

Determining *a priori* a RANS model's applicable range via global epistemic uncertainty quantification

Xinyi L D Huang^a, Naman Jain^a, Mahdi Abkar^b, Robert F Kunz^a, Xiang I A Yang^{a,*}

^a Mechanical Engineering, Pennsylvania State University, PA, 16802, USA

^b Department of Mechanical and Production Engineering, Aarhus University, 8000 Aarhus C, Denmark

ARTICLE INFO

Keywords:

Global epistemic uncertainty quantification
Reynolds-averaged Navier–Stokes equation

ABSTRACT

Calibrating a Reynolds-averaged Navier–Stokes (RANS) model against data leads to an improvement. Determining *a priori* if such an improvement generalizes to flows outside the calibration data is an outstanding challenge. This work attempts to address this challenge via global epistemic Uncertainty Quantification (UQ). Unlike the available epistemic UQ methods that are local and tell us a model's uncertainty at one specific flow condition, the global epistemic UQ method presented in this work tells us also whether a perturbation of the original model would generalize. Specifically, the global epistemic UQ method evaluates a potential improvement in terms of its “effectiveness” and “inconsistency”. Any improvement can be put in one of the following four quadrants: first, high effectiveness, low inconsistency; second, high effectiveness, high inconsistency; third, low effectiveness, low inconsistency; and fourth, low effectiveness, high inconsistency. An improvement would generalize if and only if it is in the high effectiveness, low inconsistency quadrant. To demonstrate the concept, we apply the global epistemic UQ to full Reynolds stress modeling of a stratified shear layer. The global epistemic UQ results point to a model coefficient in the pressure-strain correlation closure (among others) as effective and consistent for predicting the quantity of interest of shear layer's growth. We calibrate the model coefficients such that our RANS matches direct numerical simulation data at one flow condition. We show that the calibrated model generalizes to several other test flow conditions. On the other hand, when calibrating a high inconsistency term, the model does not generalize beyond the calibration condition.

1. Introduction

Predicting turbulence and its impact is critical to many applications in science and engineering. For example, predicting stratified wake flow is required in numerous applications including atmospheric and marine meteorology, and undersea vehicle motion [1]. Limited by the available computational resources, direct numerical simulation (DNS) and large-eddy simulation (LES) of high Reynolds number and/or high Richardson number stratified wake flow are and will remain infeasible in the foreseeable future [2,3]. Accordingly, Reynolds-averaged Navier–Stokes (RANS) modeling is the go-to tool for industrial-scale flow problems.

At a high level, a RANS model represents a mapping between the mean flow and the underlying turbulence. Because there is not a universal mapping between the mean flow and the underlying turbulence [4,5], a specific RANS model and a specific set of model coefficients exhibit suitable accuracy for only a limited range of applications. As pointed out in Ref. [5], it is hard to imagine that a RANS model calibrated to only isotropic turbulence would have predictive power

over complicated flows like stratified wakes. Hence, it is a common practice to calibrate a RANS model to a training flow before it is used for a flow of interest or a test flow. For instance, the full Reynolds stress model (FRSM) is calibrated to zero-pressure-gradient boundary-layer flow before applied to other wall-bounded flows [6].

Calibrating a RANS model requires data. At the time when the $k-\epsilon$ model, the $k-\omega$ model, and the Spalart–Allmaras (SA) model were developed [7–9], there was not a lot of high-quality data that would be used for model calibration. Things are, of course, different nowadays. The past decade has seen much progress in high-performance computing [10], and this increased computational power has enabled DNS and LES of flows at moderate and moderately high Reynolds numbers [11–13]. These DNS and LES data provide new opportunities for RANS calibration and RANS modeling in general. A notable example is the use of machine learning in RANS model calibration [14–23]. Its general methodology is to train a baseline RANS model to high-fidelity data. The baseline RANS model is usually retained, and machine learning improves upon that baseline RANS model. There are many things one

* Corresponding author.

E-mail address: xzy48@psu.edu (X.I.A. Yang).

can do to make the training process more efficient. For example, one can constrain the training so that the resulting RANS model is Galilean invariant and realizable [16,23]; one can also include as many inputs as possible to ensure that the resulting model does not underfit [20]. This machine learning approach has seen many successes, and here, we name a few. Tracey et al. [15] showed that an artificial neural network recovers the SA model from data. Ling et al. [17] showed that embedding Galilean invariance in network training greatly reduces the amount of training data needed. Wu et al. [20] extended Ling et al.'s work and incorporated rotational invariance and reflectional invariance. The main criticism of machine learning models, however, is the models' ability to generalize, or rather, a lack of knowledge about the models' applicable range.

A lack of knowledge of a model's applicable range is fundamentally due to a lack of understanding of flow physics. If one perfectly understands the flow physics, that understanding could well be used to determine whether a specific model, calibrated to a specific flow, generalizes to another specific flow. Although having a perfect understanding of flow physics is nearly impossible, it is possible to understand and quantify RANS models' uncertainties. That directly leads to epistemic uncertainty quantification (UQ). The present literature categorizes epistemic uncertainties in terms of parametric model uncertainties and non-parametric model uncertainties. Parametric uncertainties are the uncertainties in the model coefficients, and non-parametric uncertainties are the uncertainties in the model form. Both types of uncertainties can be studied by data-free methods and data-driven methods. Specifically, data-free methods consist of propagating pre-specified probability distributions of model coefficients and model terms through RANS equations and investigating the uncertainty distribution of the solution, see Refs. [24–26] for data-free UQ of parametric uncertainties and Refs. [27–31] for data-free UQ of non-parametric uncertainties. On the other hand, data-driven methods consist of assimilating data to infer the probability distributions of the model coefficients and model terms; the inferred probability distributions are available for propagating through RANS equations in a subsequent prediction step; see Refs. [32–37] for data-driven UQ of parametric uncertainties and Refs. [38–43] for data-driven UQ of non-parametric uncertainties. Although UQ of RANS is a somewhat new field, the research has led to many insights in the past few years. Here, we name a few. Margheri et al. [25] showed high-level uncertainties in $k-\epsilon$ and $k-\omega$ RANS models' channel flow results due to the uncertainties in the model coefficients. Iaccarino et al. [28] obtained a bound for the $k-\omega$ model results of flow behind a back-facing step by perturbing the shape of the Reynolds stress (we define the shape of the Reynolds stress in Section 2.6). Cheung et al. [32] found that their data-driven method leads to different model coefficients in the Spalart–Allmaras model than the conventional model coefficients. Xiao et al. [39] showed that more accurate estimates of fluid velocity can be obtained by assimilating information from data following an iterative ensemble Kalman method. A more detailed review of the literature, e.g., Refs. [44–49], falls out of the scope of this work, and the reader is directed to the review paper Ref. [50]. In all, the available epistemic UQ methods are local: they give uncertainty estimates at a given flow condition but provide very little information about a model's applicable range.

To more clearly see local UQ methods' limitations, we consider the RANS of a stratified shear layer. Stratified shear layer evolution is controlled by the Reynolds number, Re , and the Richardson number, Ri , and often other relevant parameters including the turbulence intensity TI . These flow controlling parameters (FCPs) define a FCP space. Suppose that we have a FRSM that does not accurately predict the shear layer's growth. Also, suppose that we have DNS data at one flow condition, i.e., one specific Re , Ri , and TI , and we want to make use of our DNS data to improve the RANS model. A local UQ method would help if the objective is to improve the model's performance at the DNS's condition, but it falls short if the objective is to develop an

improvement that generalizes to other flow conditions within the FCP space.

One can, of course, resort to *a posteriori* tests to determine if an improvement generalizes to other flow conditions. By comparing a model's prediction to data, *a posteriori* tests give us a definite answer to whether an improvement generalizes to a specific flow condition or not [51–54]. This process is also known as verification and validation. The difficulty, however, is that verification and validation require high-fidelity data at the test conditions, which is often not available.

The objective here is to know *a priori* whether an improvement generalizes. To know that, we need to know if the improvement has a consistent impact on a quantity of interest (QoI)—the improvement generalizes only if it has a consistent impact. This leads directly to global epistemic UQ methods, i.e., the topic of this paper. The rest of the paper is organized as follows. The methodology is presented in Section 2. In Section 3, we apply the global epistemic UQ method to the FRSM of a stratified shear layer. We conclude in Section 4.

2. Methodology

2.1. Problem statement

By definition, no RANS model can fully account for flow physics, and this leads to model uncertainty, the effects of which can be studied by perturbing the model terms. If one calibrates a model to data such that the calibrated model returns a more accurate prediction of a QoI than the original model, the calibrated model can be considered as a model improvement. The improvement may be regarded as a perturbation to the original model. We want to know the improvement's applicable range.

The problem concerns two spaces: the FCP space and the model space. A point in the FCP space defines a flow. For example, a stratified shear layer is controlled by the Richardson number and the Reynolds number. For a stratified shear layer, the Richardson number and the Reynolds number constitute a two-dimensional FCP space, and a point in this FCP space, i.e., a specific combination of the Richardson number and the Reynolds number, defines a stratified shear layer. Similarly, a point in the model space defines a RANS model. For example, a FRSM requires closures for the pressure-strain term, the dissipation term, the diffusion term, etc. (see details in Section 3.2). These closure models and the constants in these models constitute the model space. A point in this model space corresponds to a specific set of model closures and a specific set of model constants, which together define a FRSM model. Given a QoI, a FCP space, and a model space, a global epistemic UQ method maps uncertainties in the model space to uncertainties in the QoI for flows in the FCP space.

2.2. General methodology

Fig. 1 is a sketch of the general methodology. The global epistemic UQ method consists of a local epistemic UQ method and a method that screens the FCP space. A screening of the FCP space gives N sampling points or N flow conditions. The local epistemic UQ method provides uncertainty estimates at these N flow conditions. These scalar uncertainty values are defined as e_i , $i = 1, 2, 3, \dots, N$, for the N flow conditions. These local uncertainty estimates together return a global uncertainty estimate.

Following Ref. [27], we study a model's uncertainty by perturbing the model terms. We measure a perturbation in terms of its “inconsistency” and “effectiveness”. Effectiveness is measured according to

$$\mu = \frac{1}{N} \sum_{i=1}^N e_i, \quad (1)$$

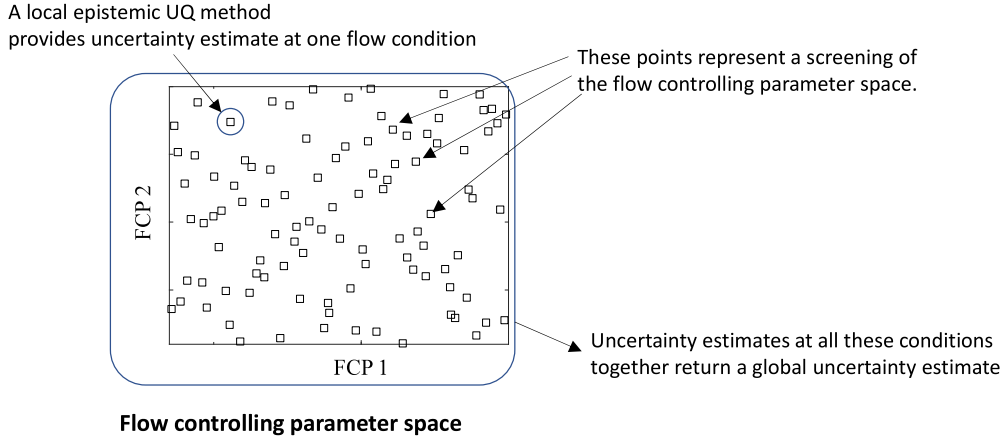


Fig. 1. A sketch of the general methodology. The sampling points in the 2D space are generated according to the “constrained” Latin hypercube method (see Section 2.5 for details).

