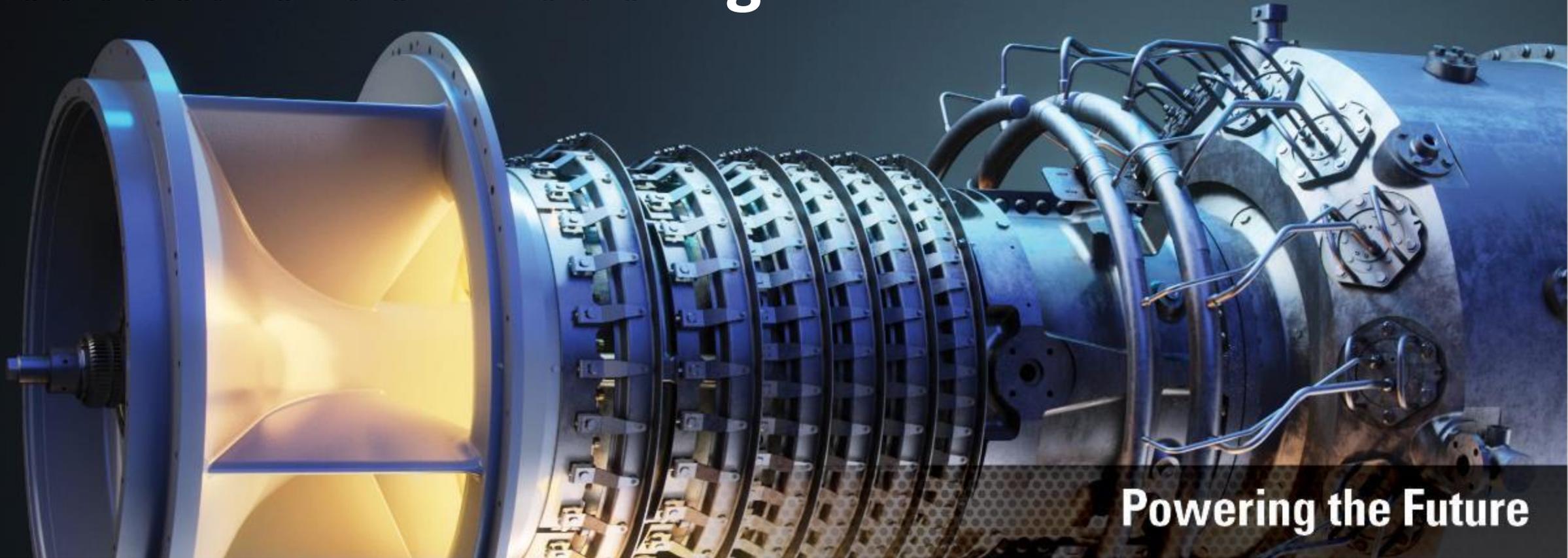


Capturing Engine Emissions (NO_x) Responses via Reduced Order Modeling

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

Malcolm Overbaugh
Solar Turbines & UC Irvine



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Outline

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

NOx Background

- NOx = Nitrogen Oxides
 - Primarily referring to NO for combustion applications, but also includes NO₂ and N₂O
- Sunlight reacts with NOx and VOCs to form tropospheric ozone and smog



