



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

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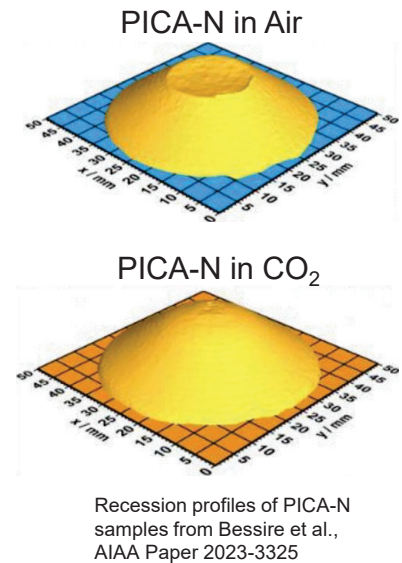


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Motivation and Introduction

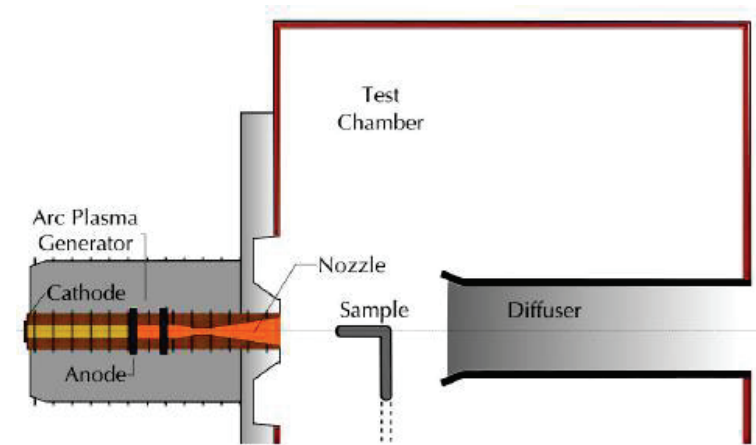
- Recent arcjet test campaigns studied the ablation processes of phenolic impregnated carbon ablator (PICA) coated with NuSil CV-1144-0 (configuration known as PICA-N) in air, N_2 , and a CO_2 -rich mixture.
- In order to quantitatively analyze material response, knowledge of the stagnation pressure and heat flux acting on the test specimen is required and must be determined computationally.
- Appropriate upstream boundary conditions must be computationally determined before experiment can be simulated.
- Boundary conditions often determined iteratively by running CFD several times per experimental point until the measured pressure and heat flux are obtained on a simulated measurement probe.

Purpose of this work is to apply an efficient approach to determining appropriate boundary conditions for any experiment within the test campaign without the need for computationally-expensive iteration.

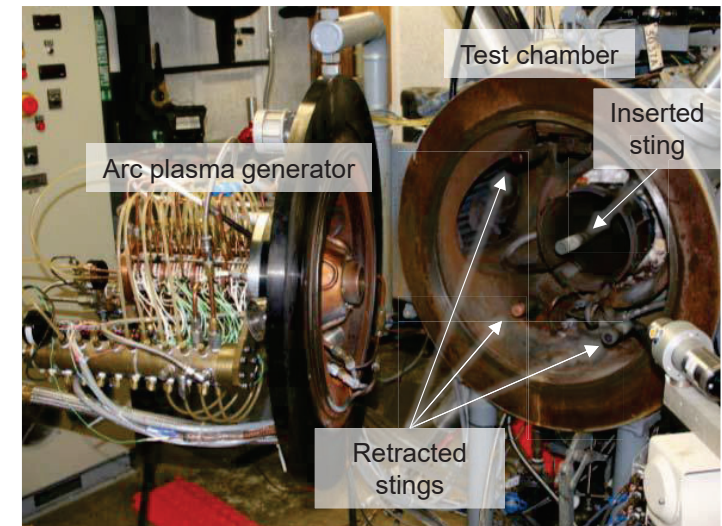


Experiment and Facility

- HyMETS (Hypersonic Materials Environmental Test System) is an arc-heated wind tunnel at NASA Langley.
- Heats test gases by flowing them across an electric arc generated between two electrodes.
- Primary facility controls: Gas flow rate and arc current
- Arc plasma generator (including nozzle) is water cooled.
- 4 arms, each with a sting for a different instrument or test specimen. For this test campaign:
 - Pitot probe (stagnation pressure)
 - Copper slug calorimeter (heat flux)
 - Gardon gauge (heat flux repeatability)
 - Test specimen (PICA-N sample)
- Gas mixture for this test campaign (by vol.):
80.5% CO₂, 14.4% N₂, 5.1% Ar
 - Facility limited in how much CO₂ it can use due to the carbon deposits that can form and damage the plasma generator.
 - Electrode damage also avoided by using Ar as shield gas.

