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Chemical Model Reduction for Negative Hydrogen Ion Density Predictions using Global Sensitivity Analysis

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Background

- Negative hydrogen ion sources (NHIS) are the preferred mode of plasma heating in tokamak devices.
  Accurate **predictions of the H^- density** are crucial for the design.

- NHIS Global Model by W. Yang et al. (GMNHIS)[1]
  involves detailed pathways composed of **~1300 reactions** to achieve high fidelity in reproducing the kinetics features.

GOAL

To **increase the computational efficiency** and
improve the predictive capabilities of the plasma chemical model by combining machine learning & uncertainty quantification tools with the modeling expertise of Princeton Collaborative Low Temperature Plasma Research Facility

[1] W. Yang et al, Physics of Plasmas 25, 113509 (2018)

Global Sensitivity Analysis

- **Reaction Parameters, $\boldsymbol{\theta}$**: Screening variables that amplify/attenuate the reaction quantities.
  Quantities of Interest, $\boldsymbol{y}$: Steady state predictions (e.g., number densities, electron temperature).

- Sensitivity analysis:
  Local SA: anchored to specific parameter values and no correlation information.
  Global SA: non-local and includes **joint effects** of parameters on quantities of interest.

- Aim is to compute the fractional variance in y attributable to each θ_i
  (i.e., Sobol total-effect sensitivity indices):

$$S_{Ti} = \frac{\mathbb{E}_{\theta \sim i}[Var_{\theta_i}(f(\boldsymbol{\theta})|\theta_i)]}{Var(f(\boldsymbol{\theta}))}$$

PCE-Based Global Sensitivity Analysis

- We can accelerate the Sobol indexes computation by invoking a smoothness assumption, and replace the model's θ_i-to-y mapping with **an orthogonal polynomial expansion**:

$$f(\boldsymbol{\theta}) \approx g(\boldsymbol{\theta}) = \sum_{k=0}^{K-1} c_k \psi_k(\boldsymbol{\xi})$$

- Now we can use training samples to construct a regression problem and learn the parameters $\boldsymbol{c}$:

$$\underset{\boldsymbol{c}}{\operatorname{argmin}} \left\| f(\boldsymbol{\theta}) - \sum_{k=0}^{K-1} c_k \psi_k(\boldsymbol{\xi}) \right\|_2^2 + \eta \|\boldsymbol{c}\|_1$$

- A remarkable feature of this polynomial construction is that we **obtain analytical access to Sobol total-order indices through the polynomial coefficients:**

$$S_{T_i} = \frac{\sum_{k \in \mathbb{I}_i} c_k^2}{\sum_{k-1}^{K} c_k^2}$$

Libraries: UQ Toolkit (UQTk)[2] and Tesuract by K. Chowdhary

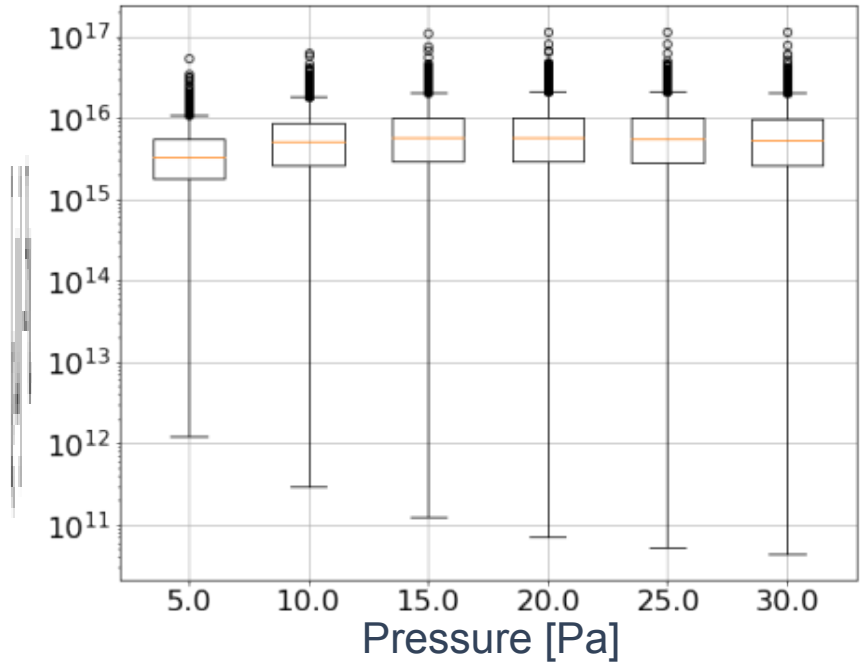
[2] Debusschere, et al., SIAM J. Sci. Comput. 26(2), pp. 698-719 (2005)

