

Statistical Calibration of the HIFiRE Flight 2 Combustion Model

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The objective of this work was to develop an approach to statistically calibrate the combustion model parameters of the HIFiRE Flight 2 combustor model. The flight experiment combustor geometry was identical to the HIFiRE Direct Connect Rig tested prior to the flight experiment to map engine operability. Pressure measurements from within the combustor were used to tune the computational fluid dynamics model of the isolator and combustor at tested dual-mode ramjet conditions. Two model parameters were considered: the turbulent Schmidt number and a parameter from the eddy dissipation concept heat release model. The calibration was performed using a Bayesian inference approach. The impact of including model discrepancy within the calibration framework was investigated. Additionally, the impact of calibrating the observation error alongside the model parameters was also evaluated. Results of the statistical calibration showed that the combustion model prior parameter distributions were significantly reduced as a result of the calibration. When including model discrepancy and calibrating the observation error alongside the model parameters, the turbulent Schmidt number posterior had a mean of 0.286 with a standard deviation of 0.015. The eddy dissipation concept parameter posterior had a mean of 0.684 and a standard deviation of 0.012. When not considering model discrepancy and calibrating the observation error, the calibrated model could not accurately capture the measurements. Mean parameter values were found to be similar to those from the full calibration, but the posterior parameter uncertainties were an order of magnitude smaller.

Nomenclature

A, B	Magnussen Model Constants	$\dot{w}$	Species Production Rate
D	Diffusion Coefficient	$\mathbf{x}$	Input Parameter
e	Observation Error	x_j	Spatial Coordinate Tensor
H	Total Enthalpy	Y	Species Mass Fraction
h	Specific Enthalpy	y^+	Nondimensional Grid Height
k	Turbulent Kinetic Energy	y_{obs}	Observation
M	Margin	δ	Model Discrepancy
P	Pressure	δ_{ij}	Kronecker Delta Function
Pr_t	Turbulent Prandtl Number	θ	Calibration Parameter
q_j	Heat Flux Vector	λ	Thermal Conductivity
R	Model Output	μ	Molecular Viscosity
$\hat{R}$	Specific Gas Constant	μ_t	Eddy Viscosity
Sc	Schmidt Number	v	Volume
Sc_t	Turbulent Schmidt Number	ρ	Density
T	Temperature	$\sigma_{\omega 1}$	Diffusion Coefficient
u	Velocity Vector	τ	Shear Stress
V	Species Diffusion Velocity	τ_t	Turbulent Time Scale
W	Molecular Weight		

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I. Introduction

The HIFiRE Flight 2 (HF2) payload was flown on May 1, 2012 from the Pacific Missile Range Facility in Hawaii to explore combustion mode transition from dual-mode combustion to supersonic combustion in a hydrocarbon-fueled scramjet engine between Mach 6 and 8. During the flight, the three-stage sounding rocket successfully accelerated the payload from Mach 6 to Mach 8+ at a nearly constant dynamic pressure. The forebody/inlet shroud was deployed at Mach 5.2, then the fuel schedule was initiated and ignition of the combustor was achieved. As the vehicle continued to accelerate, the combustor transitioned from dual-mode to scram-mode operation at a nearly constant fuel–air equivalence ratio (near unity). Data were acquired from more than 600 sensors for the entire duration of the flight test, up to and beyond the end of the experiment [1].

Prior to the HF2 experiment, a full-scale direct-connect version of the HF2 flowpath, the HIFiRE Direct-Connect Rig (HDCR), was thoroughly characterized in NASA’s Arc-Heated Scramjet Test Facility [2]. The ground test rig geometry was identical to the flight experiment from the isolator entrance to the combustor exit, including scale, with only minor differences in instrumentation. During the ground test campaign, the minimum allowable isolator margin throughout the experiment was set at 50% of the isolator length. This conservative isolator margin was assumed to be sufficient for preventing an unstart condition during the flight experiment. Robust operation of the isolator and combustor was confirmed by repeated and thorough testing at and near the expected flight fueling conditions. A description of the HDCR ground test campaign is provided by Hass et al. [3].

One of the primary test objectives of the HDCR ground test campaign was to evaluate engine performance and operability through dual-to-scram mode transition. Verifying operability was important because during dual-mode operation, the combustion induced pressure rise is upstream of the primary fuel injector. This is the condition at which an unstart event (i.e., the combustion induced shock moves into the inlet) was most likely to occur. Therefore, accurate modeling of the combustion was essential to ensure success of the flight experiment. During the flight program, a non-statistical approach was taken to calculate deterministic values of key model parameters. The values were then used to predict the flight performance [4].

Although the flight test was ultimately a success, the conservative design and analysis approaches may have resulted in a less than optimal design of the engine. Excess margin in the isolator length adds additional weight and length to the overall system. As size and weight can directly impact performance of operational systems, there is a strong need to leverage design techniques that better quantify the probability of failure modes, such as an unstart, to optimize the overall design.

Previous work by West and Bynum [5] demonstrated that the combustion induced shock location uncertainty within the isolator could be estimated based on uncertainties in ground testing, expected flight conditions, and the computational model. This was done assuming the combustion model was uncalibrated to the HDCR test data. Results indicated that although the likelihood of an engine unstart was low, uncertainty in the combustion model parameters was a significant driver in the overall reliability of the system. Building off of the previous work, the objective of this work, therefore, was to develop an approach to statistically calibrate the HF2 combustion model parameters. To date, there is no known study to have investigated calibration of a dual-mode combustion model.

The approach taken in this work was to leverage classical Bayesian inference to identify probability distributions of the model parameters that best reproduce the HDCR data. Although the overall process is not novel, calibration of such a complex physics model introduced challenges that required special consideration. Issues such as significant model-form uncertainty and large observation errors require specific strategies to identify accurate parameter distributions from the calibration. Spatially varying physics within the HF2 combustor further complicate an accurate calibration approach. The impact of these issues on the calibration process and resulting parameter probability distributions were explored in detail.

The next section describes the model calibration framework used to estimate the combustor model parameter probability distributions. Section III describes the HF2 and HDCR experiments, followed by a description of the computational modeling approach in Section IV. Results of the combustor model calibration are given in Section V along with a detailed analysis of the challenges and use of the results in future analyses. Lastly, Section VI summarizes key findings of this work.

II. Model Calibration Approach

The objective in any inference problem is to determine the calibration parameter values that enable a model to predict measured data within known measurement error. In principle, determination of the parameter values could be achieved via deterministic optimization; however, doing so may only result in best-fit parameter values. Optimization also does

not yield a statistical description of the calibration parameters without potentially significant assumptions. In the current study, the approach taken was to leverage a Bayesian framework that was modified for improved computational efficiency. The remainder of this section describes the Bayesian inference problem and calibration approach used to determine the HF2 combustor model parameters and their uncertainties based on the HDCR data.

