Calibration of nitridation reaction efficiencies from plasma wind tunnel data and beyond

Anabel del Val

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von KARMAN INSTITUTE
FOR FLUID DYNAMICS

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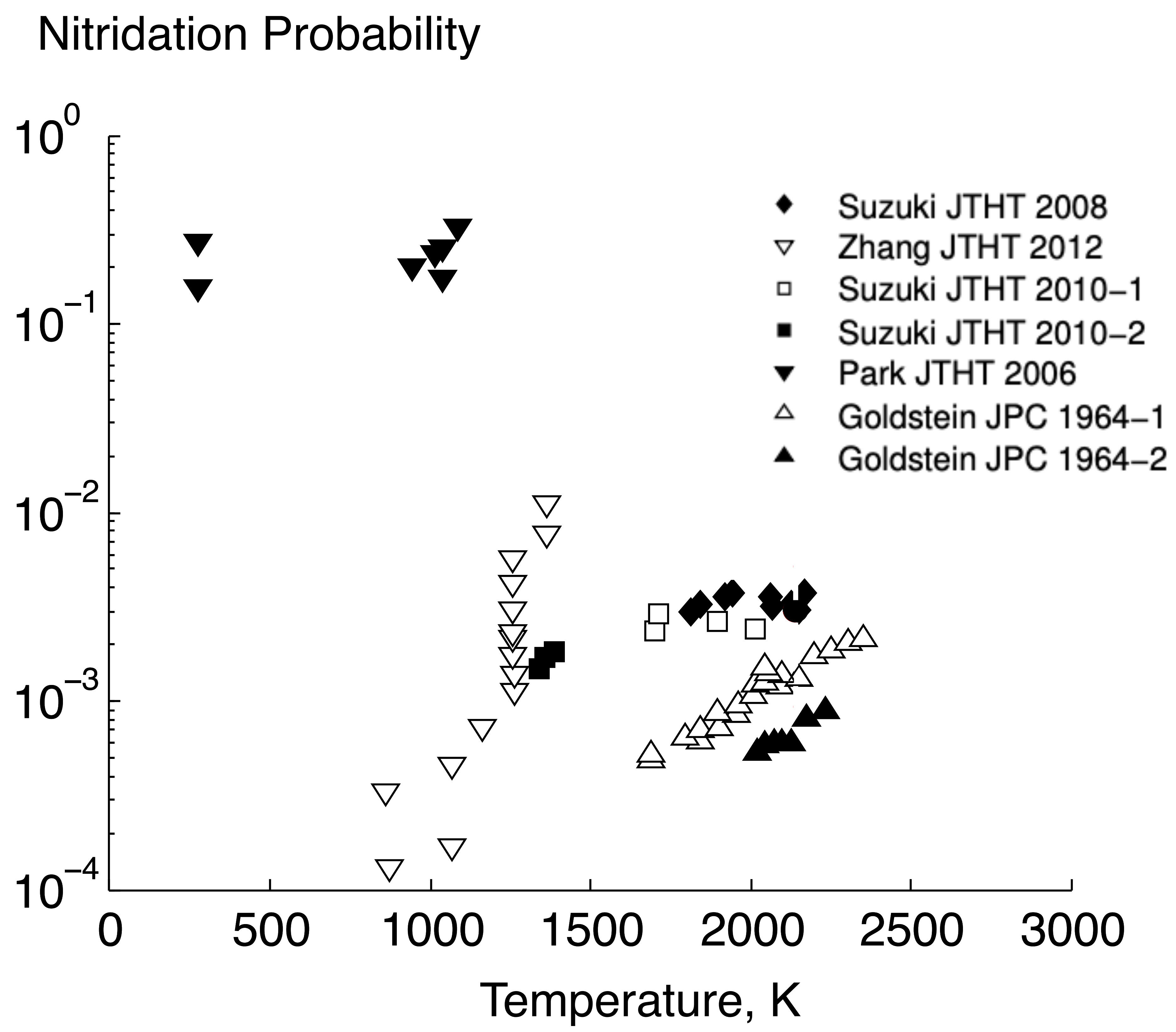
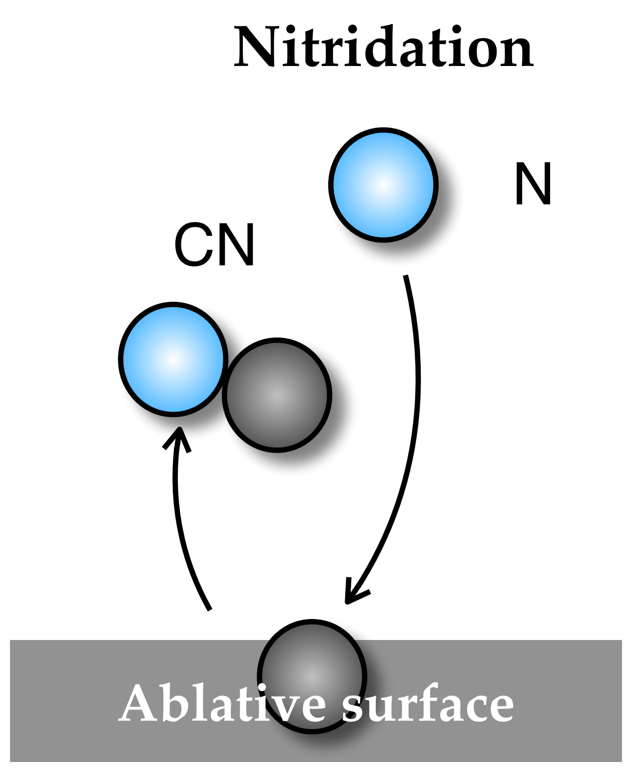
THE FRAMEWORK PROGRAMME FOR RESEARCH AND INNOVATION
HORIZON 2020

State-of-the-art nitridation efficiencies differ by several orders of magnitude





- Extension to **high temperature data**
- Models **do not account for carbon injection** in BL
- Points result from **complex numerical-experimental approaches**
- **Different** facilities and model **approximations involved**
- **Diverse** landscape in **treatment of the data**

Calibration of nitridation reaction efficiencies from plasma wind tunnel data and beyond