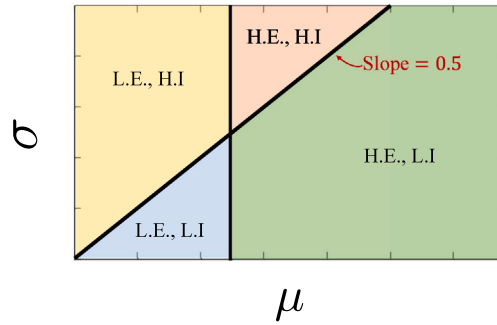


Fig. 2. $\sigma - \mu$ quadrant diagram. μ measures a perturbation's effectiveness. σ measures a perturbation's inconsistency. A large μ value corresponds to high effectiveness, i.e., H.E.. A small μ value corresponds to low effectiveness, i.e., L.E.. A large σ value corresponds to high inconsistency, i.e., H.I.. A small σ value corresponds to low inconsistency, i.e., L.I.. Here, if $\sigma/\mu > 0.5$, we say σ has a large value, and if $\sigma/\mu < 0.5$, we say σ has a small value.

i.e., the mean of e_i , and inconsistency is measured according to

$$\sigma^2 = \frac{1}{N} \sum_{i=1}^N (e_i - \mu)^2, \quad (2)$$

i.e., the standard deviation of e_i . Eqs. (1) and (2) define a quadrant diagram, as sketched in Fig. 2. If μ is large and σ is small, e_i 's have large values that vary little in the FCP space. This is high effectiveness (H.E.), low inconsistency (L.I.). It is worth noting here that σ 's value must be compared to μ : a σ value is considered large only if it is large compared to μ , and a σ 's value is considered small only if it is small compared to μ . Similarly, we can define the H.E., high inconsistency (H.I.) quadrant, the low effectiveness (L.E.), the L.I. quadrant, and the L.E., H.I. quadrant. To further illustrate the concept, we consider the following example. Suppose that we have $i=1, 2$, i.e., the FCP space contains two sampling points. Also suppose that $\mu = 10$ is high effectiveness, $\mu = 1$ is low effectiveness, $\sigma/\mu = 0$ is low inconsistency, and $\sigma/\mu = 1$ is high inconsistency. If a type of perturbation leads to $e_1 = 1, e_2 = 1$, we have $\mu = 1, \sigma/\mu = 0$, and the perturbation is in the L.E., L.I. quadrant. Because of its low effectiveness, such a perturbation is not likely to lead to any significant improvement. The same is true if the perturbation is in the L.E., H.I. quadrant. If a perturbation leads to $e_1 = 5, e_2 = 15$, we have $\mu = 10, \sigma/\mu = 1/2$, and the perturbation is in the H.E., H.I. quadrant. This perturbation will lead to improvement at the condition $i = 2$, but because of its high inconsistency, this perturbation would not generalize and work well at the condition $i = 1$. Now, if a perturbation leads to $e_1 = 10, e_2 = 10$, we have $\mu = 10, \sigma/\mu = 0$, and the perturbation is in the H.E., L.I. quadrant. We will show in Section 3.4 that an improvement will generalize only if it is in the H.E., L.I. quadrant.

2.3. Cost of global epistemic UQ

Having presented the general methodology, we now estimate the cost of global epistemic UQ. The cost of the global epistemic UQ method is roughly proportional to the times we need to evaluate the RANS model. If N' evaluations (i.e., RANS runs) are needed for local UQ at one flow condition, global epistemic UQ requires NN' evaluations of the RANS model. Again, N is the number of sampling points in the FCP space, e.g., the number of flow conditions. In the following, we estimate N and N' .

Let us consider a d -dimensional FCP space and a d' -dimensional model space. The value of d typically ranges from $\mathcal{O}(1)$ to $\mathcal{O}(10)$. For a stratified shear layer, the Reynolds number and the Richardson number give a $d = 2$ dimensional FCP space. The dimension of the FCP space will be higher if geometric parameters are involved. For example, for a stratified wake, geometric parameters that control the geometry of the wake-generating body add to FCP's dimension. The value of d' typically ranges from $\mathcal{O}(10)$ to $\mathcal{O}(100)$ depending on the number of unclosed terms and the number of model coefficients. For an eddy viscosity model, d' is about 10 [9]. d' is large for more complicated models like FRSM. For a FRSM, e.g., the one detailed in Section 3, d' is approximately 100.

If one employs a space-filling strategy [55], screening the FCP space and the model space requires $N \sim n^d$ and $N' \sim n'^{d'}$ samples, where n and n' are $\mathcal{O}(10)$ constants, and it would be prohibitively costly. To elaborate, we consider a 2D FCP space and a (tiny) 6D model space. Taking $n = 10$ and $n' = 10$ already requires 10^8 times' evaluation of the RANS model. If more efficient sampling strategies are employed, e.g., the ones described in Sections 2.4 and 2.5, screening the two space requires $N \sim n$ and $N' \sim n'd'$ samples respectively. In that case, global

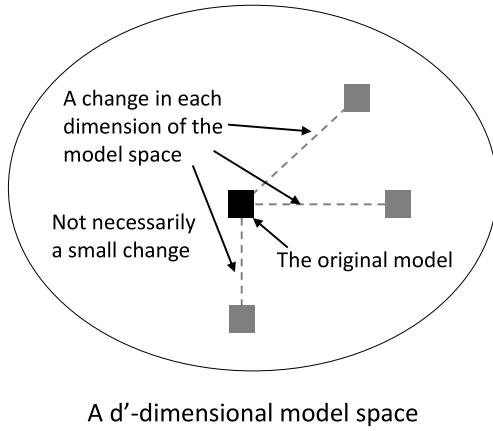


Fig. 3. A sketch of the local UQ method.

epistemic UQ requires $\mathcal{O}(100)$ times' evaluation of the RANS model for a 2D FCP space and a 6D model space.

2.4. Screening model space

We perturb the original RANS model such that the perturbed models lie in the vicinity of, but not necessarily close to the original model in the model space. Fig. 3 is a sketch of the method. Here, except for the original model, a point in the model space differs from the original model in only one dimension. This method requires $d' + 1$ evaluations of the RANS model for local UQ.

Compared to the information we can get from the recently-developed more advanced local epistemic UQ methods like the one in Ref. [34], we get less information from the method described here. We do not use these recently developed methods because they are too costly. For example, if we were to follow, e.g., Ref. [34], and propagate the PDFs of all model coefficients and all model terms through a RANS model, our global epistemic UQ would be $\mathcal{O}(100)$ times more costly. Considering that our methodology already requires about $\mathcal{O}(1000)$ RANS calculations, employing these recently-developed more advanced local UQ methods like the one in Ref. [34] is not practical.

2.5. Screening flow controlling parameter space

To keep the cost manageable, we employ the “constrained” Latin hypercube strategy to screen the FCP space. Details of the method can be found in Ref. [56]. Here, we briefly summarize the main features of the method. First, we define a Latin hypercube. A d -dimensional square grid containing sample positions is a Latin hypercube if and only if each sample is the only one in axis-aligned hyperplanes containing it. When sampling a d -dimensional space, the range of each dimension is divided into N equally probable intervals. N sample points are then placed to satisfy the Latin hypercube requirement. Fig. 4 shows two possible “designs” in a 2D space. Here, a design is a realization of the Latin hypercube. Although both designs are Latin hypercubes, the design in Fig. 4(a) is a more explorative one than the one in Fig. 4(b), making the design in Fig. 4(a) a better design. This motivated Morris and Mitchell [56] to constrain the Latin hypercube such that the distances between any two samples are maximized, leading to the “constrained” Latin hypercube method.

2.6. Physics-informed perturbations of the original model

Any change/perturbation of the original model in the model space should respect the basic physics. For example, it is desirable that if one perturbs a symmetric (or/and positive definite) tensor, the perturbed

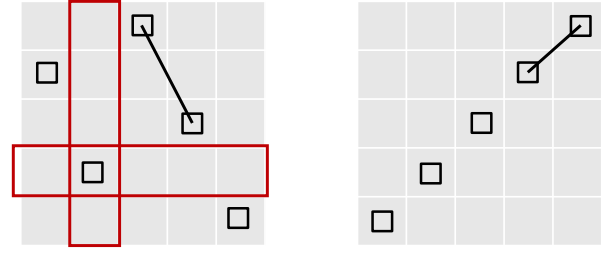


Fig. 4. Two possible Latin hypercube designs. The space is two dimensional (for visualization purposes). The thin white lines define a square grid. The black squares are sampling points. The red boxes are two hyperplanes. For a 2D space, a hyperplane is a 1D line. The two black lines indicate the smallest inter-point distance in the two designs. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

tensor remains symmetric (or/and positive definite) [20]. Following Ref. [27], perturbations of a tensor are defined in terms of the tensor's magnitude, as well as the shape and orientation of the normalized anisotropic part of that tensor:

$$a_{ij} = a_{kk} \left(\frac{1}{3} \delta_{ij} + V_{ik} \Lambda_{kl} V_{lj} \right), \quad (3)$$

where a is an arbitrary symmetric (positive definite) tensor, V is the eigenvector matrix, and Λ is the eigenvalue matrix. Perturbing a tensor's magnitude is to vary its trace a_{kk} , which adds one dimension to the model space; perturbing a tensor's shape is to vary its eigenvalues Λ , which adds two dimensions to the model space; and perturbing a tensor's orientation is to vary a tensor's eigenvectors V , which adds three dimensions to the model space. Hence, perturbing a symmetric (positive definite) tensor gives rise to a 6-dimensional model space. In addition to perturbations to a tensor term, one can also define perturbations to a vector term in terms of the vector's magnitude and its orientation:

$$b_i = \sqrt{b_k b_k} \hat{b}_i, \quad (4)$$

where b_i is an arbitrary vector, $\hat{b}_i$ is a unit vector in the direction of b_i . Perturbing a vector's magnitude is to vary its length $\sqrt{b_k b_k}$, which adds one dimension to the model space; perturbing a vector's direction is to vary $\hat{b}_i$, which adds two dimensions to the model space. Hence, perturbing a vector gives rise to a 3-dimensional model space. Thus defined perturbations to tensors and vectors are Galilean invariant. Note that perturbations of a scalar term are always Galilean invariant.

2.7. Procedure of global epistemic uncertainty quantification

The analysis begins with a baseline RANS model, a model space, a FCP space, and a QoI. We define $e_{i,j,QoI}$ as follows: a specific type of perturbation j to the original RANS model at the flow condition i gives rise to an uncertainty estimate $e_{i,j,QoI}$ for the QoI. Here, $i = 1, 2, 3, \dots, N$, and $j = 1, 2, 3, \dots, d'$. The steps of a global epistemic UQ are as follows.

1. sample the FCP space N times following the method in Section 2.5.
2. compute $e_{i,j,QoI}$ for i from 1 to N for a fixed j .
3. compute μ_j and σ_j according to

$$\mu_j = \frac{1}{N} \sum_{i=1}^N e_{i,j,QoI}, \quad \sigma_j^2 = \frac{1}{N} \sum_{i=1}^N (e_{i,j,QoI} - \mu_j)^2. \quad (5)$$

4. repeat the above three steps for $j = 1, 2, 3, \dots, d'$.

The effectiveness and inconsistency, i.e., μ_j and σ_j , contain the global uncertainty information. A specific type of perturbation j to the original model generalizes in the FCP space if and only if it is in the H.E., L.I. quadrant, i.e., only if it has a large μ value and small σ/μ value.

2.8. Discussion

In this subsection, we remark on the global epistemic UQ method.

Remark 1. We are not introducing a new sampling method. The local epistemic UQ method in Section 2.4 and the global screening method in Section 2.5 are well-established methods and require no further validation. This paper combines two established methods to address an open challenge.

Remark 2. Because of the σ - μ diagram and local epistemic UQ method in Section 2.4, an informed reader would find the global epistemic UQ method reminiscent of the Morris method. Although the difference between the two methods will become clear in Section 3, here, it is worth noting that our global epistemic UQ method differs from the Morris method in terms of the working spaces. The Morris method involves one working space, whereas our global epistemic UQ method involves two, i.e., the FCP space and the model space.

Remark 3. When we say “a UQ method is local”, we mean that the results are only applicable to the flow condition under consideration, and when we say “a UQ method is global”, we mean that the results concern all flow conditions in a FCP space. The words “local” and “global” concern the FCP only. A local UQ method may well cover a large model space. For example, the tensor perturbation methodology is a general method that may be applied to both isotropic and anisotropic eddy viscosity models [57].

Remark 4. In the current CFD literature, epistemic UQ’s overarching objective is to give a bound for RANS results. Consequently, most work does not separately study the effects of different types of model perturbations. This is not an issue for eddy-viscosity-type models, because all one can perturb is the Reynolds stress term. However, when many unclosed terms represent different physical processes in a complicated model like FRSMs, not separately studying each perturbation’s effect leads to a significant loss of information. Here, we prevent this loss of information by computing σ_j and μ_j for $j = 1, 2, \dots, d'$ separately.

3. Application

We begin our discussion by stating the general problem. We have DNS data of a temporally-evolving shear layer at one flow condition and a RANS model that does poorly in terms of predicting the shear layer’s growth. We want to calibrate the RANS model such that the calibrated model more accurately predicts the shear layer’s growth at the DNS’s condition and other conditions within a designated FCP space.

The rest of the section is organized as follows. We review the flow phenomenology of a temporally-evolving stratified shear layer in Section 3.1. The details of the FRSM are presented in Section 3.2. The details of the UQ method specific to this application are presented in Section 3.3 followed by the results in Section 3.4. In Section 3.5, we calibrate the FRSM and show that the calibrated model generalizes. The reader can skip the first two subsections if he/she is familiar with the RANS model and the flow problem. Details of the RANS and DNS codes and the simulation setup are presented in Appendices A and B.