Empirical NOx Models

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

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

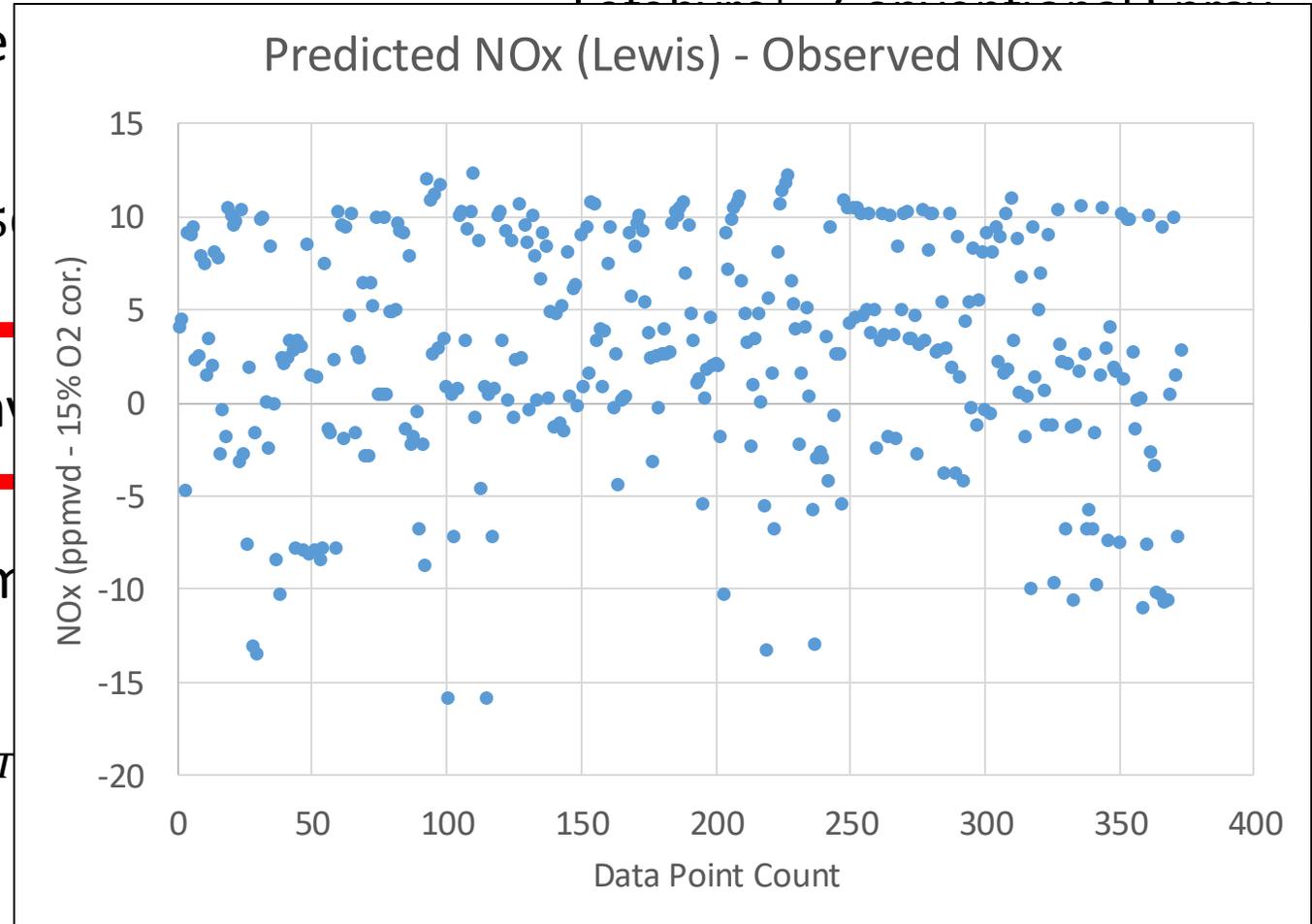
$$3. NO_x = 3.32 \cdot 10^{-6} e^{0.008 T_c} P^{0.5} \text{ (ppm)}$$

Poor Predictive Performance

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

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

(g/kg Fuel)



Generate a predictive model for NO_x 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