Development 1

High surface temperature data & deterministic model

Development 2

Stochastic model: experimental & parametric uncertainties

Development 3

Model-form uncertainties

Development 4

Merging of molecular beam & Plasmatron data

Conclusions and future outlook

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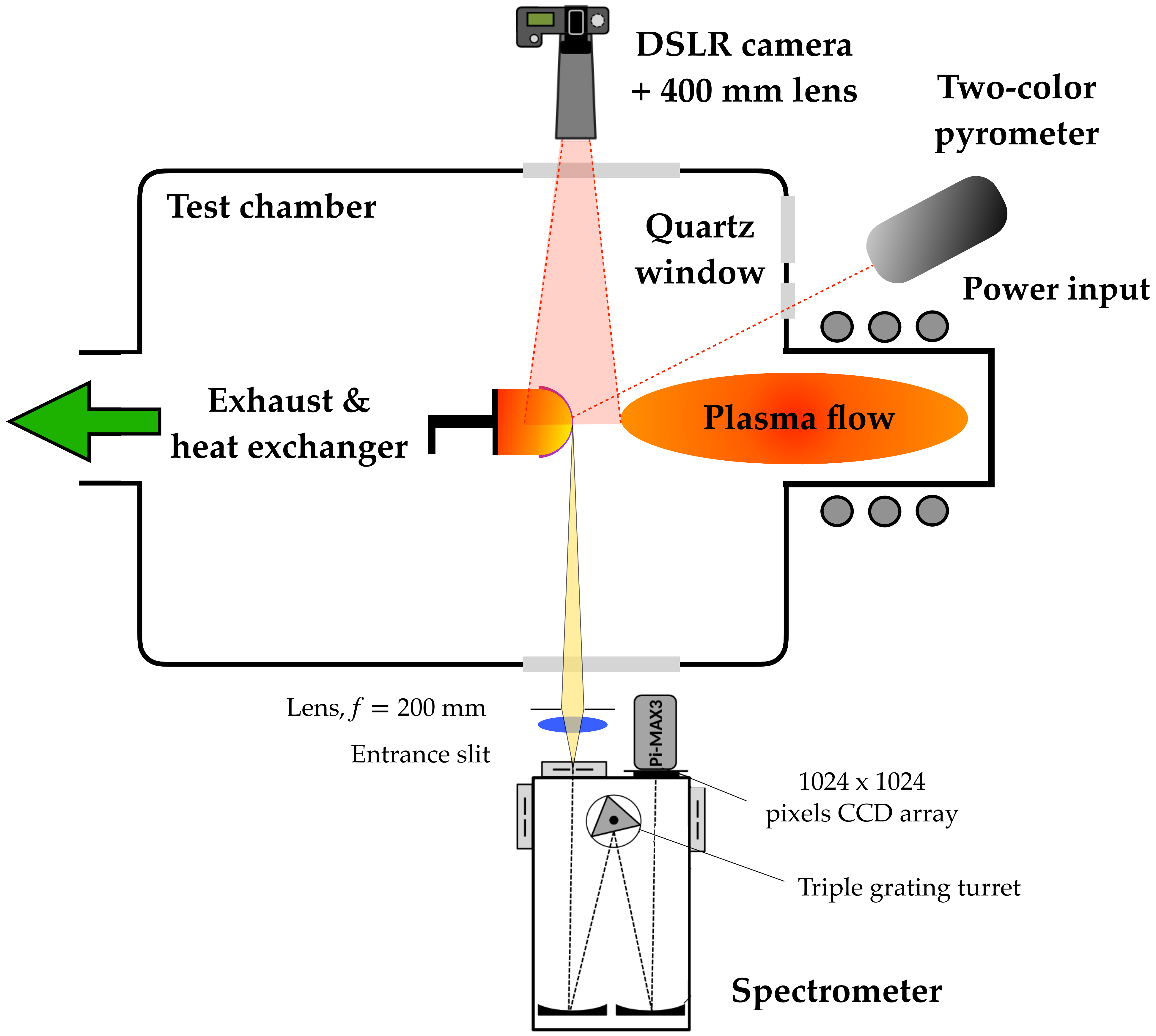
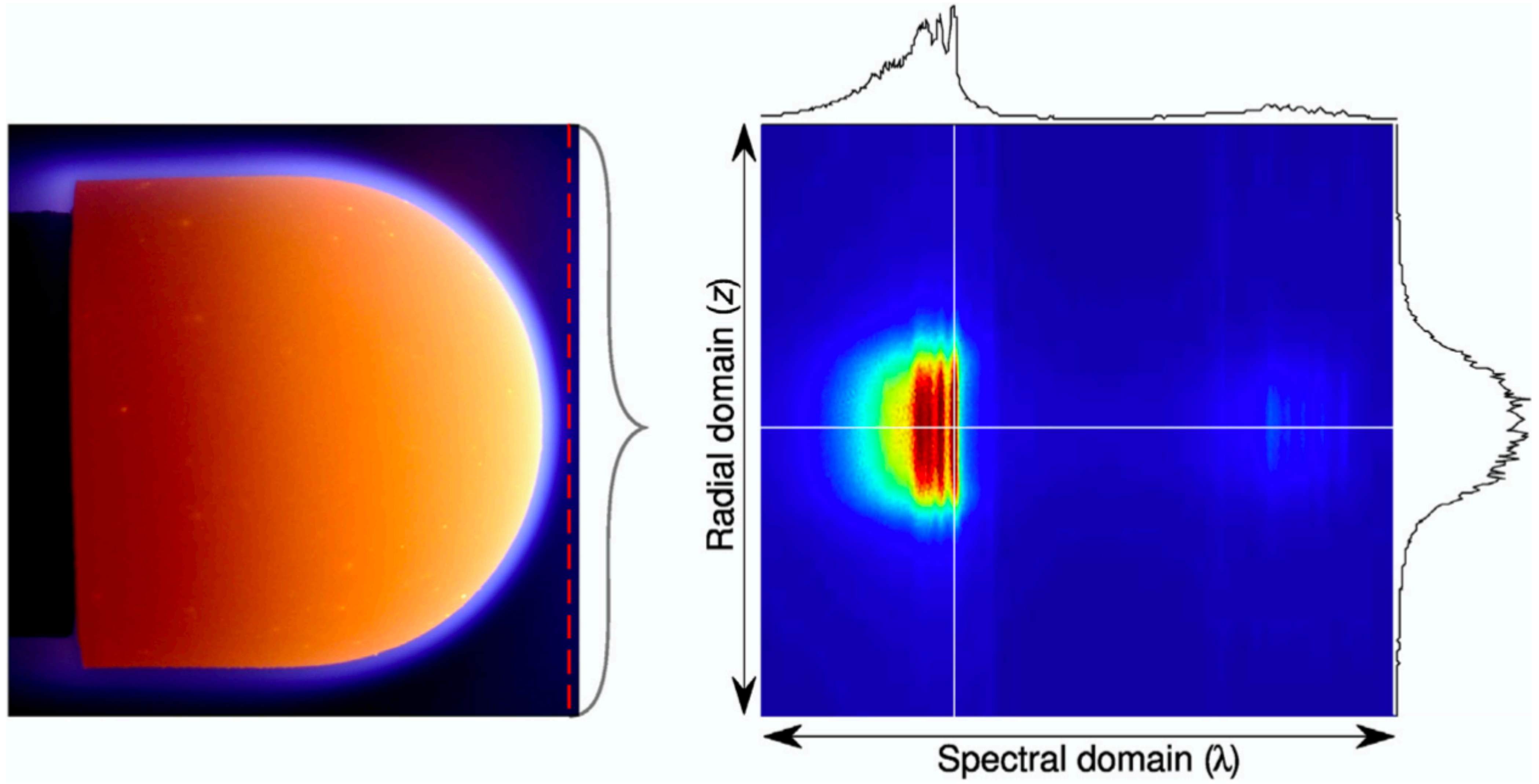


- **Graphite** samples exposed to a **subsonic plasma flow**
- **Four** conditions at different **surface temperatures** recorded [2,200-2,600K]
- **Recession rates** and **CN radiative signature** measured during steady state



Helber, Turchi, Magin. *Carbon*, 125 : 582–594, 2017

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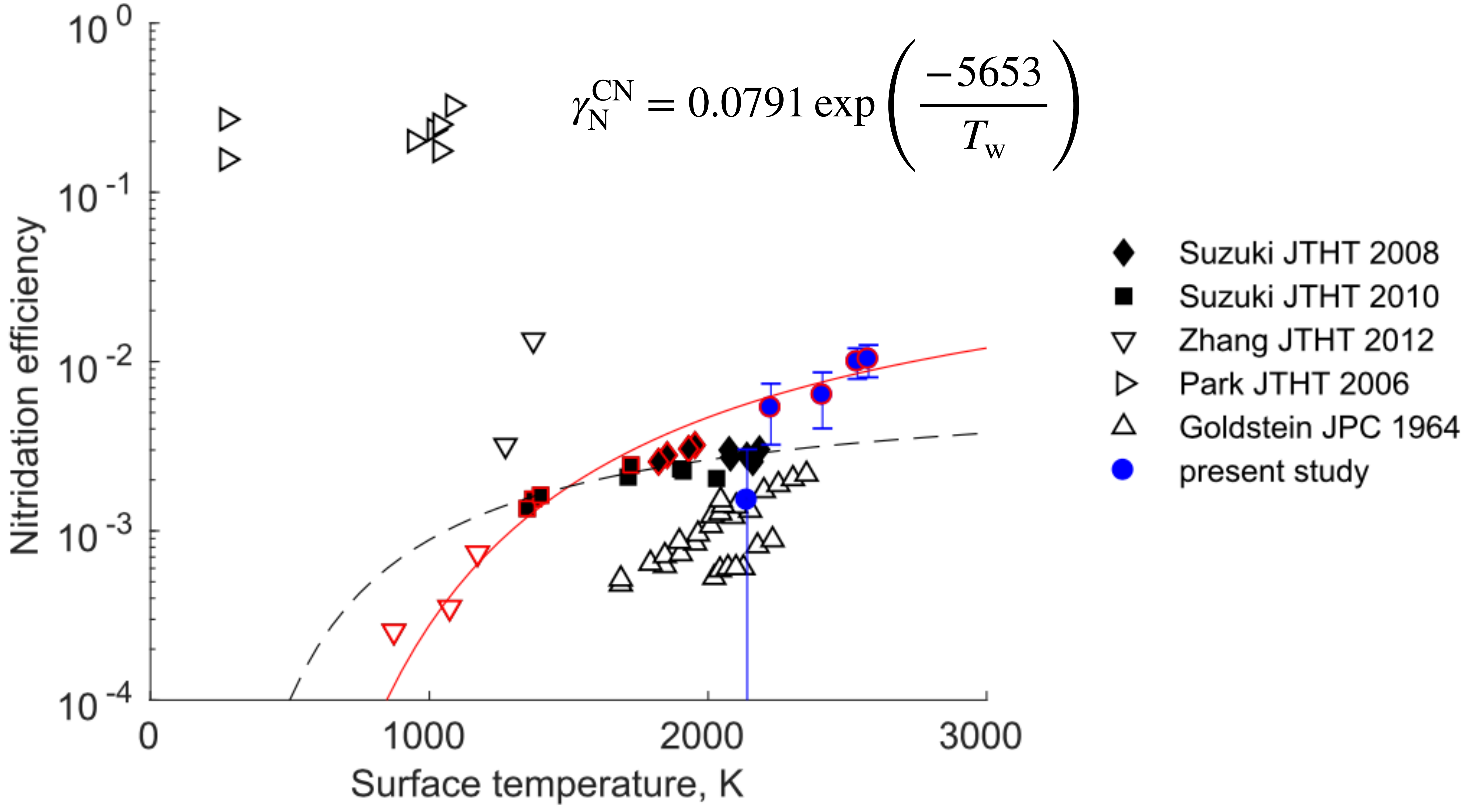