3.1. Stratified shear layer

Fig. 5(a) is a sketch of a temporally-evolving stably stratified shear layer. Such a shear layer emerges between two streams of flows that move at the same speed but in the opposite directions, with the top stream lighter than the bottom stream. Temporally evolving stratified shear layer flow has been a model problem for flows with thermal stratification, and its phenomenology has received much attention in the

published literature [58–62]. The initial state of the flow is controlled by the Reynolds number Re

$$Re = \frac{\Delta U \delta_{w,0}}{\nu}, \quad (6)$$

and the Richardson number Ri ,

$$Ri \equiv \frac{g \Delta \rho \delta_{w,0}}{\rho \Delta U^2}, \quad (7)$$

where ΔU is the velocity difference between the two streams, $\delta_{w,0} = \Delta U / \max[dU/dy]$ characterizes the shear layer thickness, g is gravity, $\Delta \rho$ is the density difference between the two streams, and ρ is the reference density. Fig. 5(b) is a qualitative sketch of stably stratified shear layer growth. When the shear layer is thin, the flow is at the “early stage”, where buoyancy does not play a very important role. As the shear layer grows, the flow enters the “late stage”, and buoyancy significantly attenuates the shear layer’s growth.

3.2. Full Reynolds stress model

Linear eddy viscosity RANS models perform poorly for stratified shear layer flow because of the strong Reynolds stress anisotropy that arises in these flows [63]. FRSMs solve the Reynolds stress transport equations, and thereby inherently accommodate Reynolds stress anisotropy. Flow memory (hysteresis) is partly accounted for by the material derivatives in the Reynolds stress transport equations in FRSM. The dissipative, diffusive, and redistributive processes in the Reynolds stress transport equations are modeled [64]. In systems where buoyancy plays an important role, the model also incorporates transport equations for the turbulent temperature fluxes, i.e., $\langle u'_i \theta' \rangle$ and temperature variance, i.e., $\langle \theta' \theta' \rangle$. A significant literature exists for these relatively complex models, see e.g., [53,65–69]. Here we provide an overview of the modeling approach. The RANS equations with the Boussinesq approximation can be written as

$$\begin{aligned} \frac{\partial U_i}{\partial x_i} &= 0, \\ \frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} &= -\frac{1}{\rho} \frac{\partial P}{\partial x_i} + \nu \frac{\partial^2 U_i}{\partial x_j \partial x_j} - \frac{\partial \langle u'_i u'_j \rangle}{\partial x_j} - \beta g_i \Theta, \\ \frac{\partial \Theta}{\partial t} + U_j \frac{\partial \Theta}{\partial x_j} &= \alpha \frac{\partial^2 \Theta}{\partial x_j \partial x_j} - \frac{\partial \langle \theta' \theta' \rangle}{\partial x_j}, \end{aligned} \quad (8)$$

where U_i is the Reynolds-averaged velocity, x_i is the spatial coordinate, t is the time, P is the Reynolds-averaged pressure, β is the thermal expansion coefficient at constant pressure, Θ is the Reynolds-averaged temperature, α is the fluid conductivity, θ' is the temperature fluctuation, u'_i is the velocity fluctuation, and $\langle \rangle$ denotes a Reynolds average. The exact transport equations for the Reynolds stresses, $R_{ij} = \langle u'_i u'_j \rangle$, temperature fluxes, $R_{\theta,i} = \langle u'_i \theta' \rangle$, and temperature variance, $R_{\theta\theta} = \langle \theta' \theta' \rangle$, are as follows

$$\begin{aligned} \frac{\partial R_{ij}}{\partial t} + U_k \frac{\partial R_{ij}}{\partial x_k} &= \underbrace{\left(-R_{ik} \frac{\partial U_j}{\partial x_k} - R_{jk} \frac{\partial U_i}{\partial x_k} \right)}_{P_{ij}} \\ &+ \underbrace{\left(\frac{\partial}{\partial x_k} \left(-\langle u'_i u'_j u'_k \rangle \right) - \frac{1}{\rho} \left\langle p' \left(u'_i \delta_{jk} + u'_j \delta_{ik} \right) \right\rangle + \nu \frac{\partial R_{ij}}{\partial x_k} \right)}_{D_{ij}} \\ &+ \underbrace{\left(-\beta \left(g_i R_{\theta,j} + g_j R_{\theta,i} \right) \right)}_{G_{ij}} + \underbrace{\left(\left\langle \frac{p'}{\rho} \left(\frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i} \right) \right\rangle \right)}_{\Phi_{ij}} \\ &- 2\nu \underbrace{\left\langle \frac{\partial u'_i}{\partial x_k} \frac{\partial u'_j}{\partial x_k} \right\rangle}_{\epsilon_{ij}}, \end{aligned} \quad (9)$$

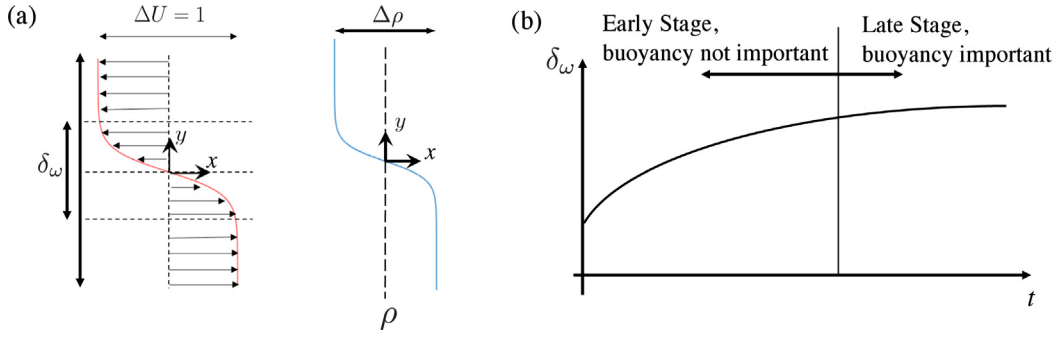


Fig. 5. (a) A sketch of a stably stratified shear layer. A stably stratified shear layer emerges between two streams moving at the same speed but in two opposite directions. The fluid velocity is in the x direction. The velocity difference between the two streams is $\Delta U = 1$ (unit). The top stream is lighter than the bottom stream. The density difference between the two streams is $\Delta \rho$. (b) A sketch of the growth of a stratified shear layer. At the early stage, buoyancy is not important. At the late stage, buoyancy becomes important.

$$\begin{aligned} \frac{\partial R_{\theta,i}}{\partial t} + U_k \left(\frac{\partial R_{\theta,i}}{\partial x_k} \right) &= \underbrace{\left(-R_{ki} \frac{\partial \Theta}{\partial x_k} - R_{\theta,k} \frac{\partial U_i}{\partial x_k} \right)}_{P_{\theta,i}} \\ &+ \underbrace{\left(\frac{\partial}{\partial x_k} \left(-\langle \theta' u'_i u'_k \rangle - \frac{1}{\rho} \langle p' \theta' \rangle \delta_{ik} + \nu \left\langle \theta' \frac{\partial u'_i}{\partial x_k} \right\rangle + \alpha \left\langle u'_i \frac{\partial \theta'}{\partial x_k} \right\rangle \right) \right)}_{D_{\theta,i}} \\ &- \underbrace{(\nu + \alpha) \left\langle \frac{\partial \theta'}{\partial x_k} \frac{\partial u'_i}{\partial x_k} \right\rangle}_{\epsilon_{\theta,i}} + \underbrace{\left(\frac{1}{\rho} \left\langle p' \frac{\partial \theta'}{\partial x_i} \right\rangle \right)}_{\Phi_{\theta,i}} + \underbrace{(-\beta g_i R_{\theta\theta})}_{G_{\theta,i}}, \end{aligned} \quad (10)$$

$$\begin{aligned} \frac{\partial R_{\theta\theta}}{\partial t} + U_k \left(\frac{\partial R_{\theta\theta}}{\partial x_k} \right) &= \underbrace{\left(-2R_{\theta,k} \frac{\partial \Theta}{\partial x_k} \right)}_{P_{\theta\theta}} + \underbrace{\left(\frac{\partial}{\partial x_k} \left(\alpha \frac{\partial R_{\theta\theta}}{\partial x_k} - \langle u'_k \theta' \theta' \rangle \right) \right)}_{D_{\theta\theta}} \\ &- \underbrace{2\alpha \left\langle \frac{\partial \theta'}{\partial x_k} \frac{\partial \theta'}{\partial x_k} \right\rangle}_{\epsilon_{\theta\theta}}, \end{aligned} \quad (11)$$

where P_{ij} , D_{ij} , G_{ij} are the Reynolds stress production, diffusion, and buoyant production tensors respectively, Φ_{ij} is the pressure-redistribution tensor, and ϵ_{ij} is the turbulence dissipation rate tensor. $P_{\theta,i}$, $D_{\theta,i}$, $\epsilon_{\theta,i}$, $G_{\theta,i}$ are the temperature flux production, diffusion, dissipation, and buoyant production vectors respectively, and $\Phi_{\theta,i}$ is the pressure-scrambling vector. $P_{\theta\theta}$, $D_{\theta\theta}$, $\epsilon_{\theta\theta}$ are the temperature variance production, diffusion and dissipation terms respectively. The production terms and the buoyancy terms, P_{ij} , $P_{\theta,i}$, $P_{\theta\theta}$, G_{ij} , $G_{\theta,i}$, do not need to be modeled at the second moment closure level, as they are comprised of the terms that are explicitly solved for in the model. The remaining terms on the right-hand side of Eqs. (9), (10) and (11) need to be modeled, as summarized below.

3.2.1. Diffusion terms modeling

The Reynolds stress diffusion term, D_{ij} , is comprised of

$$\begin{aligned} D_{ij} &= \underbrace{\left(-\frac{\partial \langle u'_i u'_j u'_k \rangle}{\partial x_k} \right)}_{D_{T,ij}} + \underbrace{\left(-\frac{1}{\rho} \frac{\partial}{\partial x_k} \left(\langle p' u'_i \rangle \delta_{jk} + \langle p' u'_j \rangle \delta_{ik} \right) \right)}_{D_{p,ij}} \\ &+ \underbrace{\left(\nu \frac{\partial^2 \langle u'_i u'_j \rangle}{\partial x_k \partial x_k} \right)}_{D_{v,ij}}, \end{aligned} \quad (12)$$

where $D_{T,ij}$ represents turbulent diffusion, $D_{p,ij}$ is the pressure-diffusion term, and $D_{v,ij}$ represents viscous diffusion. We follow the standard approach and model the diffusion terms $D_{p,ij}$ and $D_{T,ij}$ together as [65]

$$D_{p,ij} + D_{T,ij} = \frac{\partial}{\partial x_k} \left[D \frac{k^2}{\epsilon} \frac{\partial R_{ij}}{\partial x_k} \right], \quad (13)$$

where D is a diffusion model coefficient. This scalar diffusion approximation is the simplest choice of models for $D_{p,ij} + D_{T,ij}$ historically employed in the literature. Other tensorially consistent and complex models [70,71] have also been widely used, but these are not considered in this work. Similarly, for temperature flux diffusion, $D_{\theta,i}$, we have

$$\begin{aligned} D_{\theta,i} &= \underbrace{\left(-\frac{\partial \langle \theta' u'_i u'_k \rangle}{\partial x_k} \right)}_{D_{T,\theta,i}} + \underbrace{\left(-\frac{1}{\rho} \frac{\partial \langle p' \theta' \rangle \delta_{ik}}{\partial x_k} \right)}_{D_{p,\theta,i}} \\ &+ \underbrace{\left(\nu \left\langle \theta' \frac{\partial u'_i}{\partial x_k} \right\rangle + \alpha \left\langle u'_i \frac{\partial \theta'}{\partial x_k} \right\rangle \right)}_{D_{v,\theta,i}}. \end{aligned} \quad (14)$$

Consistent with Eq. (13), we adopt

$$D_{\theta,i} = D_{p,\theta,i} + D_{v,\theta,i} + D_{T,\theta,i} = \frac{\partial}{\partial x_k} \left[\left(\nu + \frac{1}{Pr_{tur,\theta,i}} \frac{k}{\omega} \right) \frac{\partial R_{\theta,i}}{\partial x_k} \right] \quad (15)$$

where $Pr_{tur,\theta,i}$ is a turbulent Prandtl number. For variance diffusion, $D_{\theta\theta}$, we adopt

$$D_{\theta\theta} = D_{v,\theta\theta} + D_{T,\theta\theta} = \frac{\partial}{\partial x_k} \left[\left(\alpha + \frac{1}{Pr_{tur,\theta\theta}} \frac{k}{\omega} \right) \frac{\partial R_{\theta\theta}}{\partial x_k} \right]. \quad (16)$$