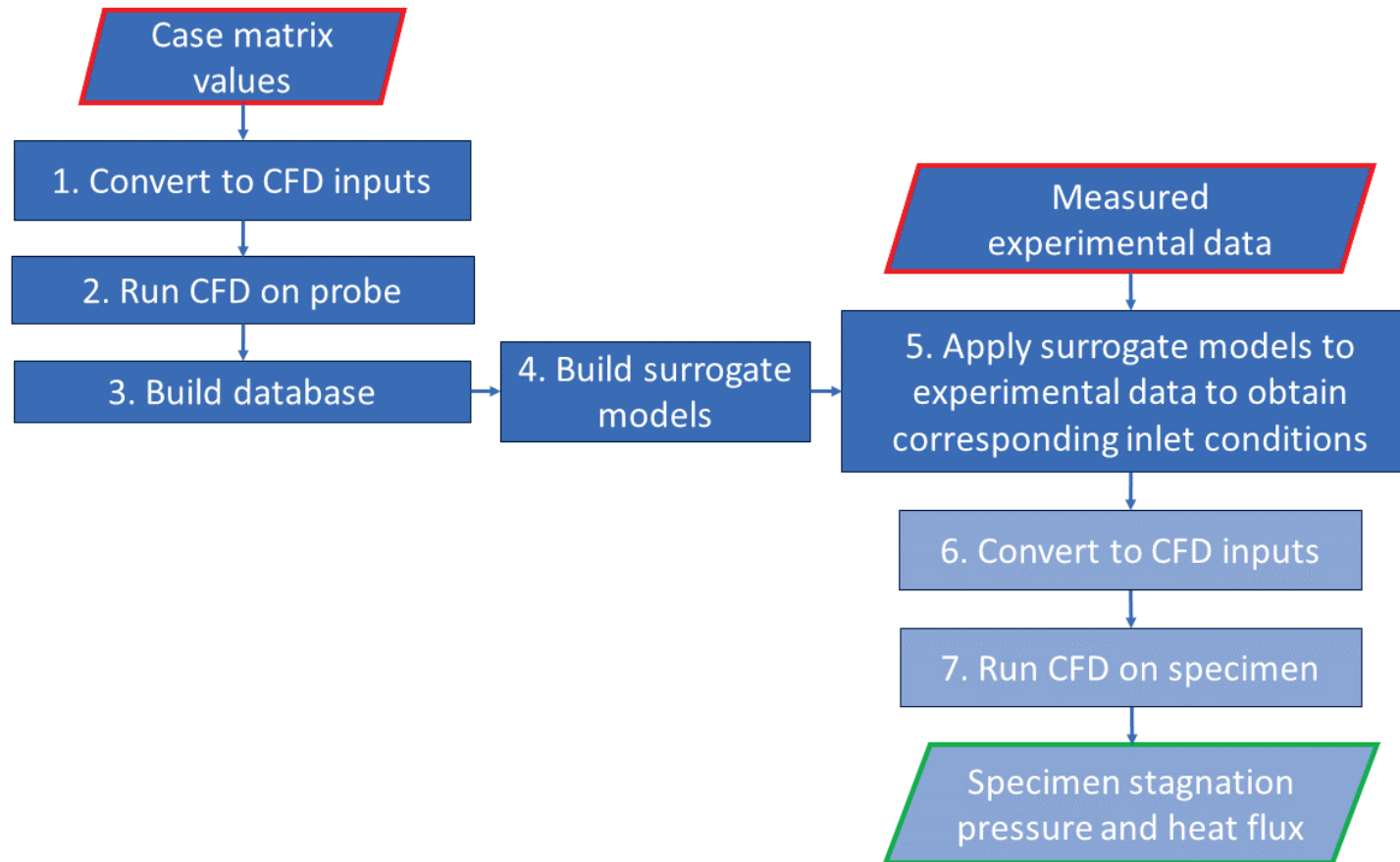


Ventura Diaz et al., AIAA Paper 2020-1710

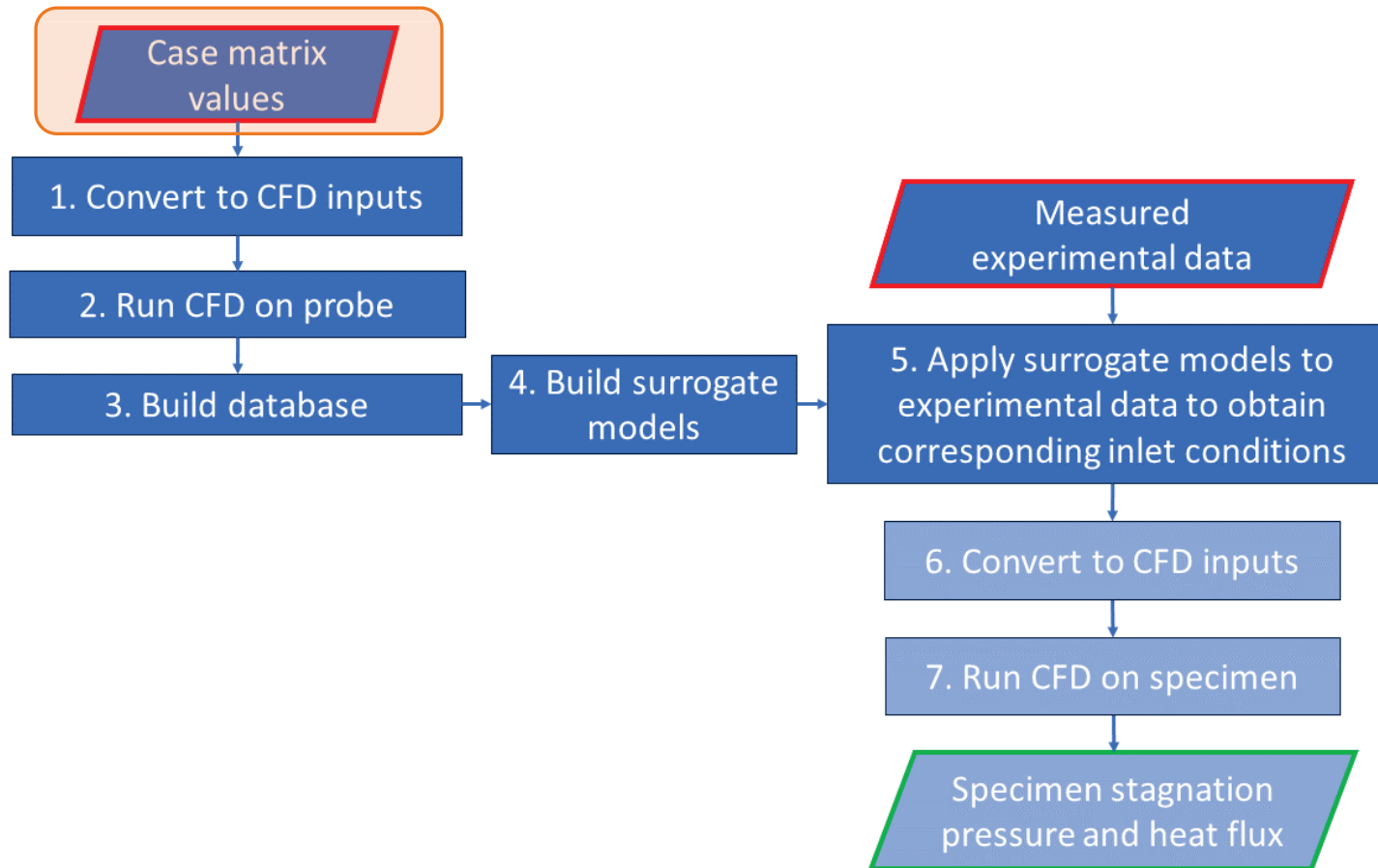


Adapted from Splinter et al., AIAA Paper 2011-1014

Computational Methods Overview

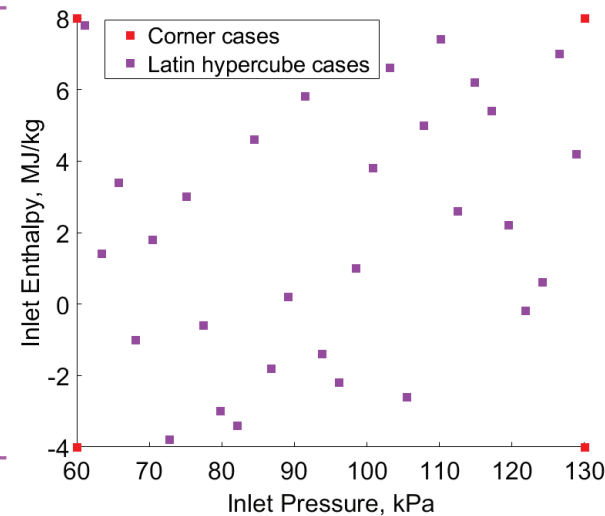
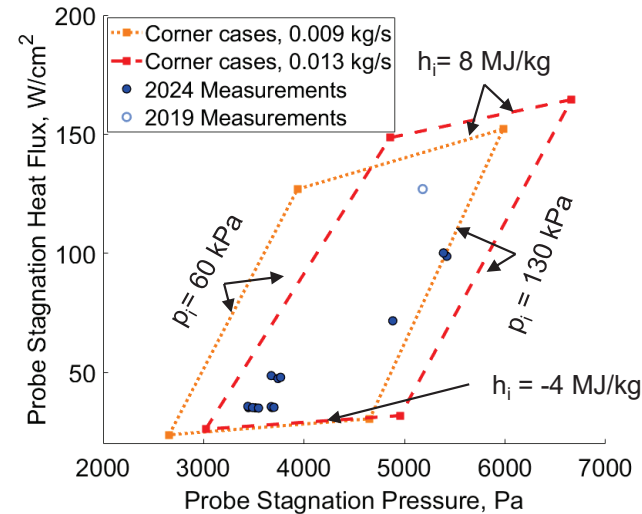


Computational Case Matrix



Computational Case Matrix

- Corners of case matrix established using experimental measurements from 2024 test campaign as well as a single case from the 2019 campaign.
 - Flow rates chosen to bound experimental flow rates.
 - Pressure and enthalpy bounds determined iteratively.
