

Arcjet Modeling for Efficient Characterization of Thermal Protection System Materials in a CO₂-Rich Environment

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The ablative heat shields on recent Mars missions had less surface recession than predicted. This deviation has been attributed to the NuSil coating that was applied to prevent particle shedding. Experiments have since shown that this coating behaves differently in a Mars-like atmosphere (rich in CO₂) than it does in an Earth atmosphere where it was initially assessed. A test campaign was conducted in 2024 at the Hypersonic Materials Environmental Test System at NASA's Langley Research Center to assess NuSil coating in a Mars-like environment. To quantitatively analyze the material response, heat flux and stagnation pressure on the test specimens are required. Due to the differences between the test specimen and the measurement probes, these quantities must be computationally determined using boundary conditions that also must be computationally determined. The purpose of this work is to apply an efficient approach of running computational cases with boundary conditions spanning the range of the experimental campaign in order to construct surrogate models to map probe measurements back to upstream boundary conditions. These surrogate models are then utilized to determine the appropriate boundary conditions for all of the experimental measurements without the need for computationally expensive iteration used in past work. For the experimental cases considered, inlet pressures are predicted with about +2/-3 kPa average uncertainty, and inlet enthalpies are predicted with about +0.6/-0.4 MJ/kg average uncertainty. The results also show that the top contributors of uncertainty are O catalytic efficiency for the high heat flux cases and CO₂-CO₂ diffusion cross section for the low heat flux cases.

I. Nomenclature

A	cross-sectional area, m ²	Δ	differential operator
C	conversion factor for volumetric flow rate, 6.309×10 ⁻⁵ (m ³ ·min)/(gal·s)	ρ	density, kg/m ³
c_p	isobaric specific heat capacity, J/(kg·K)	<i>Subscripts</i>	
E	arc voltage, V	<i>bulk</i>	calculated net heat addition to system
h	static enthalpy, J/kg	<i>CW</i>	cooling water
H	total enthalpy, J/kg	<i>exit</i>	condition at nozzle exit
I	arc current, A	<i>exp</i>	measurement from experiment
$\dot{m}$	gas mass flow rate, kg/s	<i>guess</i>	guessed value used for initiating iteration
p	pressure, Pa	<i>i</i>	static inflow condition at nozzle inlet
$\dot{q}$	heat flux, W/cm ²	<i>inj</i>	static condition at gas injection
T	temperature, K	<i>mat</i>	from CFD case matrix
u	velocity, m/s	<i>mod</i>	output of surrogate model
$\dot{V}$	cooling water volumetric flow rate, gal/min	<i>s</i>	species
X	axial distance from nozzle exit, cm	<i>STP</i>	standard temperature and pressure
Y	mass fraction	<i>w,flat</i>	wall of flat-faced Pitot probe or calorimeter
Z	radial distance from nozzle centerline, cm	<i>w,spec</i>	wall of test specimen

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II. Introduction

The Mars Science Laboratory (MSL) and Mars 2020 missions both carried a sensor suite, Mars Entry, Descent, and Landing Instrumentation (MEDLI) and MEDLI2, respectively, to collect data during entry into the Martian atmosphere. Data from both missions indicated reduced surface recession of the phenolic impregnated carbon ablator (PICA) heat shield compared to predictions [1, 2]. Both heat shields had been coated with NuSil CV-1144-0 to prevent particle shedding during assembly, testing, and launch. (The NuSil-coated PICA will hereafter be referred to as PICA-N.) Experimental work by Bessire et al. [1] at one of NASA Langley Research Center’s arcjet facilities, Hypersonic Materials Environmental Test System (HyMETS), compared PICA-N behavior in various test gases at measured heat fluxes of 126 to 140 W/cm² and measured stagnation pressures of 5.2 to 5.6 kPa. They showed that in an oxidizing environment (air or CO₂) the NuSil coating reduces the surface and in-depth temperature response to heating compared to uncoated PICA and inhibits ablation by forming a barrier against oxidation. This barrier is formed by the oxidation-resistant silicon oxycarbide that results from the pyrolysis and oxidation of PICA-N. Bessire et al. also found that the NuSil coating takes longer to decompose in environments that are high in CO₂ than it does in air or N₂ environments. These behaviors were attributed to the boundary layer having increased partial pressures of O and CO when in a CO₂ environment. The O leads to more oxidation, and the CO shifts the equilibrium of the interfacial reactions. The chemical processes responsible for these observations and attributions are discussed in more detail in Ref. [1]. These conclusions are particularly relevant for Mars missions where the atmosphere is primarily comprised of CO₂. Understanding the thermal protection system (TPS) material response to heating environments is critical for proper heat shield sizing to ensure it has sufficient reliability without having an excessive amount of margin. Understanding these processes is also key to more accurate post-flight data reconstruction. In 2024, there was another test campaign at HyMETS, to further investigate and quantify PICA-N’s response to heating in a CO₂ environment, including the effect of the NuSil coating thickness.

Arcjet facilities are capable of achieving sustained high-enthalpy flow, which makes them useful for hypersonic applications, including atmospheric entry. These facilities are used for screening TPS materials and calibrating material response models. To properly apply results from arcjet experiments, knowing the stagnation pressure and heat flux acting on the test specimen is critical. Although these values are measured by calibration probes at the test condition before injecting the specimen, the probes typically differ in shape and material from the specimen and are exposed to the flow for a much shorter time than the specimen. The aerothermal environment is greatly affected by geometry [3, 4], material properties, and wall temperature, so the measurements from flat-faced, cold-wall, metallic probes do not necessarily accurately reflect the conditions experienced by the actual rounded, hot-wall, TPS test specimen. Therefore, these specimen conditions must be determined via computational modeling of the arcjet. Proper facility boundary conditions are required to computationally model the arcjet, but because they are not measured by the facility directly, the boundary conditions must also be determined computationally, which is the focus of this work.

The general methodology presented here is to generate surrogate models of computational fluid dynamics (CFD) simulations that map flat probe stagnation pressure and heat flux measurements to upstream conditions at the nozzle inlet. These models enable the user to determine the upstream CFD boundary conditions that correspond to the measurements taken by the flat probes during the experiment. The user can then simulate the actual specimen with the proper inflow conditions to determine the conditions to which the specimen was subjected in the experiment. The methods used in this work are similar to those used in previous HyMETS work by Brune et al. [5] and Ventura Diaz et al. [3, 4], but there are differences specific to this work. For example, Brune et al. iterated with multiple CFD runs to approach specific measured stagnation pressure, $p_{w,flat}$, and heat flux, $\dot{q}_{w,flat}$, values [5], whereas the work presented here builds a more general database of $p_{w,flat}$ and $\dot{q}_{w,flat}$ values such that inflow pressure, p_i , and enthalpy, h_i , can be found for any experimental case within the bounds of the database without the need for further flat probe CFD runs. Brune et al. also used an Earth-like environment of O₂ and N₂, whereas the present work is for a Mars-like environment. Ventura Diaz et al. [3] used a database and machine learning approach similar to that presented here, but it was only for an Earth-like atmosphere. Their further work [4] included a Mars-like atmosphere very similar to that used here but only included one test condition with the Mars-like atmosphere.