3.2.2. Pressure-redistribution modeling

For the pressure-redistribution term, Φ_{ij} , we use the Speziale-Sarkar-Gatski (SSG) model [72]

$$\begin{aligned} \Phi_{ij} &= - \left(C_1 \epsilon + \frac{1}{2} C_1^* P_{kk} \right) a_{ij} + C_2 \epsilon \left(a_{ik} a_{kj} - \frac{1}{3} a_{kl} a_{kl} \delta_{ij} \right) \\ &+ (C_3 - C_3^* \sqrt{a_{kl} a_{kl}}) k S_{ij}^* \\ &+ C_4 k \left(a_{ik} S_{jk} + a_{jk} S_{ik} - \frac{2}{3} a_{kl} S_{kl} \delta_{ij} \right) \\ &+ C_5 k (a_{ik} W_{jk} + a_{jk} W_{ik}) - C_{bf} \left(G_{ij} - \frac{1}{3} G_{kk} \delta_{ij} \right). \end{aligned} \quad (17)$$

Here

$$\begin{aligned} a_{ij} &\equiv \frac{R_{ij}}{k} - \frac{2}{3} \delta_{ij}, \quad S_{ij} \equiv \frac{1}{2} \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right), \\ S_{ij}^* &\equiv S_{ij} - \frac{1}{3} S_{kk} \delta_{ij}, \quad W_{ij} \equiv \frac{1}{2} \left(\frac{\partial U_i}{\partial x_j} - \frac{\partial U_j}{\partial x_i} \right), \end{aligned}$$

and C_1 , C_1^* , C_2 , C_3 , C_3^* , C_4 , C_5 , C_{bf} are model coefficients. In anticipation of the results presented in Section 3.4, we summarize the physics

associated with each model term in Eq. (17). Pressure-redistribution is conventionally decomposed into rapid, slow, and harmonic components, and in buoyant flows (as here), an isotropization of the body forcing term [73]. The harmonic term is important only near a solid boundary and therefore is not of concern for a stratified shear layer. In Eq. (17), the first two terms model the slow pressure-redistribution (modeled from the return-to-isotropy hypothesis [74,75]), the third to the fifth terms model rapid pressure-redistribution, and the last term models the isotropization of the buoyancy force [76]. Besides the SSG model, other closure models also exist [77,78]. A fitting topic is to put all models together in the model space and study the resulting model-form uncertainty. However, measuring the effectiveness and the inconsistency for model-form perturbation is not as straightforward as that for model coefficient perturbations, because it is not entirely clear how one could define a distance between two distinctly different model forms in the model space. As such, we will leave model-form uncertainty for future investigation.

3.2.3. Pressure-scrambling modeling

The pressure-scrambling term in the flux transport equations, $\Phi_{\theta,i}$, is also decomposed into three components, $\Phi_{\theta,i,1}$, $\Phi_{\theta,i,2}$ and $\Phi_{\theta,i,3}$. We adopt a simple return-to-isotropy model [79] for $\Phi_{\theta,i,1}$, a basic isotropization of production (IP) model [76] for $\Phi_{\theta,i,2}$, and quasi-isotropic model [80] for $\Phi_{\theta,i,3}$

$$\Phi_{\theta,i} = \underbrace{-C_{\theta 1} \frac{\varepsilon}{k} R_{\theta,i}}_{\Phi_{\theta,i,1}} + \underbrace{C_{\theta 2} R_{\theta,k} \frac{\partial U_i}{\partial x_k}}_{\Phi_{\theta,i,2}} + \underbrace{C_{\theta 3} \beta g_i R_{\theta\theta}}_{\Phi_{\theta,i,3}}, \quad (18)$$

where $C_{\theta 1}$, $C_{\theta 2}$, and $C_{\theta 3}$ are model coefficients.

3.2.4. Dissipation modeling

For the Reynolds stress dissipation, we assume *local isotropy*

$$\varepsilon_{ij} = \frac{2}{3} \varepsilon \delta_{ij}, \quad (19)$$

where ε is the turbulent dissipation rate, which is related to the specific dissipation rate ω as

$$\omega = \frac{\varepsilon}{C_\mu k}, \quad (20)$$

where C_μ is a model coefficient (Prandtl-Kolmogorov constant). We solve the following transport equation for ω [8]

$$\begin{aligned} \frac{\partial \omega}{\partial t} + U_j \frac{\partial \omega}{\partial x_j} &= \frac{\alpha_\omega \omega}{2k} (P_{jj} + G_{jj}) - \beta_\omega \omega^2 + \frac{\partial}{\partial x_j} \left[\left(\nu + \sigma_\omega \frac{k}{\omega} \right) \frac{\partial \omega}{\partial x_j} \right] \\ &+ \sigma_d \frac{1}{\omega} \max \left(\frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j}, 0 \right). \end{aligned} \quad (21)$$

where α_ω , β_ω , σ_ω , σ_d are model coefficients. The temperature flux dissipation term $\varepsilon_{\theta,i}$ is modeled based on the *local isotropy* assumption as well:

$$\varepsilon_{\theta,i} = 0. \quad (22)$$

The temperature variance dissipation term $\varepsilon_{\theta\theta}$ is modeled as follows

$$\varepsilon_{\theta\theta} = C_{\theta\theta} \frac{\varepsilon}{k} R_{\theta\theta}. \quad (23)$$

where $C_{\theta\theta}$ is another model constant. Eqs. (9), (10), (11) and (21) are the eleven transport equations being solved in addition to the three RANS Eqs. (8). The 11-equation model contains four unclosed tensor terms, i.e., Φ_{ij} , $D_{p,ij}$, $D_{T,ij}$, ε_{ij} , five unclosed vector terms, i.e., $\Phi_{\theta,i}$, $D_{p,\theta,i}$, $D_{v,\theta,i}$, $D_{T,\theta,i}$, $\varepsilon_{\theta,i}$, two unclosed scalar terms, i.e., $D_{T,\theta\theta}$, $\varepsilon_{\theta\theta}$, and four terms in the specific dissipation rate equation. In sum there are twenty closure coefficients. Considering this complexity, training this model such that it generalizes beyond its calibration basis is an obvious challenge.

3.3. Global epistemic UQ details

The Reynolds number, Richardson number, and turbulence intensity define the FCP space. Specifically, $Re \times Ri \times TI = [500, 10^8] \times [0, 0.1] \times [0.01, 0.2]$, covering a wide range of flow conditions. For reference, the Reynolds number of the stratified wake behind a submarine is $Re \approx 1 \text{ [m]} \times 10 \text{ [m/s]} / 10^{-6} \text{ [m}^2\text{s}^{-1}] = 10^7$. We will use $\mathbf{F}$ to denote a point in the FCP space, and $\mathbf{F}_i$, $i = 1, 2, 3, \dots, N$, to denote the sampling points in the FCP space.

The model space is 55D. Table 1 lists the 55 perturbations that define the model space. The intention here is to include all possible perturbations one could incorporate in this baseline model. Table 1 does not include perturbations to the shape and the orientation of G_{ij} , ε_{ij} , $G_{\theta,i}$, $\varepsilon_{\theta,j}$, and $\varepsilon_{\theta\theta}$, because they do not have a notable impact on the QoIs. Varying a model coefficient is perturbing the magnitude of the corresponding term, and therefore we do not separately list magnitude perturbations in Table 1. When perturbing a model coefficient, we vary its value by 0.5%. When perturbing the shape of a tensor, we vary its eigenvalues by 0.1%. When perturbing the orientation, we rotate the tensor about one of its eigenvectors by 0.001 rad. These perturbations are sufficiently small such that $\Delta \text{QoI} / \delta$ is not a function of the perturbation's magnitude δ . It is worth noting that, for a stratified shear layer, the FRSM model, and the 9 QoIs considered in this paper, $\Delta \text{QoI} / \delta$ does not depend on δ for even large δ , as we would see in the next section. We will use $\mathbf{m}$ to denote a point in the model space and use m_j to denote $\mathbf{m}$'s j th component. For example, $m_1 = \sigma_\omega$, and $m_{54,55}$ describe the shape of P_{ij} .

We have 9 QoIs, namely, the momentum thickness δ_θ , the mean velocity U , the mean temperature T (equivalent to the mean density), the mean kinetic energy MKE, the second order moments $\langle u'u' \rangle$, $\langle v'v' \rangle$, $\langle u'v' \rangle$, $\langle v'T' \rangle$, and $\langle T'T' \rangle$. These QoIs are functions of $\mathbf{M}$ and $\mathbf{F}$. Except for the momentum thickness δ_θ , which is a function of t not y , all other 8 QoIs are functions of both y and t . Evaluating $e_{i,j,\text{QoI}}$ for a given QoI requires two evaluations of the FRSM, one at $\mathbf{M}_o$ and one at $\mathbf{M}_o + \delta_j$:

$$e_{i,j,\delta_\theta} = \sqrt{\frac{1}{t_e} \int_0^{t_e} dt \left[\frac{\delta_\theta(\mathbf{F}_i, \mathbf{M}_o + \delta_j) - \delta_\theta(\mathbf{F}_i, \mathbf{M}_o)}{\delta_j} \right]^2}, \quad (24)$$

for the QoI δ_θ , and

$$e_{i,j,\text{QoI}} = \sqrt{\frac{1}{t_e \delta_{\omega,0}} \int_{-\infty}^{\infty} dy \int_0^{t_e} dt \left[\frac{\text{QoI}(\mathbf{F}_i, \mathbf{M}_o + \delta_j) - \text{QoI}(\mathbf{F}_i, \mathbf{M}_o)}{\delta_j} \right]^2}, \quad (25)$$

for the other 8 QoIs. Here, $\mathbf{M}_o$ is the original model and δ_j is the perturbation in the j th dimension in the model space. It then follows from Eq. (5) that $\sigma_{j,\text{QoI}}$ and $\mu_{j,\text{QoI}}$ are

$$\mu_{j,\text{QoI}} = \frac{1}{N} \sum_{i=1}^N e_{i,j,\text{QoI}}, \quad \sigma_{j,\text{QoI}}^2 = \frac{1}{N} \sum_{i=1}^N (e_{i,j,\text{QoI}} - \mu_{j,\text{QoI}})^2. \quad (26)$$

For a given QoI and a give type of perturbation j , $\mu_{j,\text{QoI}}$ and $\sigma_{j,\text{QoI}}$ are two numbers.

3.4. Global epistemic UQ results

3.4.1. The number of samplings in the flow controlling parameter space

To obtain reliable estimates of $\sigma_{j,\text{QoI}}$ and $\mu_{j,\text{QoI}}$, we must sufficiently sample the FCP space. Fig. 6 shows $\sigma_{52,\delta_\theta}$ and μ_{52,δ_θ} as a function of the number of sampling N . $e_{i,52,\delta_\theta}$ varies significantly within the FCP space, and $\sigma_{52,\delta_\theta}$, μ_{52,δ_θ} is in the H.E., H.I quadrant (see Section 3.4.3). Estimating $\sigma_{52,\delta_\theta}$, μ_{52,δ_θ} is therefore more difficult than, say, estimating σ , μ in the H.E., L.I. quadrant. From Fig. 6, we observe that $N = 100$ returns reliable estimates of σ , μ . By sampling 100 times in the FCP space, each global epistemic UQ requires $N \times N' = 100 \times 56 = 5,600$ evaluations of the RANS model.

Table 1

The types of perturbations that define the model space. For indices 1–20, perturbations are for model coefficients. For indices 21–55, perturbations for tensor terms' orientation (Orn) and shape (Shp).