A. Bayesian Inference

The true output (e.g., measurement) of a physical system can be related to a model prediction as shown in Eq. (1). The model prediction, R , is a function of two parameter sets: input parameters, $\mathbf{x}$, and calibration or tuning parameters, θ . The model discrepancy, δ , is only a function of the input parameters, $\mathbf{x}$. As stated by Kennedy and O’Hagan [6], the i^{th} true observation, $y_{obs,i}$, is a sum of the model output, R , a measure of the model inadequacy or discrepancy, δ , and some observation error, e_i .

$$y_{obs,i} = R(\mathbf{x}_i, \theta) + \delta(\mathbf{x}_i) + e_i \quad (1)$$

Here, e_i accounts not only for residual model-form error not captured by the model-discrepancy term but also for the actual measurement error. Using a Bayesian framework, the calibration parameters can be estimated using Bayes’ theorem, which is stated generally in Eq. (2).

$$P(\theta|\mathbf{y}_{obs}) \propto P(\mathbf{y}_{obs}|\theta)P(\theta) \quad (2)$$

Bayes’ theorem states the joint probability distribution of the model parameters given experimental observations, $\mathbf{y}$, is proportional to the likelihood that the experimental measurements are associated with a particular value of the calibration parameters times the prior distribution of the calibration parameters. In the calibration process, the objective is to determine the posterior density of θ , $P(\theta|\mathbf{y}_{obs})$, given a belief of the prior density, $P(\theta)$, and an assumed likelihood function, $P(\mathbf{y}_{obs}|\theta)$. The likelihood function was assumed to be a multivariate Gaussian likelihood, as shown in Eq. (3).

$$P(\mathbf{y}|\theta) \propto \prod_{i=1}^N \exp \left[\frac{-(y_{obs,i} - (R_i + \delta_i))^2}{2\sigma_{obs,i}^2} \right] \quad (3)$$

Here, δ_i is the model discrepancy corresponding to $\mathbf{x}_i$, σ_{obs} is the observation error, and N is the number of observations. In the current work, uniform probability distribution priors were assumed for all calibration parameters, which is common in many engineering problems. Uniform priors are often referred to as uninformative priors. Although a uniform distribution is not truly uninformative due to bounds being placed on the distribution, the assumption here is that the chosen priors bound the true θ .

B. Modular Bayesian Framework

As described by Kennedy and O’Hagan [6], the most complete process of determining the parameter posterior distributions is referred to as a full Bayesian analysis. In such an approach, the model parameters, discrepancy model parameters, and the observation error are determined simultaneously using numerical integration. In addition to computational cost challenges with this approach, there is also an issue of identifiability. Because the model parameters and discrepancy are effectively determined simultaneously, model-form uncertainty can be incorrectly attributed to parameter uncertainty during the calibration process (or vice versa).

To alleviate these issues, a modular Bayesian framework [6] was used in the current study. This framework is illustrated in Fig. 1. Two key steps are involved that differentiate the modular approach from classical inference. First, a surrogate model of the computational model is generated over the prior parameter distributions (module 1). In this study, Gaussian process regression was used [7], but any accurate surrogate approach (e.g., polynomials, radial basis functions, neural networks, etc.) is sufficient. Secondly, the model discrepancy is determined based on an estimation of the parameter values and then fixed during the calibration process (module 2). Doing so removes the discrepancy model parameters from the calibration. Note that, in the original Kennedy and O’Hagan framework, Gaussian process regression models are used for both the simulation model and the model discrepancy term, with the hyperparameters estimated by accounting for the covariance between the two Gaussian processes. In this paper, a variant of the Kennedy and O’Hagan framework was developed that uses a parametric polynomial model for the discrepancy term, thereby improving the Bayesian inference efficiency and interpretability and extrapolation performance of the discrepancy term.

Determining the model discrepancy function was accomplished by first obtaining a *Maximum Likelihood Estimate* (MLE) of the parameter values, θ . Solving the optimization problem in Eq. (4) yields the MLE parameter values.

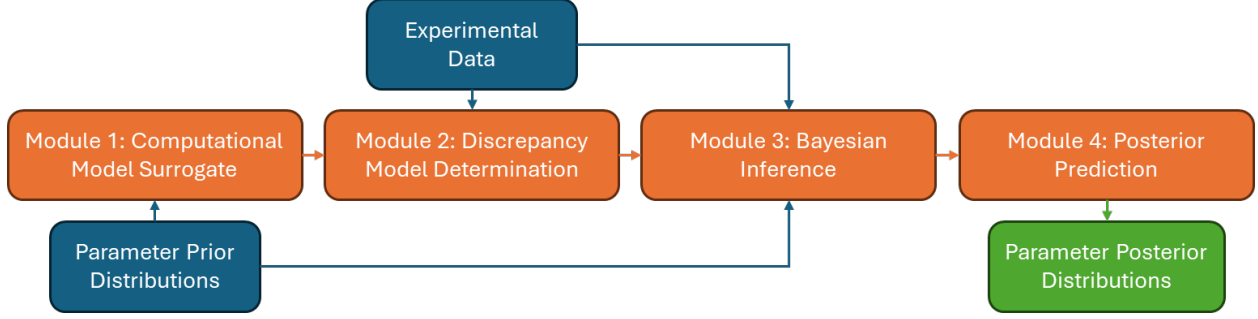


Fig. 1 Modular Bayesian framework.

Note that careful consideration should be given to ensure the global maximum is found. In this work, a multistart, gradient-based optimization approach with 10,000 starting locations was used.

$$\theta_{MLE} = \min_{\theta} [-\ln(P(\mathbf{y}_{obs}|\theta))] \quad (4)$$

Using the resulting set of model parameter values, a model discrepancy function was fit to the residuals between model predictions at the MLE parameter values and the measurements. The resulting discrepancy model was then fixed for the parameter calibration. A simple polynomial model for the discrepancy was found to be sufficiently accurate. Note that, here, the MLE of θ and the polynomial model discrepancy parameters are estimated sequentially. Future work will investigate relaxing this constraint by estimating the MLE of θ and the polynomial parameters simultaneously.

With the Gaussian process model of the expensive computational model and the polynomial discrepancy model, the calibration parameters can then be estimated (module 3). Posterior distributions, $P(\theta|\mathbf{y}_{obs})$, were approximated with a sampling routine to estimate the posterior density. The Metropolis-Hastings Markov Chain Monte Carlo (MCMC) approach was used [8]. An adaptive step size was used to improve convergence of the sampling. The target acceptance ratio was between 22% and 45% [9].