 - Ran CFD on guessed corner cases until resulting probe stagnation pressure and heat flux values enveloped all the experimental data points.
- Remaining cases determined using Latin hypercube sampling with 3 variables (flow rate, inlet pressure, and inlet enthalpy) and 30 samples (10 per variable) for a total of 38 cases.



Case matrix bounds:

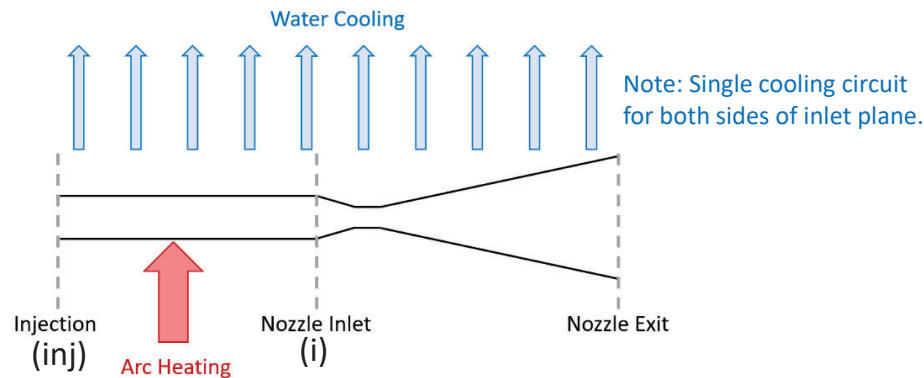
$$0.009 \frac{kg}{s} \leq \dot{m} \leq 0.013 \frac{kg}{s}$$

$$60 \text{ kPa} \leq p_i \leq 130 \text{ kPa}$$

$$-4 \frac{MJ}{kg} \leq h_i \leq 8 \frac{MJ}{kg}$$

A note about enthalpy

- Inlet enthalpy typically assumed to be the bulk enthalpy (net heat addition from the arc).



