Capturing Engine Emissions (NOx) Responses via Reduced Order Modeling

UTSR Fellowship Presentation
2024 UTSR and Advanced Turbines Program Review Meeting – University of Alabama

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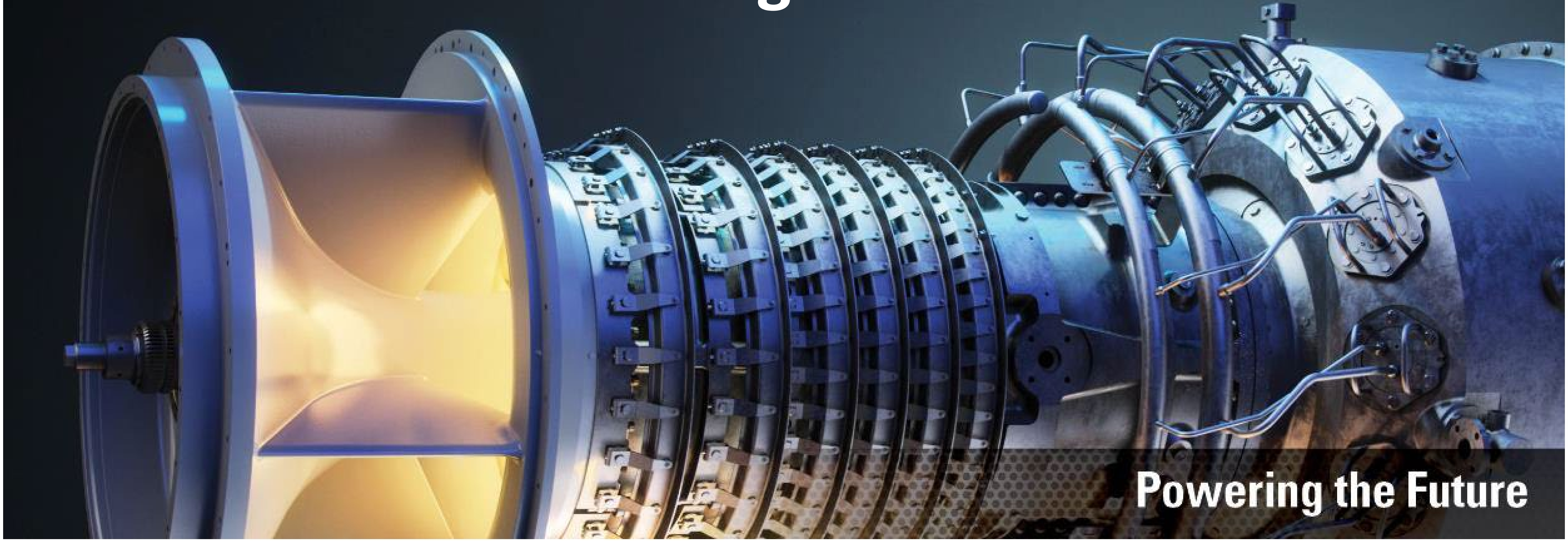

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Outline

- **Background**
  - **What is NOx?**
  - **NOx Formation Pathways**
  - **Modeling Techniques**
- NOx Modeling
- Conclusions
- Acknowledgments

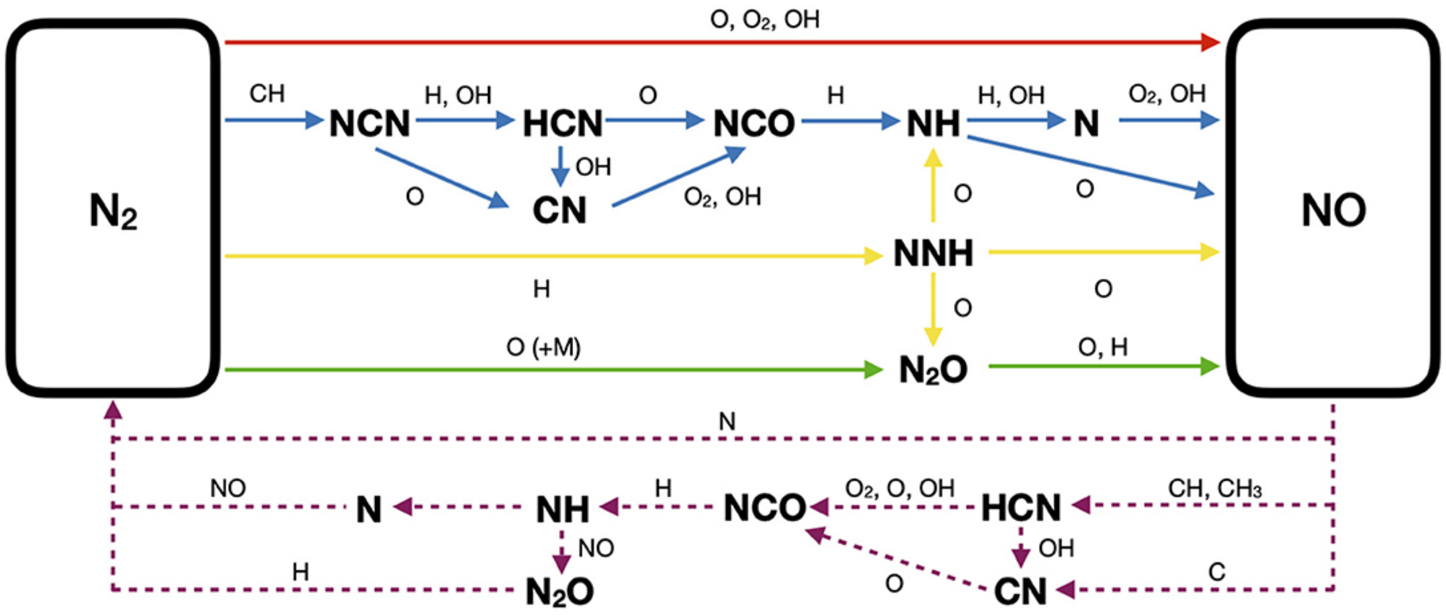
NOx Background

- NOx = Nitrogen Oxides
  - Primarily referring to NO for combustion applications, but also includes NO_2 and N_2O
- Sunlight reacts with NOx and VOCs to form tropospheric ozone and smog

NOx Formation Pathways

- Zeldovich (Thermal)
  - Dissociation of molecular nitrogen at high temperatures
  - Requires time to initiate → occurs downstream of primary reaction zone
- Fennimore (Prompt)
  - Intermediate hydrocarbon species react with molecular nitrogen in/near the flame front
- Other
  - Fuel
  - Nitrous Oxide (N2O)
  - NNH

$$NO_x = f(T, P, fuel, \tau_{res})$$



Empirical NOx Models

1. $NO_x = \frac{9*10^{-8} P^{1.25} V_c e^{(0.01 T_{st})}}{\dot{m}_a T_{PZ}}$ (g/kg Fue