The purpose of this work is to enable efficient determination of the upstream boundary conditions required to simulate the arcjet environments of the 2024 test campaign at HyMETS. These values will then be used in future work to inform material response modeling of the PICA-N samples for this test campaign. This future work will also aid in efficiently and accurately determining the facility settings and conditions required to achieve the desired stagnation pressure and heat flux in future experiments at HyMETS with this gas mixture and specimen type. This manuscript first presents an overview of the HyMETS facility and the experiments conducted in Sec. III. Section IV presents the computational models and methods used. Results are provided in Sec. V, and conclusions are discussed in Sec. VI.

III. HyMETS Arcjet Facility and Experiment

The HyMETS facility is an arc-heated wind tunnel that heats test gases by flowing them across an electric arc generated between two electrodes. Heated gases are accelerated by a converging-diverging Mach 5 nozzle and then exhausted into a test chamber. A diffuser is present to slow and cool the flow so that it may be pumped out of the facility. The entire arc plasma generator (including the nozzle) is water cooled. The HyMETS test section is illustrated in Fig. 1, and the facility is described in more detail in Ref. [6].

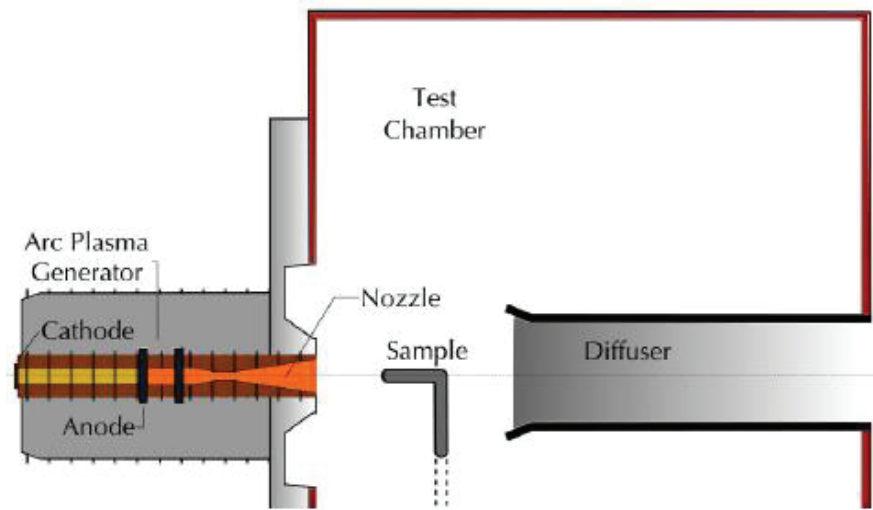


Fig. 1 Schematic diagram of HyMETS test section [3].

The facility features four arms, each with a sting holding either an instrument or a test specimen. These arms are inserted into the flow one at a time. Three instruments were mounted on the arms during this campaign: a Pitot probe for measuring stagnation pressure, a copper slug calorimeter for measuring heat flux (shown in Fig. 2), and a Gardon gauge for checking approximate heat flux and acting as a repeatability measurement. Note that the Pitot probe and slug calorimeter have the same external geometry, a cylinder with a diameter of 3.3 cm (1.3 in) and shoulder edge radius of 0.318 cm (0.125 in). They are together referred to as the calibration probe or flat probe elsewhere in this paper. The Gardon gauge readings are used to adjust facility conditions if needed until the heat flux is near the desired condition. This is because the copper slug can only be inserted into the flow once per run due to the negative effect of oxidation buildup on the slug's measurement accuracy and the time it takes for the slug to cool back down to the cold-wall condition. When the facility is at the target condition, the three instruments are sequentially inserted and removed from the flow to get pre-test measurements. Then the specimen is inserted into the flow and kept there for the desired test duration. After the specimen is removed, the Pitot probe and Gardon gauge are cycled back into the flow for post-test measurements.

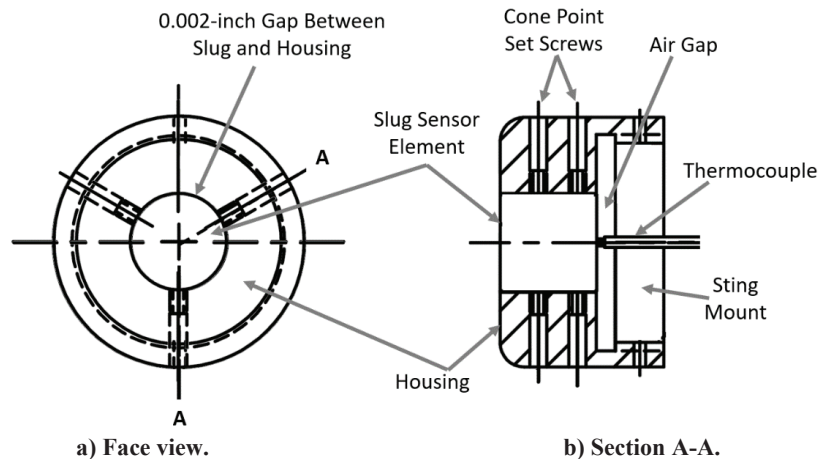


Fig. 2 Drawing of slug calorimeter.

The gas mixture composition used for this test campaign to simulate a Mars atmosphere was on average 80.5% CO₂, 14.4% N₂, and 5.1% Ar by volume. This gas composition was also used in the computational modeling. The actual composition of the Martian atmosphere is about 95% CO₂, 3% N₂, and 2% Ar by volume [7], but the facility is limited in how much CO₂ it can use, because sustained operation with CO₂ results in carbon deposits that damage the arc plasma generator [6]. The argon also functions as a shield gas to prevent damage to the electrodes. Experiments were conducted with mass flow rates ranging from 0.01160 to 0.01236 kg/s (375.9 to 400.5 standard liters per minute (SLPM)) and arc currents ranging from 121.7 to 263.3 A. These experiments resulted in measured flat probe stagnation pressures of 3.44 to 5.42 kPa and measured flat probe heat fluxes of 35.1 to 100.2 W/cm². An additional case from 2019 [1, 4] that used a very similar gas mixture (85% CO₂, 10% N₂, and 5% Ar by volume) was also considered in which a mass flow rate of 0.0093 kg/s (296 SLPM) and arc current of 236 A resulted in a measured stagnation pressure of 5.18 kPa and heat flux of 127 W/cm².