	Index	1	2	3	4	5	6	7	8	9	10	11	12	13	
	Perturbation	σ_ω	σ_d	α_ω	β_ω	C_μ	C_1	C_1^*	C_2	C_3	C_3^*	C_4	C_5	C_{bf}	
	FRSM	ω , Eq. (21)							Φ_{ij} , Eq. (17)						
Index	14	15			16		17		18	19		20			
Perturbation	D	$Pr_{tur,\theta,i}$			$Pr_{tur,\theta\theta}$		$C_{\theta 1}$		$C_{\theta 2}$	$C_{\theta 3}$		$C_{\theta\theta}$			
FRSM	D_{ij} , Eq. (13)	$D_{\theta,i}$, Eq. (15)			$D_{\theta\theta}$, Eq. (16)		$\Phi_{\theta,i}$, Eq. (18)			$\epsilon_{\theta\theta}$, Eq. (23)					
Index	21–23	24, 25	26–28		29, 30		31–33		34, 35		36–38		39,40	41–43	44, 45
Perturbation	Orn	Shp	Orn		Shp		Orn		Shp		Orn		Shp	Orn	Shp
FRSM, Eq. (17)	1st term		2nd term			3rd term			4th term			5th term			
	Index	46–48			49, 50			51–53			54, 55				
	Perturbation	Orn			Shp			Orn			Shp				
	FRSM	6th term in Eq. (17)							$\mathcal{P}_{ij}$ in Eq. (9)						

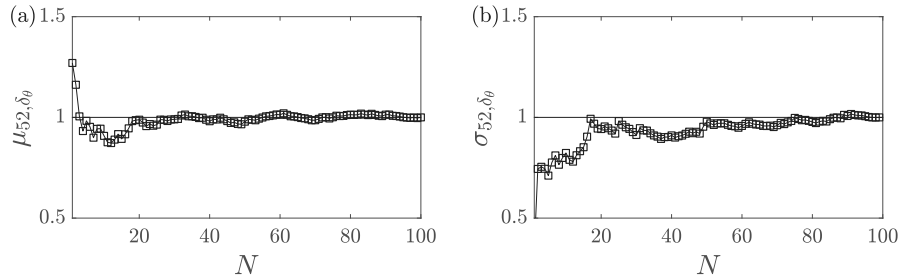


Fig. 6. (a) μ_{52,δ_θ} and (b) $\sigma_{52,\delta_\theta}$ as a function of the sampling points N in the full FCP space. The results are normalized by their respective values at $N = 100$.

3.4.2. Global epistemic UQ in a sub flow controlling parameter space

We first consider shear layers with no thermal stratification. The FCP space reduces to a 2D one, i.e., $Re \times TI = [500, 10^8] \times [0.01, 0.2]$ with $Ri = 0$, and the temperature reduces to a passive scalar. The flow physics of an unstratified shear layer is considerably simpler than a stratified one, thereby allowing us to interpret the results physically.

We sample the 2D FCP space 100 times. Fig. 7 shows $\mu_{j,QoI}$ and $\sigma_{j,QoI}$ for all QoIs. For visualization purposes, we show the σ and μ values for the 3 most effective shape perturbations, the 3 most effective orientation perturbations, and the 3 most effective model coefficient perturbations. For each QoI and a given type of perturbation (shape, orientation, or model coefficient), we normalize $\mu_{j,QoI}$ and $\sigma_{j,QoI}$ with $\max_j[\mu_{j,QoI}]$. We make the following observations. First, large perturbations and small perturbations lead to similar μ and σ values. Second, all perturbations in Fig. 7 have low inconsistency. Third, the effective perturbations are fairly consistent between different QoIs, i.e., a perturbation that is effective for one QoI is also effective for other QoIs. Specifically, perturbations 22, 32, and 52 are the most effective orientation perturbations for all 9 QoIs; perturbations 35 and 54 are among the 3 most effective shape perturbations for all 9 QoIs; perturbation 9 is the most effective model coefficient perturbation for all velocity QoIs; perturbation 5 is the most effective model coefficient perturbation for temperature QoIs, i.e., $\langle T \rangle$, $\langle v'T' \rangle$, and $\langle T'T' \rangle$.

We try to explain these results physically. Perturbations 52 and 54 correspond to the production term. Physically, the production term is responsible for turbulence generation and is one of the most important terms in the Reynolds stress transport equations. Previous UQ studies have also shown that perturbing the production term would have a big impact [27,43]. Perturbations 52 and 54 being identified as the most effective perturbations is consistent with the previous UQ studies, which also serve as a validation. Perturbations 9, 22, 32 correspond to the pressure-strain correlation term. The pressure-strain correlation is the least well-calibrated term in the FRSM model because of the

lack of high Reynolds numbers experimental data [81]. Our analysis pointing to perturbations 9, 22, 32 as an effective perturbation is consistent with the above fact: further calibration is needed for the pressure-strain correlation term. The complex nature of turbulence may also explain why pressure terms need further calibration. Generally speaking, Reynolds stresses have memory and are non-local [82]. Part of this non-locality is accounted for by the material derivatives in the Reynolds transport equations. However, considering that pressure is governed by a Poisson equation, closing the pressure strain correlation term locally is a poor approximation of the reality [83,84]. The above discussion points to a weakness of the present analysis: The analysis considers three types of perturbations; while they encompass all possible perturbations to a tensor, they do not account for non-local effects. This weakness can be addressed by considering fractional derivatives, i.e., perturbations to derivative orders [85,86], or large stencils, i.e., perturbations to numerical schemes [87,88]—a topic that we will leave for future investigation. Perturbation 5 corresponds to the dissipation term. Like measuring pressure, measuring dissipation is very hard in a laboratory experiment. As a result, there is not a lot of high Reynolds number data that one can use to calibrate the dissipation term in the Reynolds stress transport equation (at least when the FRSMs were developed). The present closure model assumes local isotropy, which is a poor approximation of the dissipation in stratified shear layers [58,59]. The analysis pointing to perturbation 5 as an effective perturbation suggests first that local isotropy is a poor approximation, and second that the dissipation term needs further calibration.

From a model calibration standpoint, global epistemic uncertainty UQ helps us identify the most effective perturbations. Because the most effective perturbations have low inconsistency, we conclude from Fig. 7, *a priori*, that for any one of the 9 QoIs, calibrating perturbations 52, 54, 9, and 5 will lead to improvements at other flow conditions in the FCP. Also, because the effective perturbations are consistent between the 9 QoIs, we conclude, *a priori*, that if one perturbs 52, 54,

9, and 5, an improvement for one QoI would lead to an improvement in other QoIs.

For a FRSM specifically, the production term P_{ij} is closed, and therefore calibrating the production term would not be a good idea. Considering that the physics is such that the production and the dissipation approximately balance [59], the results here call for a more accurate model for the dissipation term. This certainly makes sense: the purpose of a FRSM is to handle Reynolds stresses' anisotropy, but the present model for the dissipation term ε_{ij} is itself isotropic, which obviously requires improvements. When it comes to calibrating the dissipation term, directly calibrating perturbation 5 may not be a good idea — albeit being an effective and consistent perturbation. Perturbation 5 corresponds to the Prandtl–Kolmogorov constant C_μ . While there is no guarantee that the Prandtl–Kolmogorov constant is universal, its value $C_\mu = 0.09$ works well for many flows, and varying it will negatively impact the model's robustness. (Note that the global epistemic UQ does not “know” this because the other flows are not part of this analysis.) In all, model calibration is a multi-faceted problem. While effectiveness and consistency are two important aspects of the problem, model calibration must also account for, e.g., robustness and prior knowledge, which are not accounted for in our global epistemic UQ analysis.

3.4.3. Global epistemic UQ in the full flow controlling parameter space

The flow physics of a stratified shear layer is considerably more complicated than an unstratified one. As a result, interpreting the global epistemic UQ results physically would not be as straightforward as that for unstratified shear layers. Fig. 8 shows the effectiveness and inconsistency of the most effective perturbations. For visualization purposes, again, we show the 3 most effective orientation perturbations, the 3 most effective shape perturbations, and the 3 most effective model coefficient perturbations. We see that many of the effective perturbations have high inconsistency: they are in the H.I. quadrants or very close to the H.I. quadrants. Nonetheless, the effective perturbations are still consistent between different QoIs. Perturbations 9, 52, and 54 are among the most effective perturbations for all QoIs. Perturbations 35, 44, 54 are the 3 most effective shape perturbations for all but $\langle u'u' \rangle$ and $\langle u'v' \rangle$, for which, perturbation 24 replaces perturbation 44 as one of the 3 most effective shape perturbations. Perturbations 22, 32, and 52 are the 3 most effective orientation perturbations for all but $\langle u'u' \rangle$, for which 42 replaces 22 as one of the 3 most effective shape perturbations. Perturbation 9 is among the 3 most effective model perturbations for all 9 QoIs. Perturbation 10 is among the 3 most effective model coefficient perturbations for all but $\langle v'v' \rangle$, $\langle v'T' \rangle$, and $\langle T'T' \rangle$. Comparing the results in this subsection and Section 3.4.2, the most effective perturbations are similar for unstratified and stratified flows. Perturbations of the production term are still among the most effective model perturbations.

From a model calibration standpoint, high inconsistency is undesirable. If a type of model perturbation has high inconsistency, calibrating the corresponding term/coefficient is less likely to lead to improvements that generalize. In that case, the physics is such that one needs more than one model, or more than one variant of the baseline model, for the flows in the FCP space. For a stratified shear layer, the different physics is the physics of the flow in the early stage and the late stage, where the turbulent convection and the buoyancy play the dominant role, respectively. Fig. 9 shows the FRSM predicted $\delta_\theta(t)$ as a function of time at three flow conditions in the FCP space. The flow in Fig. 9(a) is still at the early stage at $t = 200$, and the flow in Fig. 9(b) is at the late stage at $t = 200$. Expecting an improvement that works for an early-stage shear layer to also work for a late-stage shear layer would be hard, and this had resulted in the high inconsistency in Fig. 8.

We can verify our interpretation of the results by studying the perturbations' effectiveness and inconsistency for flows that remain at the early stage at $t = t_e$ and for flows that enter the late stage at an early time, i.e., $t < 50$. We refer to flows that remain at the early stage

at $t = t_e$ as group 1 and flows that enter the late stage at an early time as group 2. The cases are manually grouped. We discard ambiguous cases like the one in Fig. 9(c). We compute σ , μ for the group 1 cases and the group 2 cases as follows:

$$\begin{aligned}\mu_{j,\text{QoI},\text{grp1}} &= \frac{1}{N_{\text{grp1}}} \sum_{\text{group 1 cases}} e_{i,j,\text{QoI}}, \\ \sigma_{j,\text{QoI},\text{grp1}}^2 &= \frac{1}{N_{\text{grp1}}} \sum_{\text{group 1 cases}} (e_{i,j,\text{QoI}} - \mu_{j,\text{QoI}})^2, \\ \mu_{j,\text{QoI},\text{grp2}} &= \frac{1}{N_{\text{grp2}}} \sum_{\text{group 2 cases}} e_{i,j,\text{QoI}}, \\ \sigma_{j,\text{QoI},\text{grp2}}^2 &= \frac{1}{N_{\text{grp2}}} \sum_{\text{group 2 cases}} (e_{i,j,\text{QoI}} - \mu_{j,\text{QoI}})^2,\end{aligned}\quad (27)$$

where N_{grp1} and N_{grp2} are the number of cases in groups 1 and 2, respectively, and the subscripts grp1 and grp2 are for group 1 and group 2. Fig. 10 shows the results. For visualization purposes, we show results for perturbations 52 and 9, i.e., the most effective orientation perturbation and the most effective model coefficient perturbation. The results for other perturbations are similar and are not shown here for brevity. We see significantly lower σ values for perturbations 52 and 9 when we consider cases in group 1 and group 2 separately. This directly confirms our interpretation of the results in Fig. 8.

In real-world applications, it is usually not difficult to know whether two models or two variants of the same baseline model are needed to accommodate different physics in the FCP space. For example, a fluid mechanist who has the basic knowledge of shear layers' flow phenomenology knows that the physics is different in an early-stage shear layer and a late-stage shear layer and that the different physics requires different models to accommodate. The most notable example is the modeling of wall turbulence. It is well known that the flow near a solid boundary behaves differently than flow away from a solid boundary. In RANS, one accommodates this by incorporating the distance from the wall and a wall-treatment [89]. When it comes to a stratified shear layer, one could incorporate, say, the local Richardson number and a low/high-Richardson-number treatment, a topic that we will leave for future investigation. Accordingly, in practice, it can be problematic to include too many flows for model training, in which case, model training would needlessly trade-off accuracy for robustness.