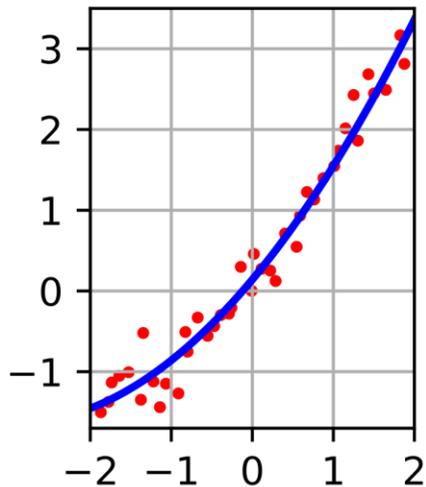
Problem Definition

Modeling with HEEDs



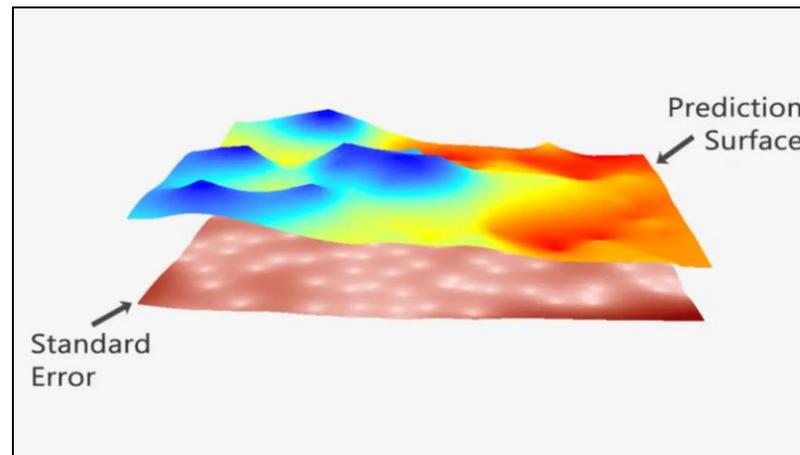
- Regression

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



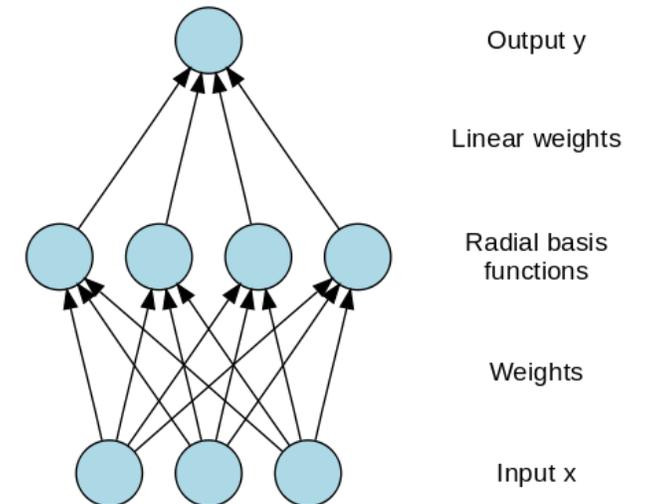
- Kriging

- 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