Note that the observation error, $\sigma_{obs,i}$, is often a critical part of the calibration process. If there is a reliable estimate for the observation error and assuming that the discrepancy term can fully recover the unmodeled physics in the simulation model, $\sigma_{obs,i}$ may be fixed during the calibration process. Otherwise, $\sigma_{obs,i}$ may be determined as part of the parameter calibration. If the latter approach is used, $\sigma_{obs,i}$ may be fixed at a small value when determining the MLE parameter values for the discrepancy model in the modular Bayesian framework. During the MCMC parameter estimation, $\sigma_{obs,i}$ can then be determined alongside the model parameters. Both approaches are explored later in Section V.

The above approach is a computationally efficient strategy for performing Bayesian inference. Estimating the posterior distributions with a sampling approach like an MCMC requires numerous evaluations of the computational model. Using an expensive model, such as the one described in the next section, was deemed impractical. However, the above approach is only one of many that may be considered, or even required. Jiang et al. [10] describe multiple approaches and potential implications of each. The approach used here was found to be sufficient for the current study.

III. HIFiRE Flight 2 and HDCR Data Overview

This section describes the HF2 experiment and connectivity to the HDCR ground test. A brief overview of the HDCR measurements is then provided, along with supporting references for further details of the testing.

A. Flowpath Geometry

The HF2 flowpath geometry can be divided into three main components: the forebody and inlet, the isolator, and the combustor. Figure 2 shows a three-dimensional view of the HF2 flowpath integrated into the flight test article. The forebody and inlet geometry were only used in the HF2 experiment. The isolator and combustor, however, were identical to the HDCR ground test experiment. Inflow for the HDCR ground test came from the direct-connect facility nozzle, which is connected to the isolator.

Figure 3 shows a two-dimensional schematic of the isolator and combustor flowpath. The coordinate frame origin for the flight test article was located in the center of the flowpath, at the forebody virtual leading edge. The isolator

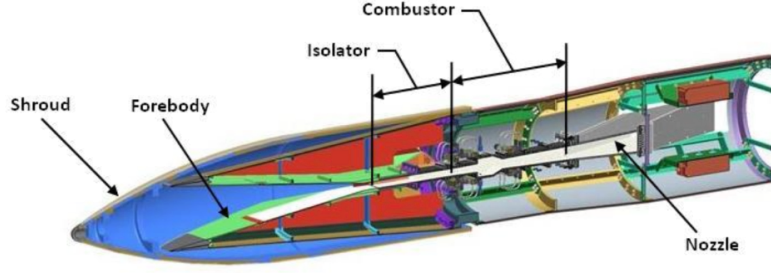


Fig. 2 HIFiRE Flight 2 forebody and inlet geometry integrated with the flight vehicle.

entrance was located 40.438 in. downstream of the forebody virtual leading edge. The flowpath was symmetric about the $z = 0$ and $y = 0$ planes. Port and starboard isolator and combustor surfaces were constant z -planes separated by a width of 4 in. Table 1 lists the x and y values for several key geometric features on the cowl wall.

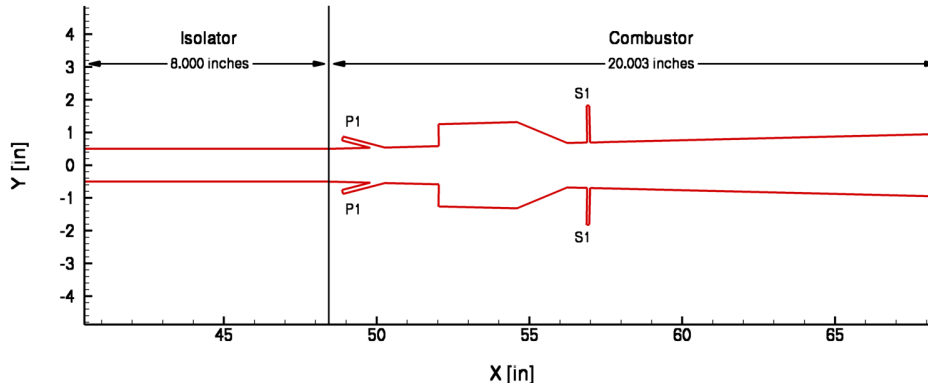


Fig. 3 Two-dimensional profile of the HIFiRE Flight 2 isolator and combustor geometry.

Table 1 HIFiRE Flight 2 as-designed cowl wall flowpath geometry specifications

Feature	x [in]	y [in]
Isolator Start	40.438	0.500
Isolator End	48.438	0.500
Combustor Start	48.438	0.500
P1 Injectors	50.034	0.536
Cavity Step Start	52.034	0.582
Cavity Step End	52.019	1.256
Cavity Closeout Start	54.588	1.315
Cavity Closeout End	56.232	0.677
S1 Injectors	56.938	0.693
Combustor End	68.441	0.954

Injectors used in both the ground and flight experiments were installed at the P1 and S1 injector stations (Fig. 3). The P1 injector station, located upstream of the cavity, consisted of eight injectors (four on the body-side and four on the cowl-side) equally spaced apart at 1 in. and at 1/2 in. from the side walls with diameters of 1/8 in. The S1 injector station, located downstream of the cavity, consisted of eight injectors (four on the body-side and four on the cowl-side)

equally spaced apart at 1 in. and at 1/2 in. from the side walls with diameters of 0.094 in. P1 injectors were inclined at 15° to the flowpath surface, and S1 injectors are normal to the flowpath surface.

B. HDCR Measurements

Prior to the HF2 experiment being flown, the two phase HDCR ground test campaign was conducted to map engine performance. The engine was tested at Mach numbers ranging from about 6 to 8. Instrumentation within the engine included 144 static pressure ports, 19 thermocouples, and four heat flux gauges. Detailed overviews of the model, test objectives, instrumentation, and measured data are provided by Hass et al. [3, 11, 12]

Because dual-mode ramjet operation of the HF2 experiment was considered a stressing condition for the engine, the model calibration effort in this work focused on the Mach 6.5 test condition. A scatter plot of the wall pressure measurements is shown in Fig. 4. These data cover about 1.3 seconds of fuel-on testing taken during steady-state conditions. Note that the spatial zero (x-axis) is the start or entrance of the isolator.

