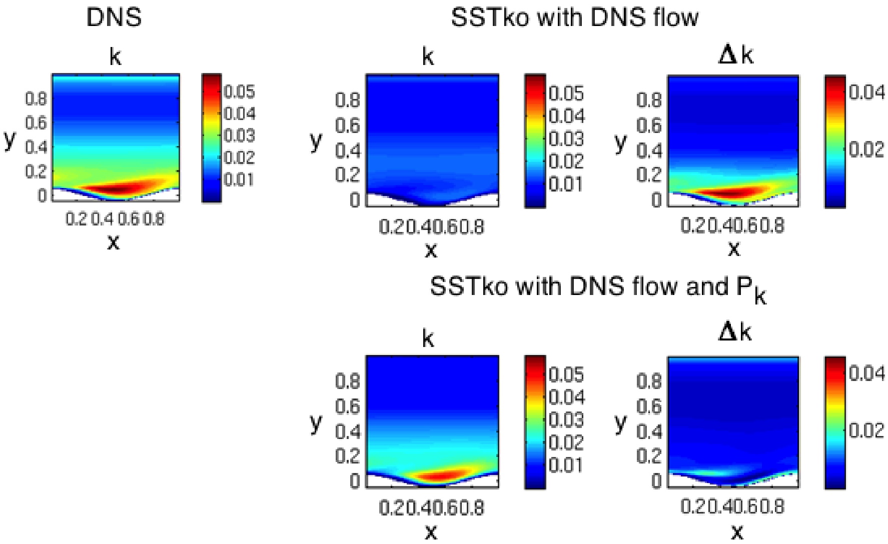

Figure 3. Comparison of k from DNS and SST $k-\omega$ (SSTko) models.

those resolved in a LES and subsequently solving an optimization problem to identify the maximum QoI. In the present study it is investigated whether a more general approach for defining the perturbation functions, similar to the one outlined above for the Reynolds stresses, can be used to represent the uncertainty in the downstream mixing.

RESULTS

In order to correctly quantify the uncertainty in the scalar field, it is necessary to 1. adequately represent the uncertainty in the mean flow field and 2. adequately represent the uncertainty in the turbulent scalar fluxes. The first subsection presents the uncertainty predicted in the mean velocity field using the methodology described in Gorlé *et al.* (2012) and summarized above. The second subsection presents an a priori investigation of the turbulent scalar flux model alignment to investigate whether the EUQ method for the turbulent scalar fluxes presented above could capture the uncertainty for the dispersion from the point source over the wavy wall.

Uncertainty in the Flow Field

Figure 4 presents the velocity contours over one wave length for the DNS, the unperturbed $k-\omega$ SST model and the perturbed $k-\omega$ SST model, with eigenvalue perturbations towards the C1 and C3 corners of the Barycentric map. The plots show that quantitatively the uncertainty in the velocity field is well represented, especially in the region below the crest of the wave.

A more quantitative comparison is presented in Figure 5. The plots show the DNS profiles for the horizontal and vertical velocities, and the lines that present the maximum and minimum values obtained from the perturbed runs. The plots confirm the observations from Figure 4, with the uncertainty in the velocity field being well represented by the two perturbed runs. For the horizontal velocity it is only on top of the wave crest that the uncertainty in the velocity field is less well represented. For the vertical velocity, the two runs do not seem to capture the maximum value on top of the wave crest and the negative peak below the wave crest.

As a starting point for analyzing the uncertainty in the scalar flux field, the representation of the uncertainty in the flow field using these two runs is found to be sufficient. If the initial UQ results for the scalar field would show insufficiently large bounds that can be related to the mean velocity field, it is expected that the uncertainty in the flow field could be further increased to fully encompass the DNS result by either increasing the area in which the perturbations are introduced or by increasing the magnitude of the perturbations.

Evaluation of Discrepancies in the Scalar Flux Field

The method for quantifying the uncertainty in the scalar flux model is based on introducing perturbations in the Reynolds stresses used in the GGDH model formulation (Eq. 5). The results of this approach can only represent the uncertainty correctly if the perturbations in the Reynolds stresses induce sufficient rotation in the turbulent scalar flux vector. In a future analysis we will investigate whether this can realistically be achieved using the two perturbed runs presented above by verifying the orientation of the perturbed scalar flux vectors.

In the initial analysis presented below we verified the original model form alignment for the SGDH and GGDH models. Figure 6 presents the results for the cosine of the angle between the actual turbulent scalar flux vector obtained from the DNS database and the modeled scalar flux vector, computed using the DNS Reynolds stresses and DNS mean scalar field as input. The plot clearly demonstrated the superior performance of the GGDH model, which is an indication that, provided we introduce sufficient uncertainty in the Reynolds stresses, we can get an adequate representation of the uncertainty in the scalar flux vector using 5.