Deterministic inverse problem

$$\arg\min_{\boldsymbol{c}} J(\boldsymbol{p}) = \|\boldsymbol{y}_{\mathrm{obs}} - \boldsymbol{f}(\boldsymbol{X}_{\mathrm{obs}}, \boldsymbol{c}, \boldsymbol{p})\|^2 + \mathscr{R}(\boldsymbol{X}_{\mathrm{obs}}, \boldsymbol{c}, \boldsymbol{p})$$

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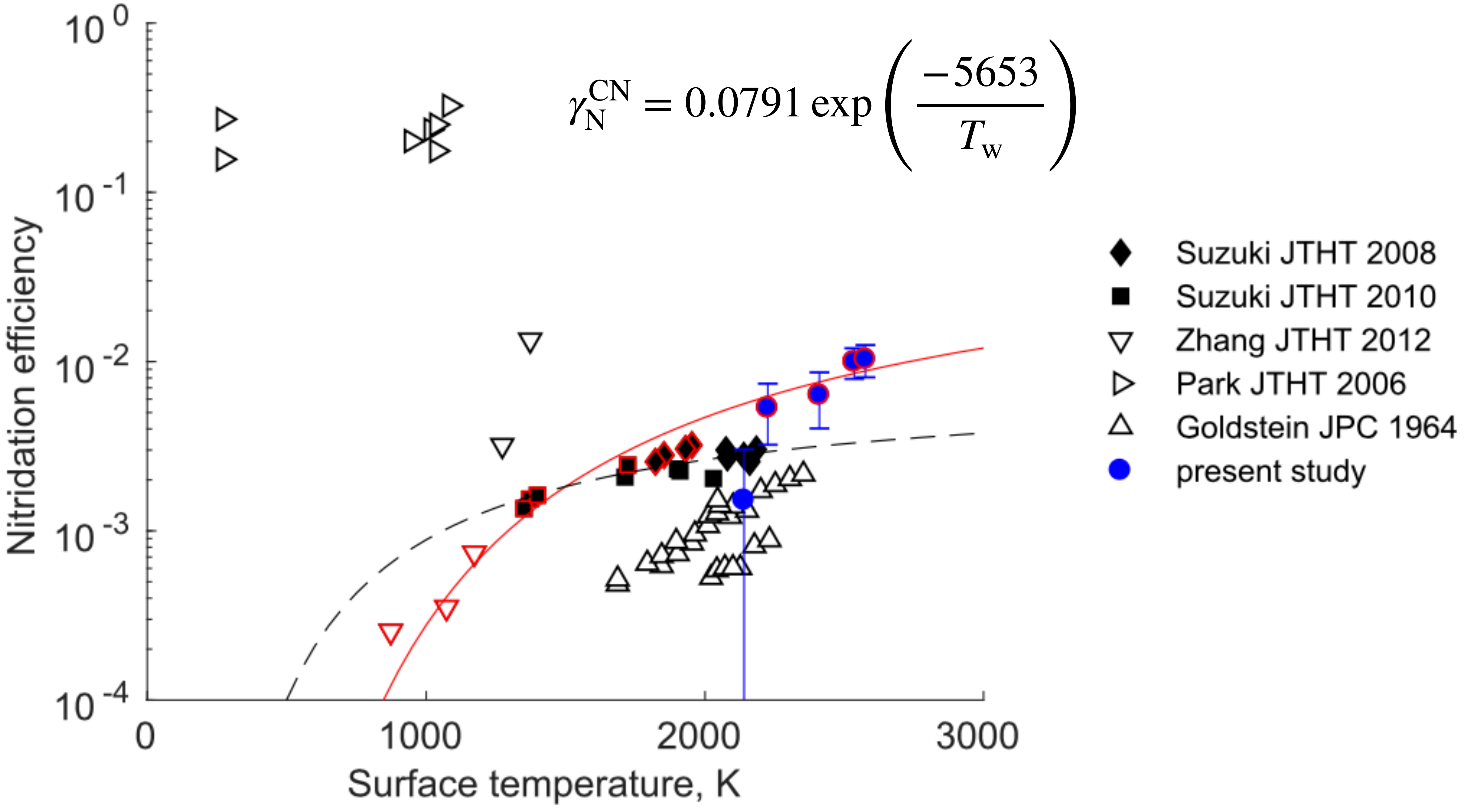

Deterministic inverse problem

$$\arg\min_{\boldsymbol{c}} J(\boldsymbol{p}) = \|\boldsymbol{y}_{obs} - \boldsymbol{f}(\boldsymbol{X}_{obs}, \boldsymbol{c}, \boldsymbol{p})\|^2 + \mathscr{R}(\boldsymbol{X}_{obs}, \boldsymbol{c}, \boldsymbol{p})$$

Different surface temperatures

Everything else…

Recession rate

Reacting flow model w/ surface reaction

γ_N^{CN}

- What if $\boldsymbol{y}_{obs}$ is noisy?
- What if we don't really know parameters $\boldsymbol{p}$?
- What if $\boldsymbol{f}$ is wrong?

Helber, Turchi, Magin. *Carbon*, 125 : 582–594, 2017.

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- What if $\boldsymbol{y}_{\text{obs}}$ is noisy? → Aleatory uncertainty
- What if we don't really know parameters $\boldsymbol{p}$? → Epistemic uncertainty
- What if f is wrong? → Model-form uncertainty

Development 3

Stochastic inverse problem

$$\boldsymbol{y}_{\text{obs}} = f(\boldsymbol{Q}, \boldsymbol{X}_{\text{obs}}) + \boldsymbol{E}$$

$$\boldsymbol{Q} = \{\boldsymbol{C}, \boldsymbol{P}\} \qquad \boldsymbol{Q} \sim \mathscr{P}(\boldsymbol{q}),\ \boldsymbol{E} \sim \mathscr{P}(\boldsymbol{e})$$

Development 1	**Development 2**	Development 3	Development 4
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Bayesian formalism

$$\underbrace{\mathscr{P}\,(\boldsymbol{Q}\,|\,\boldsymbol{y}_{\mathrm{obs}})}_{\text{Posterior distribution}} = \frac{\underbrace{\mathscr{P}\,(\boldsymbol{y}_{\mathrm{obs}}\,|\,\boldsymbol{Q})}_{\text{Likelihood function}} \times \underbrace{\mathscr{P}\,(\boldsymbol{Q})}_{\text{Prior distribution}}}{\mathscr{P}(\boldsymbol{y}_{\mathrm{obs}})}$$

How to **efficiently combine models, experiments** and **stochastic inference methods** to **extract accurate nitridation models** with **estimation** of their **uncertainty**?