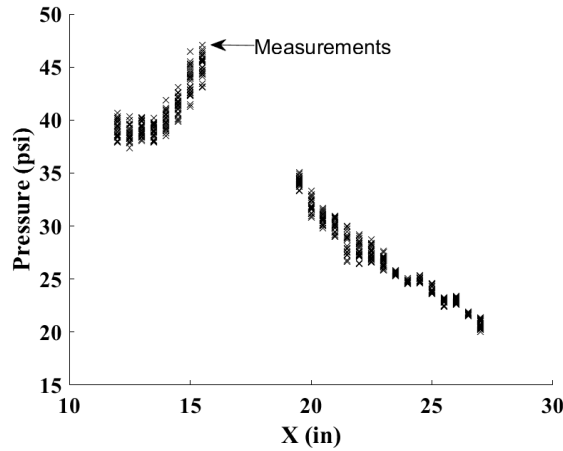


Fig. 4 HDCR data for the Mach 6.5 test condition.

Pressure measurements were taken at a rate of 10 Hz. There were eight pressure taps within the cavity and 16 in the expansion section of the test rig. In total, there were 288 individual measurements both spatially and in time. The measurement uncertainty for each pressure port was determined to be about 0.1 psi during the testing.

An important note about the data used for the calibration should be made. Other than the measurement locations above, there were additional pressure ports upstream of the cavity and four measurements between the cavity and expansion regions. The primary goal of the calibration in this work was to target the combustion. Upstream of the cavity is mostly the effects of combustion (e.g. shocks and separated flow) but not explicitly the combustion process. Between the cavity and expansion regions, there were significant unsteady processes occurring due to the geometry. As capturing these processes was not the purpose of the current calibration effort and the measurements would dilute the results, these measures were omitted from the current study.

IV. Computational Model Description

In this section, the computational modeling approach is presented. A detailed overview of the flow solver is given followed by a description of the computational grid. Lastly, the model calibration parameters are identified.

A. Flow Solver

The computational modeling for this effort was performed using VULCAN-CFD 7.1 [13]. VULCAN-CFD is a compressible, turbulent, Navier-Stokes flow solver with allowances for finite-rate chemistry and/or thermodynamic non-equilibrium. Multi-block structured or mixed element (tetrahedral, prismatic, pyramid, and hexahedral) unstructured grids can be used for discretization of the computational domain, and solutions can be obtained using explicit or implicit time advancement schemes. Wall matching functions and multigrid methods for elliptic and space marching schemes are available to reduce computational cost. Flow solver capabilities include models for compressibility, Reynolds

stress anisotropies, turbulent diffusivity, finite-rate chemistry, and turbulence-chemistry interaction effects. Available turbulence models include several one- and two-equation models, as well as Large Eddy Simulation (LES) and hybrid Reynolds-Averaged Navier-Stokes (RANS)/LES options. Mathematical details of the various Vulcan-CFD models are described by Baurle et al. [14].

For the current work, the flow was assumed to be steady. The Reynolds-averaged conservation equations and equation of state reduce to Eqs. (5)-(9).

$$\frac{\partial}{\partial x_j} (\bar{\rho} \tilde{u}_j) = 0 \quad (5)$$

$$\frac{\partial}{\partial x_j} (\bar{\rho} \tilde{u}_i \tilde{u}_j + \bar{\rho} \widetilde{u_i'' u_j''}) + \frac{\partial}{\partial x_j} (\delta_{ij} \bar{P} - \bar{\tau}_{ij}) = 0 \quad (6)$$

$$\frac{\partial}{\partial x_j} (\bar{\rho} \tilde{H} \tilde{u}_j + \bar{\rho} \widetilde{H'' u_j''}) + \frac{\partial}{\partial x_j} (\bar{q}_j - \bar{\tau}_{ij} \tilde{u}_i - \overline{\tau_{ij} u_i''}) = 0 \quad (7)$$

$$\frac{\partial}{\partial x_j} (\bar{\rho} \tilde{Y}_m \tilde{u}_j + \bar{\rho} \widetilde{Y_m'' u_j''}) + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{Y}_m \tilde{V}_j^{(m)} + \overline{\rho Y_m'' V_j^{(m)''}}) = \bar{w}_m \quad (8)$$

$$\bar{P} = \bar{\rho} \hat{R} \tilde{T} \quad (9)$$

In this set of governing equations, $(\bar{\cdot})$ is a time-averaged variable, $(\tilde{\cdot})$ is a mass-weighted or Favré-averaged variable, and $(\cdot'')$ is the Favré-averaged fluctuating component of a variable. The Reynolds stress tensor was modeled using the Boussinesq approximation, given in Eq. (10).

$$\bar{\rho} \widetilde{u_i'' u_j''} = \frac{2}{3} \delta_{ij} \bar{\rho} \tilde{k} - \mu_t \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \mu \frac{\partial \tilde{u}_k}{\partial x_k} \right) \quad (10)$$

Here, $\tilde{k}$ is the turbulent kinetic energy given as $\frac{1}{2} \widetilde{u_i'' u_i''}$, δ_{ij} is the Kronecker delta function, and μ_t is the eddy viscosity. The molecular stress tensor was approximated by using only mean temperature and composition to determine the molecular viscosity and ignoring differences in time and Favré-averaged velocity components, as shown in Eq. (11).

$$\bar{\tau}_{ij} = \mu \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \mu \frac{\partial \tilde{u}_k}{\partial x_k} \quad (11)$$

Here, μ is the molecular viscosity, which was determined using polynomial curve fits by Gordon and McBride [15, 16]. The functional form of μ is defined in Eq. (12), where the polynomial coefficients are given in Table 2.

$$\mu = \exp \left[a \ln \tilde{T} + \frac{b}{\tilde{T}} + \frac{c}{\tilde{T}^2} + d \right] \quad (12)$$

Table 2 Molecular viscosity model coefficients

Species	T_{min}	T_{max}	a	b	c	d
N ₂	200.0	1000.0	6.25265770E-01	-3.17796520E+01	-1.64079830E+03	1.74549920E+00
	1000.0	5000.0	8.73952090E-01	5.61522220E+02	-1.73948090E+05	-3.93359580E-01
O ₂	200.0	1000.0	6.09161800E-01	-5.22448470E+01	-5.99740090E+02	2.04108010E+00
	1000.0	5000.0	7.22164860E-01	1.75508390E+02	-5.79748160E+04	1.09010440E+00
Fuel	200.0	6000.0	6.34569909E-01	-6.81950096E+01	-4.71743313E+03	1.33311546E+00
Products	200.0	6000.0	5.95245776E-01	-3.23829843E+02	3.32381117E+04	2.17623143E+00

In the energy equation, the high-order correlation, $\bar{\rho} \widetilde{H'' u_j''}$, was determined with gradient diffusion approximations on the first and third terms, as shown in Eq. (13). The second term is the vector dot product of the mean velocity and the Reynolds stress tensor.