From Perturbed Reactions to Sensitivity Indexes

1. Divided the reactions in families and exposed their (initially hard-coded) parameters

2. Drawn 3000 samples of $\boldsymbol{\theta}$ from independent uniform distributions (i.e., $\theta_i = \mathcal{U}[0,2]$, with $i = 1{:}1303$)

GMNHIS

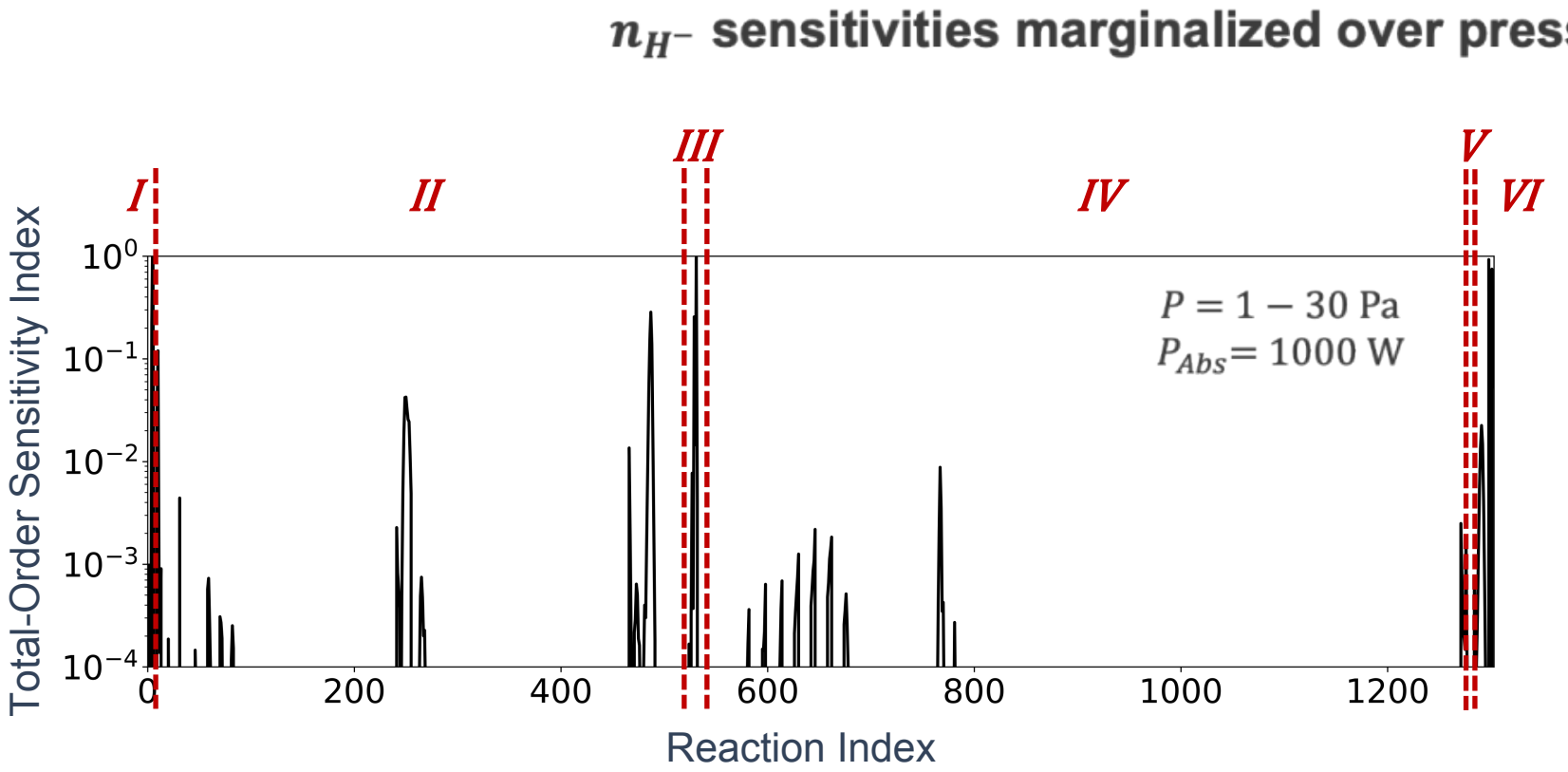


What is the percentage of n_{H^-} variations attributable to each parameter?