Lefebvre[1] – Conventional Spray

2. $NO_x = 29 e^{-(21670/T_c)} P^{0.66} [1 - e^{-(25}$

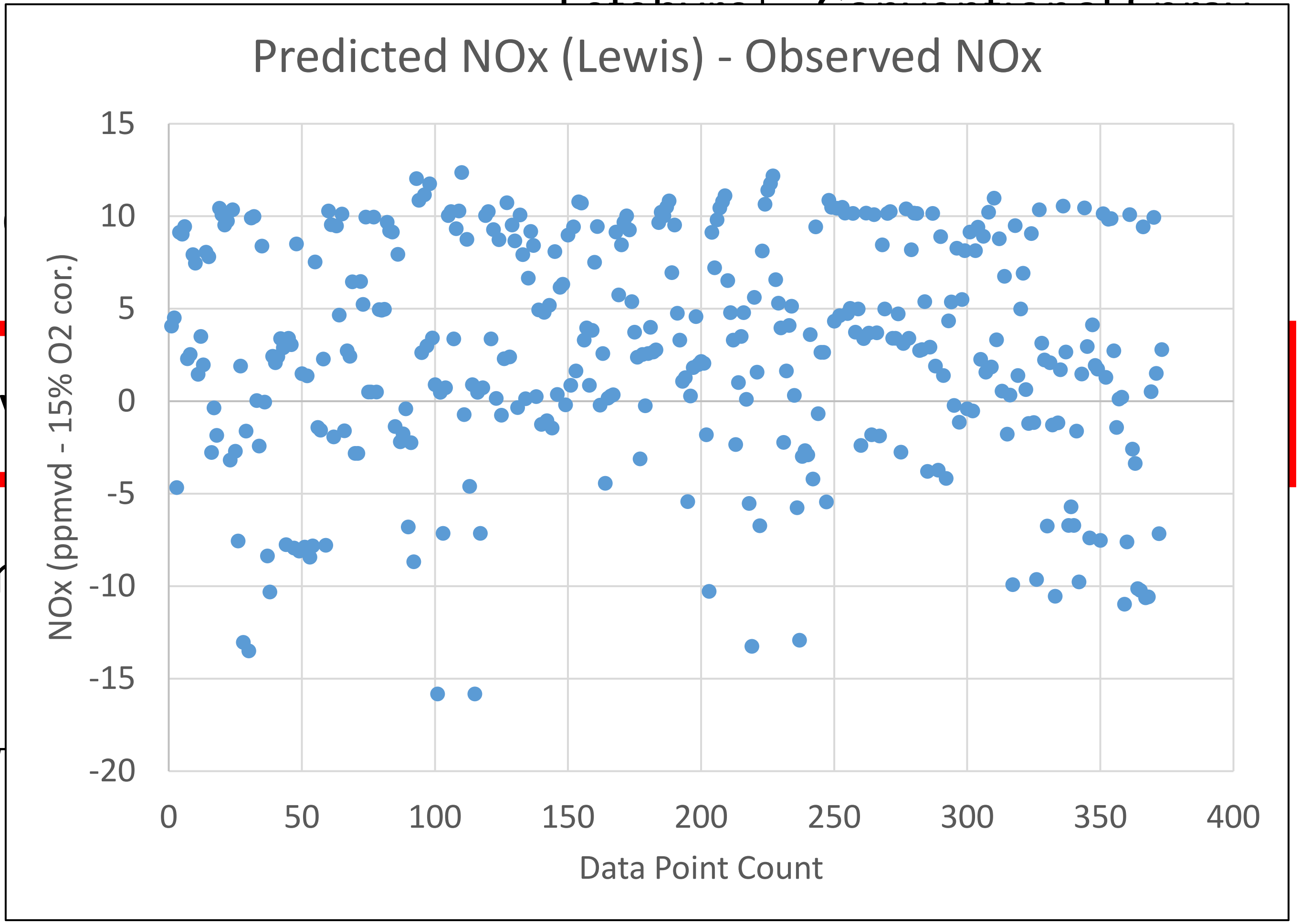
3. $NO_x = 3.32 * 10^{-6} e^{0.008 T_c} P^{0.5}$ (ppm

Poor Predictive Performance

4. $NO_x = 18.1 (P_2/P_1)^{1.42} \dot{m}_a^{0.3} q^{0.72}$ (ppm

5. $NO_x = 15.1^{14} (t - 0.5 t_e)^{0.5} e^{(-71000/T}$

(g/kg Fuel)



Problem Definition

Generate a predictive model for NOx that

i. Is grounded on the formation physics (kinetics-based and empirical models)

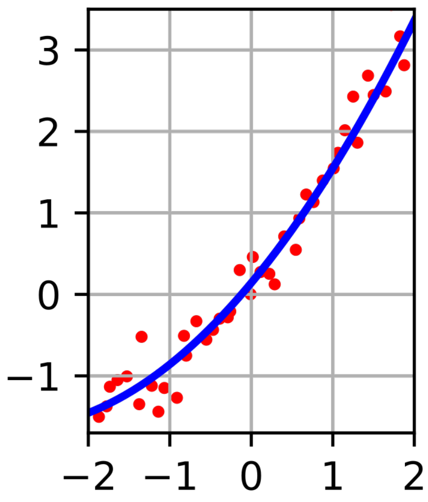
ii. Is based on instrumentation & hardware data

iii. Meets predictive performance standards

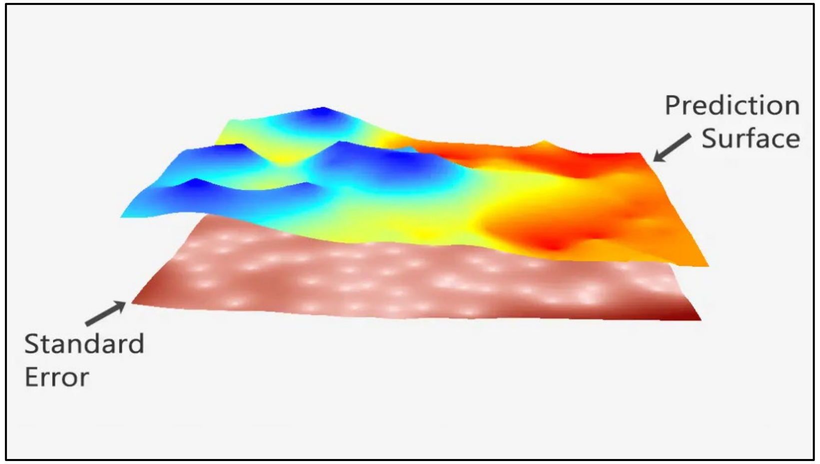
Modeling with HEEDs

HEEDS

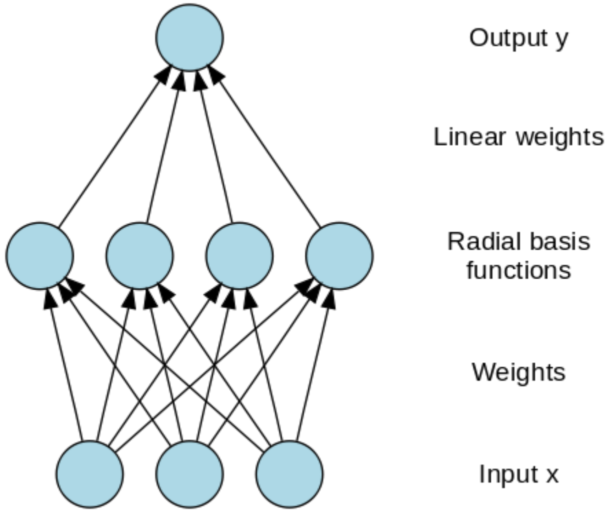
- Regression
  - Method of least squares, minimizes residuals between data and a defined base function



- Kriging
  - Method of spatial interpolation to estimate a variable over a continuous spatial field
  - Exact Interpolator



- Radial Basis
  - Predicts an output by calculating the distance between a point within the design space and a center
  - Exact Interpolator



Modeling Process

1. Data Pre-processing

2. Model Shape Definition

3. Model Generation

4. Analysis

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Outline

- Background
- **NOx Modeling**
  - **23001S Data Set Analysis**
  - **23001S Results**
  - **Summary**
- Conclusions
- Acknowledgments