3.5. Machine learning aided RANS modeling

We have DNS data at one training condition, where the growth of the shear-layer thickness is shown in Fig. 11(a). We want to calibrate our FRSM to our data such that the calibrated model predicts shear layer growth more accurately at the training condition and at the other three test conditions, whose shear layer growth is shown in Fig. 11 (b, c, d). To verify that the calibrated model does/does not work at the test conditions, we will compare the FRSM results to DNSs at the test conditions. Obviously, we do not use the DNSs at the test conditions for model calibration. Again, the QoI is δ_θ . We see from Fig. 8(a) that perturbation 9 has high effectiveness and low inconsistency. Calibrating the corresponding model coefficient C_3 to data would therefore lead to improvements that generalize. On the other hand, perturbation 22 has high effectiveness and high inconsistency. Calibrating the corresponding model term, i.e., the shape of the first term in Eq. (17), would lead to improvements that work for the calibration data but do not generalize. Although not shown in Fig. 8(a), perturbation 1 has low effectiveness and low inconsistency. Calibrating the corresponding model coefficient, σ_ω , would not have a notable effect on the QoI. Hence, from Fig. 8, we conclude, a priori, that calibrating C_3 would lead to an improvement at both the training condition and the test conditions, calibrating the shape of the first term in Eq. (17) would lead to an improvement at the training condition but not necessarily at the test conditions, and varying σ_ω would not lead to much improvement. In the following, we calibrate C_3 , σ_ω , and the shape of the first term in

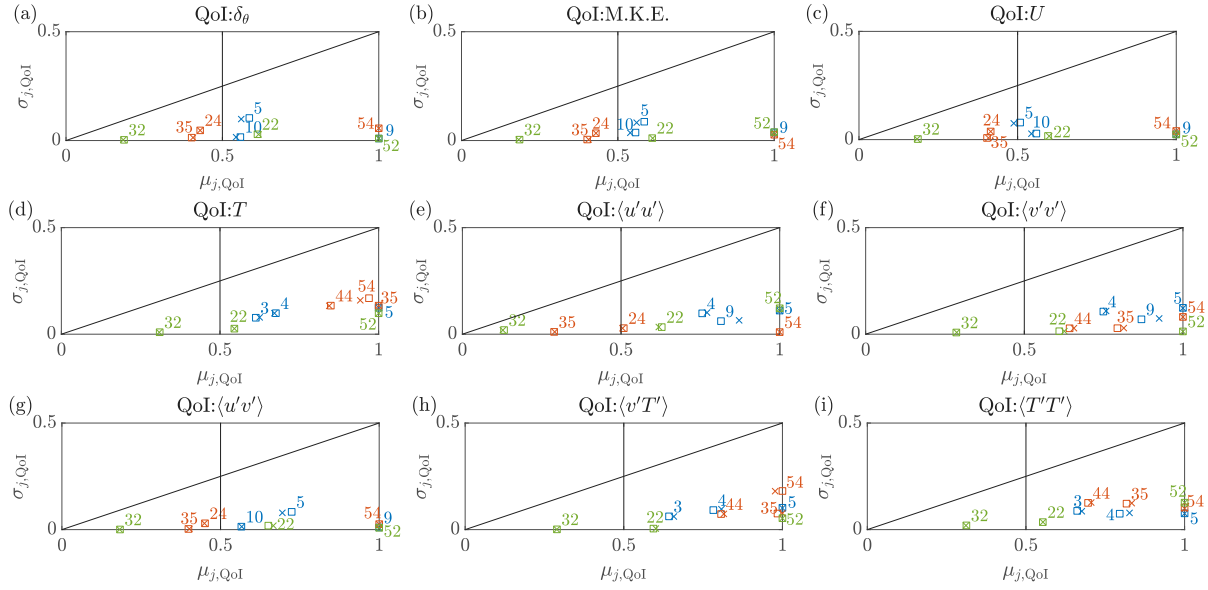


Fig. 7. $\sigma - \mu$ diagrams for unstratified shear layer. For visualization purposes, we show σ, μ for the 3 most effective shape perturbations, the 3 most effective orientation perturbations, and blue for model-coefficient perturbations. Perturbation types are color-coded. We use green for orientation perturbations, red for shape perturbations, and blue for model-coefficient perturbations. For a given QoI and a given type of model perturbation, the σ, μ values are normalized with $\max_j[\sigma_j]$ among the given type of model perturbation (shape/orientation/model-coefficient). Square symbols are results due to small perturbations, and cross symbols are due to large perturbations. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

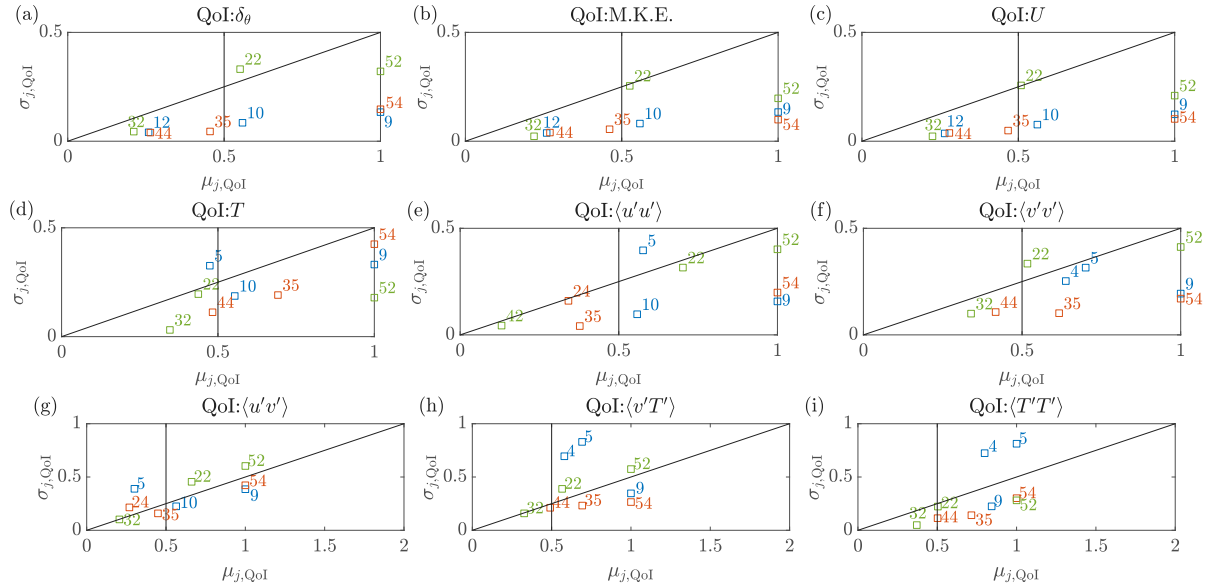


Fig. 8. $\sigma - \mu$ diagram for stratified shear layer. The legends are the same as in Fig. 7.

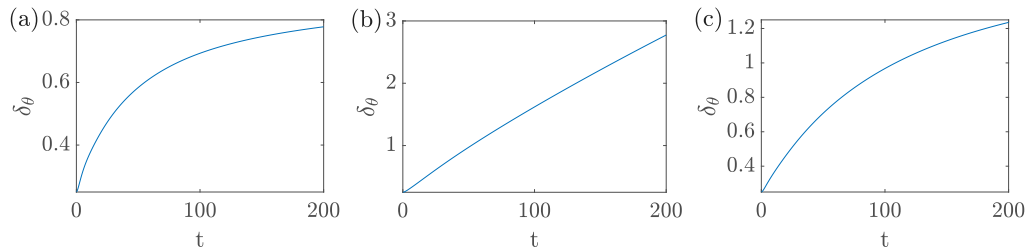


Fig. 9. The FRSM predicted time evolution of the shear layer thickness δ_θ at three flow conditions in the FCP space. The exact Re , TI , and Ri are not important. The shear layer thickness is normalized with its value at $t = 0$. (a) The shear layer has entered the late stage at $t = 200$. (b) The shear layer remains at the early stage at $t = 200$. (c) The shear layer is somewhat ambiguous in terms of whether it is at the early stage or late stage at $t = 200$.

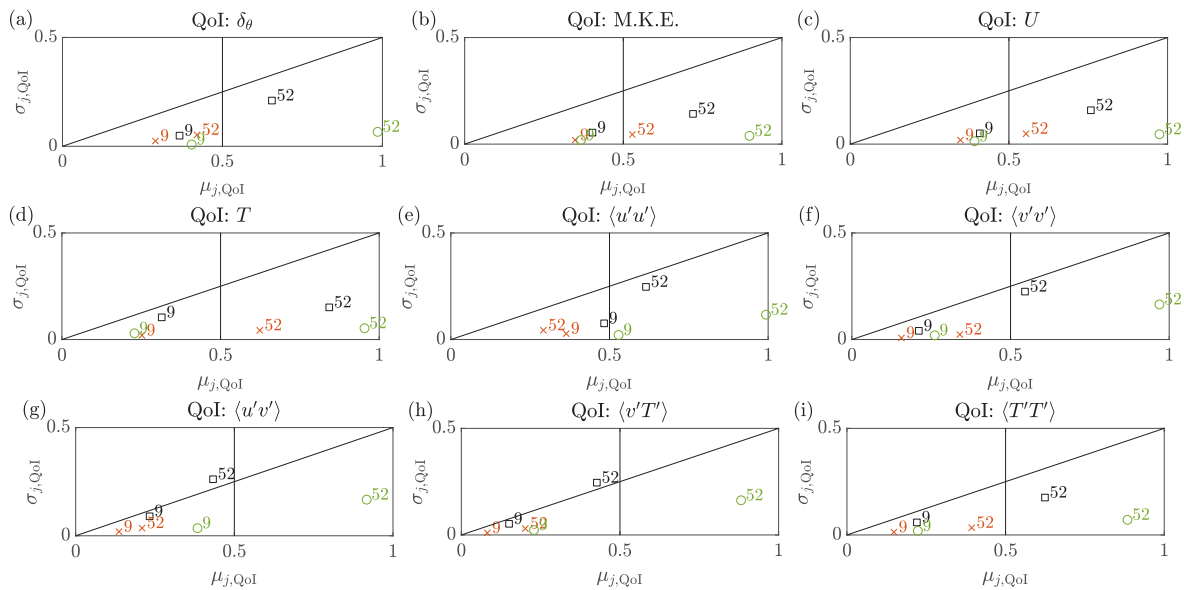


Fig. 10. $\sigma - \mu$ diagram. We use square symbols for un-grouped results, round symbols for group 1 results and cross symbols for group 2 results.

Eq. (17) so that the model matches the data as closely as possible at the training condition and see if the calibrated model performs as expected at the other three test conditions.

Fig. 11 shows the calibration results. Fig. 11(a) shows the shear layer growth results at the training condition, and Fig. 11 (b, c, d) shows the shear layer growth results at the test conditions. We see that by calibrating C_3 such that the calibrated FRSM matches the DNS at the training condition, the calibrated FRSM model agrees more closely with the DNS at all test conditions. We also see that matching the DNS at the training condition by calibrating the shape of the first term in Eq. (17), the calibrated FRSM does not perform consistently at the three test conditions. Lastly, varying σ_{ω} , even by 50% (which is a large perturbation), does not lead to a notable change in the shear layer growth. In all, the results confirm our expectation, and we can indeed determine *a priori* the applicable range of an improvement from global epistemic uncertainty quantification.

The discussion here is limited to stratified shear layer, however, the same method can well be applied to other flows with a gradient in fluid density, including stratified wakes [1,90] and turbulence mixing as a result of Rayleigh–Taylor and Richtmyer–Meshkov instability [91–93]. Like stratified shear layer, isotropy and eddy viscosity are poor modeling choices for these flows [94,95], and the presence of flow anisotropy calls for FRSM type of models [96]. However, because the model coefficients in many, if not all, of the existing FRSMs are calibrated to flows that are weakly anisotropic [97], an engineer needs to re-calibrate the existing models before the models can be used for, e.g., flows in the vicinity of shock waves. Re-calibration is usually not straightforward, particularly when there are $\mathcal{O}(100)$ possible terms/coefficients. Like FRSM of stratified shear layers, the global epistemic uncertainty quantification methodology can help re-calibrate FRSM for other variable property flows like Rayleigh–Taylor and Richtmyer–Meshkov instability induced flows by identifying terms and coefficients that are in the high effective and low inconsistency quadrant.

4. Conclusions

We develop a global epistemic UQ method that allows us to determine *a priori* a RANS model's applicable range, more specifically, to determine if a RANS model is able to extrapolate to a flow condition outside the training data. The method consists of a local UQ method and a global screening method. It evaluates a model perturbation (not necessarily a small perturbation) in terms of its effectiveness and

inconsistency. A perturbation that improves a RANS model's performance at one condition is going to generalize to other conditions in the flow controlling parameter space if and only if the perturbation has high effectiveness and low inconsistency. We apply the method to FRSM of a stratified shear layer. For this particular model, the model space has 55 dimensions; the FCP space is three-dimensional; and 9 quantities of interest are considered. A global epistemic UQ analysis of the FRSM model in this FCP space requires $\mathcal{O}(10^3)$ RANS calculations. The results point to the production term, the pressure strain term, and the coefficients C_μ , C_3 as the most effective terms for model calibration among the 55 model perturbations for the 9 quantities of interest. Following the global epistemic UQ results, we calibrate our FRSM to DNS at one flow condition by calibrating an effective and consistent model perturbation. The calibrated model works well in the training condition. More importantly, as expected from the global epistemic UQ analysis, the calibrated model generalizes to three other test conditions outside the training dataset.