Note here the importance of making proper SLPM-to-kg/s conversions as the computational results are sensitive to mass flow rate. Conversions should use the gas density at standard temperature and pressure (STP) per Eq. (1) rather than the conventional method of using local pressure and temperature as a substitute for density change from STP based on the ideal gas law as in Eq (2). For typical applications where no reactions are taking place, these two methods are equivalent, but the arc heating in this application significantly changes the composition of the gas between what was injected and what enters the nozzle. This changes the molecular weight of the gas and thus the specific gas constant at the nozzle inlet from what it was at the point of injection where the SLPM was measured. Therefore, nozzle inlet pressure and temperature describe a different density and gas than what was injected and are not suitable to use in the SLPM-to-kg/s conversion. Equation (1) is insensitive to flow properties changing at different locations and test conditions and requires fewer inputs.

$$\frac{kg}{s} = SLPM \left(\frac{\rho_{STP}}{\rho_{inj}} \right) \left(\frac{1 m^3}{1000 L} \right) \left(\frac{1 min}{60 s} \right) \rho_{inj} = SLPM \left(\frac{1 m^3}{1000 L} \right) \left(\frac{1 min}{60 s} \right) \rho_{STP} \quad (1)$$

$$\frac{kg}{s} = SLPM \left(\frac{T_{inj}}{T_{STP}} \right) \left(\frac{p_{STP}}{p_{inj}} \right) \left(\frac{1 m^3}{1000 L} \right) \left(\frac{1 min}{60 s} \right) \rho_{inj} \neq SLPM \left(\frac{T_i}{T_{STP}} \right) \left(\frac{p_{STP}}{p_i} \right) \left(\frac{1 m^3}{1000 L} \right) \left(\frac{1 min}{60 s} \right) \rho_i \quad (2)$$

Another crucial point when making these conversions is to ensure that the STP used to obtain ρ_{STP} for the calculation is the same as the STP to which the flowmeter calibrations are referenced. For HyMETS, this was 273.15 K and 101.325 kPa, but “standard” conditions can vary by company, country, and application, so it is important to verify as this has a strong impact on the calculated flow rate and the computational results.

IV. Computational Methods

In this section, the CFD grid, settings, and assumptions are first presented. Then the process of establishing the database bounds, building the database, and building the initial surrogate models is described. The approach used for uncertainty quantification and its subsequent implementation into additional surrogate models is then presented. Finally, the last subsection discusses the prediction of boundary conditions that include uncertainty and how these boundary conditions will be used in future work to calculate specimen wall conditions.

A. Computational Fluid Dynamics

CFD was performed using the Langley Aerothermodynamic Upwind Differencing Algorithm (LAURA) [8], which is a structured, viscous Reynolds-Averaged Navier-Stokes solver used to model high-energy, chemically reacting flows. The HyMETS facility was modeled as axisymmetric, and the model included the nozzle, test cabin, and flat-faced calibration probe as shown in Fig. 3. The outer wall of the test cabin was modeled with a radius of 12.13 cm rather than the actual 30.58 cm (1 ft) radius. Modeling the wall closer to the centerline reduced the size of the grid and was shown to not compromise the results. A similar grid was used by Brune et al. [5] who also performed a grid convergence study to ensure grid independence of solutions. The grids are topologically the same with only the slight geometric difference of probe position. Brune et. al modeled the probe face 5.08 cm (2 in) from the nozzle exit plane versus 7.3025 cm (2.875 in) in the present grid. Both grids correctly use a nozzle cone half-angle of 12° despite previous papers [5, 6, 9] mistakenly listing 8°.

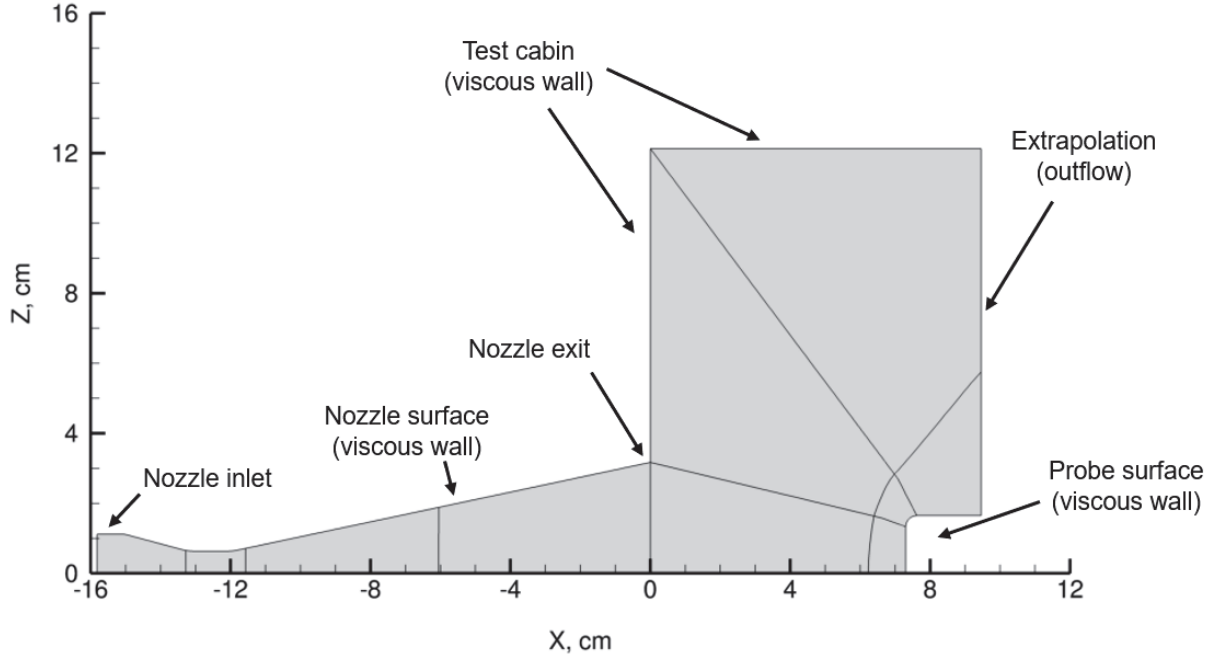


Fig. 3 Computational domain for flat probe CFD cases.

The flat probe was analyzed using a catalytic efficiency of 10% for O and N per Ref. [5] and a constant wall temperature of 350 K. The effect of deviation from this assumed catalytic efficiency is addressed in Sec. IV.C as part of a parametric uncertainty analysis. All other walls, including the nozzle wall, were treated as non-catalytic with a temperature of 300 K. Despite previous work by Brune et al. that showed sensitivity of predicted probe pressure to nozzle catalysis [9], the nozzle in HyMETS is known to have a CuO layer on the surface, which inhibits oxidation. The Mars-like environment was simulated with a nine-species gas model [10] consisting of CO₂, N₂, CO, NO, O₂, C, N, O, and Ar. Note that other common species, such as CN and C₂, were not found to form in noticeable quantities for the probe simulations at the considered test conditions and were, therefore, neglected. These species may be more critical when simulating the PICA-N samples. Thermal non-equilibrium was modeled using a two-temperature model [11] in which translational and rotational energy modes are equilibrated at a different temperature than the vibrational and electronic energy modes. An initial case at representative conditions was run with this grid and converged so that the actual cases of interest could be run as restarts from this pre-converged case. This reduced computational time and facilitated easier automation.

B. Database and Model Generation

The full computational approach to finding specimen stagnation pressure and heat flux is illustrated in Fig. 4. The scope of the current work, however, is only to find the boundary conditions corresponding to the experimental measurements (steps 1 through 5). Steps 6 and 7 are included below for context only and will be performed in future work. This subsection discusses steps 1 through 4, and Sec. IV.D discusses steps 5 through 7.