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

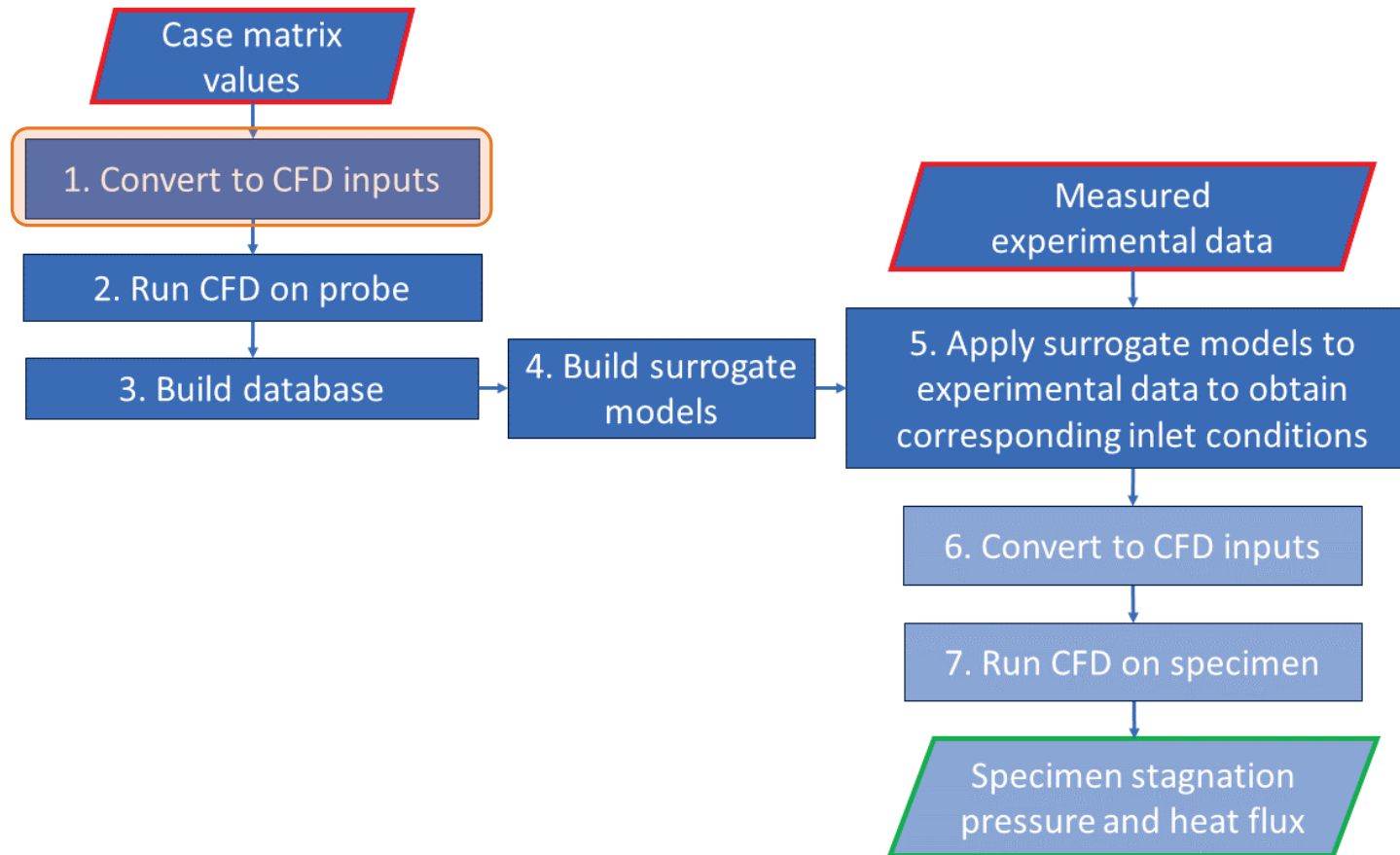
Water cooling

$$H_{exit} = H_{inj} + h_{bulk}$$

- However, this neglects the enthalpy in the flow at injection (prior to the arc).
 - Fine for N_2 or air where the heat of formation is zero or negligible.
 - Not fine for CO_2 where the heat of formation is significant and negative.
- Bulk enthalpy equation also assumes all the cooling has already occurred (more fitting for nozzle exit).
- Considering h_{inj} (includes heat of formation) and the fact that only some of the cooling takes place upstream of the nozzle inlet, we can establish limits on possible inlet enthalpy h_i .

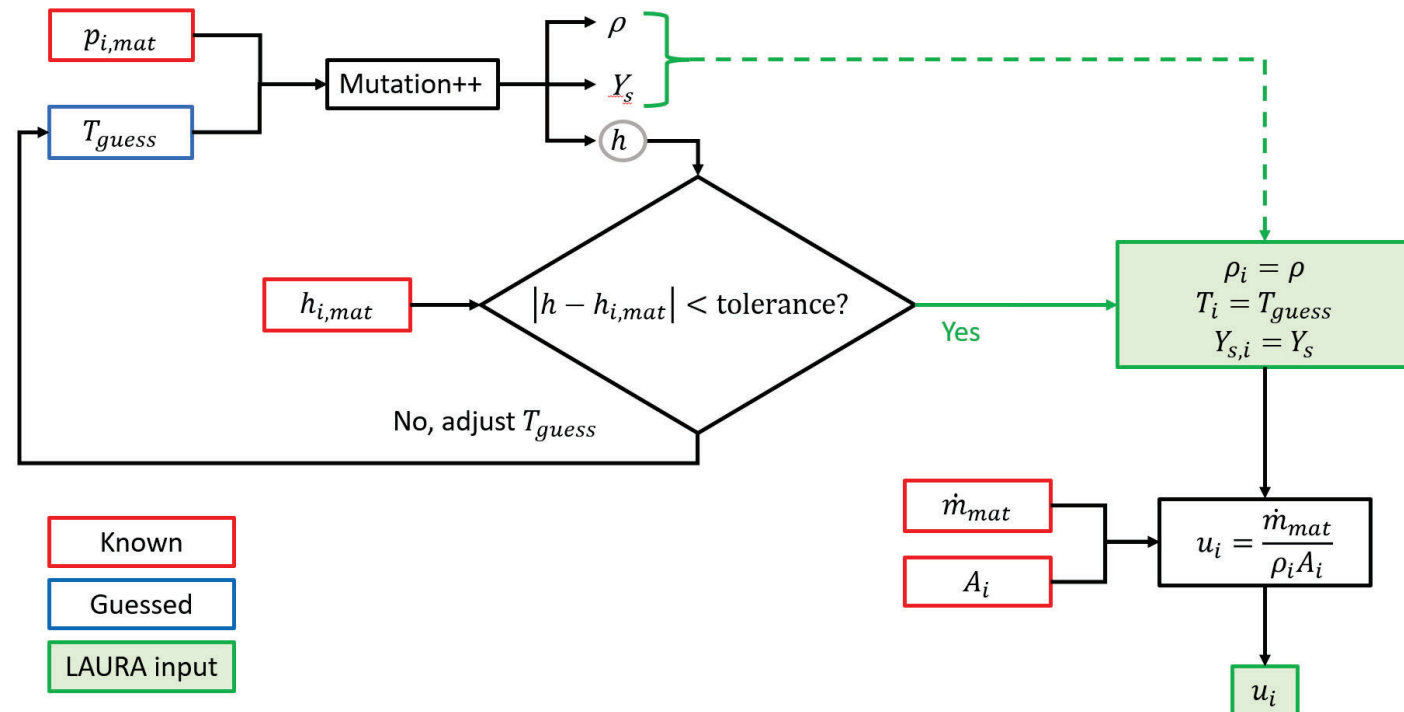
$$h_{inj} + \overset{\text{heating - cooling}}{h_{bulk}} < h_i < h_{inj} + \overset{\text{heating only}}{\frac{EI}{\dot{m}}}$$