Data Interpretation in Context

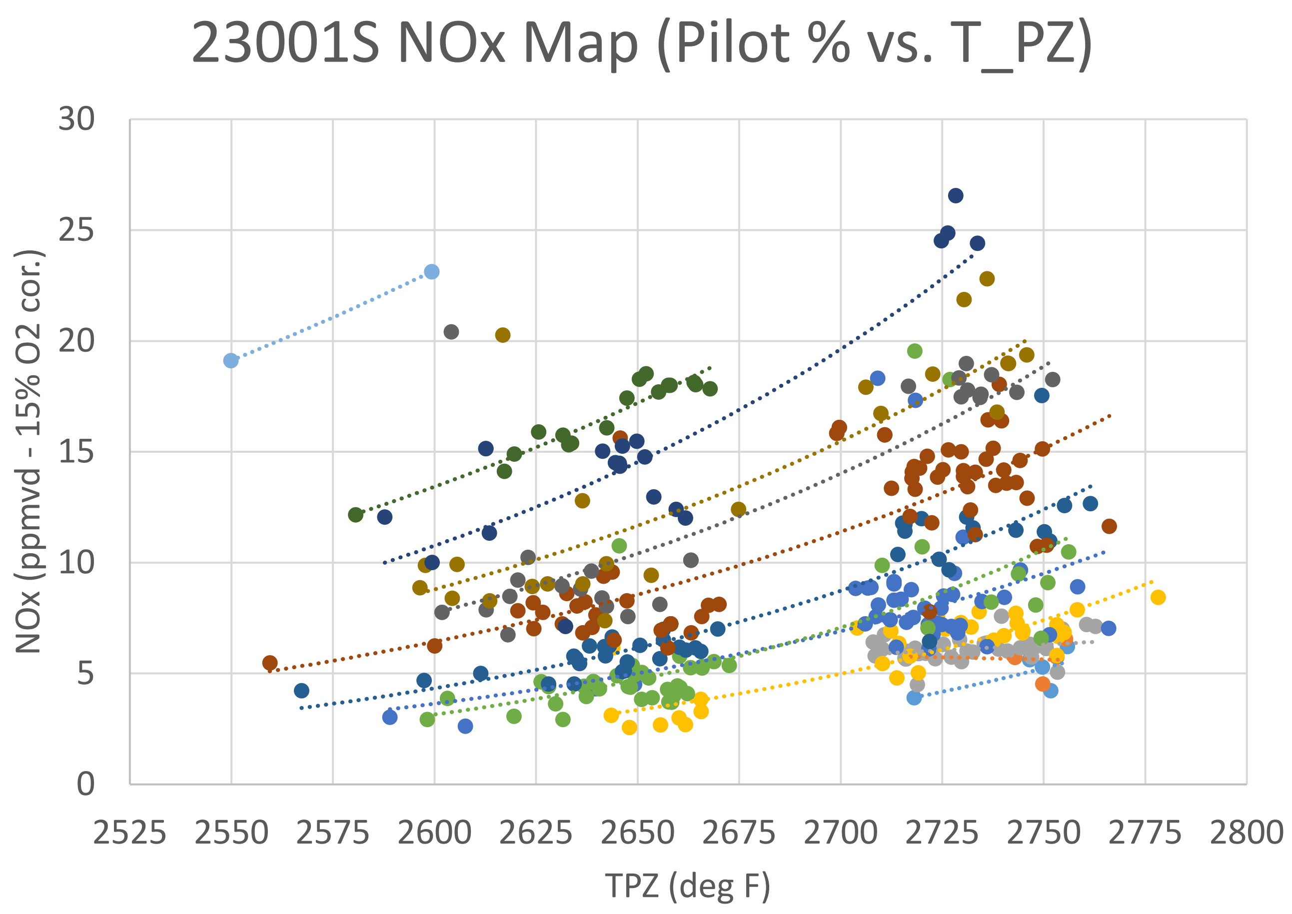
Engine Controls
- % Load
- % GP Speed

Hardware
- Rating
- Injector/Liner Spec
- Injector Eff. Area
- Liner Eff. Area

Compressor
- T1
- T2
- P2

Combustion
- % Pilot
- Cmb. Primary Zone Temp.
- Cmb. ΔP
- TRIT (T3)
- T5

NOx Performance Context

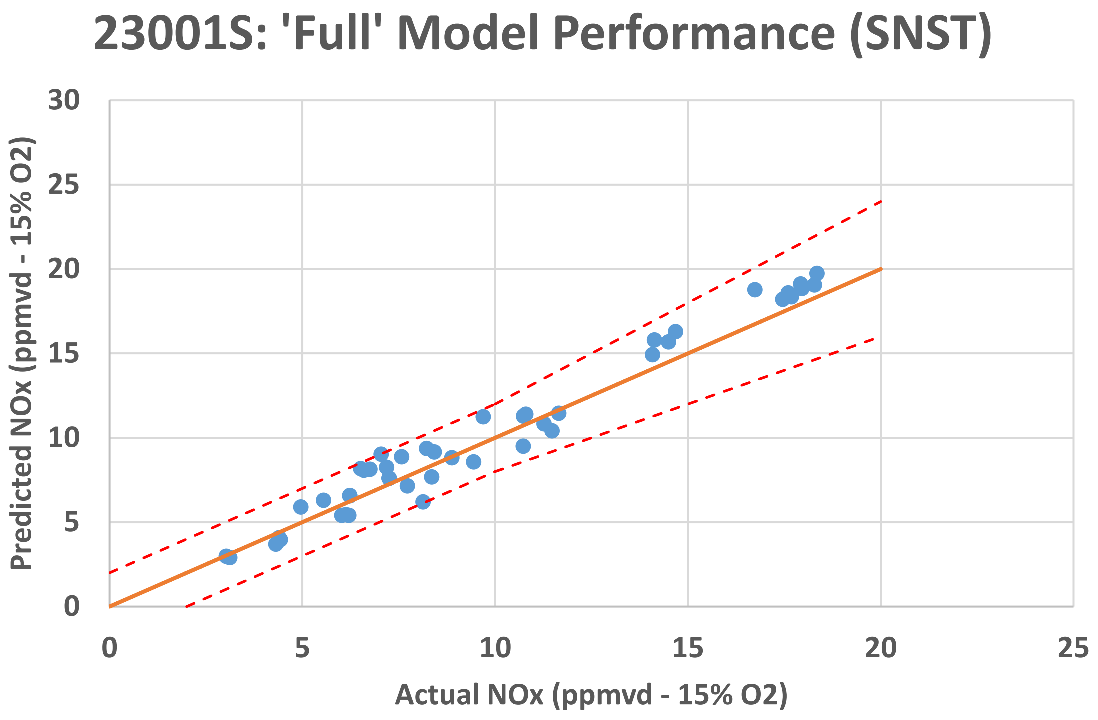


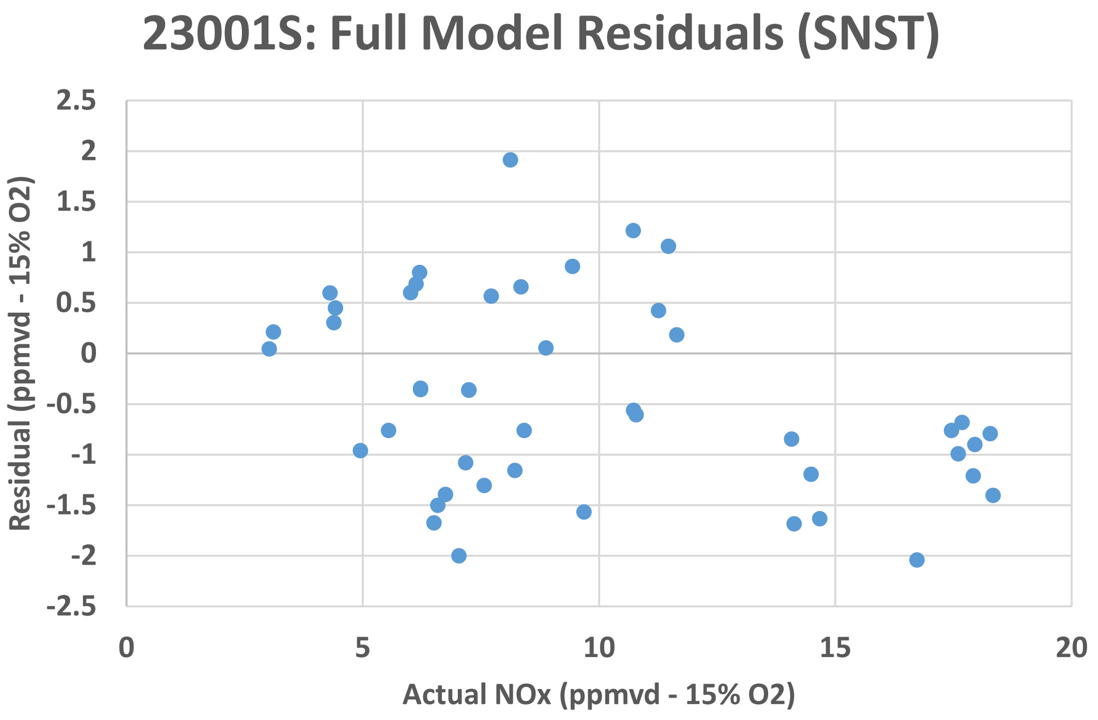
- Pilot % and Cmb. Primary Zone Temp. (TPZ) are highly influential
- Other influential parameters are unclear