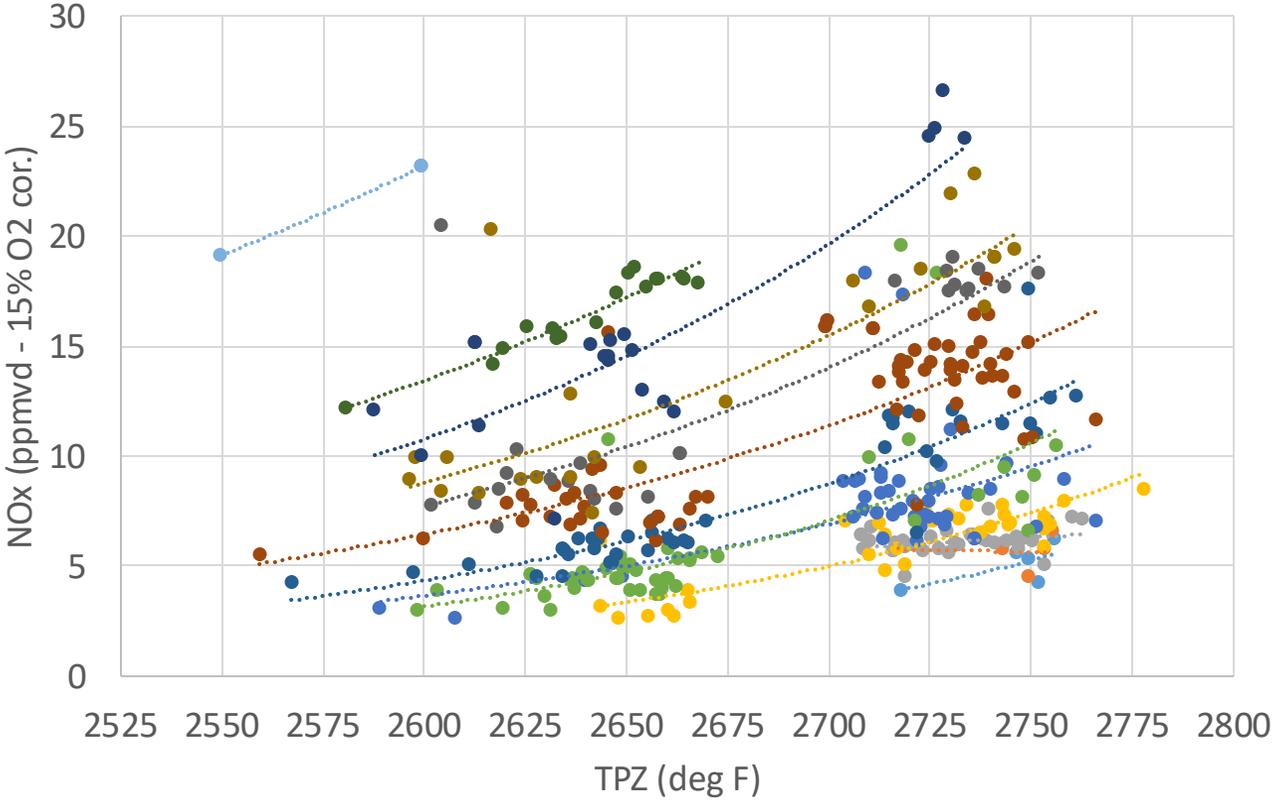


Combustion

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

NOx Performance Context

23001S NOx Map (Pilot % vs. T_PZ)



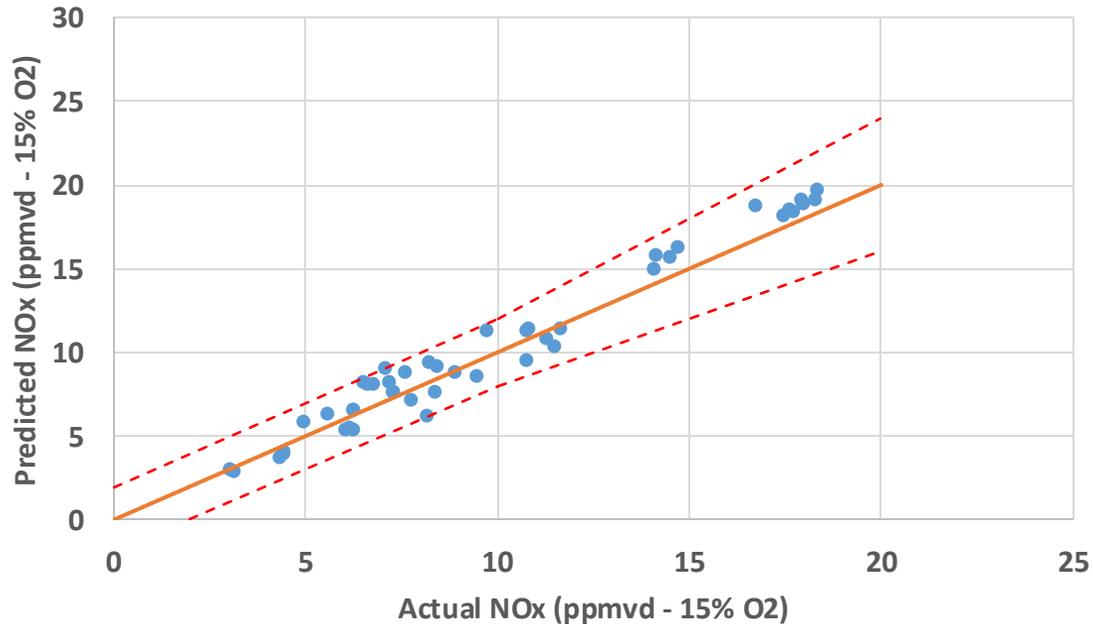
- Pilot % and Cmb. Primary Zone Temp. (TPZ) are highly influential
- Other influential parameters are unclear