Note: The perturbations propagate through a complex network of reactions. The contribution to n_{H^-} creation/depletion of high rate reaction could be negligible due to bottle necks in the chemical chain.

From Perturbed Reactions to Sensitivity Indexes

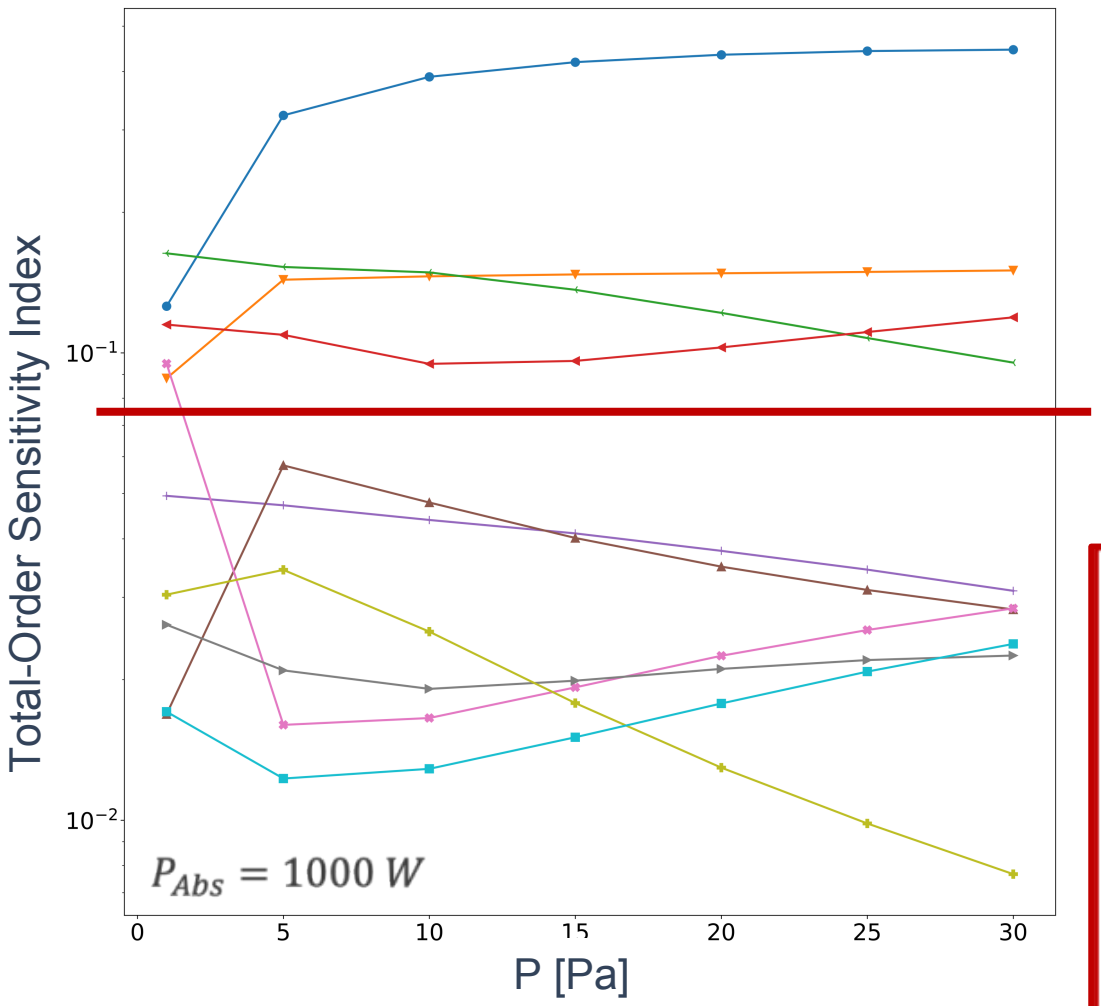
3. Constructed a polynomial chaos expansion
4. Used the expansion coefficients for retrieving Sobol total-order sensitivity indexes