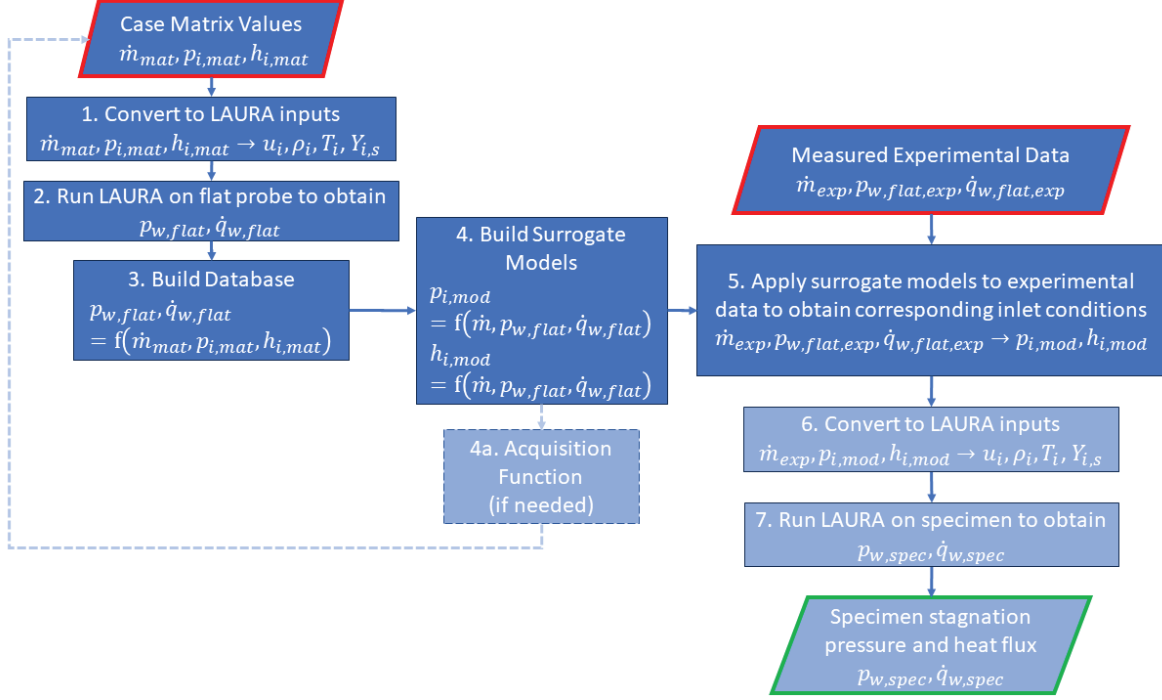


Fig. 4 Flowchart of computational approach to finding specimen stagnation pressure and heat flux.

Before step 1 could begin, a case matrix needed to be established. The first cases of interest analyzed in LAURA were at the eight corners of the eventual case matrix. These corner cases were run first to verify that the bounding values of $\dot{m}_{mat}$, $p_{i,mat}$, and $h_{i,mat}$ resulted in flat probe $p_{w,flat}$ and $\dot{q}_{w,flat}$ values that bounded the $p_{w,flat,exp}$ and $\dot{q}_{w,flat,exp}$ values measured during the experiments. Setting appropriate case matrix bounds ensured that the training data for the surrogate models would cover the entire experimental range to prevent the need for extrapolation. Additionally, running the corner cases also acted as a spot check of solution convergence and informed the number of solver iterations to perform on subsequent LAURA cases.

Bounding values of $\dot{m}_{mat}$ were based on experimental data from the 2024 campaign as well as a single point from the 2019 test campaign [1, 4]. Appropriate $p_{i,mat}$ and $h_{i,mat}$ bounds to envelop the experimental results without creating an excessively broad input range were determined iteratively using LAURA runs, but initial guesses were needed. The initial upper bound guesses for $p_{i,mat}$ and $h_{i,mat}$ came from a set of LAURA runs that had previously been performed to try to match the 2019 test mentioned above. The lower bound for $p_{i,mat}$ was initially guessed based on an approximation of total pressure upstream of the normal shock formed in front of the probe. This was found using the measured $p_{w,flat,exp}$ (total pressure downstream of the shock) and the total pressure ratio across a normal shock at Mach 5 (the nozzle exit Mach number taken to be the approximate Mach number upstream of the shock). The lower bound for $h_{i,mat}$ was initially guessed using bulk enthalpy according to the energy change in Eq. (3), consisting of power fed into the arc minus the rate of energy removal by water cooling [12]. The corresponding energy balance is written in Eq. (4) and illustrated in Fig. 5.

$$h_{bulk} = \frac{EI - \dot{V}_{CW} \rho_{CW} c_{p,CW} \Delta T_{CW} C}{\dot{m}} \quad (3)$$

$$H_{exit} = H_{inj} + h_{bulk} \quad (4)$$

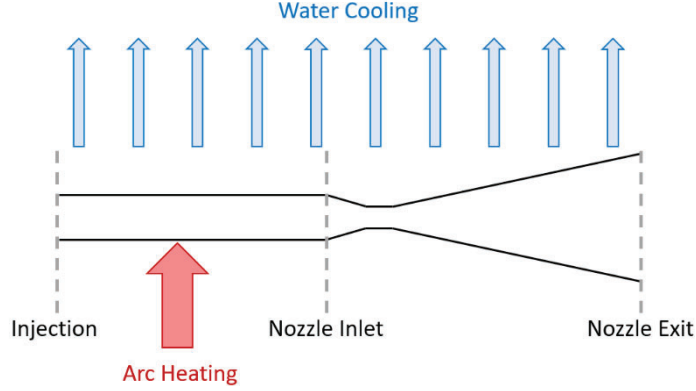


Fig. 5 Schematic of net energy change.

However, the h_{bulk} estimate for inlet enthalpy was found to be insufficient to yield stagnation heat flux values low enough to bound the $\dot{q}_{w,flat,exp}$ measurements. This is because it neglects the enthalpy at the point of injection, H_{inj} , and therefore does not account for heat of formation. This neglect is logical for air systems where this equation is typically used, but accounting for the large negative heat of formation of CO_2 is crucial when using a Mars-like gas mixture. Therefore, a more appropriate way to estimate the lower bound on inlet enthalpy is illustrated in Fig. 6 and expressed mathematically in Eqs. (5-7). The use of h_{bulk} from Eq. (3) in these equations assumes that all of the cooling (the second term in the numerator of Eq. (3)) happens upstream of the nozzle inlet. In reality, the same cooling water circuit actually cools both the upstream portion of the arc plasma generator and the nozzle together, so assuming this cooling is confined to only the upstream portion results in a conservative minimum enthalpy value.

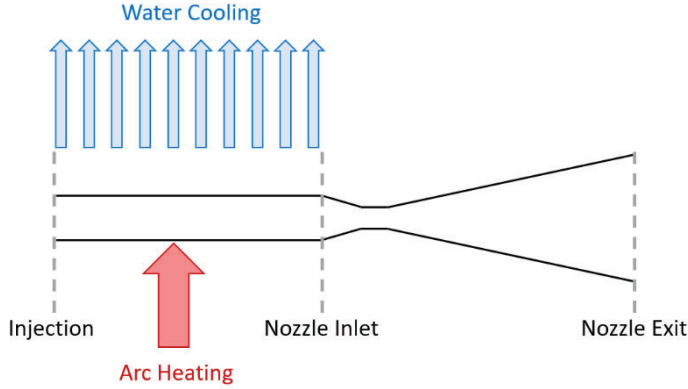


Fig. 6 Schematic of minimum energy change between injection and nozzle inlet.

$$H_i > H_{inj} + h_{bulk} \quad (5)$$

Expanding Eq. (5) to show the components of total enthalpy yields Eq. (6).

$$h_i + \frac{u_i^2}{2} > h_{inj} + \frac{u_{inj}^2}{2} + h_{bulk} \quad (6)$$

Neglecting velocities due to their insignificant contributions at the injection and inlet stations for the cases considered yields Eq. (7).

$$h_i > h_{inj} + h_{bulk} \quad (7)$$

Conversely, an upper limit on inlet enthalpy can be found by assuming that none of the cooling happens upstream of the nozzle inlet and that all cooling is confined to the nozzle. The resulting energy balance is illustrated in Fig. 7 and expressed mathematically in Eqs. (8-10).