$$\bar{\rho} \widetilde{H'' u_j''} = -\frac{\mu_t}{Pr_t} \frac{\partial \tilde{h}}{\partial x_j} + \bar{\rho} \tilde{u}_i \widetilde{u_i'' u_j''} - \frac{\mu_t}{\sigma_k} \frac{\partial \tilde{k}}{\partial x_j} \quad (13)$$

The turbulent Prandtl number, Pr_t , was assumed to be 0.9. σ_k is a closure coefficient that depends on the turbulence model, which is discussed later. The molecular diffusion term was approximated by

$$\frac{\partial}{\partial x_j} (\overline{\tau_{ij} u_i''}) = \frac{\partial}{\partial x_j} \left(\mu \frac{\partial \tilde{k}}{\partial x_j} \right) \quad (14)$$

Similar to the mean molecular stress tensor, the heat flux vector was approximated as

$$\bar{q}_j = -\lambda \frac{\partial \tilde{T}}{\partial x_j} - \bar{\rho} D \sum_{m=1}^{ns} h_m (\tilde{T}) \frac{\partial \tilde{Y}_m}{\partial x_j} \quad (15)$$

where h_m is the enthalpy of species m , ns is the number of species in the mixture, λ is the thermal conductivity, and D is the diffusion coefficient. λ is of the same functional form as Eq. (12). Coefficients for the λ model are given in Table 3.

Table 3 Thermal conductivity model coefficients

Species	T_{min}	T_{max}	a	b	c	d
N ₂	200.0	1000.0	8.54394360E-01	1.05732240E+02	-1.23478480E+04	4.77931280E-01
	1000.0	5000.0	8.84071460E-01	1.33572930E+02	-1.14296400E+04	2.44170190E-01
O ₂	200.0	1000.0	7.72291670E-01	6.84632100E+00	-5.89333770E+03	1.22103650E+00
	1000.0	5000.0	9.09173510E-01	2.91241820E+02	-7.96501710E+04	6.48516310E-02
Fuel	200.0	6000.0	6.19217798E-01	-6.96353233E+02	5.96425297E+04	3.61603514E+00
Products	200.0	6000.0	7.01728893E-01	-6.72400225E+02	9.13828329E+04	2.43508477E+00

Diffusion was modeled with Fick's law such that the molecular Schmidt number, Sc , defines the mass diffusivity constant given the viscosity, as shown in Eq. (16). Here, Sc was assumed to be a constant 0.72.

$$D = \frac{\mu}{Sc \bar{\rho}} \quad (16)$$

Lastly, in the species mass continuity equation, the Reynolds mass flux vector was approximated with a gradient diffusion approximation, as shown in Eq. (17).

$$\bar{\rho} \widetilde{Y_m'' u_j''} = -\frac{\mu_t}{Sc_t} \frac{\partial \tilde{Y}_m}{\partial x_j} \quad (17)$$

Here, Sc_t is the turbulent Schmidt number. Molecular mass diffusion was approximated by neglecting diffusion coefficient turbulent fluctuations and gradients of Favré mass fraction fluctuations, as shown in Eq. (18).

$$\bar{\rho} \tilde{Y}_m \tilde{Y}_j^{(m)} + \overline{\rho Y_m'' V_j^{(m)''}} = \bar{\rho} D \frac{\partial \tilde{Y}_m}{\partial x_j} \quad (18)$$

The last term in the species mass continuity equation, $\tilde{w}_m$, is the time-averaged species production rates. The base combustion model used was the eddy dissipation concept (EDC) of Magnussen and Hjertager [17]. With the EDC model, time-averaged species production rates were approximated by Eq. (19).

$$\tilde{w}_m = \nu_m W_m \frac{A}{\tau_t} \text{MIN} \left[\frac{\bar{\rho}_f}{\nu_f W_f}, \frac{\bar{\rho}_a}{\nu_a W_a}, \frac{B \bar{\rho}_p}{\nu_p W_p} \right] \quad (19)$$

Here, A and B are closure coefficients where A controls the rate of heat release and B limits the combustion product production rate. This model results in significantly reduced computational requirements and is valid for mixing-limited combustor operation, such as in the current work. The base Magnussen model was modified according to the methods prescribed by Norris [18]. This modified Magnussen model attempts to incorporate the predictive capabilities of a finite-rate kinetics model with the computational cost of the Magnussen model. The constant τ_t was added to the base Magnussen model to limit the turbulent mixing time scale, which functions to set an upper limit for the reaction rate in regions of high turbulence. The chemical composition of the fuel was a 64%/36% molar mixture of ethylene and methane. Combustion products were modeled as 54.945% H₂O and 45.055% CO₂.

The turbulence model used was the blended 1988 Wilcox $k - \omega$ and the Jones Launder $k - \epsilon$ model of Menter [19] in conjunction with the wall matching functions of Wilcox [20]. Wall matching functions reduce the overall number of grid points required and reduce the aspect ratio of the cells near the walls. Inviscid fluxes were evaluated using the low-diffusion flux splitting scheme of Edwards [21]. To ensure the solution satisfied the total variation diminishing (TVD) property, the van Leer flux limiter [22] was used. The monotone upstream centered scheme for conservation laws (MUSCL) [22] interpolation coefficient was chosen to be one-third.

The wall boundary condition used was a no-slip wall with a one-dimensional, wall-normal heat transfer model. This model requires a wall thickness over conductivity specification and a back side wall temperature. Thickness to conductivity values matched the vehicle wall hardware. Back side wall temperatures for the isolator and combustor were set to values obtained in the ground tests using sub-surface thermocouples as described by Cuda and Hass [23].

B. HDCR Computational Grid

A three-dimensional, structured, quarter-symmetry computational grid was created for the HDCR as-designed geometry. The grid contained 8.7 million cells and was clustered near the wall to maintain an average y^+ of 10 throughout the flowpath with a maximum y^+ of 50. Simulation convergence was declared when the integrated forces on the surfaces in the x, y, and z directions, the integrated wall heat flux, and the mass flow conservation were nominally invariant with iteration history (unsteady variations of no more than 0.5 percent); and when the L_2 -norm of the residual error had dropped by at least 2.5 orders of magnitude from the initial residual.

C. Calibration Parameters

Two calibration parameters were identified within the computational fluid dynamics model of the HDCR. These parameters are listed in Table 4, along with their prior uncertainties. Note that both prior distributions were assumed to be uniform and, therefore, uninformative for the model calibration. Within the EDC combustion model, the A constant controls the rate of heat release. The turbulent Schmidt number, Sc_t , effectively controls mixing in the combustor. A and Sc_t uncertainties are taken from expert opinion regarding the possible ranges of these combustion model parameters in the absence of calibration data. Other parameters in the EDC model considered were B and τ_t , as well as turbulence model closure coefficients. However, the model was found to be relatively insensitive to the uncertainty in these parameters at the studied flow conditions. Therefore, to reduce complexity of the calibration, these parameters were omitted.