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Prior distribution

$\mathscr{P}(\boldsymbol{q})$

1 Surrogate modeling

GPR $(\boldsymbol{q})$

2 Sensitivity analysis

Sobol indices

3 Likelihood building

$$\mathscr{L}(\boldsymbol{d}_{\mathrm{obs}}\,|\,\boldsymbol{q}) \propto \prod_{i\in\mathscr{I}} \prod_{\substack{j\in\mathscr{S}\\ j\notin\mathscr{I}}} \exp\left[-\frac{|d_i - q_i|^2}{2\sigma_{d_i}^2}\right] \exp\left[-\frac{|d_j - \bar{d}_j(q_j)|^2}{2\sigma_{d_j}^2}\right]$$

$$\boldsymbol{d}_{\mathrm{obs}} - f(\boldsymbol{Q},\boldsymbol{X}) = E$$

4 Posterior sampling

MCMC algorithm with adaptation of the covariance matrix with an initial burn-in phase (50% samples)

Posterior distribution

$\mathscr{P}(\boldsymbol{q}\,|\,\boldsymbol{d}_{\mathrm{obs}})$

del Val, Le Maître, Congedo, Magin. *Carbon*, 200 : 199–214, 2022

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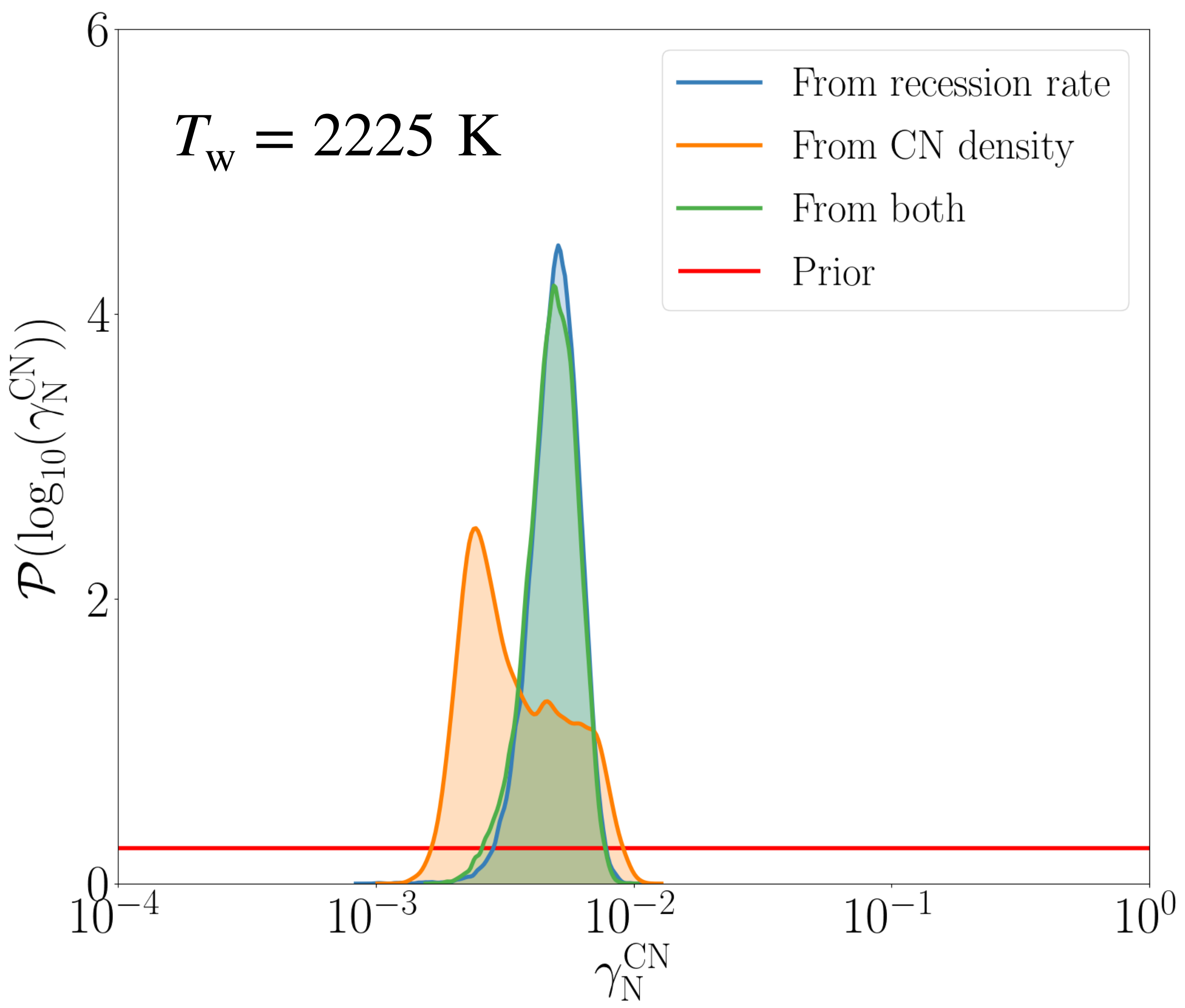
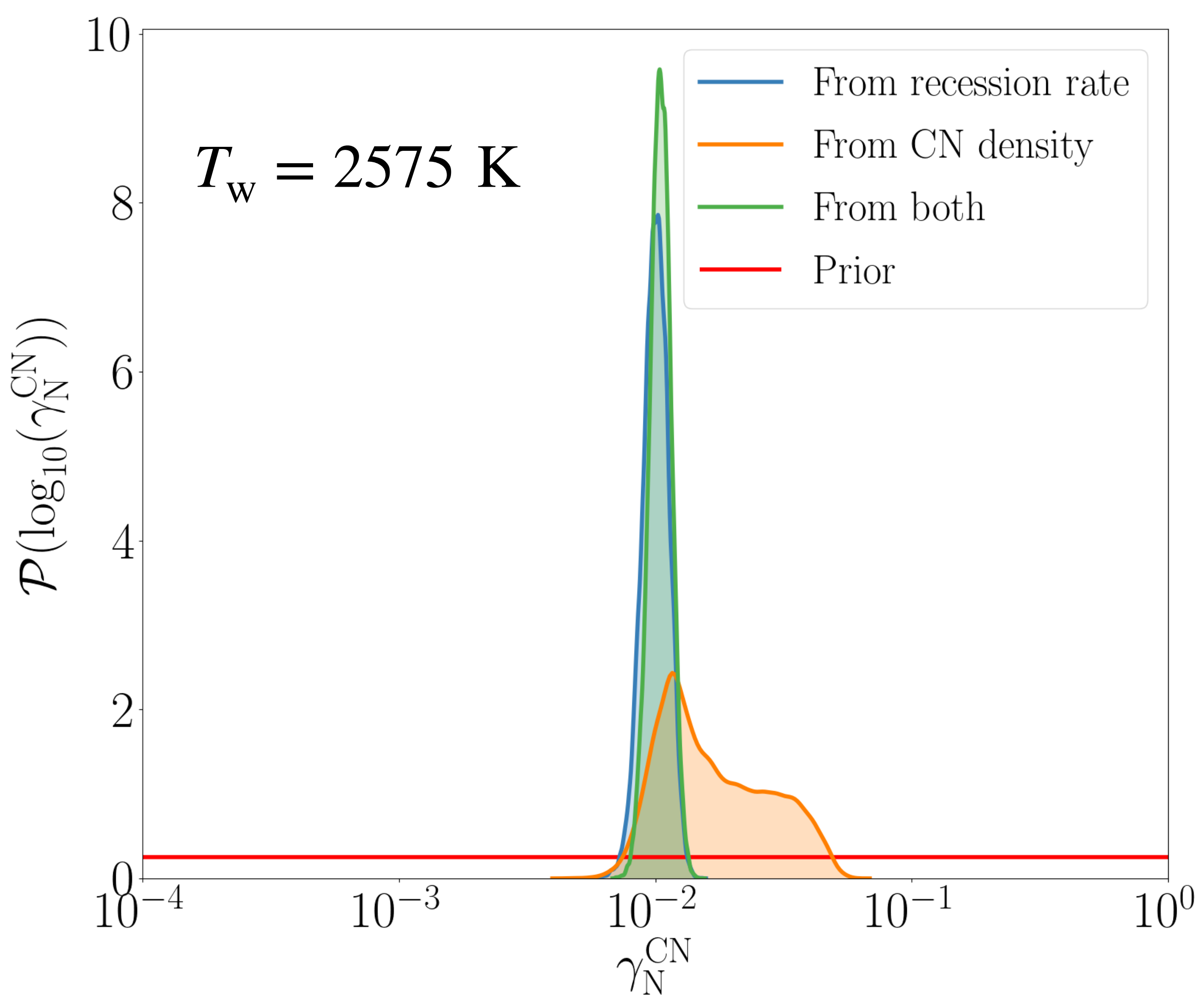
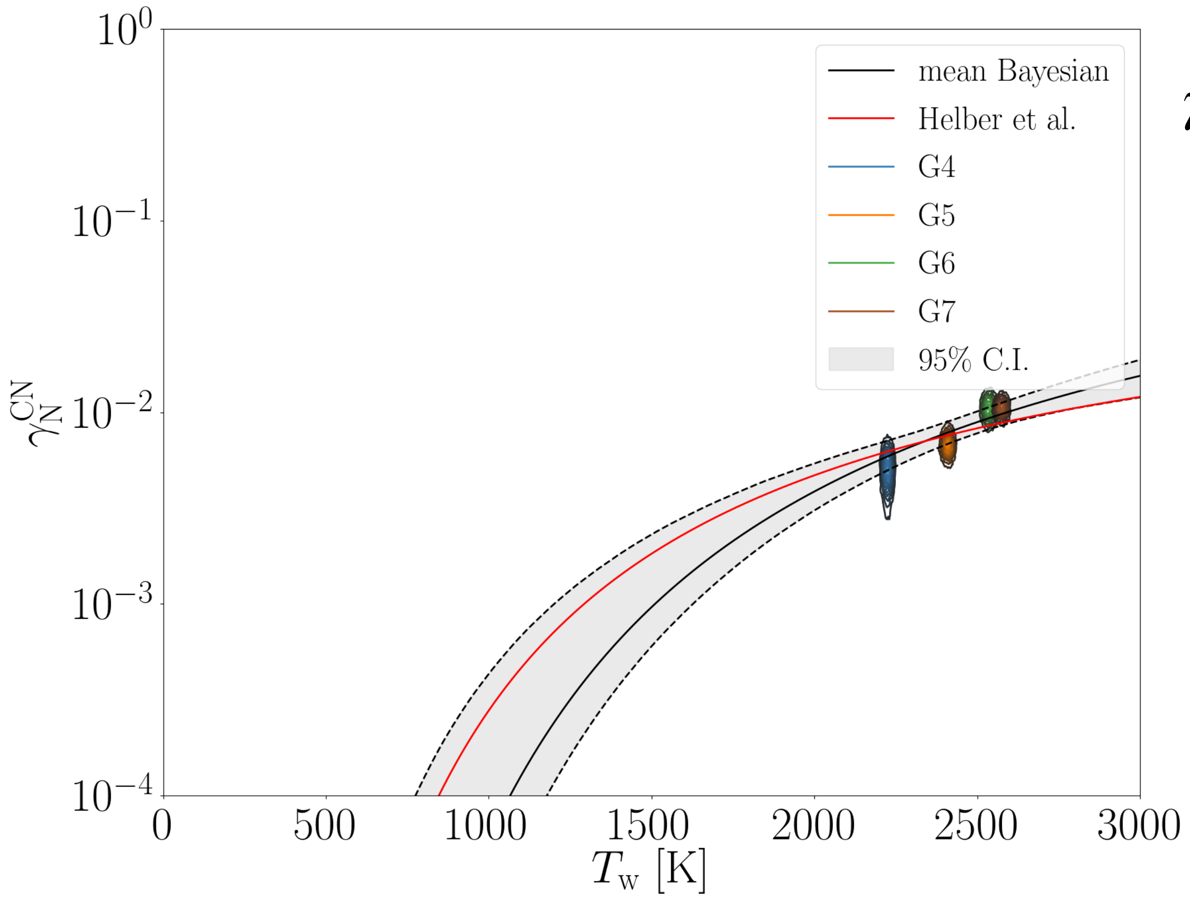
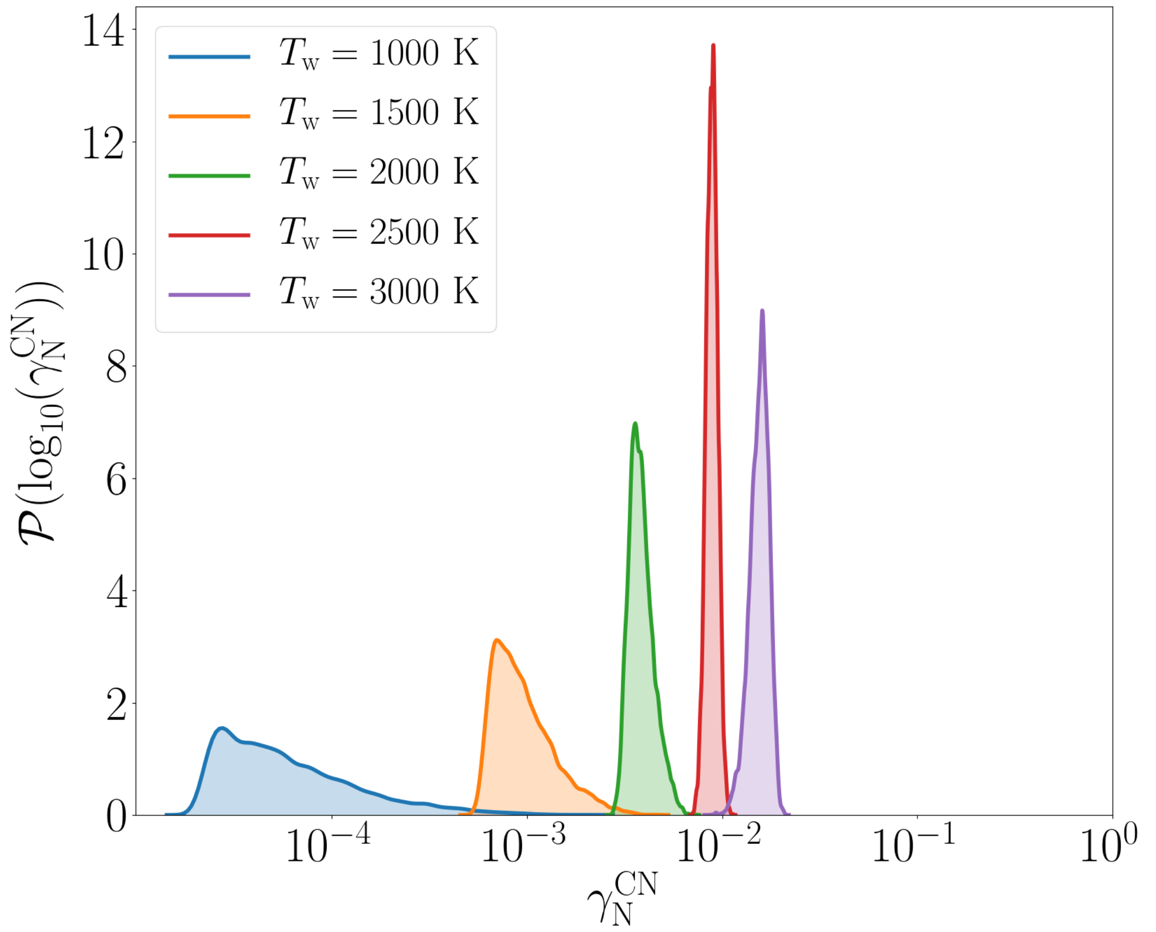