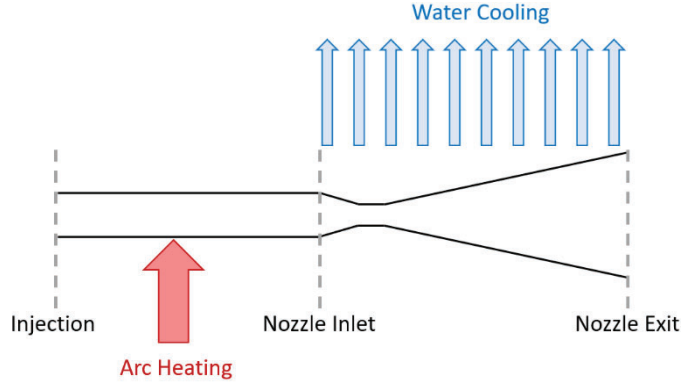


Fig. 7 Schematic of maximum energy change between injection and nozzle inlet.

$$H_i < H_{inj} + \frac{EI}{\dot{m}} \quad (8)$$

Expanding Eq. (8) to show the components of total enthalpy yields Eq. (9).

$$h_i + \frac{u_i^2}{2} < h_{inj} + \frac{u_{inj}^2}{2} + \frac{EI}{\dot{m}} \quad (9)$$

Neglecting velocities due to their insignificant contributions at the injection and inlet stations for the cases considered yields Eq. (10).

$$h_i < h_{inj} + \frac{EI}{\dot{m}} \quad (10)$$

After some iteration, the final selected bounds of $\dot{m}_{mat}$, $p_{i,mat}$, and $h_{i,mat}$ were 0.009 to 0.013 kg/s, 60 to 130 kPa, and -4 to 8 MJ/kg, respectively. These variable ranges were used to construct a list of the next LAURA flat probe cases to execute. Cases were selected via Latin hypercube sampling with three variables ($\dot{m}_{mat}$, $p_{i,mat}$, and $h_{i,mat}$) and 30 samples (10 per variable), which with the corner cases made a total of 38 cases for constructing the surrogate models. This number of samples was later determined to be sufficient.

Required LAURA inputs include velocity, density, temperature, and species mass fractions at those conditions, so step 1 of Fig. 4 was to determine these values from $\dot{m}_{mat}$, $p_{i,mat}$, and $h_{i,mat}$ using the iterative and automated process shown in Fig. 8. A temperature guess was made, and the MULTicomponent Thermodynamic And Transport properties for IONized gases (Mutation++) program [13] was used to calculate the enthalpy corresponding to that temperature guess and pressure. The temperature guess was varied until the resulting enthalpy matched the target enthalpy, $h_{i,mat}$. Mutation++ output from that pressure and temperature provided the corresponding density and mass fractions present at the nozzle inlet. The density and nozzle inlet area were used with $\dot{m}_{mat}$ to calculate velocity at the nozzle inlet. For simplicity, uniform inflow velocity and enthalpy profiles were assumed. Brune et. al [5] assumed parabolic profiles but later found the impact of profile shape on the surface conditions of the calibration probe to be negligible [9].

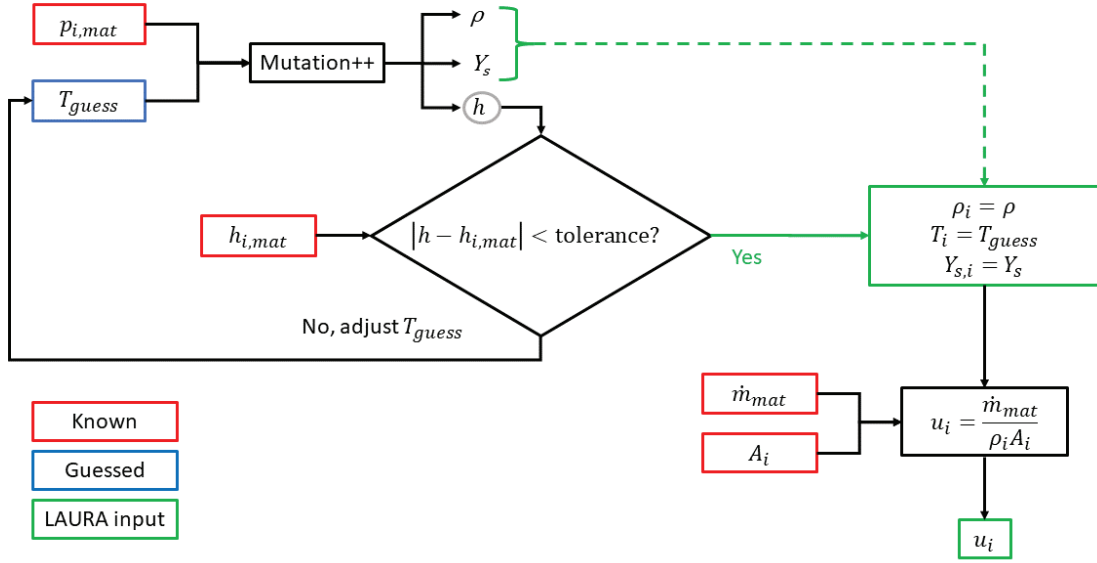


Fig. 8 Flowchart for determining LAURA inputs.

Once these inputs were established, LAURA was run for these cases (step 2 in Fig. 4), and the stagnation pressure and convective heat flux values, $p_{w,flat}$ and $\dot{q}_{w,flat}$, respectively, were harvested and stored in a database of flat probe LAURA results (step 3 in Fig. 4). The database was then used to generate Gaussian process (Kriging) surrogate models [14] to predict $p_{i,mod}$ and $h_{i,mod}$ as a function of $\dot{m}$, $p_{w,flat}$, and $\dot{q}_{w,flat}$ (step 4 in Fig. 4). Figure 9 shows a map of the of the cases used to build the surrogate models. In both Figs. 9.a and 9.b, mass flow rate would be the third dimension in the direction normal to the page. Figure 9.b is overlaid with experimental measurements to illustrate the models' coverage of the region of interest.