“Full” Model Performance – 23001S, Any Liner, Any Injector

- Linear-Gaussian Kriging Model
- Meets performance standards

- Slight overprediction above 12 ppm
  - $Res. = NOx_{actual} - NOx_{predicted}$





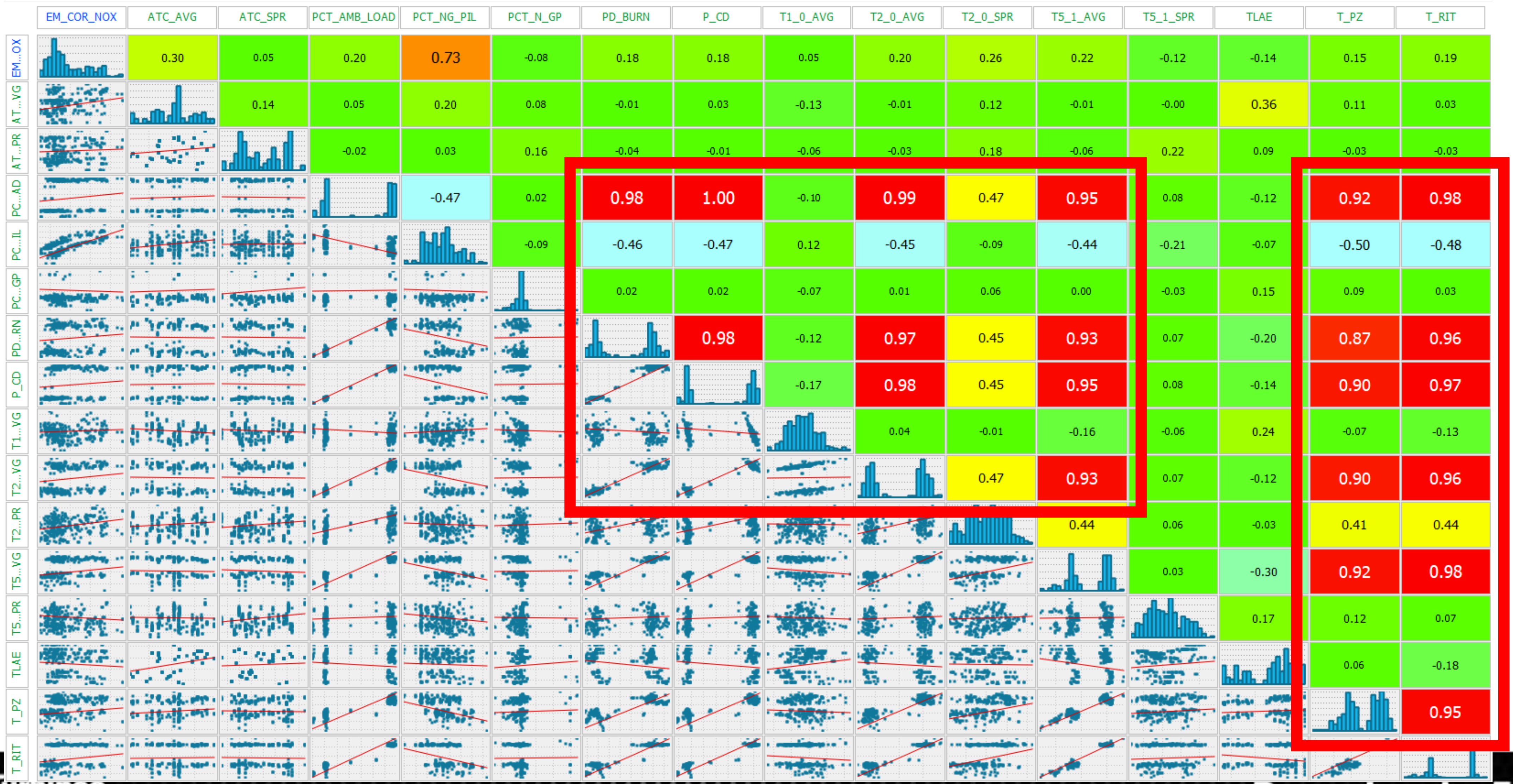
Full Model Conclusions

Full model performs *well*

Data is derived from Test → Increased amount of instrumentation

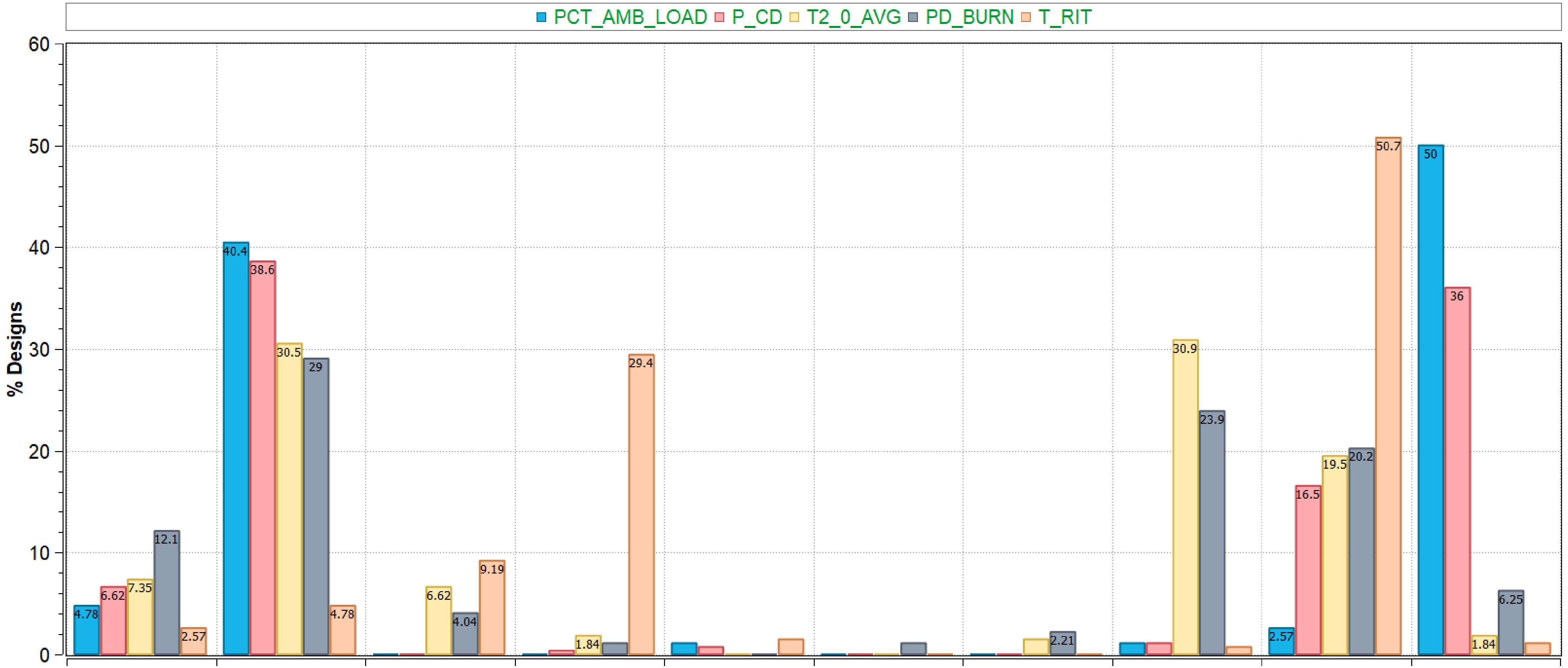
Can the number of inputs be reduced while preserving model efficacy?

Dataset Analysis – Input Correlation



Dataset Analysis – Input Correlation

- P_CD (P2) = Compressor Discharge Pressure
- PD_Burn (Cmb. ΔP) = Combustor Pressure Drop
- TRIT = Turbine Rotor Inlet Temperature