Table 4 HDCR model calibration parameters and prior distributions

Parameter	Distribution	Min	Max
Sc_t	Uniform	0.5	0.9
A	Uniform	1.5	4.0

V. Results and Discussion

This section contains the model calibration results and supporting discussion. First, uncalibrated model predictions are shown. The calibration with and without model discrepancy was performed to highlight the impact of including, or rather acknowledging, the presence of model-form uncertainty. Then, calibration of the observation error alongside the model parameters was performed to further refine the parameter posterior estimate.

A. Uncalibrated Model Predictions

Before performing the model calibration, an accurate surrogate model of the expensive HDCR computational model over the full range of the parameter prior distributions was needed. Recall from Fig. 4 that the measurements cover two geometrically and physically different regions of data: the cavity and the expansion. Instead of trying to fit a singular Gaussian process to both regions, two separate models were generated to better approximate both regions.

The Gaussian process models were created with 12 evaluations of the computational model distributed over the calibration parameter domains. The four corner points of the domain were used along with space-filling points chosen with a Latin hypercube design. A leave-one-out verification approach was used to determine the predictive accuracy of

the model. The cavity model had an error of about 7%, and the model of the expansion region had an error of about 3%. Note that these errors in the Gaussian process models are not carried forward through the parameter calibrations as they are acceptably small and were assumed to have minimal impact.

With accurate surrogates of the HDCR model, the full prior parameter distributions were propagated through the Gaussian process models. Figure 5 shows the resulting combustor pressure model predictions compared to the HDCR measurements.

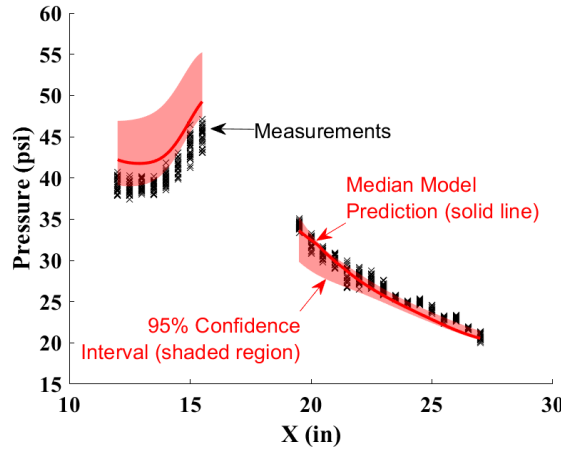


Fig. 5 Uncalibrated predictions of combustor pressure in the HDCR combustor and expansion regions.

There are a couple of important notes to make about this comparison. First, the prediction uncertainty is the result of using the full prior distribution of both model parameters. Second, there is an obvious bias to the predictions. In the combustor region, the model generally over predicts the pressure, so much so that even using the full prior information of the two calibration parameters, the model predictions do not bound the HDCR measurements. Downstream, the predictions are qualitatively better, but the model underpredicts pressure within much of the expansion region.

The model predictions not falling within the full prior distributions of the model parameters is a sign of two possible issues: calibration parameters are missing from the prior uncertainty space or the model is inherently deficient. No other parameters could be identified that would allow the model predictions to bound the data. Therefore, the presence of model-form uncertainty was considered later in the calibration process.

B. Impact of Model Discrepancy

Following the calibration procedure described in Section II, the computational model was first calibrated to the measurements assuming no model-form uncertainty (i.e., no module 2). The observation error was also fixed to the measurement error, which had a standard deviation of 0.1 psi. The resulting calibrated model prediction compared to the HDCR data is shown in Fig. 6. Figure 7 shows the calibration parameter posterior distributions.

From these figures, the parameter calibration results in a model prediction that generally fits within the measured data. At nearly all locations, the predictions touch at least a subset of the data. However, there is an obvious bias in the combustor region where the prediction is above the majority of the measurements after about x of 14 in. In the expansion region, the model under predicts the pressure at 19.5 in. and again around 24 in. This resulting model prediction is effectively a least squares fit to the data within the prior parameter distribution domains. Also, Fig. 6 does contain a 95% confidence interval of the median model prediction; however, the interval is extremely small. This issue is the result of assuming a fixed observation error and is addressed later. An inability of the model to globally capture the data is an indication of the model inadequacy, which needs to be addressed.

To acknowledge the presence of model-form uncertainty and improve the results, calibration was repeated with the model dependency term included. Again the observation error was fixed at a standard deviation of 0.1 psi. The resulting model predictions compared to the HDCR data and the posterior parameter distributions are shown in Figs. 8 and 9, respectively.

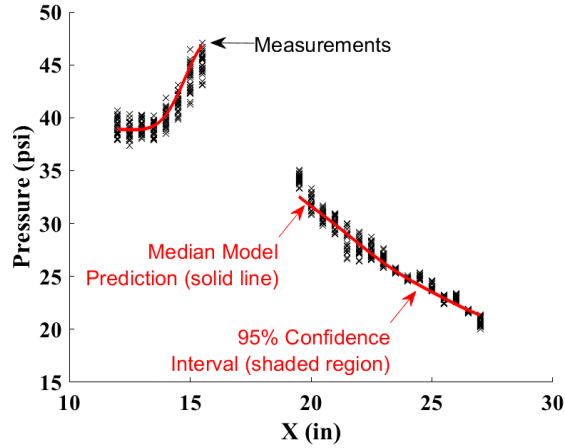


Fig. 6 Model predictions without discrepancy using calibrated parameters and fixed observation errors.