Computational Inlet Conditions

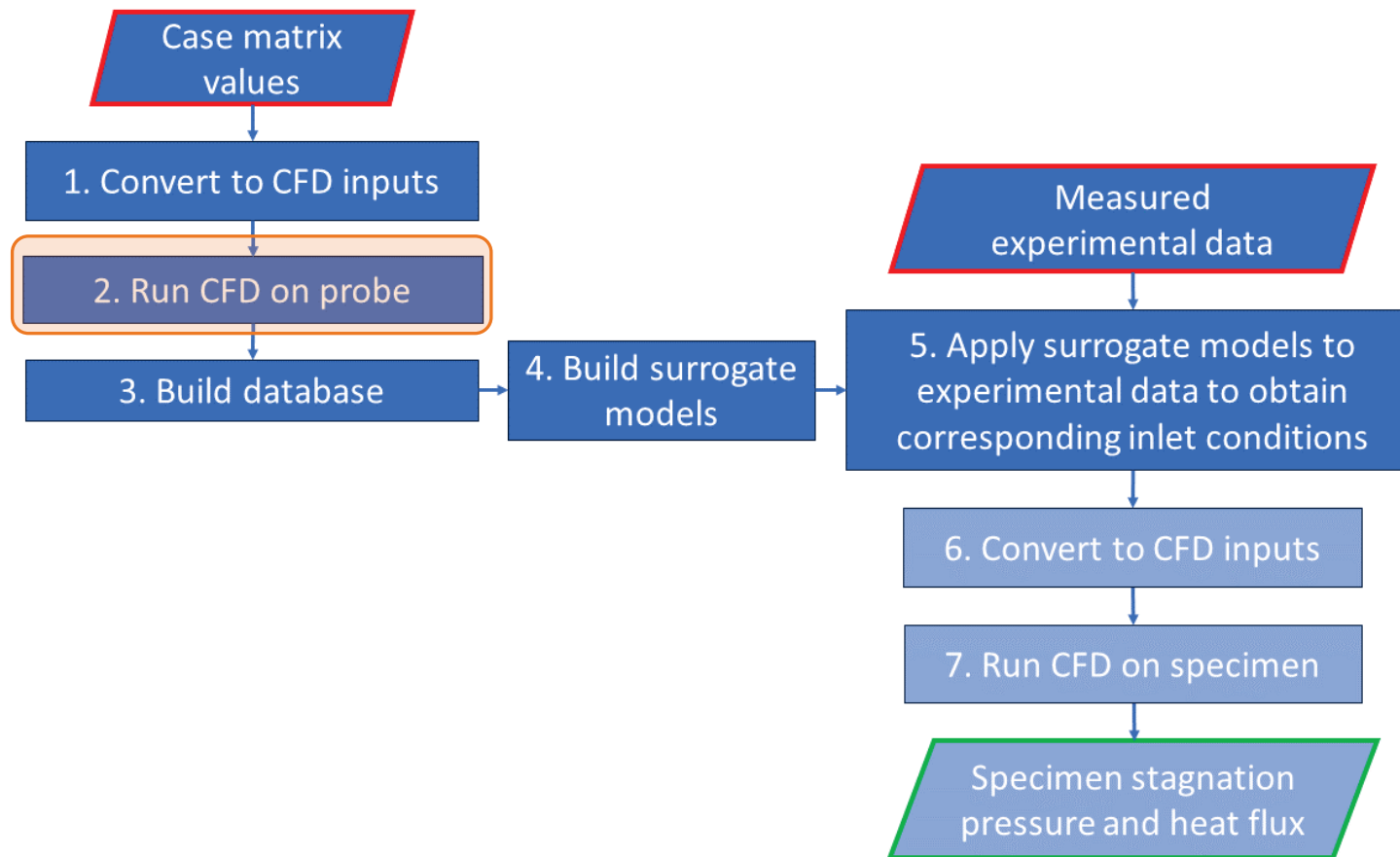


Computational Inlet Conditions

- LAURA (CFD solver) needs input conditions of density, temperature, velocity, and species mass fractions at the nozzle inlet.
- Density, temperature, and mass fractions are computed using Mutation++ thermochemical library by iterating on temperature until enthalpy matches desired value from case matrix.
- Velocity computed using area of nozzle inlet, mass flow rate from case matrix, and computed gas density at inlet.