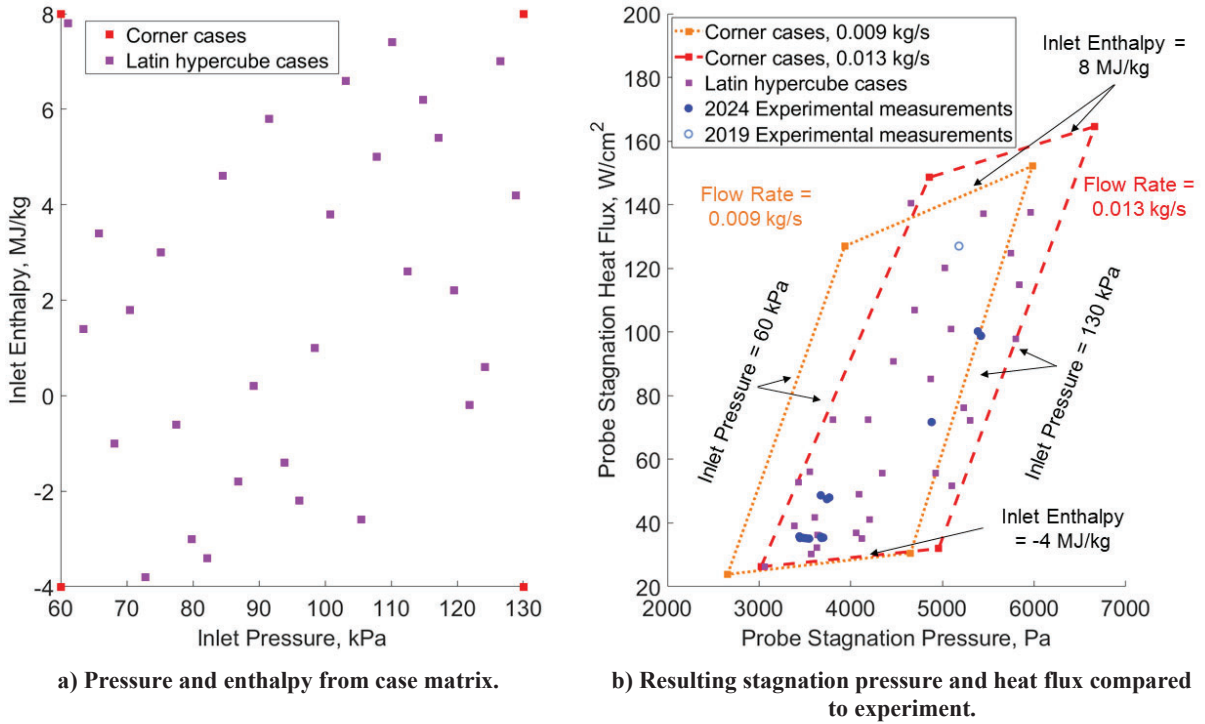


Fig. 9 Values used to build surrogate models overlaid with experimental measurements of interest.

More sample points could have been added in step 4a of Fig. 4 as part of surrogate model refinement, although that was deemed unnecessary based on the verification results presented in Sec. V. If model refinement were necessary, however, more LAURA cases would be added to the database, and the Kriging models would be regenerated with each iteration of the database. Cases to be added would be selected using adaptive sampling based on an acquisition function of Kriging model predictions. The acquisition function would identify the part of the Kriging model with the highest uncertainty in the prediction and add a point there. This model refinement loop would continue until some criterion was satisfied.

C. Uncertainty Quantification and Additional Models

Uncertainties in the model were addressed by running LAURA's built-in functionality for efficient parametric uncertainty quantification and sensitivity analysis. The methods used are described in Ref. [15]. The process begins by restarting an existing case several times with uncertain quantities set to distributed values within their specified bounds and uses the new results to build a polynomial chaos expansion (PCE) of the CFD model. The uncertainty in all the uncertain parameters is then propagated through the PCE using a Monte Carlo sampling approach to determine the upper and lower bounds of heat flux. Additionally, global nonlinear sensitivities to each parameter are determined analytically from the PCE model. In this work, 50 samples at each of the 38 database cases were determined to be sufficient to accurately estimate the uncertainty and sensitivities. A total of 61 uncertain quantities were considered including catalytic efficiencies, reaction rates, and diffusion cross sections. Reaction rate uncertainties are described in Ref. [15]. Wright et al. [16] detailed the uncertainty in the diffusion cross sections. Oxygen catalytic efficiencies (nominally set to 10%) considered were 3% to 20% based on Ref. [17] values for an unoxidized copper surface. Similarly, N catalytic efficiencies (nominally set to 10%) considered were 5% to 15% based on the same source, although N catalysis had no significant impact on the heat flux results. The same process described above was also used to find upper and lower bounds of stagnation pressure for each corner case, but the percent difference between the upper and lower stagnation pressure never exceeded 2.2% for any of the corner cases, so the pressure sensitivity to the considered uncertainties was deemed negligible compared to the heat flux sensitivity and was not considered further. For reference, heat flux had 12% to 26% difference between upper and lower values.

Four new Kriging surrogate models were built using the upper and lower bound heat flux values for each database case. One predicts p_i corresponding to upper bound heat flux, another predicts h_i corresponding to upper bound heat flux, another predicts p_i corresponding to lower bound heat flux, and the last one predicts h_i corresponding to lower bound heat flux. The purpose of these additional surrogate models was to see how uncertainty propagates from the assumptions in the CFD model to heat flux results to inlet conditions predicted. This is critical to eventually quantifying the uncertainty in CFD results for the specimen since those cases will be fed inlet conditions from the surrogate models presented.

Note that facility-related uncertainties were neglected in the present work but should be considered when applying the surrogate models to experimental measurements in future work. The most notable facility uncertainty is in the heat flux measured by the slug calorimeter, which is typically assumed to be $\pm 10\%$ [6, 9, 18], although Brune and Morrow found it to be only up to $\pm 4\%$ [19].

D. Calculations Corresponding to Experiment

The surrogate models were used to infer the $p_{i,mod}$ and $h_{i,mod}$ conditions corresponding to each experimental case using the measured $\dot{m}_{exp}$, $p_{w,flat,exp}$, and $\dot{q}_{w,flat,exp}$ (step 5 in Fig. 4). In future work, there will be another round of LAURA runs using these inferred conditions for each experimental case but with the geometry and material properties of the test specimen (PICA-N sample) rather than the flat probe. Each case will start from a pre-converged LAURA solution. The inferred $p_{i,mod}$ and $h_{i,mod}$ will be used with the measured $\dot{m}_{exp}$ to calculate the required LAURA inputs per step 6. After each case is complete (step 7), $p_{w,spec}$ and $\dot{q}_{w,spec}$ will be harvested from the LAURA results and will serve as the inferred stagnation pressure and heat flux that acted on the actual test specimen. These values will then be used to analyze the material response of the specimen.

V. Results

Figures 10 and 11 show results from a sample case using the flat calibration probe. This was one of the cases that came from the Latin hypercube part of the case matrix. The temperature field is shown in Fig. 10. Figure 11 shows the stagnation pressure and heat flux profiles along the centerline slice of the probe. The stagnation point ($Z = 0$ cm) results are what were used to build the databases and surrogate models.