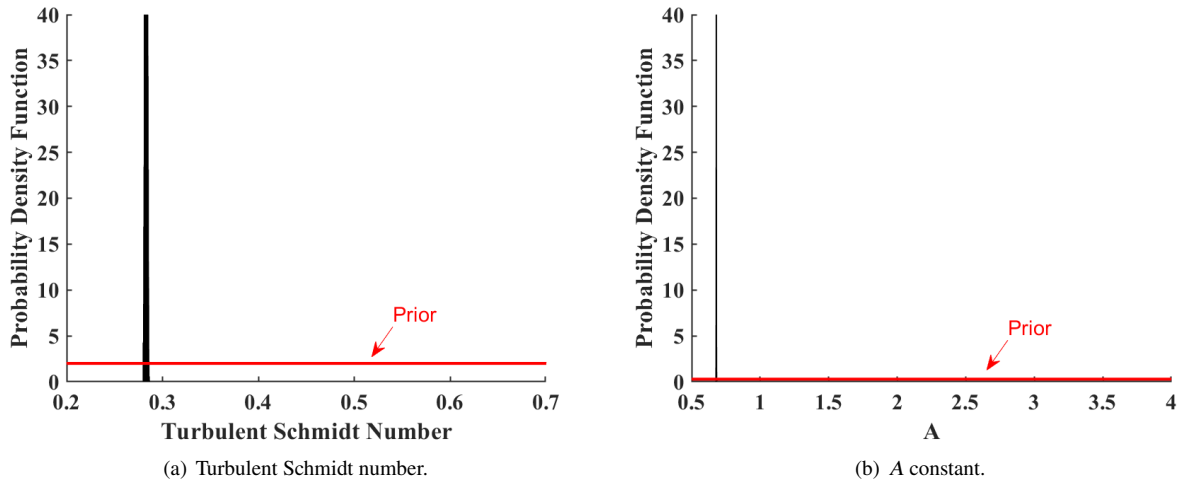


Fig. 7 Posterior parameter distributions without discrepancy using calibrated parameters and fixed observation errors.

Notice now that the model posterior prediction in Fig. 8(a) runs right through the measured data. In both regions, there are significant improvements to the predictions. The model discrepancy, shown in Fig. 8(b), confirms the observations from Fig. 6. However, there are two issues to identify. First, similar to the calibration with no discrepancy, the posterior parameter uncertainties are unreasonably small. Given the complexities of the model and measurement spread, this does not seem reasonable. Further investigation was needed. Second, and related, is that the resulting model predictions do not bound the measurements at each x location. This suggests that the calibration is “too confident.” The primary issue is the assumption of a small, fixed observation error.

C. Observation Error Calibration

In the previous calibration results, the posterior predictions do not bound the HDCR data. Although the resulting median qualitatively fits through the data well, the prediction uncertainty does not capture all of the possible measurements. This overly confident result is due to the observation error being assumed to be the measurement error. In reality, there is significant scatter in the measurements due to more than just measurement error. Unsteady facility operation, unseen flow transients, or other uncharacterized phenomena may result in measurement variability. If these processes were well-understood, they could perhaps be modeled. In the limit, the observation error may then reduce to the measurement

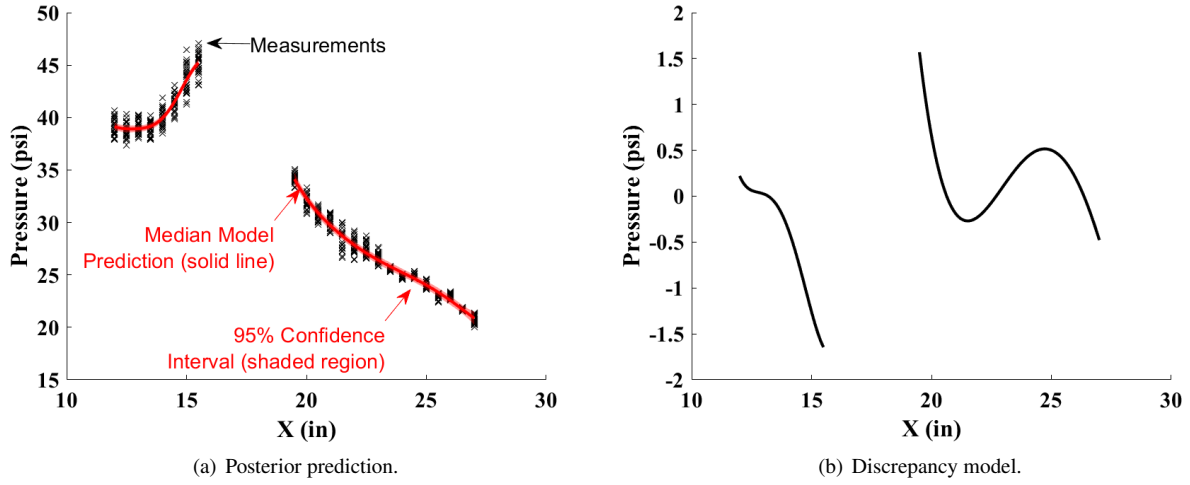


Fig. 8 Model predictions with discrepancy using calibrated parameters and fixed observation errors.

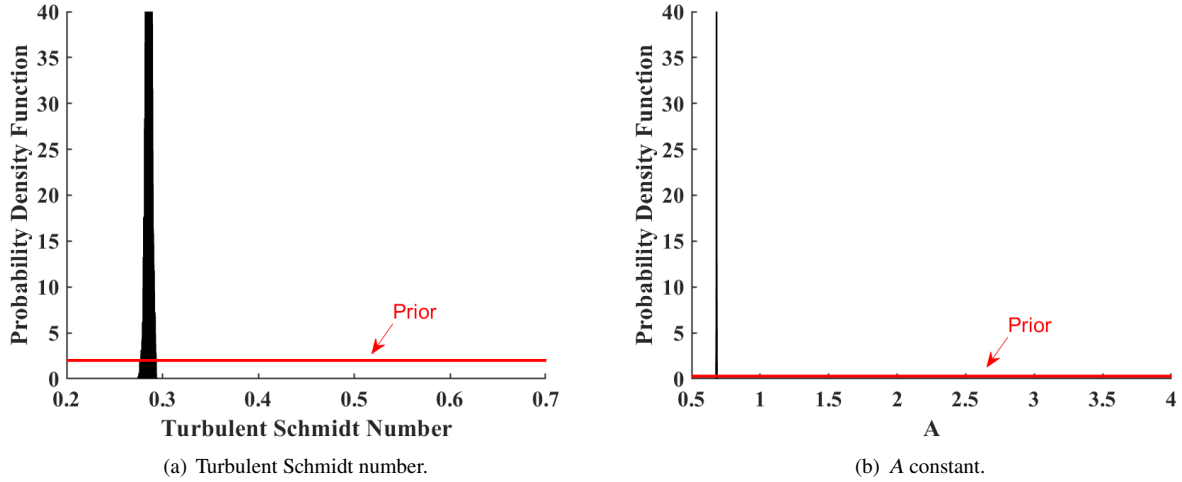


Fig. 9 Posterior parameter distributions with discrepancy using calibrated parameters and fixed observation errors.

error. However, the root cause of the measurement variation is not known, so the measurement spread is accepted as epistemic observation error that must be acknowledged in a parameter calibration.