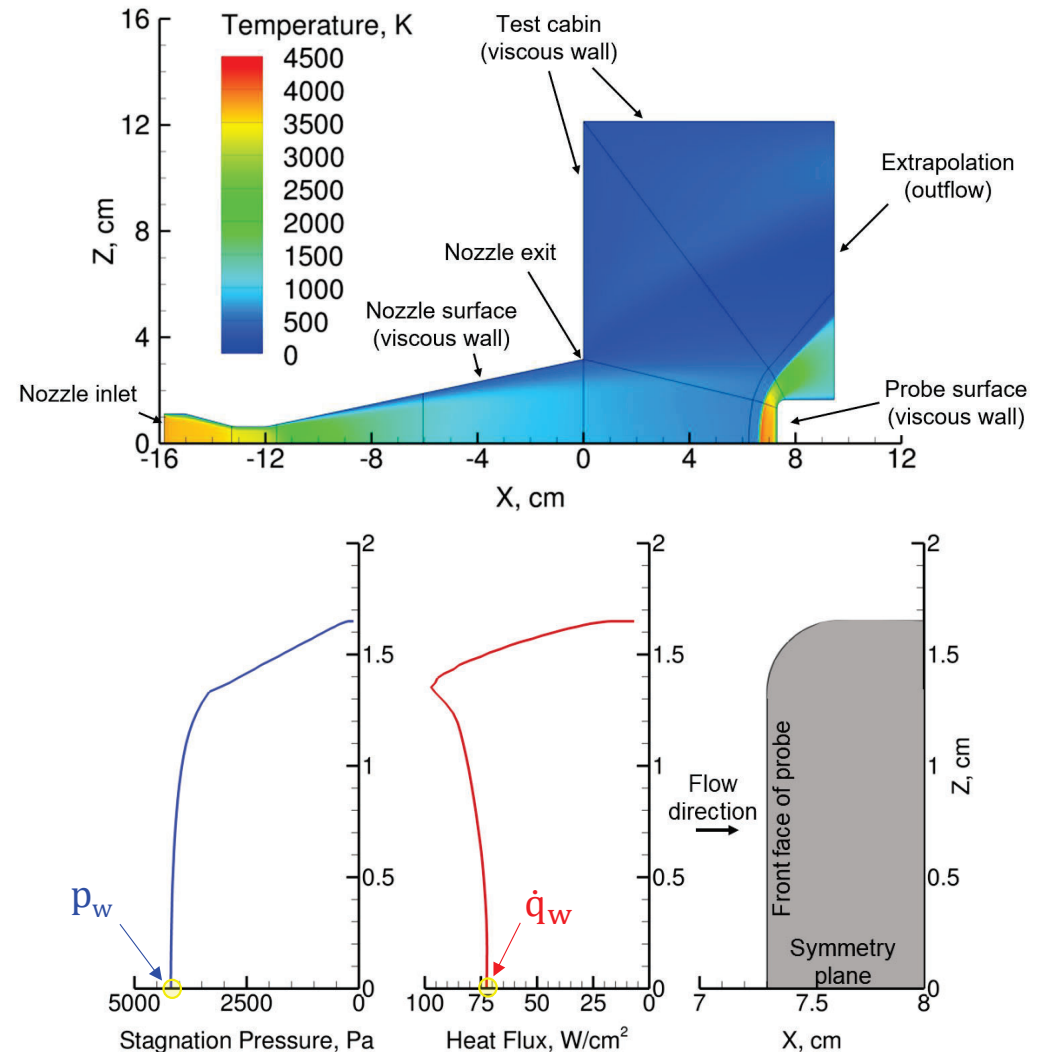


CFD



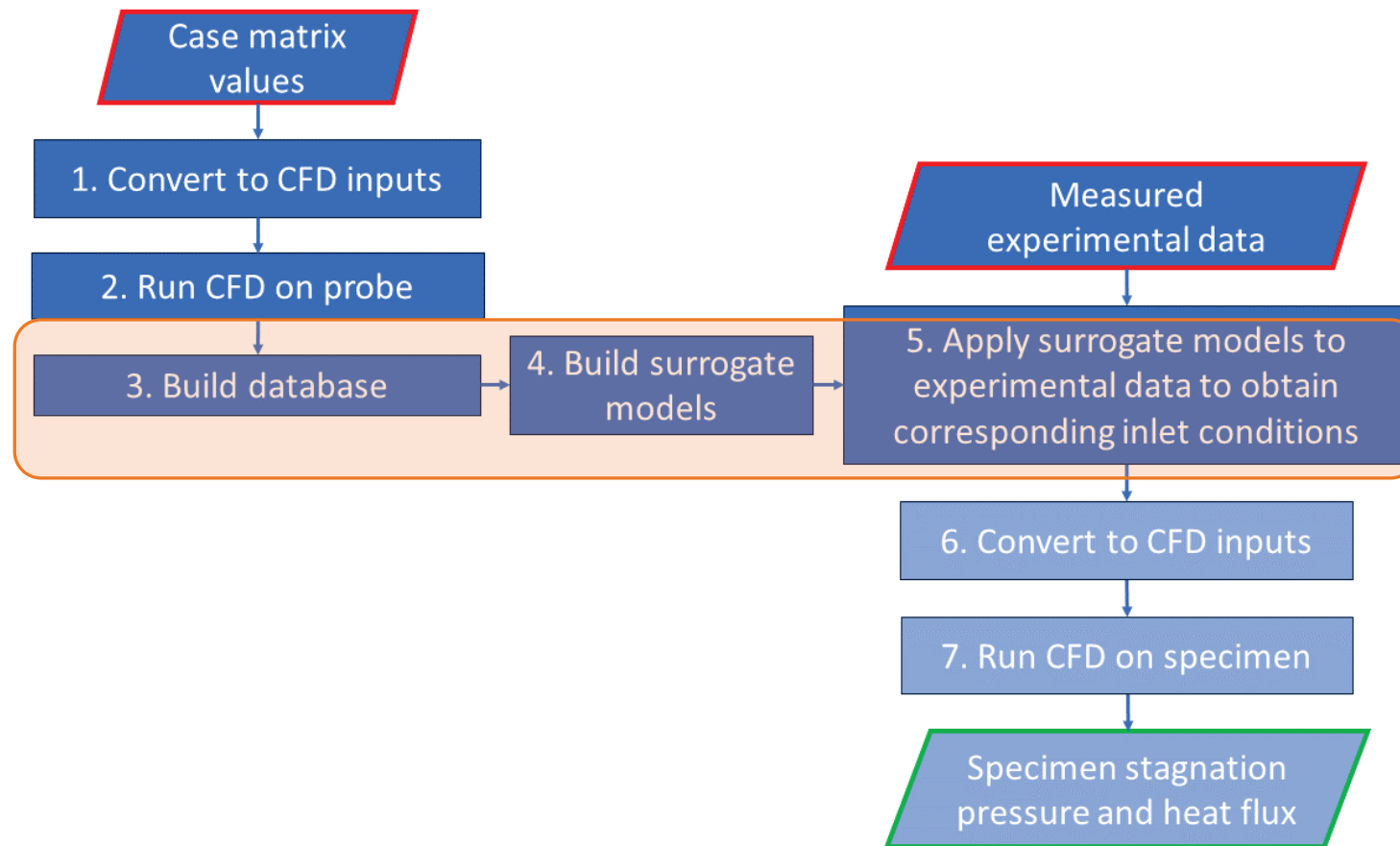
CFD

- LAURA is a structured, viscous, RANS solver for modeling high-energy, chemically reacting flows.
- HyMETS facility modeled by axisymmetric grid.
 - Walls of calibration probe assumed to have temperature of 350 K and catalytic efficiency of 10% for both O and N.
 - All other walls assumed to be 300 K and non-catalytic.
- Considered 9 gas species:
 CO_2 , N_2 , CO , NO , O_2 , C , N , O , and Ar
- Thermal non-equilibrium modeled with two-temperature model in which $T_{\text{translational}} = T_{\text{rotational}}$ and $T_{\text{vibrational}} = T_{\text{electronic}}$.
- Stagnation pressure and heat flux values taken from center point of probe ($Z = 0$).



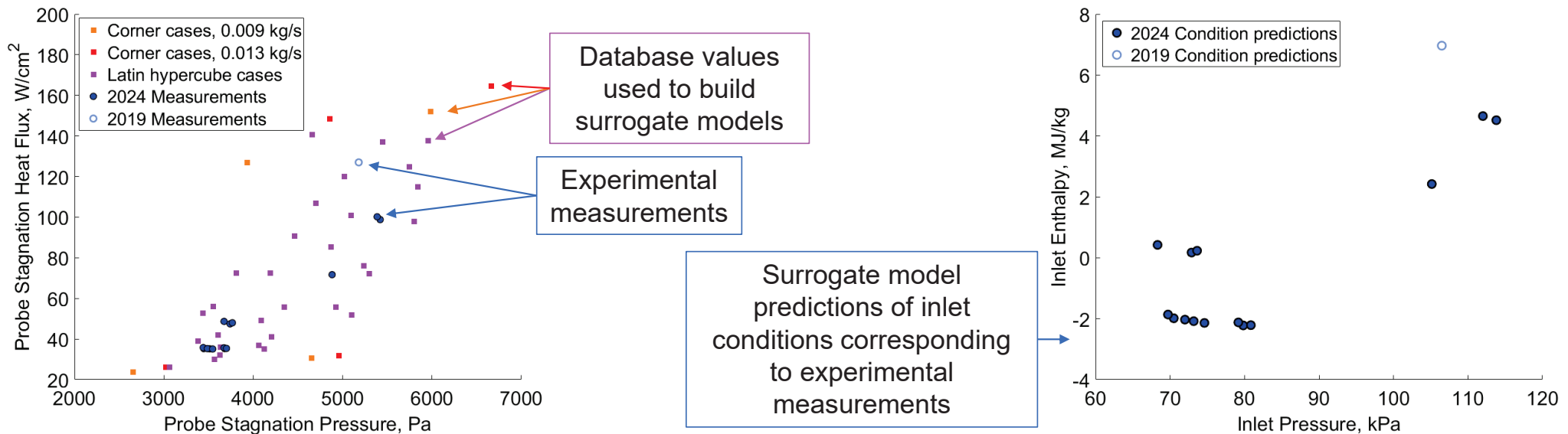
Sample results from case with inlet conditions of $\dot{m} = 0.01213 \text{ kg/s}$, $p_i = 75.17 \text{ kPa}$, and $h_i = 3 \text{ MJ/kg}$