$$\gamma_N^{CN} = 0.28^{+0.22}_{-0.21} \exp\left(\frac{8337.8^{+1608.2}_{-3308.3}}{T_w}\right)$$



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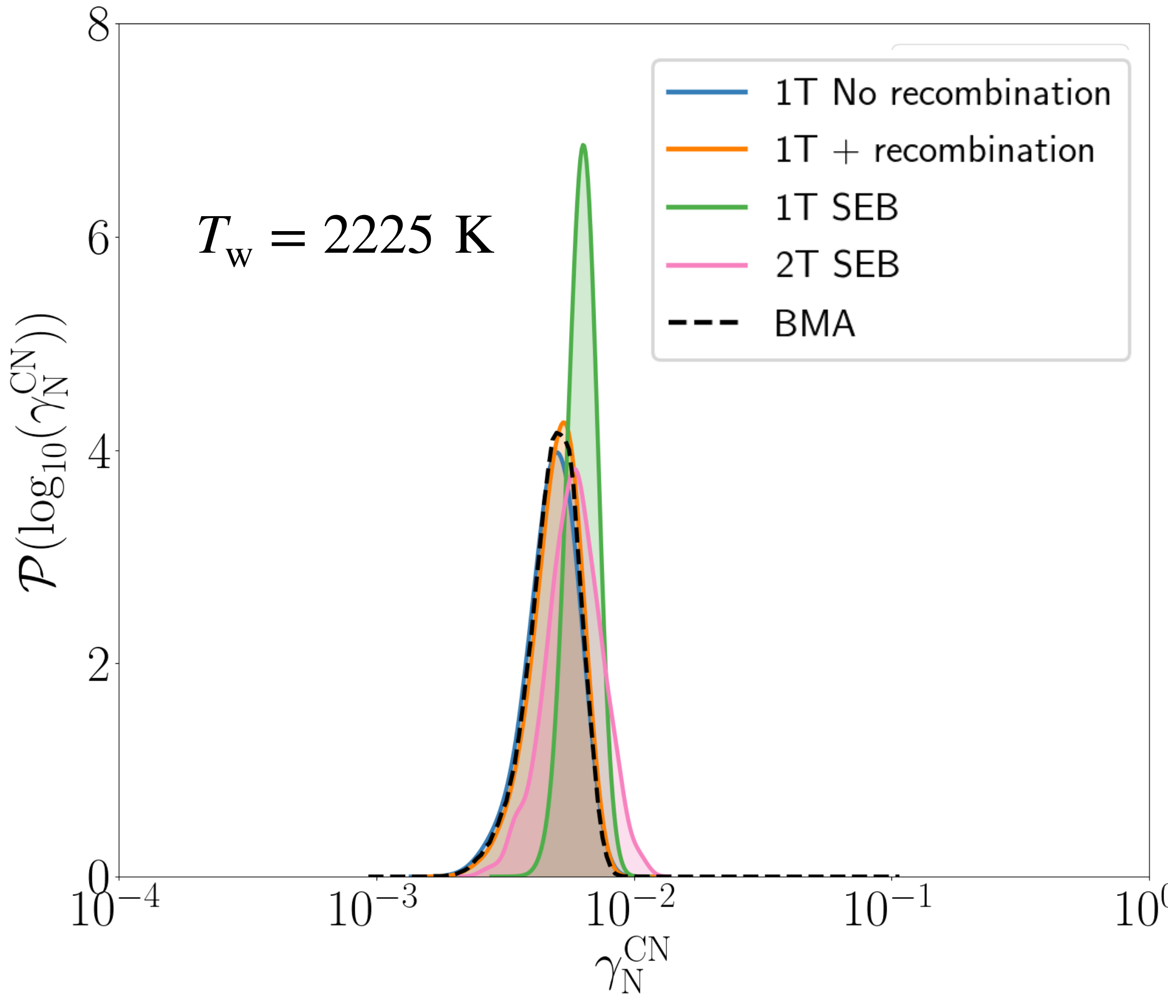
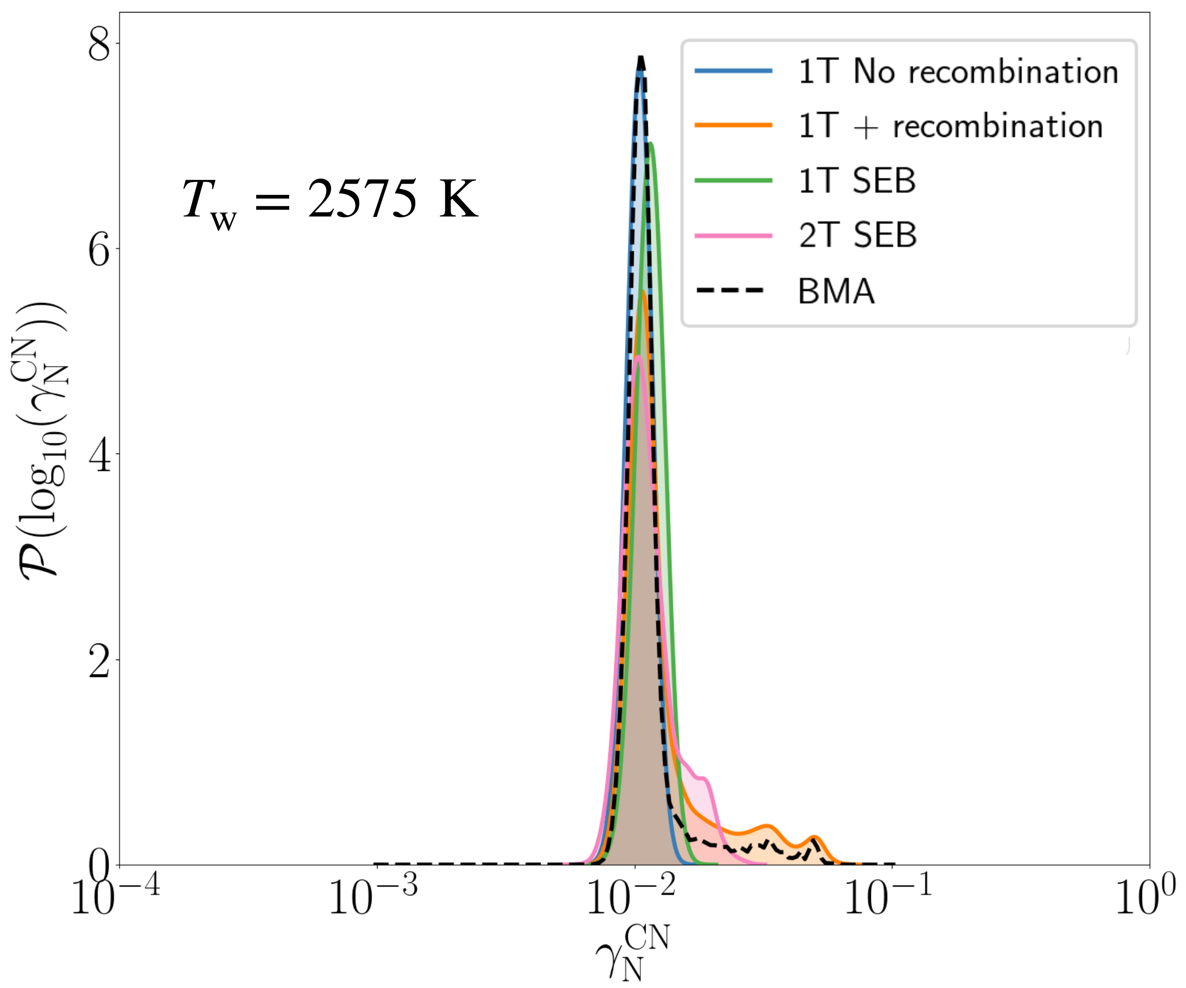
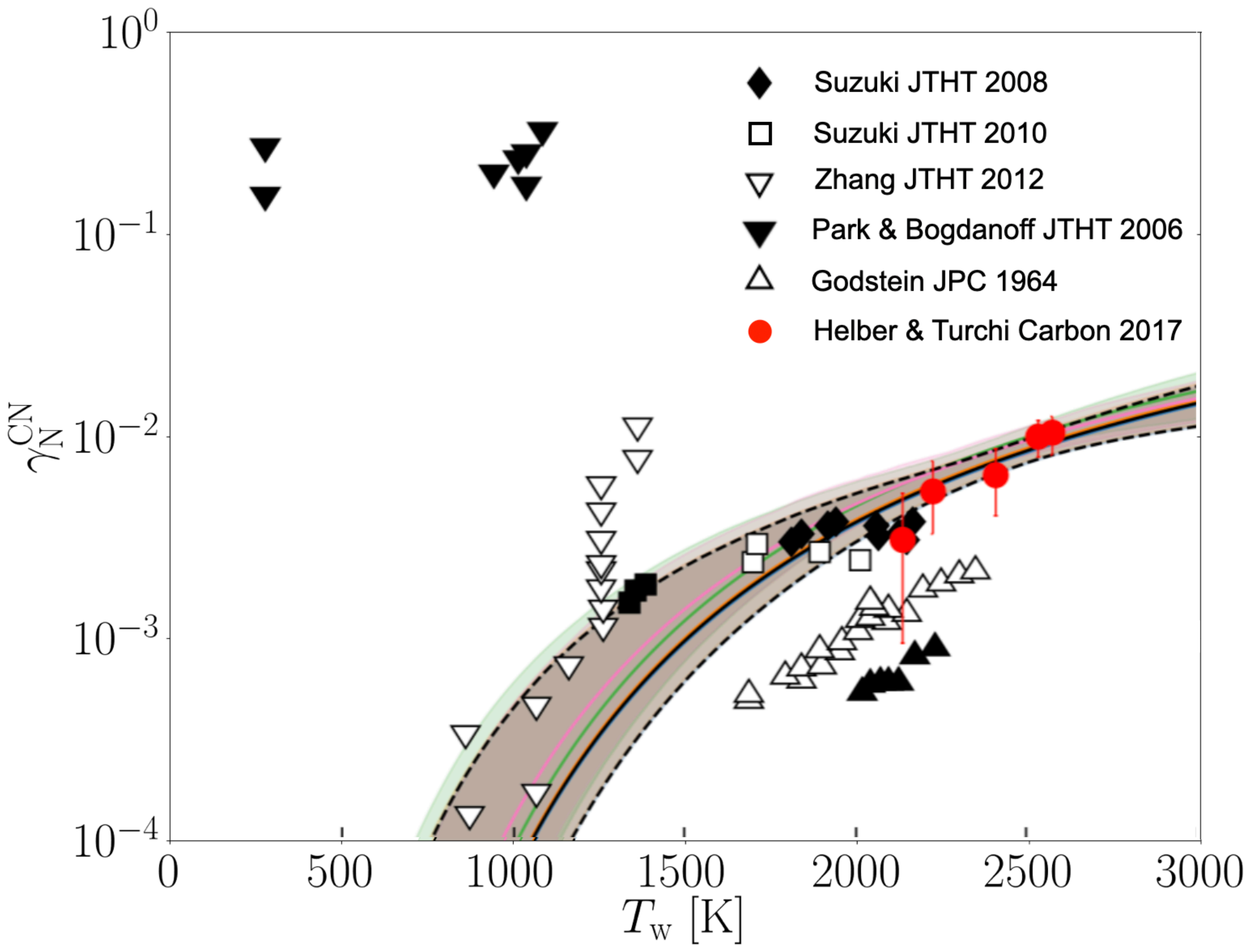
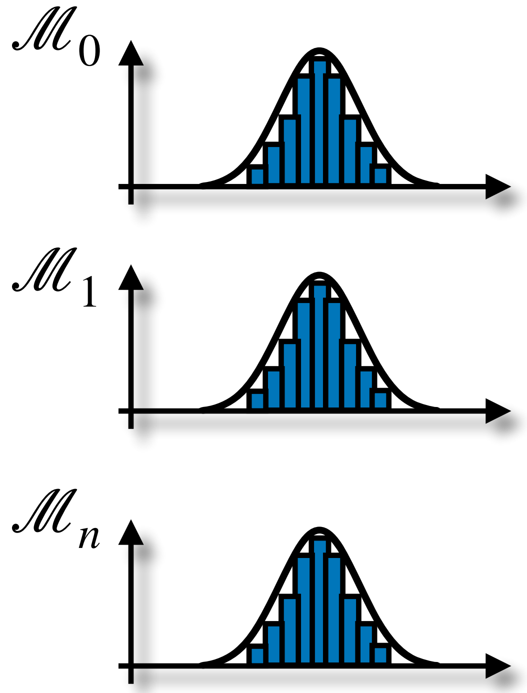