To account for the measurement variability and the residual model-form error that has not been captured by the discrepancy term beyond just the measurement error, the observation error was added to the set of calibration parameters. The resulting model predictions compared to the HDCR data and the posterior parameter distributions are shown in Figs. 10 and 11, respectively. Note that in the modular Bayesian framework used in this study, the observation error was fixed at the measurement error value when determining the model dependency function. Then, as part of the parameter calibration step, the observation error was calibrated alongside the two model parameters.

Notice now that the model prediction uncertainty bounds the HDCR data tightly. The resulting posterior parameter distributions are now, perhaps, more realistic for such a complex model and experiment. Compared to the previous calibrations, these results account for both the presence of model-form uncertainty and variability in the measurements that is greater than the measurement error. A summary of all the calibrations is provided in Table 5. Notice that the mean parameter values are captured well, even using the simplest calibration approach. However, the uncertainty in the parameters is under predicted by an order of magnitude. A possible reason that the posterior distribution means are

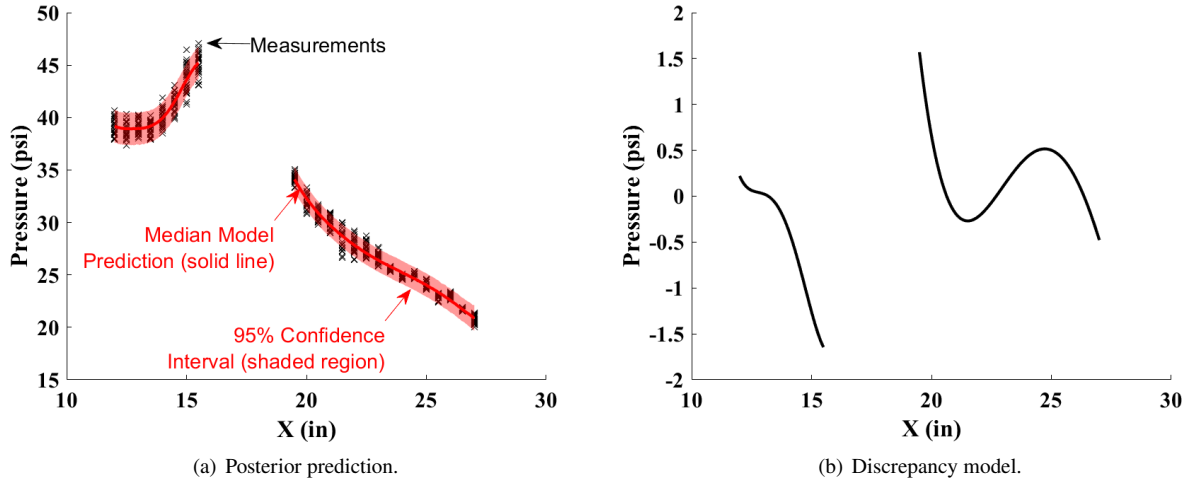


Fig. 10 Model predictions with discrepancy using calibrated parameters and observation errors.

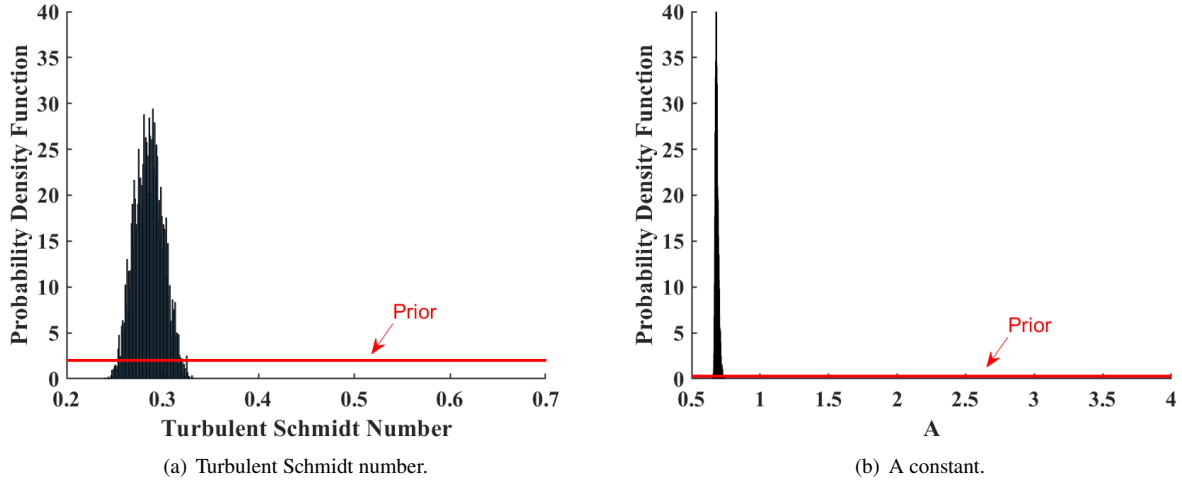


Fig. 11 Posterior parameter distributions with calibrated parameters and observation errors.

similar across different approaches is that the discrepancy term parameters are estimated after the MLE of θ . In future work, as mentioned previously, investigating the estimation of discrepancy polynomial model parameters simultaneously with the MLE of θ by modifying Eq. (4) may be considered.

Table 5 HDCR model calibration results

Approach	S_{cT}	A
No discrepancy, fixed observation error	$\mu = 0.283, \sigma = 0.001$	$\mu = 0.680, \sigma = 0.001$
With discrepancy, fixed observation error	$\mu = 0.286, \sigma = 0.003$	$\mu = 0.682, \sigma = 0.002$
With discrepancy, calibrated observation error	$\mu = 0.286, \sigma = 0.015$	$\mu = 0.684, \sigma = 0.012$

A discussion of the physical meaning and significance of these results is warranted as the parameter distributions may be used in future works. The above results are subject to the identified model discrepancy. That means if the

parameter values in Table 5 are used to predict, for example, the flight vehicle combustor pressures, the discrepancy through the combustor must also be included. This is a very important fallacy of the parameter distributions above.

VI. Conclusions

Calibration of accurate hypersonic air-breathing combustion models using available and relevant ground test data is critical to accurately predicting flight vehicle performance. The complexity of both the physics models and ground testing make statistical calibration challenging. In this work, an efficient strategy for calibrating a dual-mode ramjet combustion model was developed that leveraged a Bayesian inference based approach. The framework efficiently addressed the issues of the model having significant model-form uncertainty and the measurements having variability much greater than the measurement error. The impacts of both model discrepancy and calibrating the observation error alongside the model parameters were investigated. Although the mean values of the calibration parameters were found to be largely insensitive to including the model-form uncertainty and observation error in the calibration, the parameter uncertainties were greatly impacted. Overall, the strategies investigated in this work outline a traceable and rigorous approach to calibrating hypersonic air-breathing combustion model parameters.

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