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

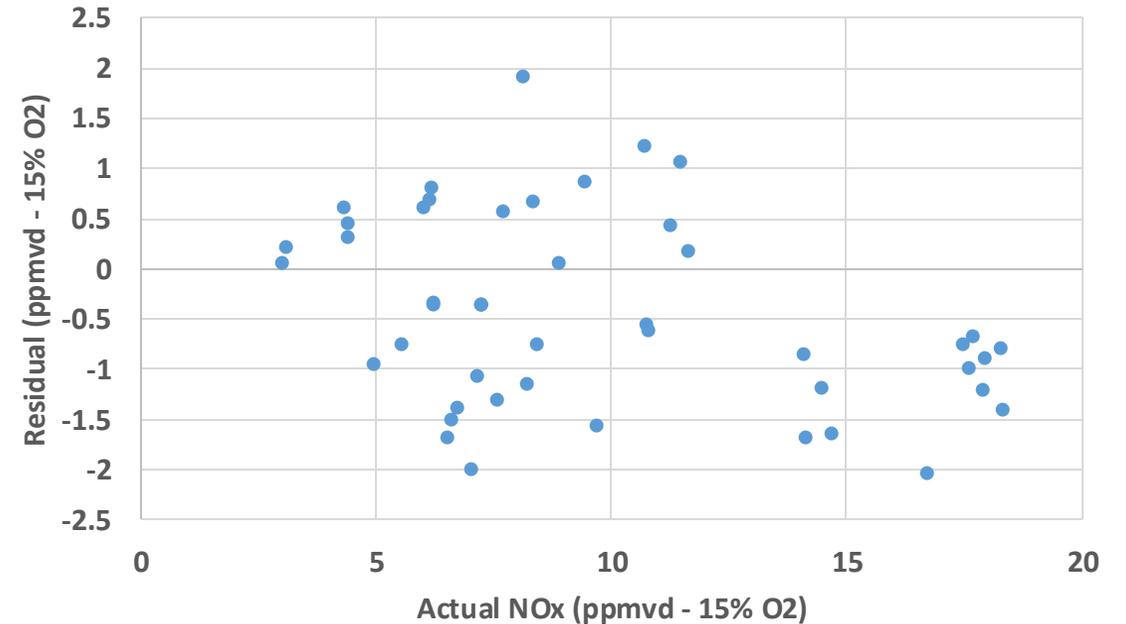
- Linear-Gaussian Kriging Model
- Meets performance standards

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

23001S: 'Full' Model Performance (SNST)



23001S: Full Model Residuals (SNST)



Full Model Conclusions



Full model performs well



Data is derived from Test → Increased amount of instrumentation



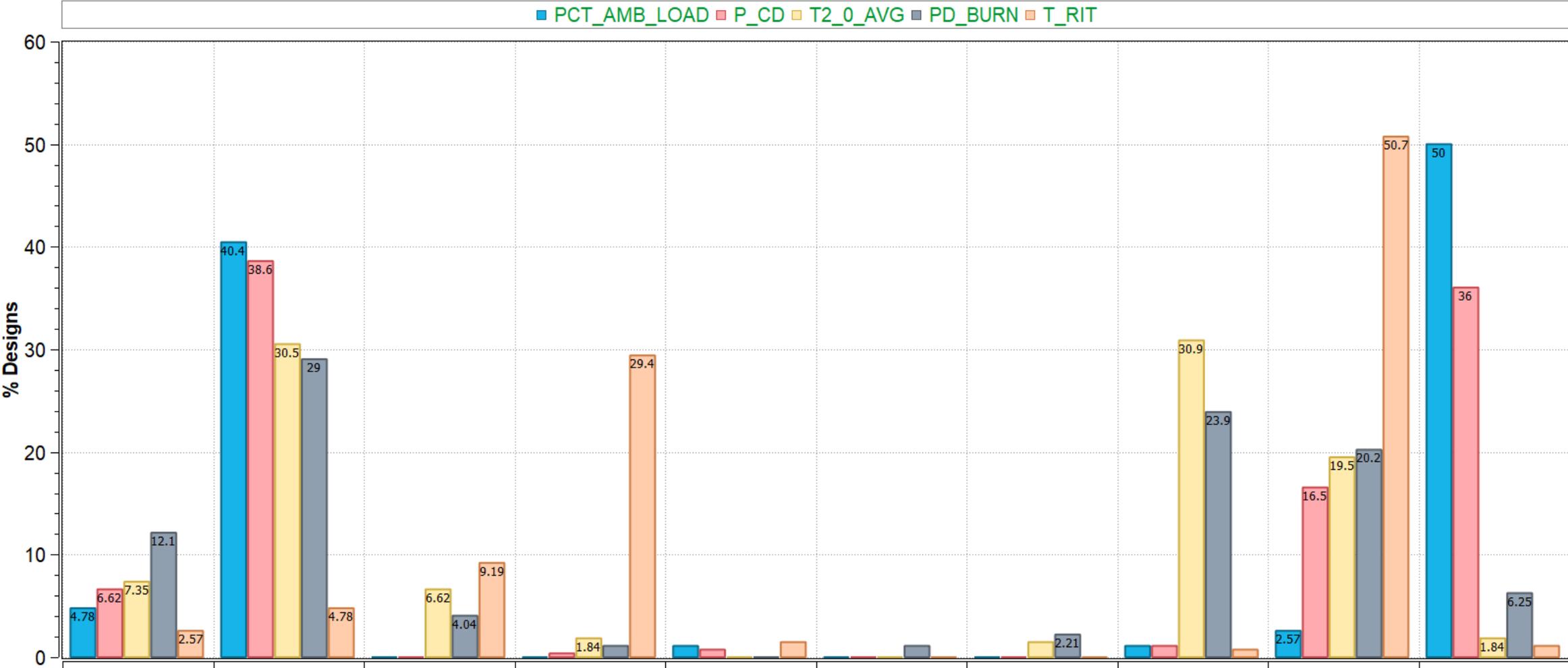
Can the number of inputs be reduced while preserving model efficacy?