Database and Surrogate Models



Database and Surrogate Models

- Stagnation pressures and heat fluxes from CFD collected in a database with the mass flow rates, inlet pressures, and inlet enthalpies used to achieve them.
- Database used to construct 2 Gaussian process (Kriging) surrogate models to predict inlet pressure and enthalpy.
 - $p_i = f(\dot{m}, p_w, \dot{q}_w)$
 - $h_i = f(\dot{m}, p_w, \dot{q}_w)$
- Experimental measurements fed into surrogate models to generate inlet condition predictions.



Model Verification

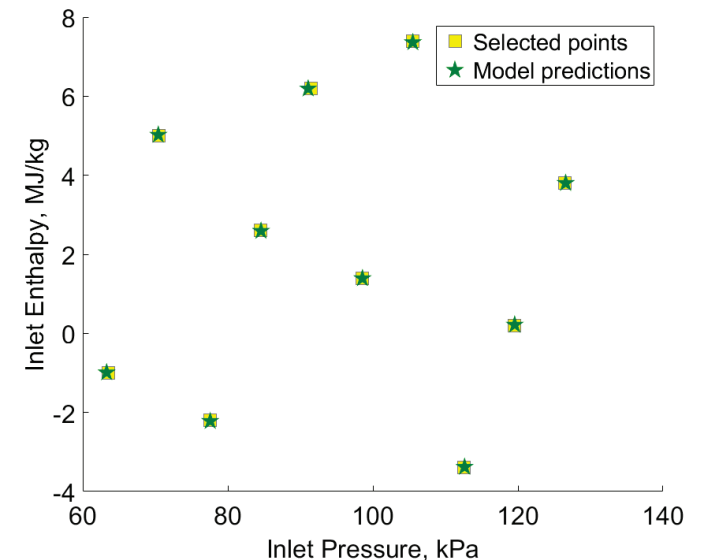
- Leave one out cross validation (LOOCV) performed to ensure predictions not overly dependent on any single training point in the database.

	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%

- Also verified using 10 new cases (combinations of $\dot{m}$, p_i , h_i) not included in training data.

- Selected via Latin hypercube sampling and run in CFD to get stagnation pressure (p_w) and heat flux ($\dot{q}_w$) results.
- Surrogate models applied to CFD results to get p_i and h_i predictions. Compared to the actual p_i and h_i values selected.

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



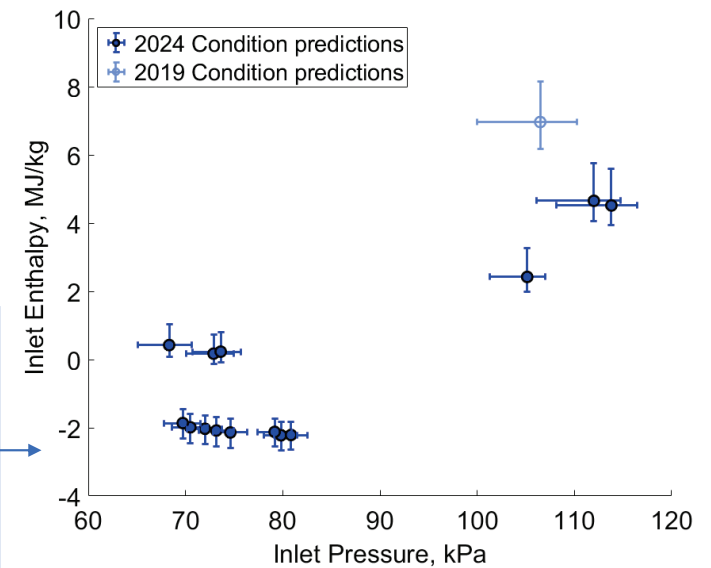
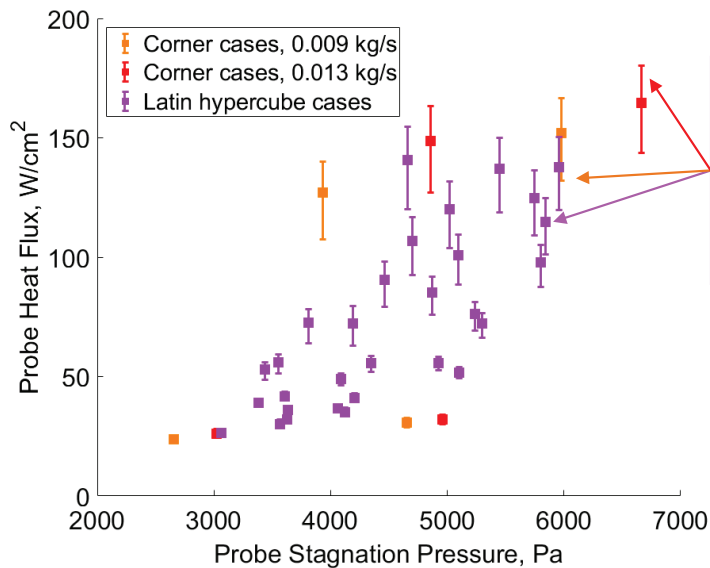
Uncertainty Quantification

- Model uncertainties addressed using LAURA's built-in functionality for efficient parametric uncertainty quantification and sensitivity analysis.
 - Total of 61 uncertain quantities considered including catalytic efficiencies, reaction rates, and diffusion cross sections.
 - Reported out upper and lower bounds of heat flux for each of the 38 database cases.
 - Stagnation pressure bounds also considered but later neglected due to small sensitivity compared to heat flux.
 - For corner cases, lower bound and upper bound of stagnation pressure never differed by more than 2.2%. Heat flux bounds, however, differed by 12-26%.
- Main driver of uncertainty for *high* enthalpy cases (where overall uncertainty was also the greatest) was O catalytic efficiency, followed by CO-O diffusion cross section.
 - Together account for 95-97% of heat flux uncertainty.
- Main driver of uncertainty for *low* enthalpy cases was CO₂-CO₂ diffusion cross section, followed by CO₂-N₂ and CO₂-CO diffusion cross sections.
 - Together account for 93-95% of heat flux uncertainty, although uncertainty for these low enthalpy cases is very small anyway.