CONCLUSIONS AND FUTURE WORK

In a previous study (Gorlé *et al.* , 2012), we showed that the uncertainty in the size of the separated region and

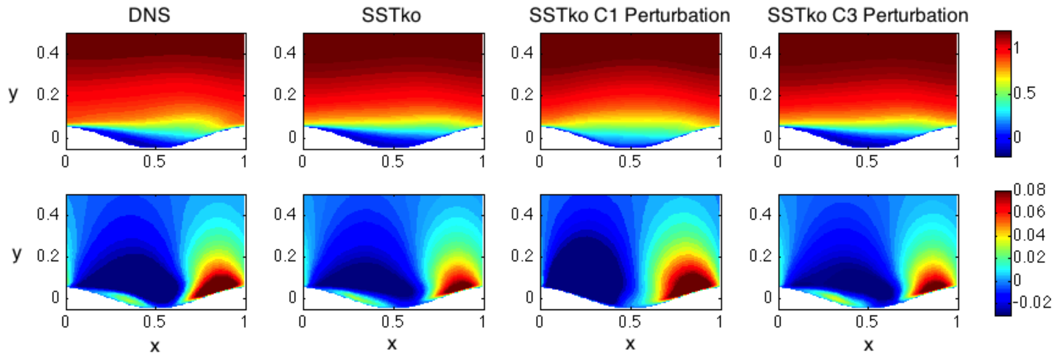

Figure 4. Contours of the horizontal (top) and vertical (bottom) velocity from DNS, unperturbed SST $k-\omega$ (SSTko) model, and perturbed SST $k-\omega$ model.

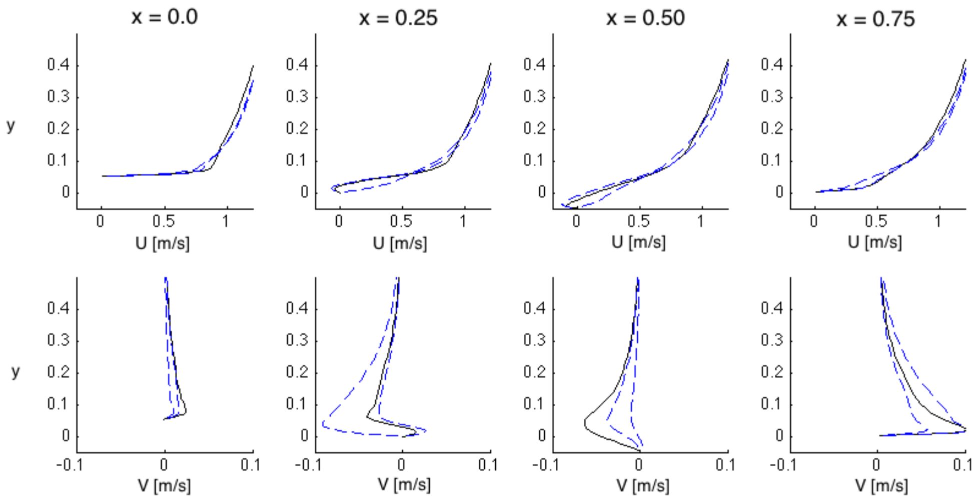

Figure 5. Comparison of velocity profiles at 4 different horizontal locations along the wave length. DNS result (black solid line) and maximum and minimum of the perturbed SST $k-\omega$ (SSTko) simulations (blue dotted lines).

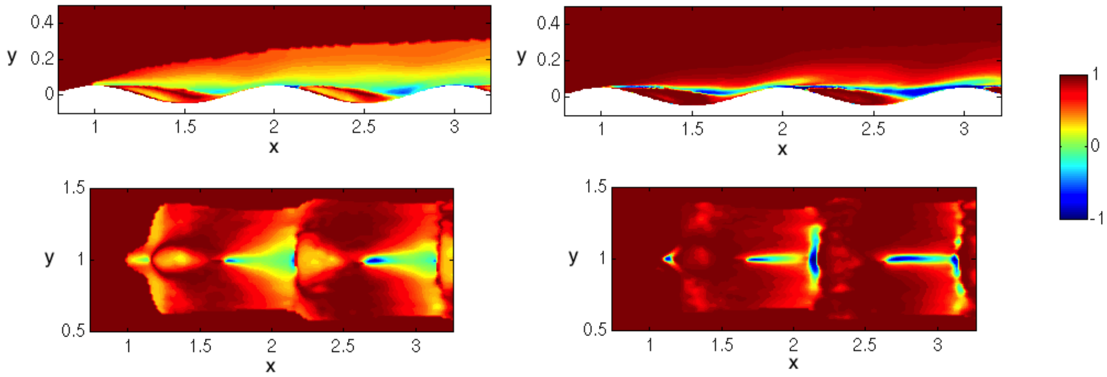

Figure 6. Comparison of k from DNS and SST $k-\omega$ (SSTko) models.

in the wall shear stress for the row over a wavy wall can be captured by introducing perturbations in the Reynolds stress tensor .

In the present study we are investigating extending this approach to quantify the uncertainty in the scalar field resulting from dispersion from a point source over the wavy wall. It was shown that the representation of the uncertainty in the flow field using the two runs which allowed quantifying the uncertainty in the wall shear stress is sufficient to serve as a starting point to quantify the uncertainty in the advection of the scalar. An a priori analysis of the scalar flux model alignment showed the benefits of using the tensorial diffusion coefficient formulations (2) and indicates that, provided we introduce sufficient uncertainty in the Reynolds stresses, we could get an adequate representation of the uncertainty in the scalar flux vector using 5.

In a further analysis, we will verify the rotations induced in the turbulent scalar flux vector by introducing the Reynolds stress perturbations used in the two perturbed $k-\omega$ SST models. Based on this result, a UQ study will be formulated where Reynolds stress perturbations will be introduced both the momentum equations and the scalar transport equation to quantify the uncertainty in the scalar dispersion.

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