CRedit authorship contribution statement

Xinyi L D Huang: Data curation, Software, Writing. **Naman Jain:** Data curation, Software, Writing. **Mahdi Abkar:** Formal analysis, Writing. **Robert F Kunz:** Conceptualization, Methodology, Project administration, Resources, Supervision, Writing. **Xiang I A Yang:** Conceptualization, Methodology, Project administration, Resources, Supervision, Writing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

This work was sponsored by the US Office of Naval Research under contract N000142012315, with Dr. Peter Chang as Technical Monitor. The DNSs are performed on ACI-ICS at Penn State.

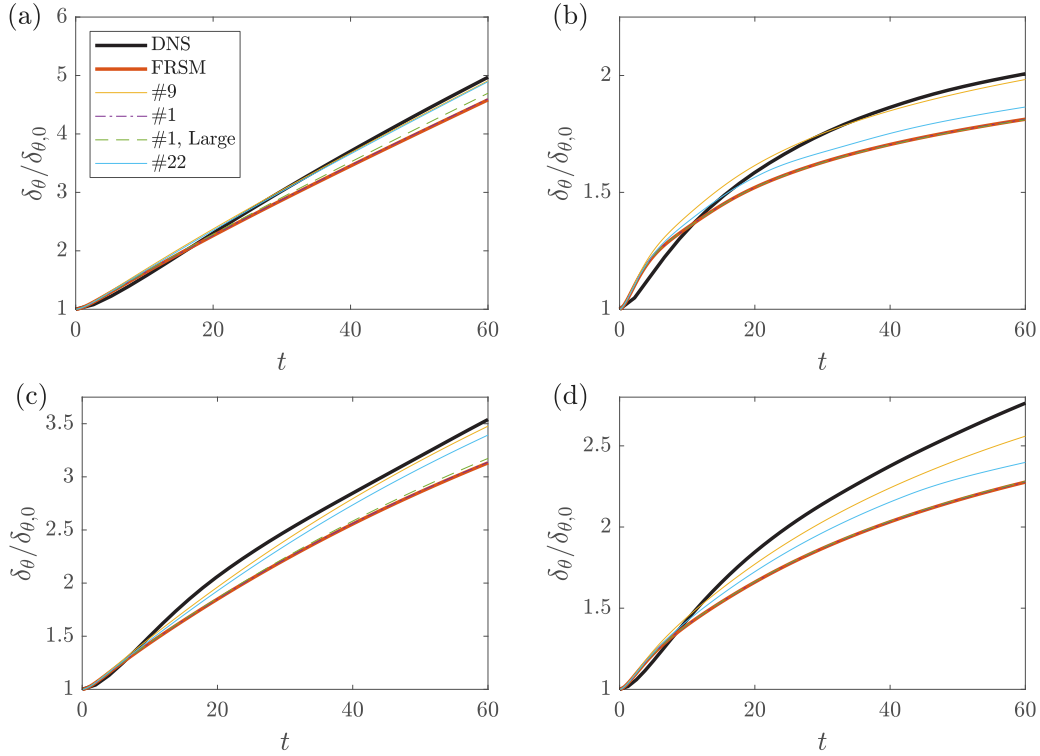


Fig. 11. Shear-layer growth as a function of time. (a) the training condition, and (b,c,d) the test conditions. Here, we calibrate the FRSM via perturbation 1, 9, and 22. Perturbation 1 is in the LE, LI quadrant. Perturbation 9 is in the HE, LI quadrant. Perturbation 22 is in the HE, HI quadrant. The legends are shown in (a). “#1 Large” is where we vary σ_ω by 50%. Perturbation #1 does not have a notable impact on the QoI δ_θ , and “#1”, “#1, Large”, and “FRSM” collapse in (a). “#1” and “FRSM” collapse in (b, c, d).

Appendix A. RANS details

The RANS code we use is the in-house finite-volume unstructured solver NPHASE [98]. The algorithm follows the established segregated pressure-based methodology. We use a collocated variable arrangement and apply a lagged coefficient linearization [99]. Continuity is imposed through pressure correction, based on the SIMPLE-C algorithm [100]. In constructing cell face fluxes, a momentum interpolation scheme [101] is employed.

For the stratified shear layer calculations, we use a Cartesian mesh for a grid size of $N_x \times N_y \times N_z = 4 \times 401 \times 2$. We refine the mesh near the centerline, using 28 grid points to resolve $2\delta_{\omega,0}$. The flow is periodic in the streamwise direction, and we apply a symmetric condition at the side and top and the bottom boundaries. The initial conditions are given as follows

$$\begin{aligned}
 U &= -\frac{1}{2}\Delta U \tanh\left(\frac{2y}{\delta_{\omega,0}}\right), \quad T = \frac{1}{2}\Delta T \tanh\left(\frac{2y}{\delta_{\omega,0}}\right), \\
 \langle u'u' \rangle &= \langle v'v' \rangle = \langle w'w' \rangle = \left[\Delta U \text{TI} \exp\left(-0.67y^2/\delta_{\omega,0}^2\right) \right]^2, \\
 \langle u'v' \rangle &= -0.023C_\mu^{-1/4}\delta_{\omega,0} \Delta U \frac{dU}{dy} \text{TI} \exp\left(-1.35y^2/\delta_{\omega,0}^2\right), \\
 \langle u'w' \rangle &= 0, \quad \langle v'w' \rangle = 0, \\
 \langle u'\theta' \rangle &= 0, \quad \langle v'\theta' \rangle = 0, \quad \langle w'\theta' \rangle = 0, \quad \langle \theta'\theta' \rangle = 0,
 \end{aligned} \tag{A.1}$$

where a Gaussian profile is used for the Reynolds stresses and the coefficients 0.67, 0.023, 1.35 are obtained by fitting to our DNS. We integrate the RANS equations to $t_e = 200$.

Appendix B. DNS details

We use the open-source finite-difference solver AFiD for our DNS. The code uses a second-order finite difference scheme and solves for

fluid velocities on a staggered grid. Time discretization uses a second-order Adams–Bashforth method. Further details of the solver can be found in Ref. [102] and the references cited therein [103–105].

For the stratified shear layer calculation, we apply a periodic condition in the streamwise and the spanwise directions and a free-slip condition at both the top and bottom boundaries. We use a Cartesian mesh for the two DNSs. For the DNS with $Ri = 0.1$, the domain size is $L_x \times L_y \times L_z = 64.50 \times 21.50 \times 48.38$, and the grid count, $N_x \times N_y \times N_z = 384 \times 128 \times 512$. The other flow controlling parameters are $Pr = 1.0$, $Re = 1280$. For the DNS with $Ri = 0.0$, the domain size is $L_x \times L_y \times L_z = 64.50 \times 21.50 \times 32.25$, and the grid count $N_x \times N_y \times N_z = 384 \times 128 \times 192$. The other flow controlling parameters are $Pr = 1.0$, $Re = 640$. Our grid resolution is the same as [59]. The initial conditions are also the same as in Ref. [59]. Because the flow is transient, we run the same case 100 times for the ensemble average.

References

- [1] Lin J-T, Pao Y-H. Wakes in stratified fluids. *Annu Rev Fluid Mech* 1979;11(1):317–38.
- [2] Choi H, Moin P. Grid-point requirements for large eddy simulation: Chapman's estimates revisited. *Phys Fluids* 2012;24(1):011702.
- [3] Yang X, Griffin K. Grid-point and time-step requirements for direct numerical simulation and large-eddy simulation. *Phys Fluids* 2020;33(1):015108.
- [4] Frisch U. *Turbulence: the legacy of A.N. Kolmogorov*. Cambridge University Press; 1995.
- [5] Spalart PR. Philosophies and fallacies in turbulence modeling. *Prog Aerosp Sci* 2015;74:1–15.
- [6] Mellor GL, Yamada T. A hierarchy of turbulence closure models for planetary boundary layers. *J Atmos Sci* 1974;31(7):1791–806.
- [7] Jones W, Launder BE. The prediction of laminarization with a two-equation model of turbulence. *Int J Heat Mass Transfer* 1972;15(2):301–14.
- [8] Menter FR. Two-equation eddy-viscosity turbulence models for engineering applications. *AIAA J* 1994;32(8):1598–605.
- [9] Spalart P, Allmaras S. A one-equation turbulence model for aerodynamic flows. In: *AIAA paper*, 1992. p. 439.
- [10] Messina P. The exascale computing project. *Comput Sci Eng* 2017;19(3):63–7.