$$\arg\min_{c} J(\boldsymbol{p}) = \|\boldsymbol{y}_{\text{obs}} - \boldsymbol{f}(\boldsymbol{X}_{\text{obs}}, \boldsymbol{c}, \boldsymbol{p})\|^2 + \mathscr{R}(\boldsymbol{X}_{\text{obs}}, \boldsymbol{c}, \boldsymbol{p})$$

- What if f is wrong? → Model-form uncertainty





$$\frac{\mathscr{P}(\boldsymbol{y}_{\text{obs}} \mid \mathscr{M}_0)}{\sum_i \mathscr{P}(\boldsymbol{y}_{\text{obs}} \mid \mathscr{M}_i)} \longrightarrow \text{Denominator of Bayes' rule}$$

$$\frac{\mathscr{P}(\boldsymbol{y}_{\text{obs}} \mid \mathscr{M}_1)}{\sum_i \mathscr{P}(\boldsymbol{y}_{\text{obs}} \mid \mathscr{M}_i)}$$

$$\frac{\mathscr{P}(\boldsymbol{y}_{\text{obs}} \mid \mathscr{M}_n)}{\sum_i \mathscr{P}(\boldsymbol{y}_{\text{obs}} \mid \mathscr{M}_i)}$$

del Val, Magin, Congedo. *Int J Heat Mass Transfer (under review), 2022.* Preprint available on RG

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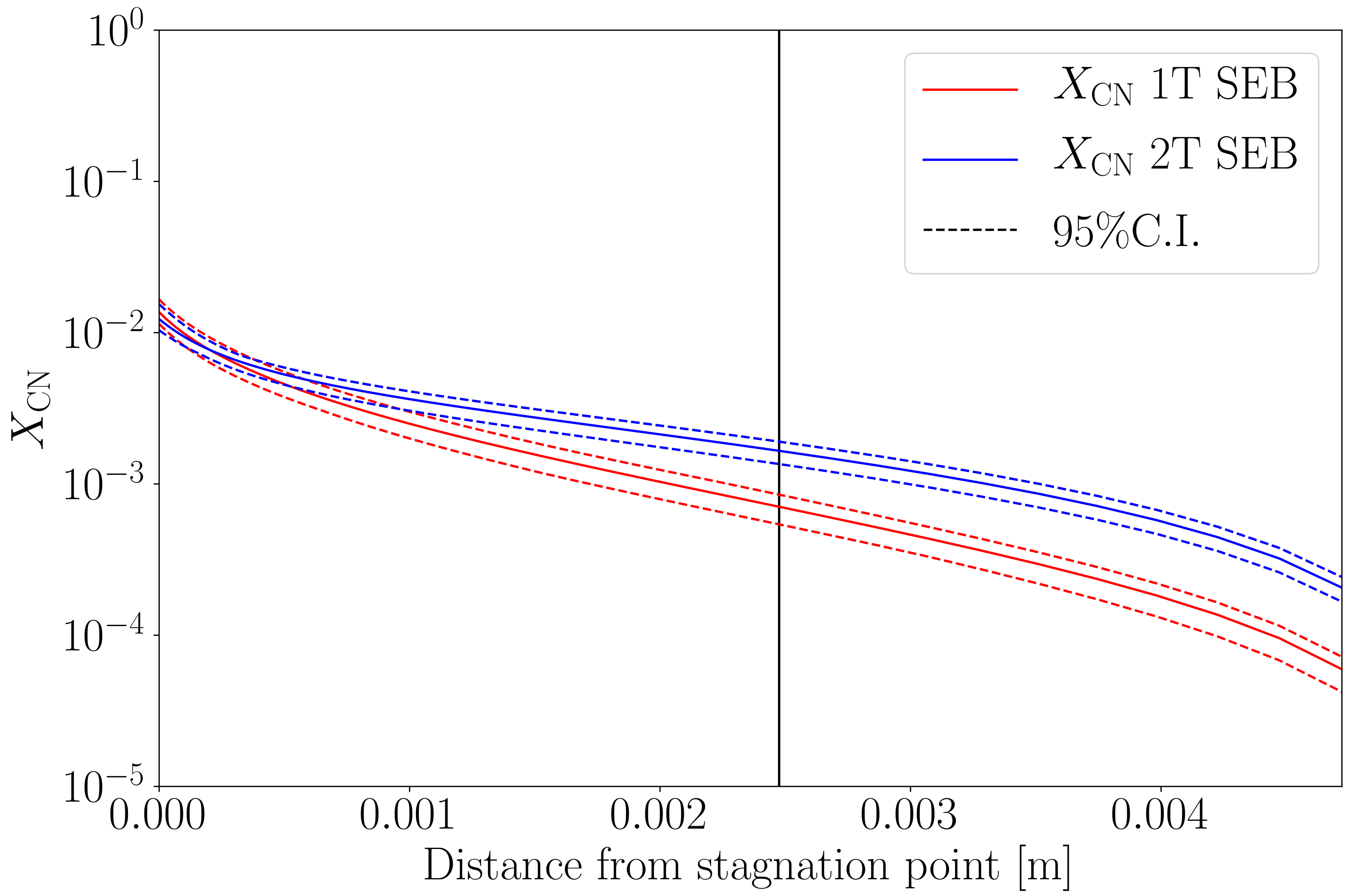