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

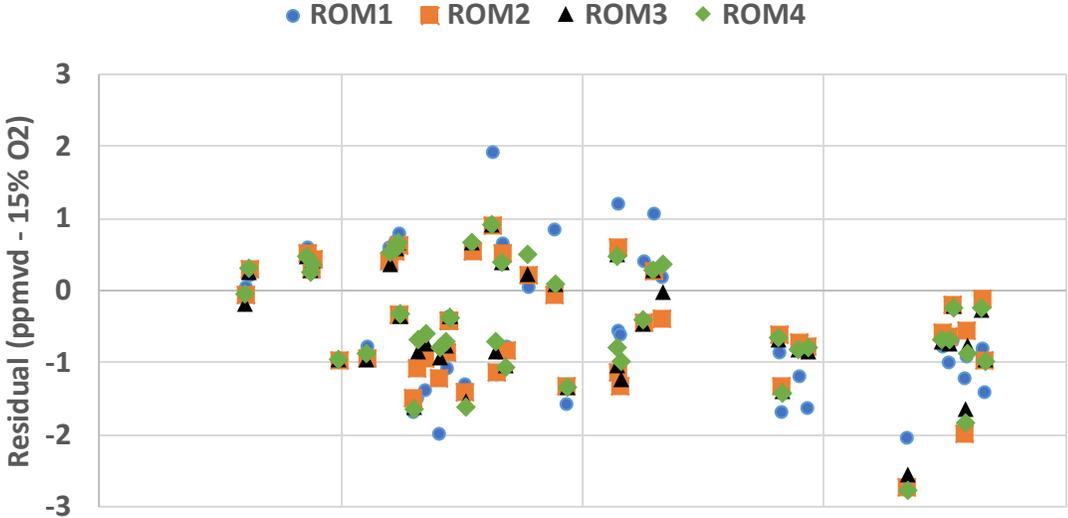
Model Name	Model Input Reductions
Full (ROM 1)	N/A
ROM 2	PD_BURN, P_CD, T2_avg, T2_spr, T_RIT
ROM 3	PCT_AMB_LOAD
ROM 4	T_PZ

Reduced Model Performance

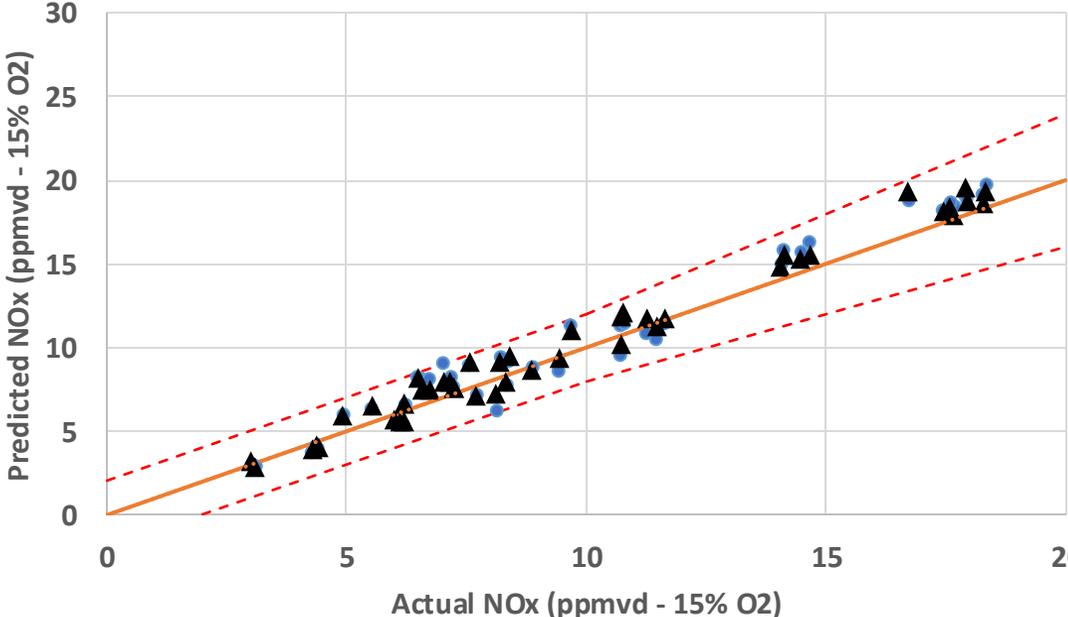
- ~18% overall improvement of model performance
- Some outliers show reduced predictive accuracy