- [11] Graham J, Kanov K, Yang X, Lee M, Malaya N, Lalescu C, et al. A web services accessible database of turbulent channel flow and its use for testing a new integral wall model for LES. *J Turbul* 2016;17(2):181–215.
- [12] Lee M, Moser RD. Direct numerical simulation of turbulent channel flow up to $Re_\tau = 5200$. *J Fluid Mech* 2015;774:395–415.
- [13] Yamamoto Y, Tsuji Y. Numerical evidence of logarithmic regions in channel flow at $Re_\tau = 8000$. *Phys Rev Fluids* 2018;3(1):012602.
- [14] Duraisamy K, Zhang ZJ, Singh AP. New approaches in turbulence and transition modeling using data-driven techniques. In: AIAA paper, 2015. p. 1284.
- [15] Tracey BD, Duraisamy K, Alonso JJ. A machine learning strategy to assist turbulence model development. In: AIAA paper, 2015. p. 1287.
- [16] Ling J, Jones R, Templeton J. Machine learning strategies for systems with invariance properties. *J Comput Phys* 2016;318:22–35.
- [17] Ling J, Kurzwski A, Templeton J. Reynolds averaged turbulence modelling using deep neural networks with embedded invariance. *J Fluid Mech* 2016;807:155–66.
- [18] Ray J, Lefantzi S, Arunajatesan S, Dechant L. Bayesian parameter estimation of a $k-\epsilon$ model for accurate jet-in-crossflow simulations. *AIAA J* 2016;54(8):2432–48.
- [19] Wang J-X, Wu J-L, Xiao H. Physics-informed machine learning approach for reconstructing Reynolds stress modeling discrepancies based on DNS data. *Phys Rev Fluids* 2017;2(3):034603.
- [20] Wu J-L, Xiao H, Paterson E. Physics-informed machine learning approach for augmenting turbulence models: A comprehensive framework. *Phys Rev Fluids* 2018;3(7):074602.
- [21] Zhang X, Wu J, Coutier-Delgosha O, Xiao H. Recent progress in augmenting turbulence models with physics-informed machine learning. *J Hydrodyn* 2019;31(6):1153–8.
- [22] Milani PM, Ling J, Eaton JK. Turbulent scalar flux in inclined jets in crossflow: counter gradient transport and deep learning modelling. 2020, arXiv preprint arXiv:2001.04600.
- [23] Zhao Y, Akolekar HD, Weatheritt J, Michelassi V, Sandberg RD. RANS turbulence model development using CFD-driven machine learning. *J Comput Phys* 2020;109413.
- [24] Dunn MC, Shotorban B, Frendi A. Uncertainty quantification of turbulence model coefficients via Latin hypercube sampling method. *J Fluid Eng* 2011;133(4).
- [25] Margheri L, Melli M, Salvetti MV, Sagaut P. Epistemic uncertainties in RANS model free coefficients. *Comput Fluids* 2014;102:315–35.
- [26] Schaefer J, Hosder S, West T, Rumsey C, Carlson J-R, Kleb W. Uncertainty quantification of turbulence model closure coefficients for transonic wall-bounded flows. *AIAA J* 2017;55(1):195–213.
- [27] Emory M, Larsson J, Iaccarino G. Modeling of structural uncertainties in Reynolds-averaged Navier-Stokes closures. *Phys Fluids* 2013;25(11):110822.
- [28] Iaccarino G, Mishra AA, Ghili S. Eigenspace perturbations for uncertainty estimation of single-point turbulence closures. *Phys Rev Fluids* 2017;2(2):024605.
- [29] Mishra AA, Iaccarino G. Uncertainty estimation for Reynolds-averaged Navier-Stokes predictions of high-speed aircraft nozzle jets. *AIAA J* 2017;55(11):3999–4004.
- [30] Edeling WN, Iaccarino G, Cinnella P. Data-free and data-driven RANS predictions with quantified uncertainty. *Flow Turbul Combust* 2018;100(3):593–616.
- [31] Xiao H, Wang J-X, Ghanem RG. A random matrix approach for quantifying model-form uncertainties in turbulence modeling. *Comput Method Appl M* 2017;313:941–65.
- [32] Cheung SH, Oliver TA, Prudencio EE, Prudhomme S, Moser RD. Bayesian uncertainty analysis with applications to turbulence modeling. *Reliab Eng Syst Safe* 2011;96(9):1137–49.
- [33] Kato H, Obayashi S. Approach for uncertainty of turbulence modeling based on data assimilation technique. *Comput Fluids* 2013;85:2–7.
- [34] Edeling W, Cinnella P, Dwight RP. Predictive RANS simulations via Bayesian model-scenario averaging. *J Comput Phys* 2014;275:65–91.
- [35] Edeling WN, Cinnella P, Dwight RP, Bijl H. Bayesian estimates of parameter variability in the $k-\epsilon$ turbulence model. *J Comput Phys* 2014;258:73–94.
- [36] Kato H, Yoshizawa A, Ueno G, Obayashi S. A data assimilation methodology for reconstructing turbulent flows around aircraft. *J Comput Phys* 2015;283:559–81.
- [37] Papadimitriou DI, Papadimitriou C. Bayesian uncertainty quantification of turbulence models based on high-order adjoint. *Comput Fluids* 2015;120:82–97.
- [38] Singh AP, Duraisamy K. Using field inversion to quantify functional errors in turbulence closures. *Phys Fluids* 2016;28(4):045110.
- [39] Xiao H, Wu J-L, Wang J-X, Sun R, Roy C. Quantifying and reducing model-form uncertainties in Reynolds-averaged Navier-Stokes simulations: A data-driven, physics-informed Bayesian approach. *J Comput Phys* 2016;324:115–36.
- [40] Wu J-L, Wang J-X, Xiao H. A Bayesian calibration–prediction method for reducing model-form uncertainties with application in RANS simulations. *Flow Turbul Combust* 2016;97(3):761–86.
- [41] Wang J, Wu J-L, Xiao H. Incorporating prior knowledge for quantifying and reducing model-form uncertainty in RANS simulations. *Int J Uncertain Quantif* 2016;6(2).
- [42] Parish EJ, Duraisamy K. A paradigm for data-driven predictive modeling using field inversion and machine learning. *J Comput Phys* 2016;305:758–74.
- [43] Gorlé C, Zeoli S, Emory M, Larsson J, Iaccarino G. Epistemic uncertainty quantification for Reynolds-averaged Navier-Stokes modeling of separated flows over streamlined surfaces. *Phys Fluids* 2019;31(3):035101.
- [44] Zadeh LA, Klir GJ, Yuan B. Fuzzy sets, fuzzy logic, and fuzzy systems: selected papers. vol. 6, World Scientific; 1996.
- [45] Klir GJ, Harmanec D. Generalized information theory. *Kybernetes* 1996;25(7–8):50–67.
- [46] Person S, Hajagos JG. Arithmetic with uncertain numbers: rigorous and (often) best possible answers. *Reliab Eng Syst Safe* 2004;85(1–3):135–52.
- [47] Yang X, Zafar S, Wang J-X, Xiao H. Predictive large-eddy-simulation wall modeling via physics-informed neural networks. *Phys Rev Fluids* 2019;4(3):034602.
- [48] Huang XL, Yang XI, Kunz RF. Wall-modeled large-eddy simulations of spanwise rotating turbulent channels—Comparing a physics-based approach and a data-based approach. *Phys Fluids* 2019;31(12):125105.
- [49] Huang XL, Yang XI. A Bayesian approach to the mean flow in a channel with small but arbitrarily directional system rotation. *Phys Fluids* 2021;33(1):015103.
- [50] Xiao H, Cinnella P. Quantification of model uncertainty in RANS simulations: A review. *Prog Aerosp Sci* 2019;108:1–31.
- [51] Rumsey CL, Gatski T, Sellers III W, Vasta V, Viken S. Summary of the 2004 computational fluid dynamics validation workshop on synthetic jets. *AIAA J* 2006;44(2):194–207.
- [52] Vassberg J, Tinoco E, Mani M, Brodersen O, Eisfeld B, Wahls R, et al. Summary of the third AIAA CFD drag prediction workshop. In: AIAA paper, 2007. p. 260.
- [53] Eisfeld B, Rumsey C, Togiti V. Verification and validation of a second-moment-closure model. *AIAA J* 2016;54(5):1524–41.
- [54] Roy CJ, Rumsey CL, Tinoco EN. Summary data from the sixth AIAA computational fluid dynamics drag prediction workshop: Code verification. *J Aircr* 2018;55(4):1338–51.
- [55] Santner TJ, Williams BJ, Notz WI, Williams BJ. The design and analysis of computer experiments. vol. 1, Springer; 2003.
- [56] Morris MD, Mitchell TJ. Exploratory designs for computational experiments. *J Statist Plann Inference* 1995;43(3):381–402.
- [57] Mishra A, Iaccarino G. Theoretical analysis of tensor perturbations for uncertainty quantification of Reynolds averaged and subgrid scale closures. *Phys Fluids* 2019;31(7):075101.
- [58] Basak S, Sarkar S. Dynamics of a stratified shear layer with horizontal shear. *J Fluid Mech* 2006;568:19.
- [59] Brucker KA, Sarkar S. Evolution of an initially turbulent stratified shear layer. *Phys Fluids* 2007;19(10):105105.
- [60] Pham HT, Sarkar S, Brucker KA. Dynamics of a stratified shear layer above a region of uniform stratification. *J Fluid Mech* 2009;630:191–223.
- [61] Pham HT, Sarkar S. Transport and mixing of density in a continuously stratified shear layer. *J Turbul* 2010;(11):N24.
- [62] Pham HT, Sarkar S. Large eddy simulations of a stratified shear layer. *J Fluid Eng* 2014;136(6).
- [63] Launder BE. Second-moment closure: present...and future? *Int J Heat Fluid Flow* 1989;10(4):282–300.
- [64] Durbin PA. Some recent developments in turbulence closure modeling. *Annu Rev Fluid Mech* 2018;50:77–103.
- [65] Shir C. A preliminary numerical study of atmospheric turbulent flows in the idealized planetary boundary layer. *J Atmos Sci* 1973;30(7):1327–39.
- [66] Gibson M, Launder B. Ground effects on pressure fluctuations in the atmospheric boundary layer. *J Fluid Mech* 1978;86(3):491–511.
- [67] Craft T, Ince N, Launder B. Recent developments in second-moment closure for buoyancy-affected flows. *Dynam Atmos Oceans* 1996;23(1–4):99–114.
- [68] Eisfeld B. Steps towards a Reynolds stress model for the prediction of separated flows. In: AVT-307 symposium on separated flow: prediction, measurement and assessment for air and sea vehicles, paper, no. 9, 2019. p. 7–9.
- [69] Eisfeld B, Rumsey CL. Length-scale correction for Reynolds-stress modeling. *AIAA J* 2020;58(4):1518–28.
- [70] Daly BJ, Harlow FH. Transport equations in turbulence. *Phys Fluids* 1970;13(11):2634–49.
- [71] Hanjalic K, Launder B, et al. A Reynolds stress model of turbulence and its application to thin shear flows. *J Fluid Mech* 1972;52(4):609–38.
- [72] Speziale CG, Sarkar S, Gatski TB. Modelling the pressure-strain correlation of turbulence: an invariant dynamical systems approach. *J Fluid Mech* 1991;227:245–72.
- [73] Pope SB. Turbulent flows. IOP Publishing; 2001.
- [74] Rotta J. Statistische theorie nichthomogener turbulenz. *Z Phys* 1951;129(6):547–72.
- [75] Lumley JL, Newman GR. The return to isotropy of homogeneous turbulence. *J Fluid Mech* 1977;82(1):161–78.
- [76] Launder B. The prediction of force field effects on turbulent shear flows via second-moment closure. In: Advances in turbulence 2. Springer; 1989, p. 338–58.

- [77] Launder BE, Reece Jr G, Rodi W. Progress in the development of a Reynolds-stress turbulence closure. *J Fluid Mech* 1975;68(3):537–66.
- [78] Johansson AV, Hallbäck M. Modelling of rapid pressure–strain in Reynolds-stress closures. *J Fluid Mech* 1994;269:143–68.
- [79] Monin A. On the symmetry properties of turbulence in the surface layer of air. *Isv Atmos Ocean Phys* 1965;1:45–54.
- [80] Launder B. Heat and mass transport. In: *Turbulence*. Springer; 1975, p. 231–87.
- [81] Panda J. A review of pressure strain correlation modeling for Reynolds stress models. *Proc Inst Mech Eng* 2020;234(8):1528–44.
- [82] Kraichnan RH. Lagrangian-history closure approximation for turbulence. *Phys Fluids* 1965;8(4):575–98.
- [83] Mishra AA, Girimaji SS. Toward approximating non-local dynamics in single-point pressure–strain correlation closures. *J Fluid Mech* 2017;811:168–88.
- [84] Hamlington PE, Dahm WJ. Nonlocal form of the rapid pressure-strain correlation in turbulent flows. *Phys Rev E* 2009;80(4):046311.
- [85] Samko SG. Fractional integrals and derivatives, theory and applications. Minsk: Nauka i Tekhnika; 1987.
- [86] Lischke A, Pang G, Gulian M, Song F, Glusa C, Zheng X, et al. What is the fractional Laplacian? 2018, arXiv preprint [arXiv:1801.09767](https://arxiv.org/abs/1801.09767).
- [87] Zhou X-H, Han J, Xiao H. Learning nonlocal constitutive models with neural networks. 2020, arXiv preprint [arXiv:2010.10491](https://arxiv.org/abs/2010.10491).
- [88] Zhou X-H, Han J, Xiao H. Frame-independent vector-cloud neural network for nonlocal constitutive modelling on arbitrary grids. 2021, arXiv preprint [arXiv:2103.06685](https://arxiv.org/abs/2103.06685).
- [89] Eisfeld B, Brodersen O. Advanced turbulence modelling and stress analysis for the DLR-F6 configuration. In: *AIAA Paper*, 2005. p. 4727.
- [90] Spedding GR. Wake signature detection. *Annu Rev Fluid Mech* 2014;46:273–302.
- [91] Zhou Y. Rayleigh–Taylor and Richtmyer–Meshkov instability induced flow, turbulence, and mixing. I. *Phys Rep* 2017;720–722:1–136.
- [92] Zhou Y, Clark TT, Clark DS, Gail Glendinning S, Aaron Skinner M, Huntington CM, et al. Turbulent mixing and transition criteria of flows induced by hydrodynamic instabilities. *Phys Plasmas* 2019;26(8):080901.
- [93] Zhou Y, Remington BA, Robey HF, Cook AW, Glendinning SG, Dimits A, et al. Progress in understanding turbulent mixing induced by Rayleigh–Taylor and Richtmyer–Meshkov instabilities. *Phys Plasmas* 2003;10(5):1883–96.
- [94] Cabot W, Zhou Y. Statistical measurements of scaling and anisotropy of turbulent flows induced by Rayleigh–Taylor instability. *Phys Fluids* 2013;25(1):015107.
- [95] Zhou Y, Cabot WH, Thornber B. Asymptotic behavior of the mixed mass in Rayleigh–Taylor and Richtmyer–Meshkov instability induced flows. *Phys Plasmas* 2016;23(5):052712.
- [96] Zhou Y. Rayleigh–Taylor and Richtmyer–Meshkov instability induced flow, turbulence, and mixing. part II. *Phys Rep* 2017;723:1–160.
- [97] Souffland D, Soulard O, Griffond J. Modeling of Reynolds stress models for diffusion fluxes inside shock waves. *J Fluid Eng* 2014;136(9).
- [98] Kunz R, Yu W-S, Antal S, Ertorre S. An unstructured two-fluid method based on the coupled phasic exchange algorithm. In: *AIAA paper*, 2001. p. 2672.
- [99] Clift SS, Forsyth PA. Linear and non-linear iterative methods for the incompressible Navier–Stokes equations. *Internat J Numer Methods Fluids* 1994;18(3):229–56.
- [100] Van Doormaal JP, Raithby GD. Enhancements of the SIMPLE method for predicting incompressible fluid flows. *Numer Heat Transfer* 1984;7(2):147–63.
- [101] Rhie C, Chow WL. Numerical study of the turbulent flow past an airfoil with trailing edge separation. *AIAA J* 1983;21(11):1525–32.
- [102] Van Der Poel EP, Ostilla-Mónico R, Donners J, Verzicco R. A pencil distributed finite difference code for strongly turbulent wall-bounded flows. *Comput Fluids* 2015;116:10–6.
- [103] Ostilla-Mónico R, Yang Y, Van Der Poel EP, Lohse D, Verzicco R. A multiple-resolution strategy for direct numerical simulation of scalar turbulence. *J Comput Phys* 2015;301:308–21.
- [104] Kooij GL, Botchev MA, Frederix EM, Geurts BJ, Horn S, Lohse D, et al. Comparison of computational codes for direct numerical simulations of turbulent Rayleigh–benard convection. *Comput Fluids* 2018;166:1–8.
- [105] Zhu X, Mathai V, Stevens RJ, Verzicco R, Lohse D. Transition to the ultimate regime in two-dimensional Rayleigh–Benard convection. *Phys Rev Lett* 2018;120(14):144502.