Reduced Model Key

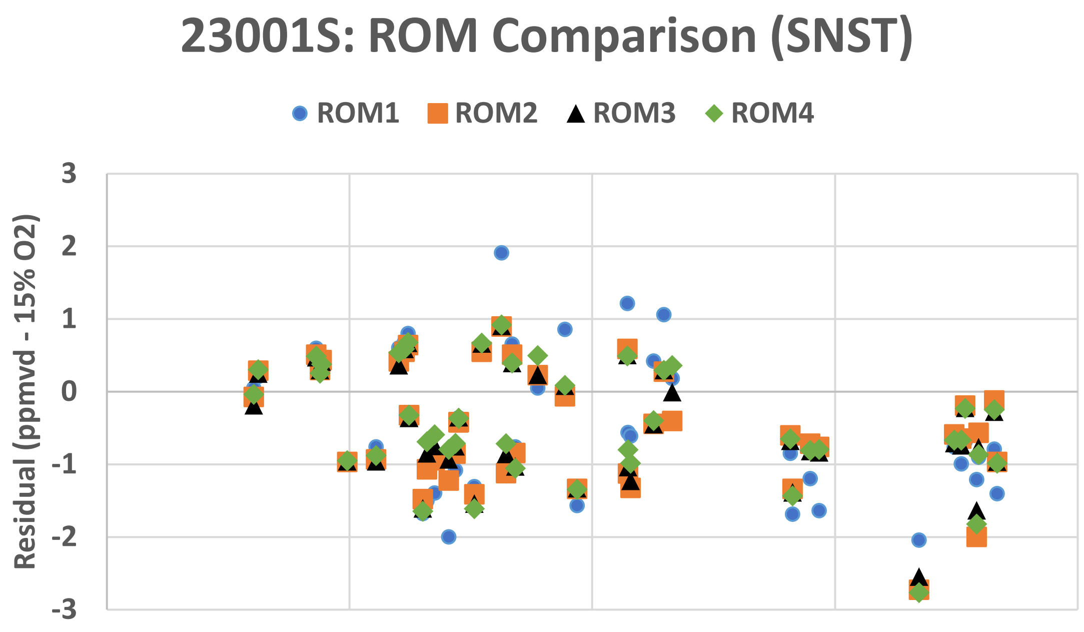
- Model Inputs:
  - Engine Controls: PCT_AMB_LOAD, PCT_N_GP
  - Hardware: ATC_avg, ATC_spr, TLAE
  - Compressor: T1, T2_avg, T2_spr, P_CD
  - Combustion: PCT_NG_PIL, T_PZ, PD_BURN, T_RIT, T5_avg, T5_spr

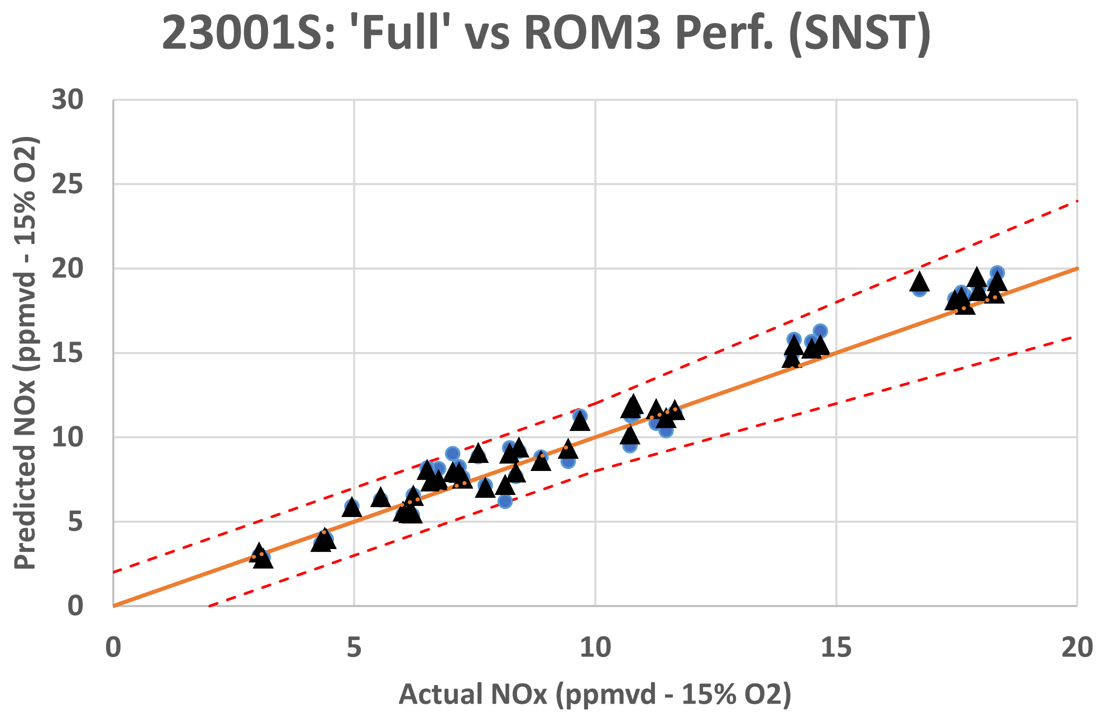
Model Name	Model Input Reductions
Full (ROM 1)	N/A
ROM 2	PD_BURN, P_CD, T2_avg, T2_spr, T_RIT
ROM 3	PCT_AMB_LOAD
ROM 4	T_PZ

Reduced Model Performance

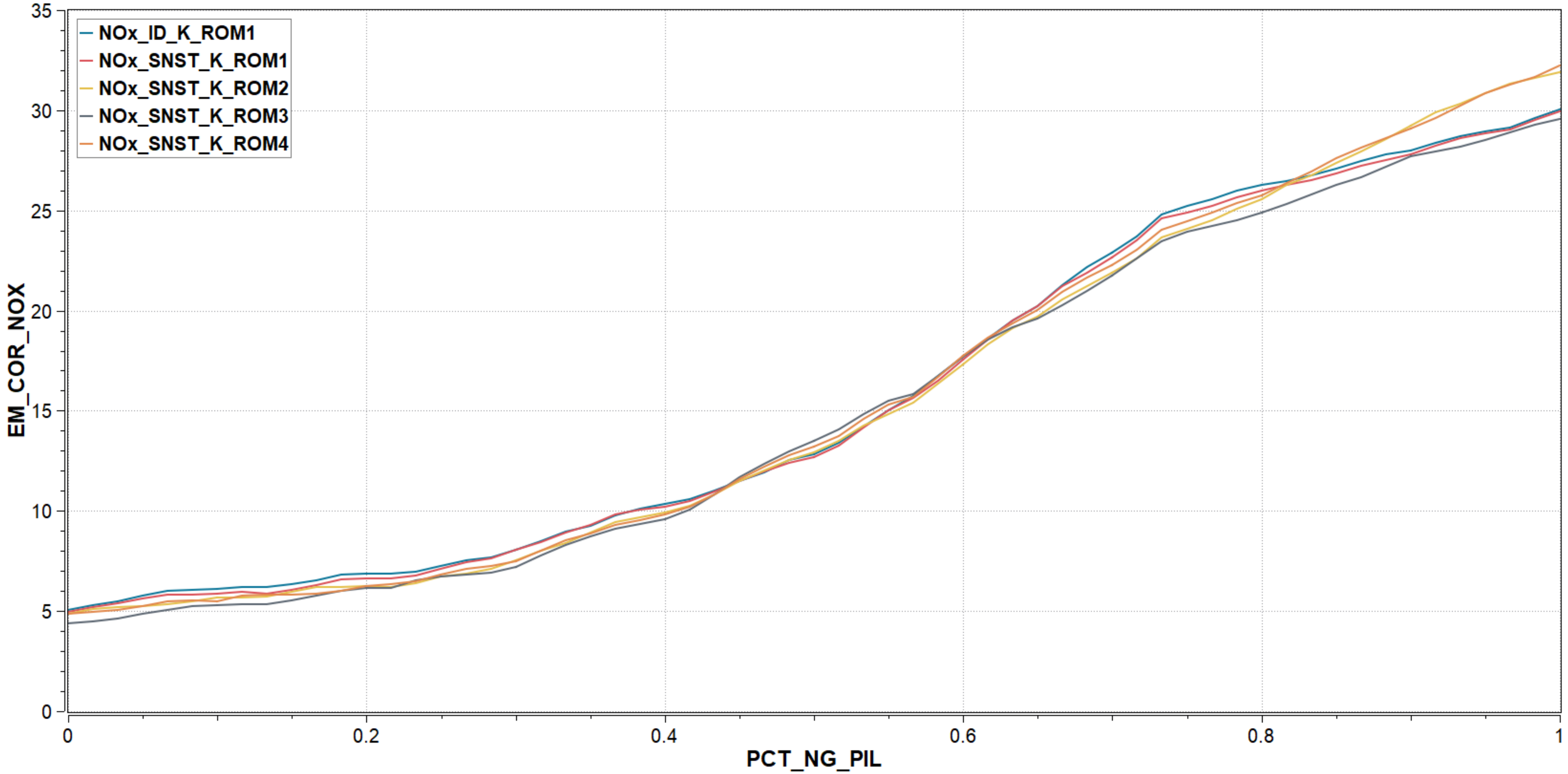
- ~18% overall improvement of model performance
- Some outliers show reduced predictive accuracy