Families of Exposed Reactions:

I. $e + M \rightarrow \cdots$, **with** $M \neq H_2(v)$
II. $e + M \rightarrow \cdots$, with $M = H_2(v)$
III. **e and $H_2(v)$ not in reactants**
IV. $H_2(v) + \mathrm{M} \rightarrow \cdots$, with $M \neq e$
V. Electronic excitations of H_2
VI. **Surface interactions**

Sensitivities of n_{H^-} as Functions of Pressure and Power



- $e + H_2 \rightarrow H + H + e$
- $H + H^- \rightarrow H_2 + e$
- $2H + Wall \rightarrow H_2$
- $H_3^+ + Wall \rightarrow H_2 + H$
- $e + H_2(8) \rightarrow H + H^-$
- $H_3^+ + H^- \rightarrow 4H$
- $e + H_2 \rightarrow H_2^+ + 2e$
- $e + H_2(7) \rightarrow H + H^-$
- $e + H_2(9) \rightarrow H + H^-$
- $e + H \rightarrow H(n = 2) + e$

Independently on pressure and absorption power, there is a clear cut below the four main reactions.

Exceptions:

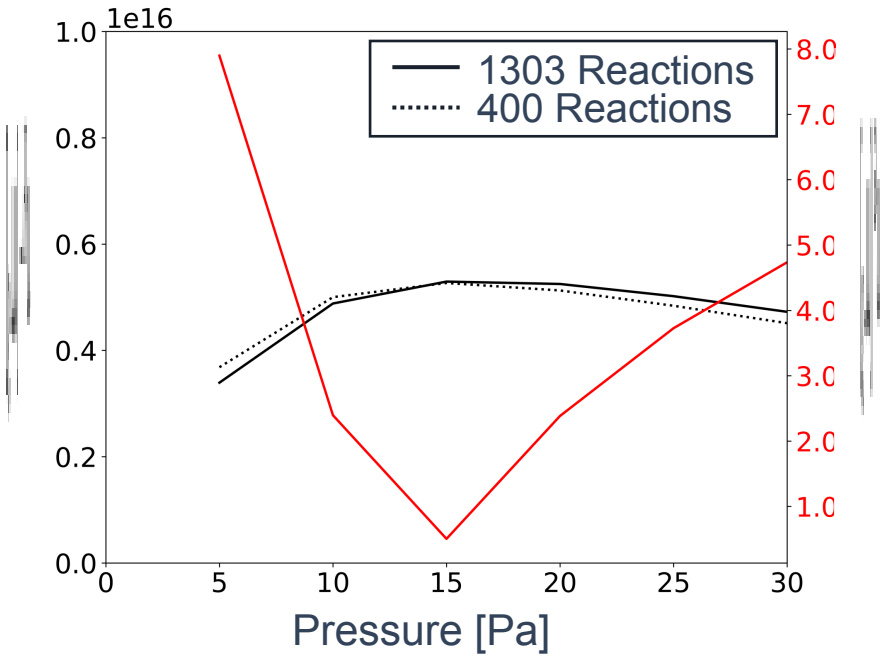
- Ionization (at low P and/or P_{Abs})
- Electronic excitation and Dissociative attachment v=9 (at high P_{Abs})