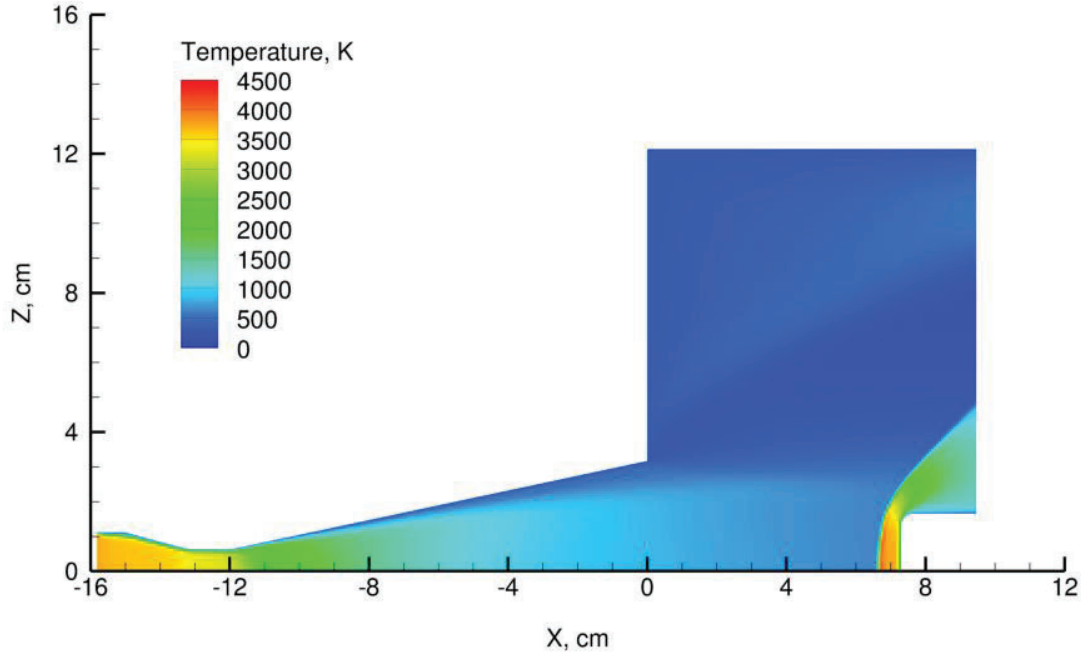
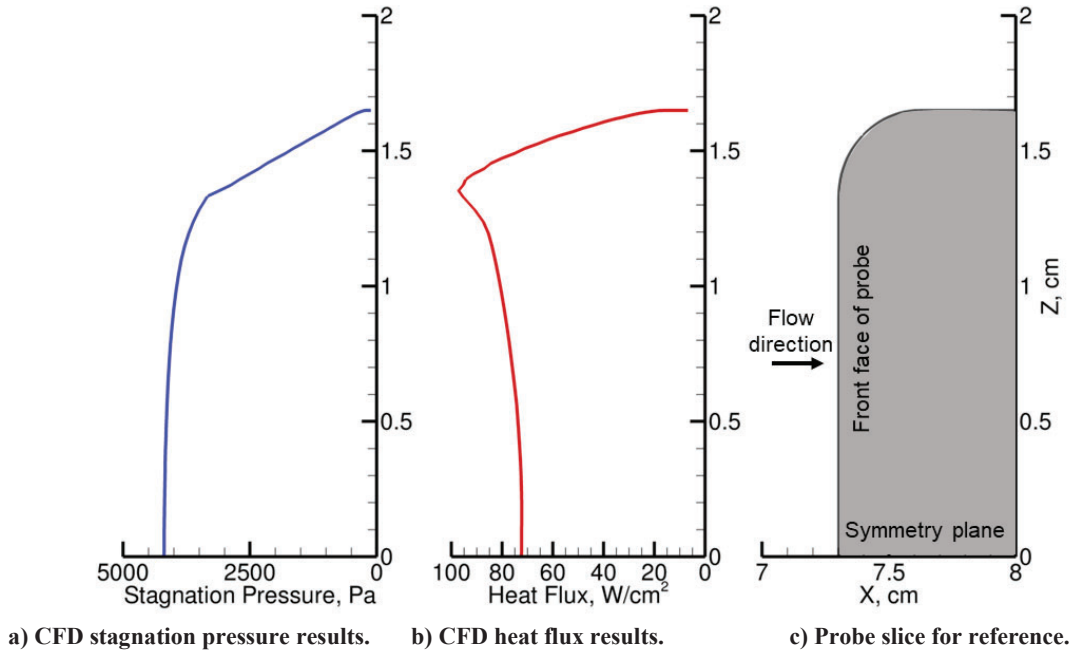


Fig. 10 Flowfield temperature for inflow conditions of $\dot{m} = 0.01213$ kg/s, $p_i = 75.17$ kPa, and $h_i = 3$ MJ/kg.



a) CFD stagnation pressure results. b) CFD heat flux results. c) Probe slice for reference.

Fig. 11 Probe surface pressure and heat flux for $\dot{m} = 0.01213$ kg/s, $p_i = 75.17$ kPa, and $h_i = 3$ MJ/kg.

Verification of the initial surrogate models involved leave one out cross-validation (LOOCV) to ensure that predictions were not overly dependent on any single training point. The results are presented in Table 1. Error is the root mean square of the difference between the LOOCV predictions and the training data values. Both models had errors less than 1% of the range of the variable of interest. Standard error (error divided by the standard deviation of the training data values) was also computed in order to make the error independent of scale and was deemed sufficiently low.

Table 1 Leave one out cross-validation results

	Pressure Model	Enthalpy Model
Error	423.8 Pa	70,114 J/kg
Standard Error	0.0174	0.0168
Variable Range	60 to 130 kPa (70 kPa)	-4 to 8 MJ/kg (12 MJ/kg)
Error as Percent of Range	0.61%	0.58%

A second approach to verify the initial surrogate models was employed in which 10 new $\dot{m}$, p_i , and h_i combinations were selected via Latin hypercube sampling. These cases were executed in LAURA, and the resulting $p_{w,flat}$ and $\dot{q}_{w,flat}$ were harvested. The existing surrogate models were then used to predict $p_{i,mod}$ and $h_{i,mod}$ based on $\dot{m}$ and these $p_{w,flat}$ and $\dot{q}_{w,flat}$ results. The $p_{i,mod}$ and $h_{i,mod}$ predictions were compared to the p_i and h_i values used to generate the LAURA inputs. This tested the models' ability to make predictions consistent with CFD at points other than the ones used to train the models. The key results are presented in Table 2. Among the 10 cases assessed, the pressure and enthalpy predicted by the models never deviated more than 0.43 kPa and 0.0445 MJ/kg, respectively, from the CFD inputs. All absolute differences between predictions and CFD input values were less than 1% of the variable range and, on average, less than 0.2% of the variable range.

Table 2 Verification results using additional 10 cases

	Pressure Model	Enthalpy Model
Average Absolute Difference	119 Pa	15,023 J/kg
Avg Difference as Percent of Range	0.17%	0.13%
Maximum Absolute Difference	430 Pa	44,460 J/kg
Max Difference as Percent of Range	0.61%	0.37%