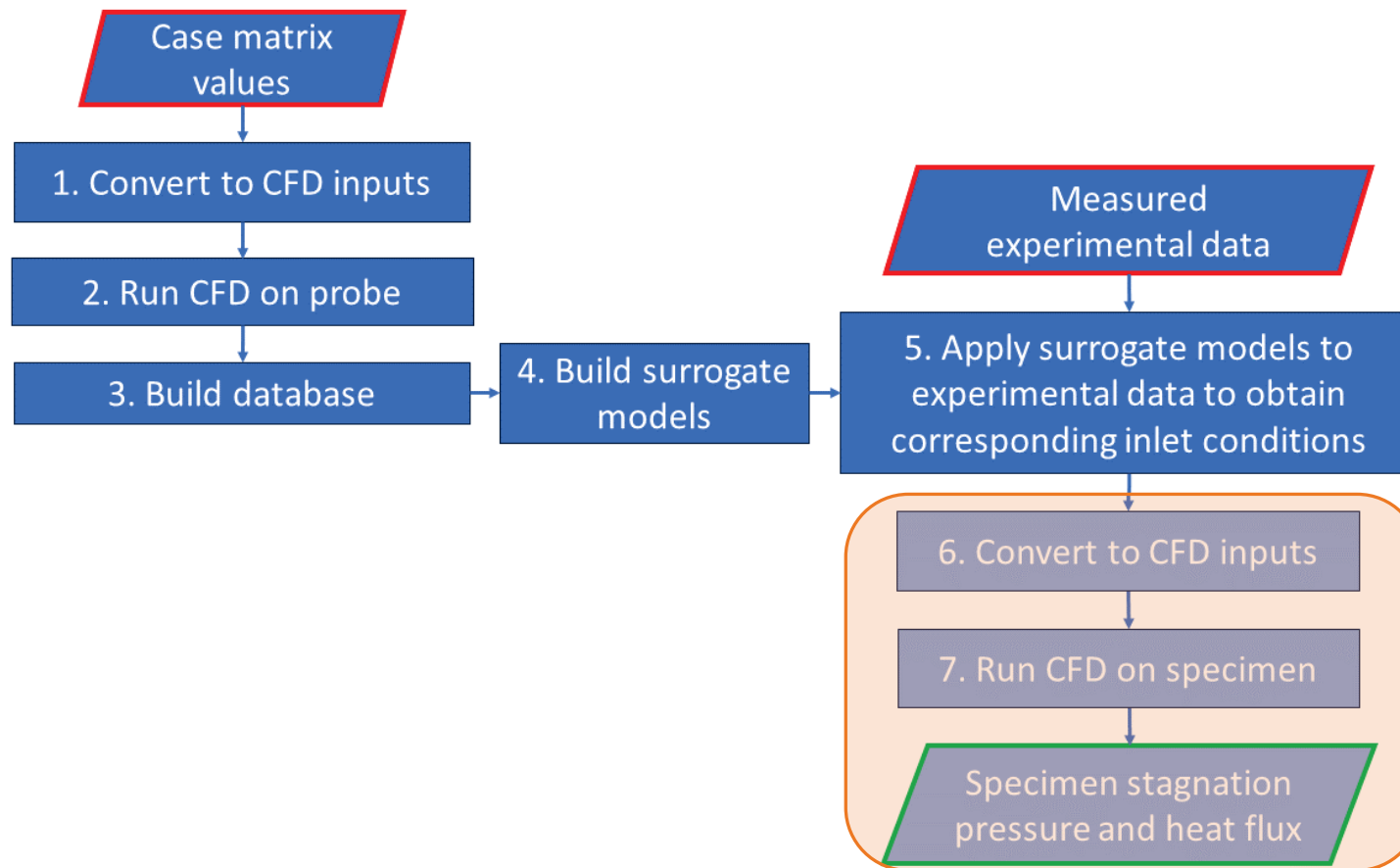
Enthalpy, MJ/kg	Top Sources of Heat Flux Uncertainty	Percent of Total Uncertainty
-4	CO ₂ -CO ₂ diffusion cross section	64.8%-68.0%
	CO ₂ -N ₂ diffusion cross section	14.9%-16.1%
	CO ₂ -CO diffusion cross section	10.5%-13.3%
8	O catalytic efficiency	58.8%-69.7%
	CO-O diffusion cross section	27.3%-36.9%

Uncertainty Quantification (cont'd)

- Used lower and upper bounds of heat flux from the 38 database cases to build 4 new Kriging surrogate models.
 - $p_{i,lower} = f(\dot{m}, p_w, \dot{q}_w)$
 - $p_{i,upper} = f(\dot{m}, p_w, \dot{q}_w)$
 - $h_{i,lower} = f(\dot{m}, p_w, \dot{q}_w)$
 - $h_{i,upper} = f(\dot{m}, p_w, \dot{q}_w)$
- Inlet conditions predicted as before for the experimental cases.
- Average prediction uncertainty was about +2/-3 kPa for inlet pressure and +0.6/-0.4 MJ/kg for inlet enthalpy.



Future Work



Conclusions

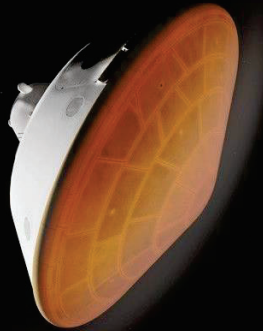
- CFD performed on several cases spanning facility conditions of recent test campaign to simulate the HyMETS environment with a calibration probe inserted and CO₂-rich atmosphere.
- Surrogate models developed to map measured stagnation pressures and heat fluxes to nozzle inlet conditions.
 - Average prediction uncertainty was about +2/-3 kPa for inlet pressure and +0.6/-0.4 MJ/kg for inlet enthalpy.
 - The primary driver of uncertainty for the high enthalpy cases with the greatest uncertainty was O catalytic efficiency. More precise knowledge of O catalysis will allow for reduced uncertainty in predictions.
- The ability to efficiently determine nozzle inlet conditions (CFD boundary conditions) for any experiment within the database bounds will enable more efficient computational material response modeling of the PICA-N test specimens in future work.



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