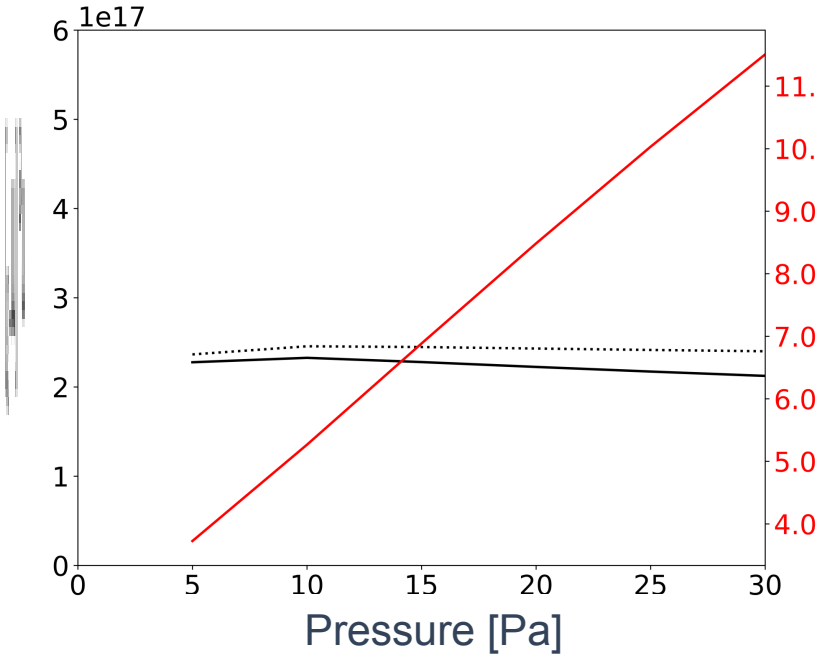
$\mathbf{n_{H^-}}$ sensitivities of the 10 most influential reactions as function of pressure

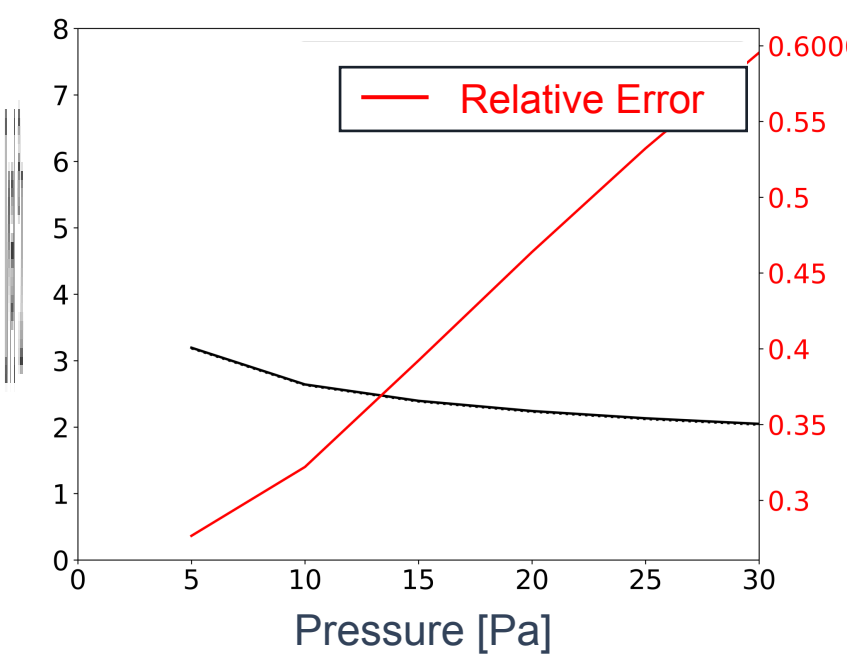
GSA-Based Reduction of the Chemical System

Global sensitivity analysis can inform the construction of reduced chemical systems composed by:

- Reactions characterized by Sobol total-order indexes larger than specified thresholds
- Species involved in those reactions