Model	RMSE
Full (ROM 1)	1.030
ROM 2	0.869
ROM 3	0.845
ROM 4	0.857

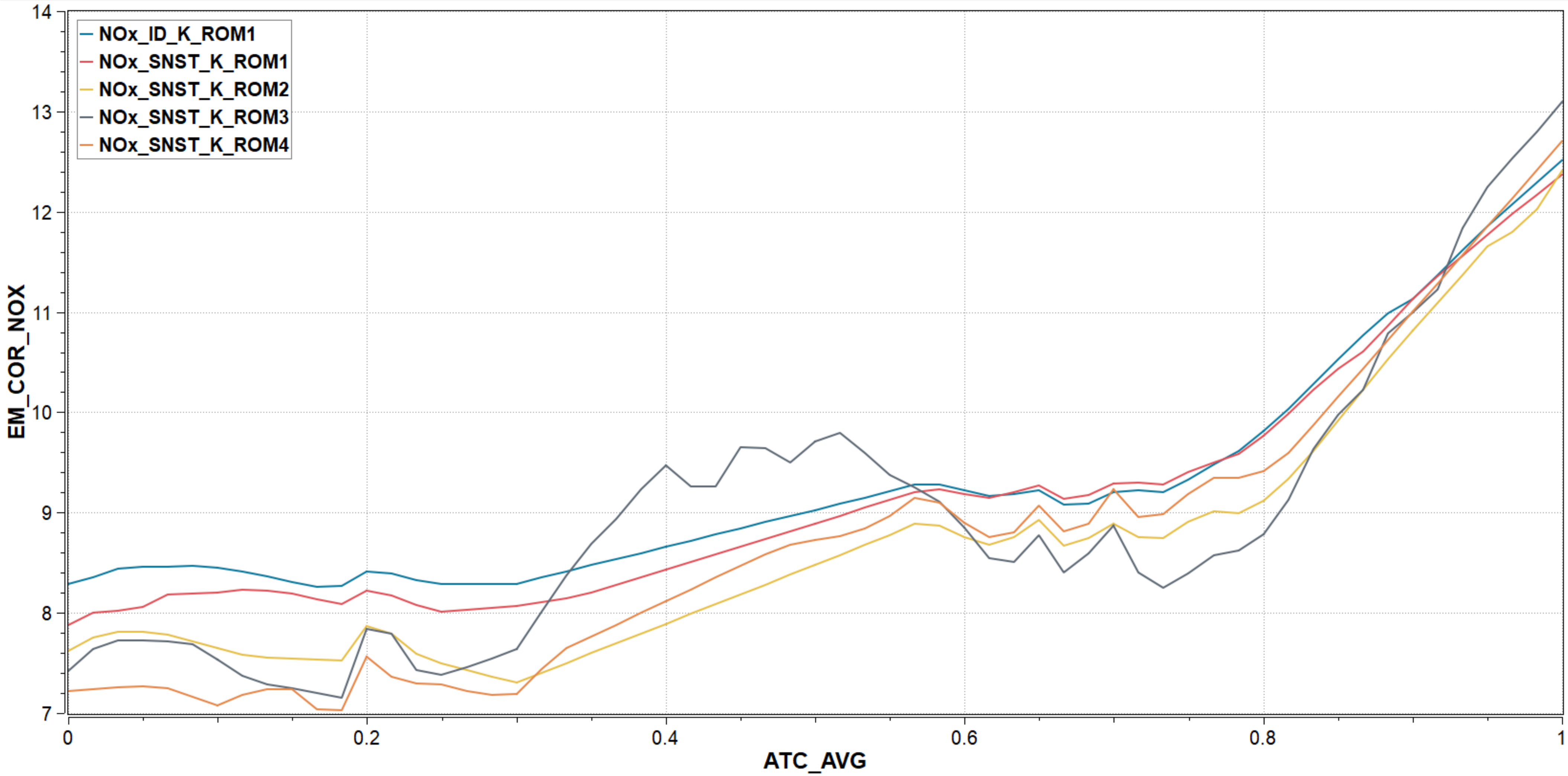




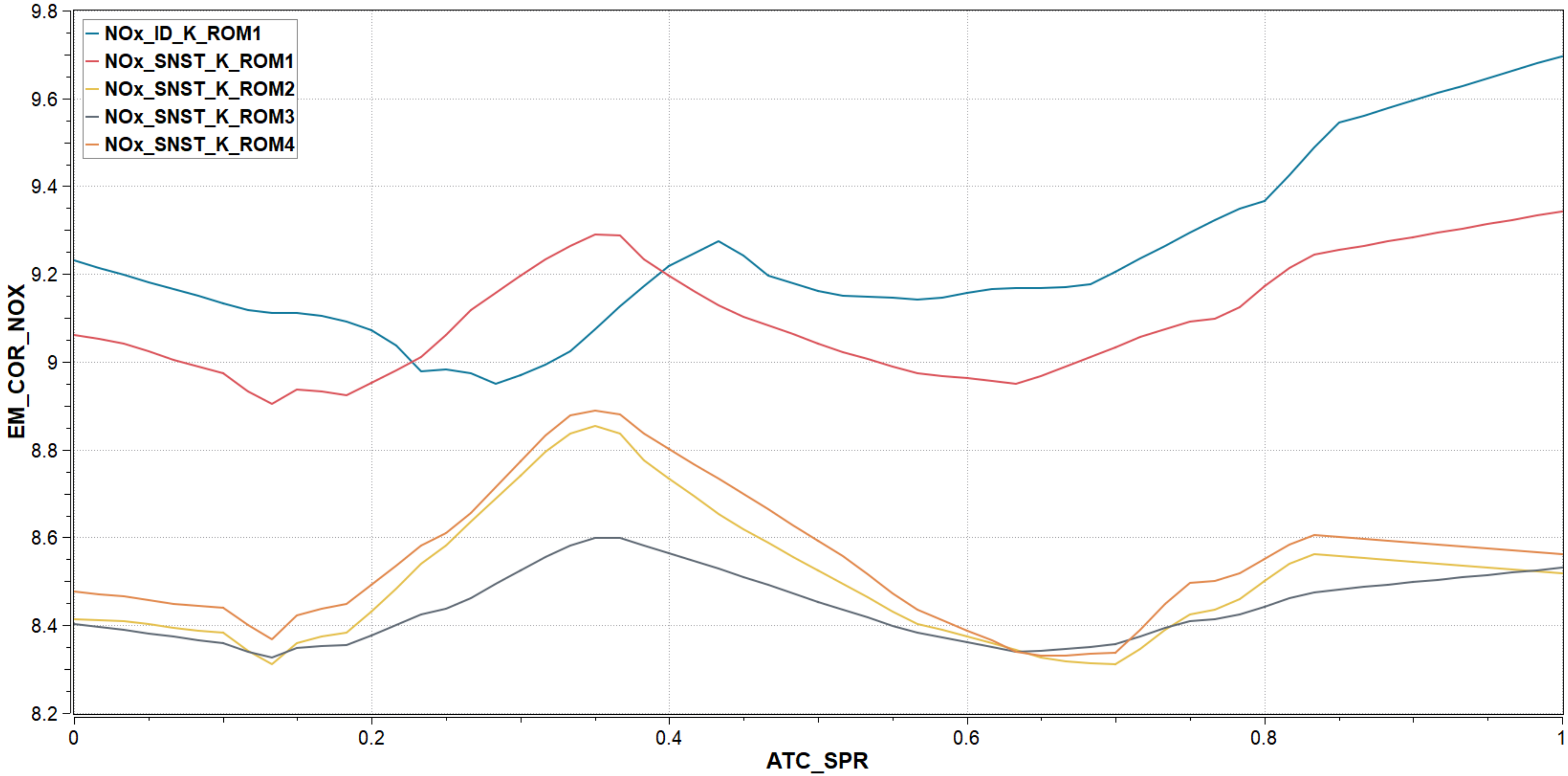
Reduced Model Shape Comparison - % Pilot