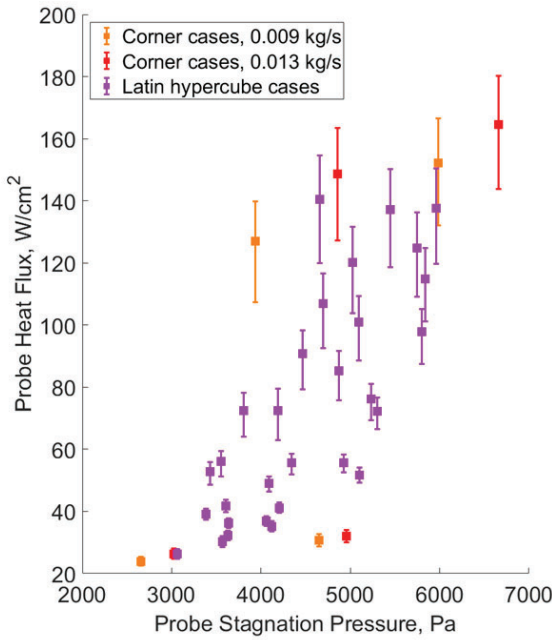
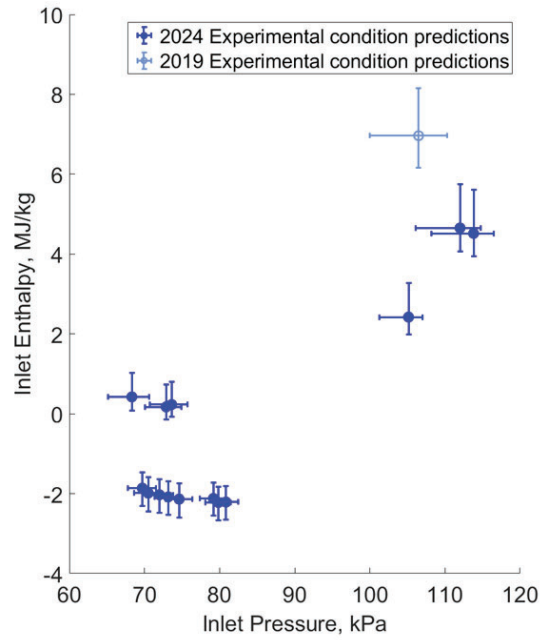
A parametric uncertainty analysis was performed as described in Sec. IV.C, and results for the corner cases are given in Table 3. For all the corner cases where $h_i = -4$ MJ/kg, the top contributor to uncertainty was the CO₂-CO₂ diffusion cross section, followed by the CO₂-N₂ and CO₂-CO diffusion cross sections. These sensitivities changed at higher enthalpies, however, where the uncertainty was also greater overall. For all the corners where $h_i = 8$ MJ/kg, the top contributor to uncertainty was the O catalytic efficiency, followed by the CO-O diffusion cross section. The higher enthalpy cases have much more O available to combine to O₂ at the probe surface than the lower enthalpy cases. Oxygen recombination is a strongly exothermic reaction, so it is not surprising that uncertainty in the efficiency of this reaction would contribute so heavily to heat flux uncertainty for higher enthalpy cases with more abundant O.

Figure 12 illustrates the impact of considering the uncertainty in the CFD. Figure 12.a shows the uncertainty in heat flux values from CFD that were used to build the additional surrogate models. Although the effect is minimal for cases with low heat fluxes (low enthalpy cases), it becomes extremely significant at higher heat fluxes (high enthalpy cases). For example, the CFD case with $\dot{m} = 0.013$ kg/s, $p_i = 130$ kPa, and $h_i = 8$ MJ/kg (top right of Fig. 12.a) had a heat flux uncertainty of +9% and -13%. Note that these percentages do not yet account for the already significant measurement uncertainty in the slug calorimeter, which could be as much as $\pm 4\%$ or $\pm 10\%$ depending on the source [6, 9, 18, 19].

This sizable uncertainty in heat flux translates to significant uncertainty in the prediction of inlet pressure and enthalpy required to achieve a given stagnation pressure and heat flux on the calibration probe. Figure 12.b shows how the heat flux uncertainty from Fig. 12.a propagated through the surrogate model to the enthalpy and pressure predictions for the experimental cases. For example, using the surrogate models developed here, the 2019 case has a predicted inlet pressure uncertainty of +3.6% and -6.1% and a predicted inlet enthalpy uncertainty of +17.0% and -11.5%. Considering all the experimental cases, the average prediction uncertainty was about +2/-3 kPa for inlet pressure and about +0.6/-0.4 MJ/kg for inlet enthalpy. The uncertainty in inlet conditions will be carried into the eventual CFD runs on the test specimen and result in further uncertainty in the heat flux and stagnation pressures acting on the specimen. Although the method presented here provides a good framework, it also highlights the importance of future work to reduce uncertainty bounds by better quantifying catalytic efficiencies and diffusion cross sections.

Table 3 Uncertainty quantification results for corner cases of case matrix

Mass Flow Rate, kg/s	Inlet Pressure, kPa	Inlet Enthalpy, MJ/kg	Heat Flux, W/cm ²			Top Sources of Uncertainty in Heat Flux	Percent of Total Uncertainty
			Low	Nominal	High		
0.009	60	-4	22.5	23.9	25.5	CO ₂ -CO ₂ diff. cross sec.	66.0%
						CO ₂ -N ₂ diff. cross sec.	14.9%
						CO ₂ -CO diff. cross sec.	12.8%
0.013	60	-4	24.8	26.2	28.0	CO ₂ -CO ₂ diff. cross sec.	64.8%
						CO ₂ -N ₂ diff. cross sec.	15.9%
						CO ₂ -CO diff. cross sec.	13.3%
0.009	130	-4	28.8	30.6	32.7	CO ₂ -CO ₂ diff. cross sec.	68.0%
						CO ₂ -N ₂ diff. cross sec.	16.0%
						CO ₂ -CO diff. cross sec.	10.5%
0.013	130	-4	30.1	31.9	34.1	CO ₂ -CO ₂ diff. cross sec.	67.7%
						CO ₂ -N ₂ diff. cross sec.	16.1%
						CO ₂ -CO diff. cross sec.	11.0%
0.009	60	8	107.3	127.0	139.9	O catalytic efficiency	69.7%
						CO-O diff. cross sec.	27.3%
0.013	60	8	127.2	148.5	163.4	O catalytic efficiency	65.6%
						CO-O diff. cross sec.	30.6%
0.009	130	8	132.0	152.2	166.5	O catalytic efficiency	61.1%
						CO-O diff. cross sec.	34.0%
0.013	130	8	143.8	164.6	180.1	O catalytic efficiency	58.8%
						CO-O diff. cross sec.	36.9%

**a) Stagnation pressure and heat flux results with incorporated model uncertainty.****b) Inlet pressure and enthalpy predictions for the experimental cases.****Fig. 12 Uncertainty in heat flux and resulting uncertainty in boundary condition predictions.**

VI. Conclusions

A method to efficiently determine upstream conditions corresponding to a recent arcjet test campaign was presented. This involved executing CFD cases of the calibration probe over a range of facility conditions and then creating surrogate models to map the probe stagnation results back to upstream conditions. This is a significant improvement over the previous method of manually iterating through boundary conditions and running several CFD cases per experiment until CFD results match the experimental measurements. Model verification and uncertainty quantification of the current surrogate models were also presented. The uncertainty analysis demonstrated the need for more precise knowledge of model parameters, specifically O catalysis, which is the primary driver of uncertainty at high enthalpy conditions where uncertainty is the greatest, and CO₂-CO₂ diffusion cross section, which drives the uncertainty at low enthalpy. These surrogate models serve as a map of experimentally measured stagnation pressures and heat fluxes to upstream conditions. In a future work, these upstream conditions will be used for CFD runs of the test specimen. The resulting stagnation pressures and heat fluxes will inform material response analysis of the PICA-N samples. They can also be used to build another surrogate model to map specimen stagnation pressure and heat flux back to required facility settings (mass flow and arc current) in order to more efficiently and precisely meet the desired test conditions.

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