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

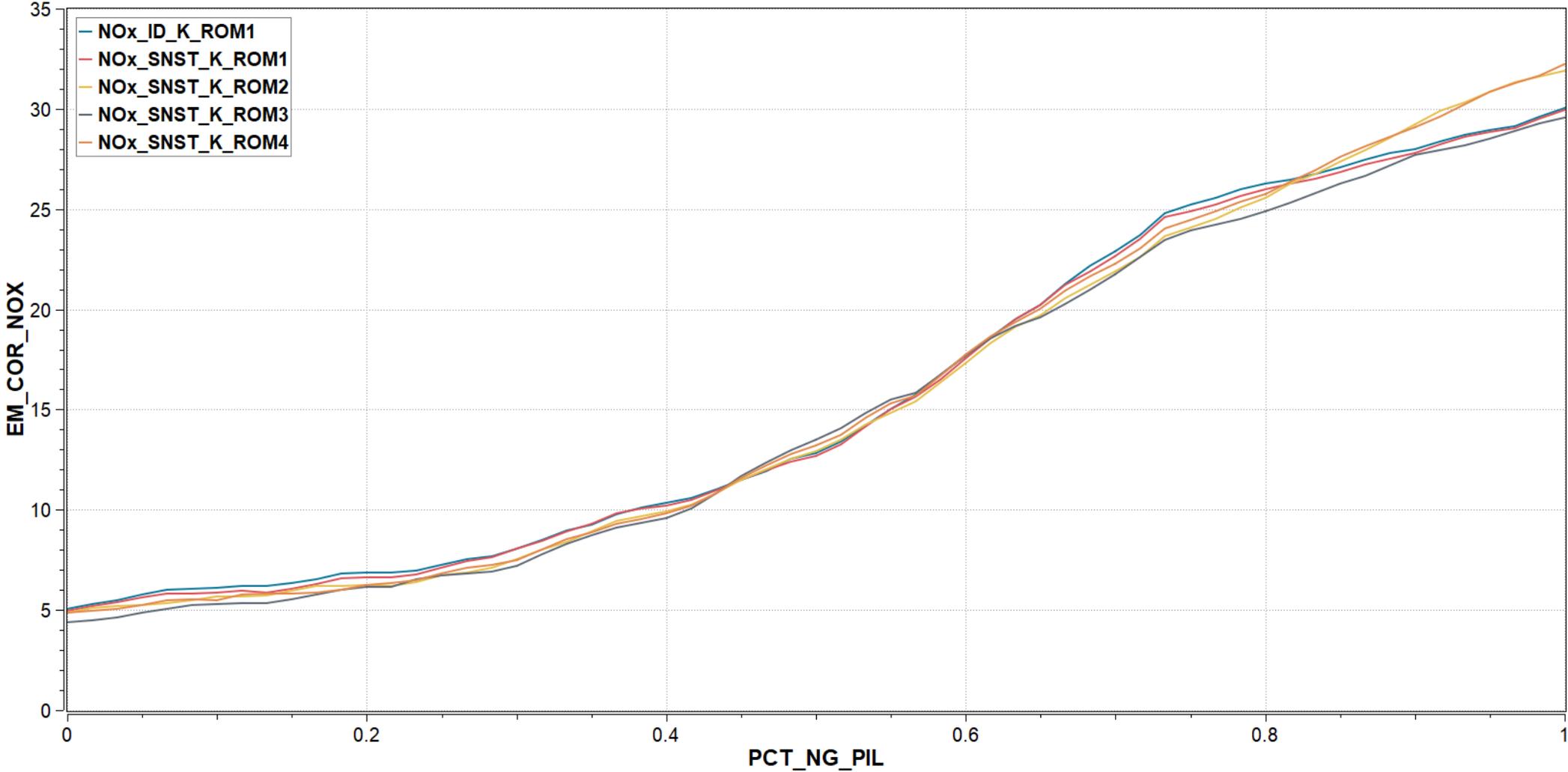
23001S: ROM Comparison (SNST)