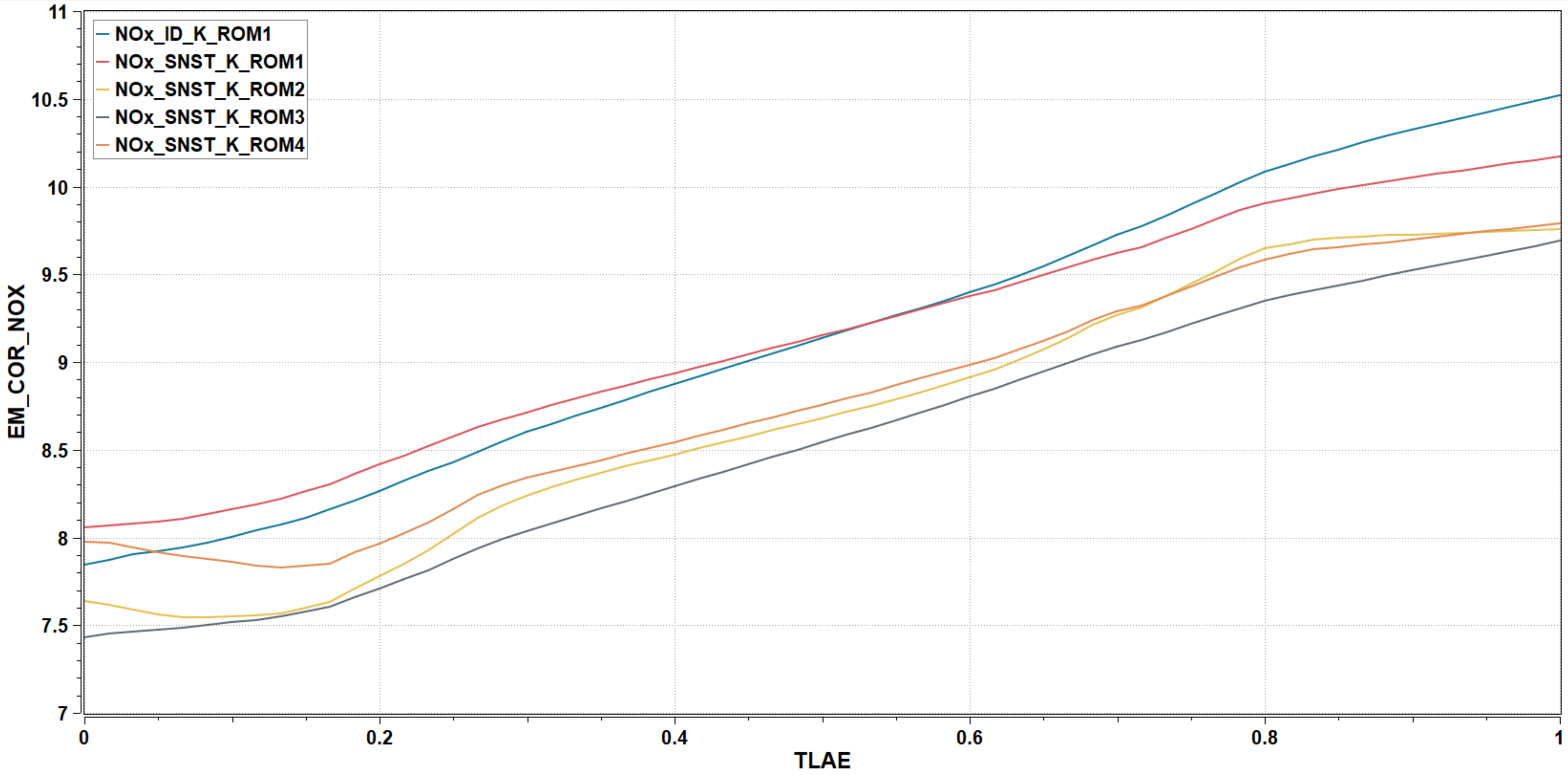
Reduced Model Shape Comparison – Inj. Eff. Area Avg.



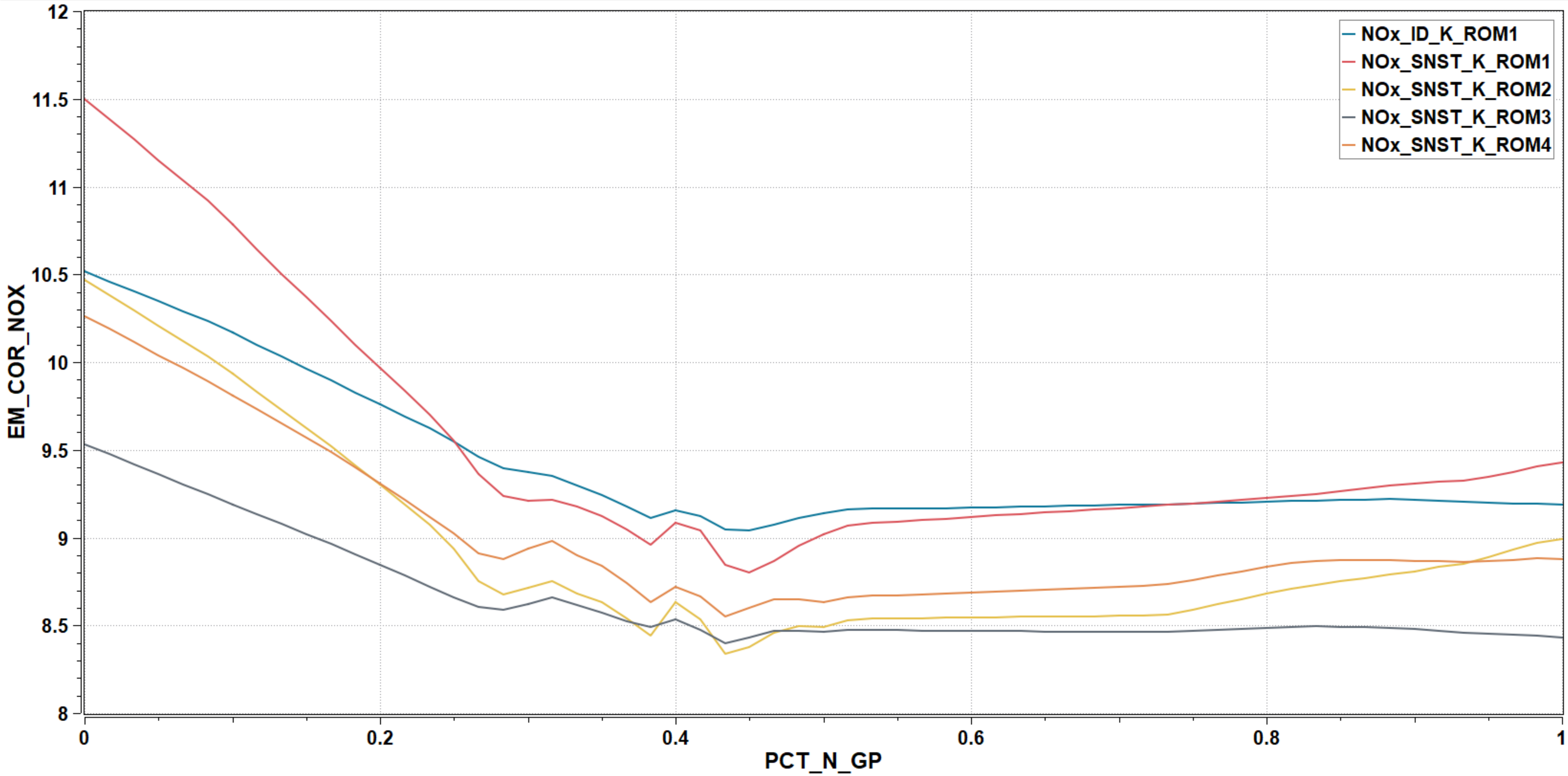
Reduced Model Shape Comparison – Inj. Eff. Area Spread