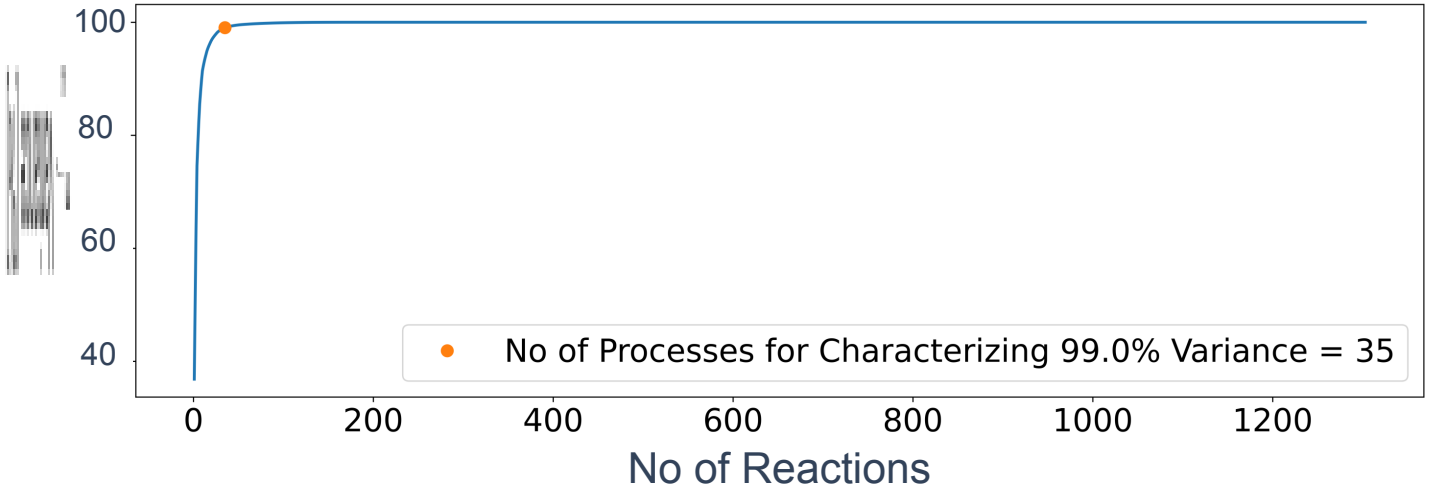




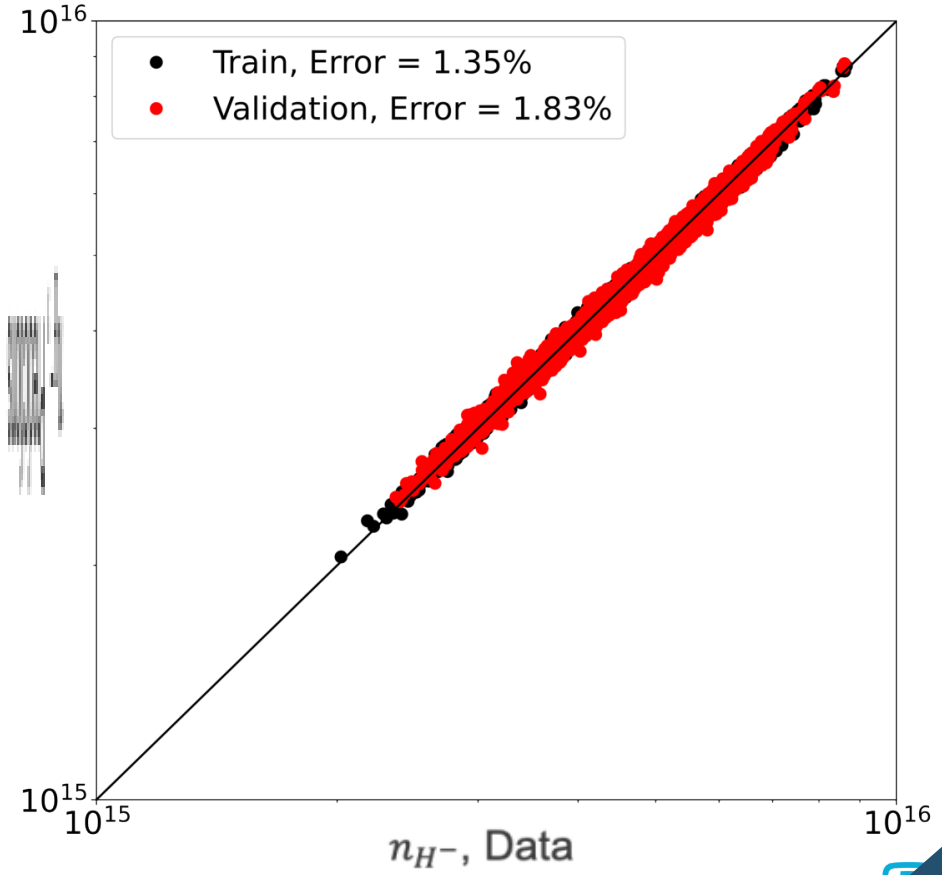
Advantages:

- **Reduction of the computational cost** due to lower dimensionality and decreased stiffness
- **Increase in the predictive capabilities,** as ad hoc experiments can be focused on the calibration of the most descriptive parameters

High-accuracy Reduced Order Model Surrogate



Selected the 35 highest-sensitivity reactions. Overall, these are able to characterize 99% of the y variance.



Constructed a **36-dimensional 3rd order PCE.**

- 35 reaction perturbations, in the range $\pm 20\%$
- Pressure, in the range 5-30 Pa;

The surrogate can be used for efficiently calibrating the reaction parameters from n_{H^-} experimental data

Conclusions

- Exposed GMNHIS' reactions, performed polynomial chaos expansion-based global sensitivity analysis, and identified the most import processes as function of P and P_{Abs}

Independently on P or P_{Abs}:
- $e + H_2 \rightarrow H + H + e$
- $H + H^- \rightarrow H_2 + e$
- $2H + Wall \rightarrow H_2$
- $H_3^+ + Wall \rightarrow H_2 + H$

At low P or P_{Abs}:
- $e + H_2 \rightarrow H_2^+ + 2e$

At high P_{Abs}:
- $e + H_2(v = 9) \rightarrow H + H^-$
- $e + H \rightarrow H(n = 2) + e$

- Constructed sensitivity-driven reduced models, robust under rate coefficient uncertainties
  From ~1300 reactions to 400 with errors below 10% for n_{H^-}, n_e, T_e

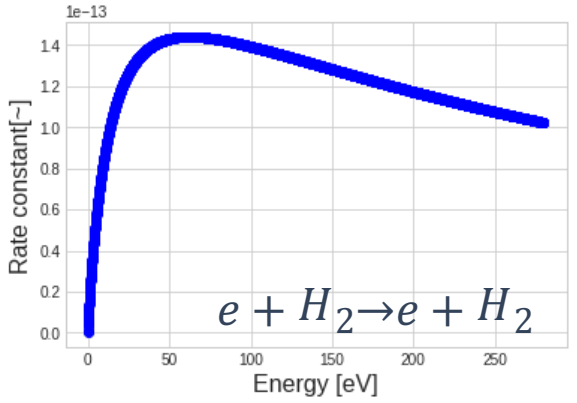
- Generated low-dimensional surrogates for speeding up the inverse problem solution (i.e., calibration and optimization under uncertainties)
  The surrogate is more that 2 orders of magnitude faster than the full model.

Final Remarks

- Increasing model complexity does not have to be the first direction of effort
- Once the critical reactions are identified, experiments and literature review should focus on them to make first order improvements
- From the prospective of increasing the model predictive capabilities, accounting for uncertainties in reaction parameters and forward propagating them to the quantities of interest is as important as adding more reactions for refining the model fidelity
- Model reductions depend on the application (i.e., $f(\text{uncertainties}, t, \dots)$)
- The framework is **automated** and **general.** It can be applied to **different chemical systems**

Ongoing and Future Work

- Calibrating rate coefficients using fake and experimental data via Bayesian inference
- Comparing global sensitivity analysis-based reductions to graph ensemble-based techniques
- Comparing polynomial chaos expansion to alternative surrogate techniques (e.g. neural networks)
- Working with Dr. Yang on improving the GMNHIS implementation (e.g., code versatility, code robustness, dynamic simulations, …)
- Analyze the time-dependent sensitivity
- Perturb the parameter model forms rather than their magnitude



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QUESTIONS?

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