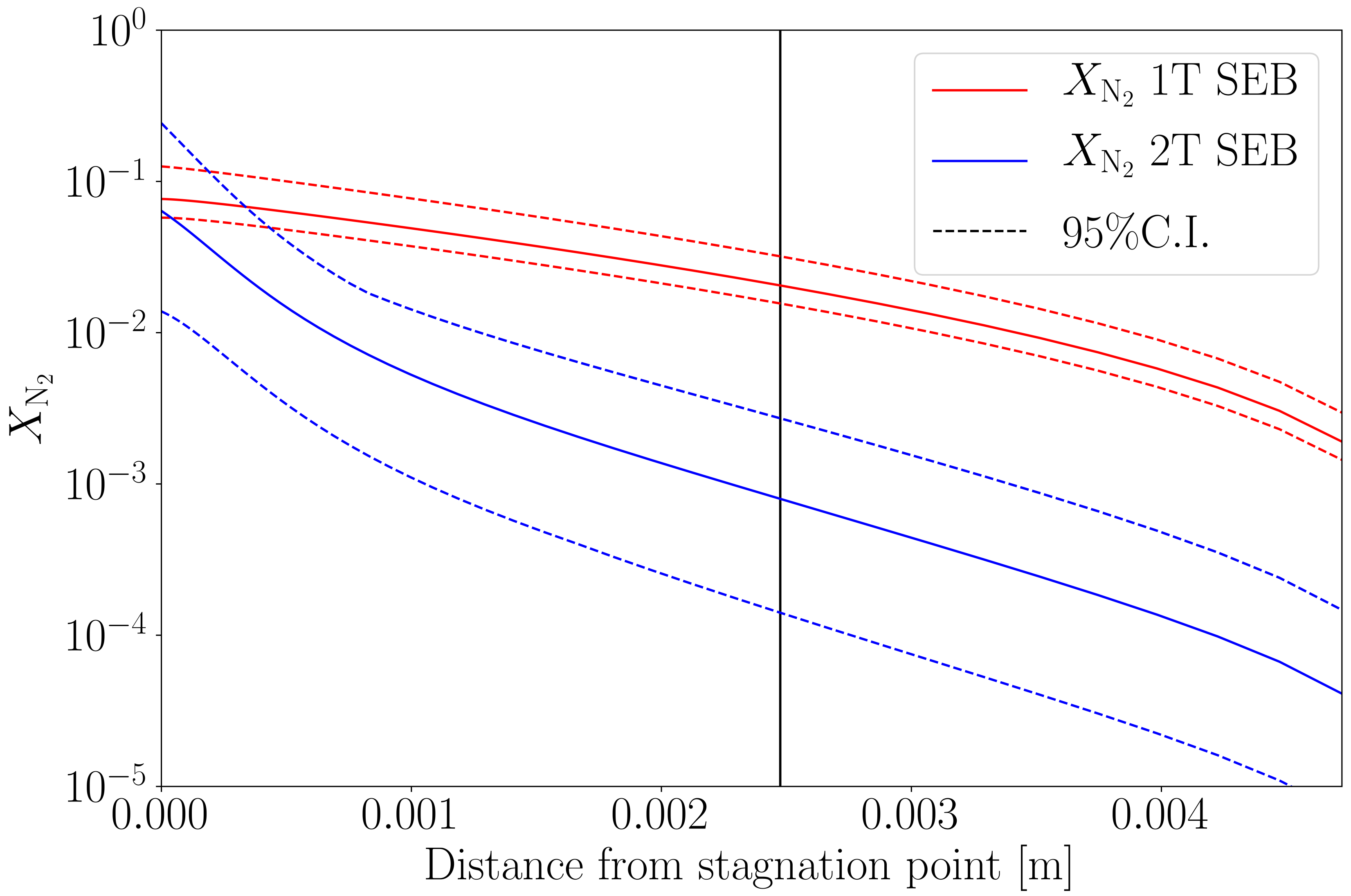

More informative experiments can be **proposed** based on these insights

del Val, Magin, Congedo. *Int J Heat Mass Transfer (under review), 2022.* Preprint available on RG

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Set of reactions [1]:

Absorption-Desorption

$$N + s \rightarrow N_s \qquad (k_{abs})$$
$$N_s \rightarrow N + s \qquad (k_{des})$$

Nitridation

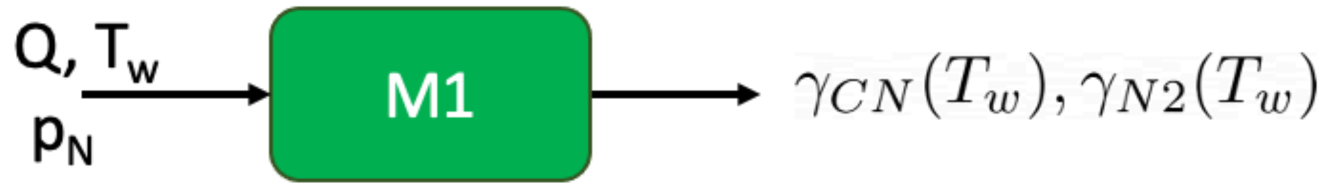
$$N + N_s + C_b \rightarrow CN + N + s \qquad (k_{nit,1})$$
$$N_s + C_b \rightarrow CN + s \qquad (k_{nit,2})$$

Recombination

$$N + N_s \rightarrow N_2 + s \qquad (k_{rec,1})$$
$$N_s + N_s \rightarrow N_2 + 2s \qquad (k_{rec,2})$$

Models:

1. Molecular beam experiments

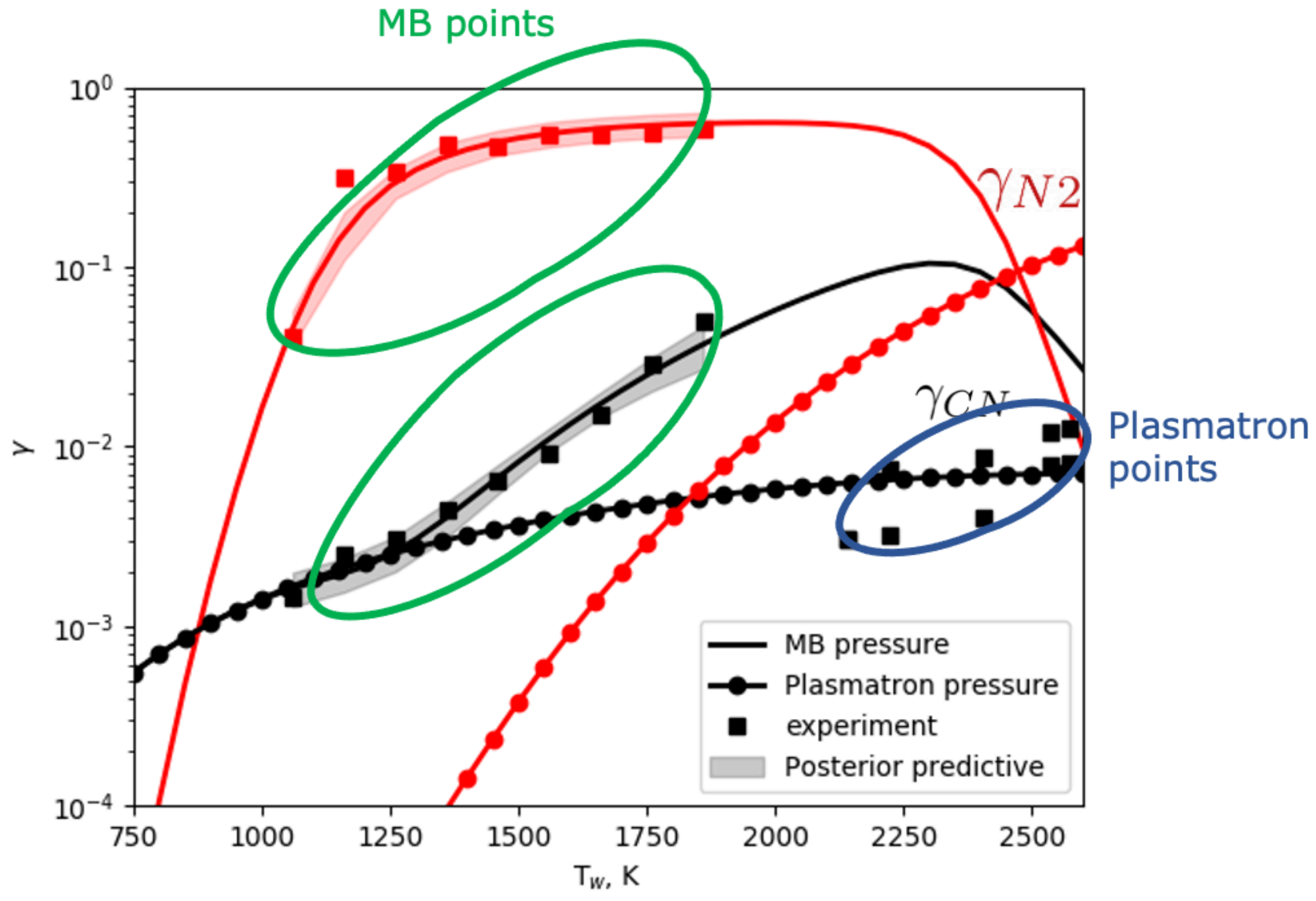


Analytical formulation

2. Plasmatron experiments

Approximated by a low-fidelity analytical formulation

(Future: Surrogate model from CFD stagnation line simulations)



[1] Prata, Schwartzentruber, Minton. *AIAA Journal 60:2, 627-640, 2022*

Capriati, del Val, Congedo, Minton, Schwartzentruber, Magin. *(ongoing…)*

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Take home messages

Uncertainty modeling/stochastic inverse problems

- Uncertainty is a necessary component that should be modeled in addition to the physical problem of interest
- Incorporating uncertainties in inverse problems requires the overhaul of deterministic inverse techniques
- The Bayesian formalism computes an objective measure of uncertainty, informed by experimental data

Development of Bayesian inference frameworks for the stochastic calibration of graphite nitridation

- A stochastic methodology has been developed to incorporate uncertainties affecting the calibration of nitridation
- Recession rates and CN densities used jointly to infer nitridation efficiencies
- Model-form uncertainties incorporated through a Bayesian Model Averaging method

Finite-rate nitridation model calibrated using molecular beam and Plasmatron data

- Detailed mechanism can get information from both experiments at low and high pressures
- Calibrated model seems to fit well the experimental data
- Still early in the work but hope to have results with a CFD model soon

THANK YOU

Questions?

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