Reduced Model Shape Comparison – Total Liner Eff. Area



Reduced Model Shape Comparison – % GP Speed

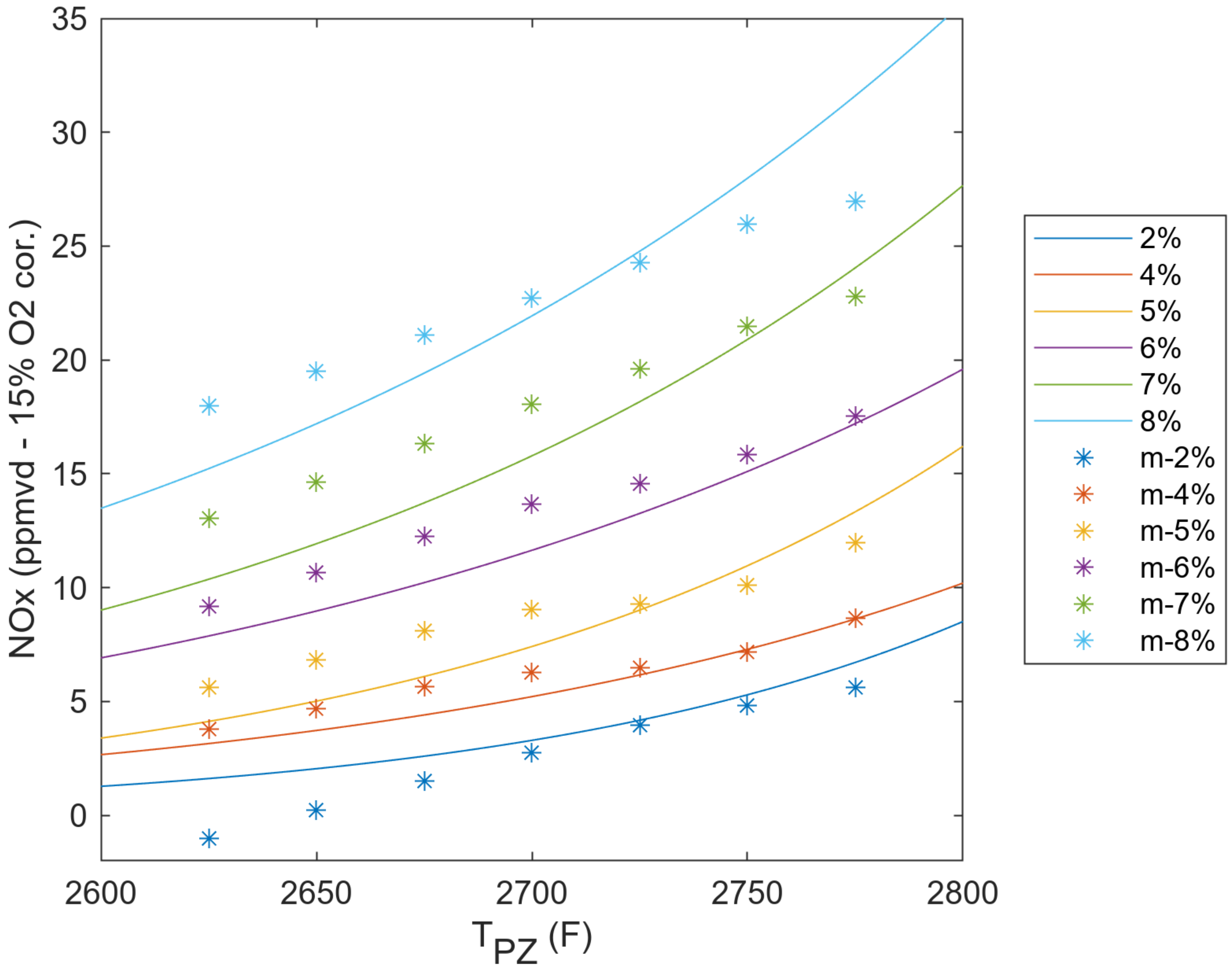


Reduced Model Performance Comparison

Study No.	Rating	Liner	Injector	Data Point Count	Best Model	RSME	Improvement (%)
1	23001S	Any	Any	373	ROM3	0.845 (1.035)	18.36
2	23001S	Any	372240	272	ROM3	0.934 (1.119)	16.53
3	23001S	376445	Any	209	ROM3	0.943 (1.006)	6.26
4	23001S	372784	Any	164	ROM3	0.862 (0.864)	0.23
5	23001S	376445	372240	187	ROM2	1.032 (1.126)	8.35
6	23502S	Any	372240	355	ROM4	0.746 (1.024)	27.15
7	23502S	376445	372240	239	ROM3	1.593 (1.960)	18.72
8	23502S	372784	372240	116	ROM3	0.539 (0.418)	-22.45

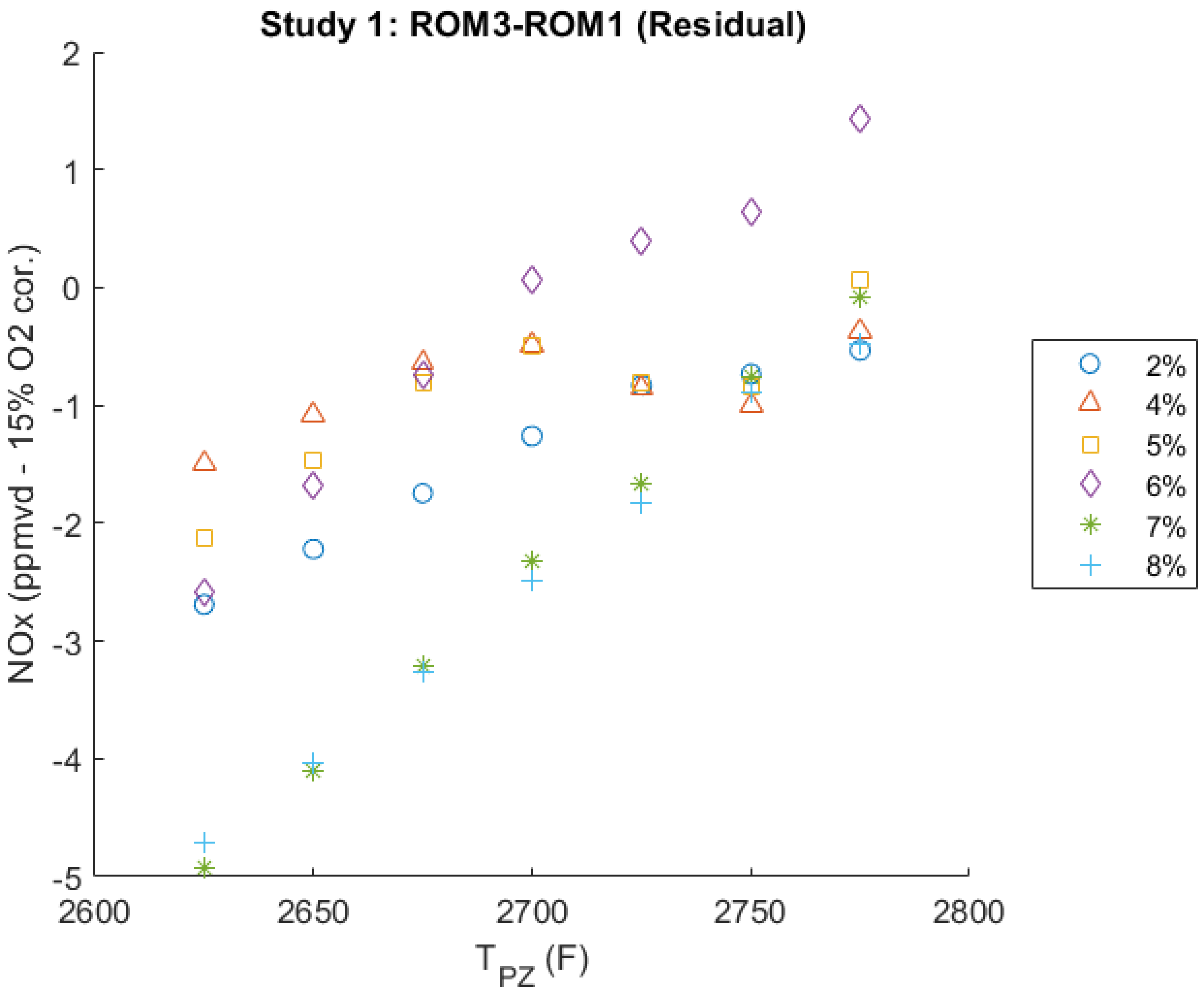
23001S Combustion Map Comparison

- Lines = Jan. 2022 – Jun. 2024 Test Data contours
- Stars = 23001S General ROM3 Predicted NOx
  - Input with ‘dummy’ data
- Larger error at extremes



ROM Compare in Context

- ROM1 generally overpredicts NOX
  - Further overpredicts at low T_PZ, high PCT_PIL vs. ROM3



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Conclusions

- ROMs performed better than ‘full’ models
  - Overfitting to highly correlated data
- Hardware agnostic, rating specific models performed best
  - Likely due to quantity of data
  - ~300-pt. datasets are sufficient to generate NOx models using Kriging methods
- Good models generally abide by trends defined by physics, despite error in raw predicted value

Recommendations for Future Work

- Automate pre-processing
- Continue to build out datasets
  - More data → Better models
- Further validation with various, other hardware versions
  - Determine need for Rating and/or Hardware Specific NOx Models

Acknowledgements

- Dr. Vince McDonell
- Stephen Theron
- Mason Westmoreland
- Shaun Ho
- Tim Caron
- Jon Duckers
- The Solar Combustion Department
- Ryan Ehlig
- John Mason
- Dan Reitz
- Miller Robison
- DOE and SWRI

THANK YOU

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