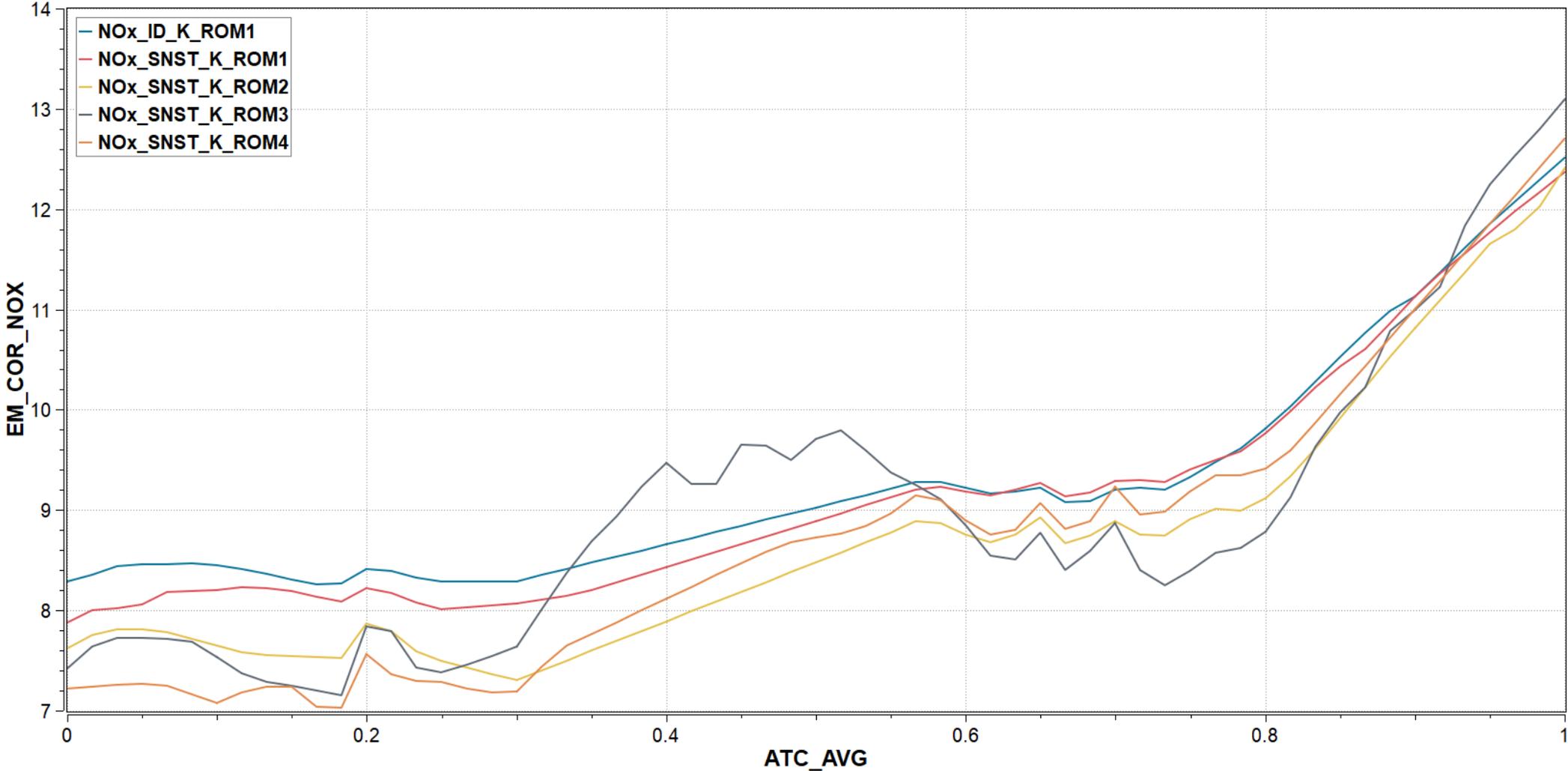
23001S: 'Full' vs ROM3 Perf. (SNST)



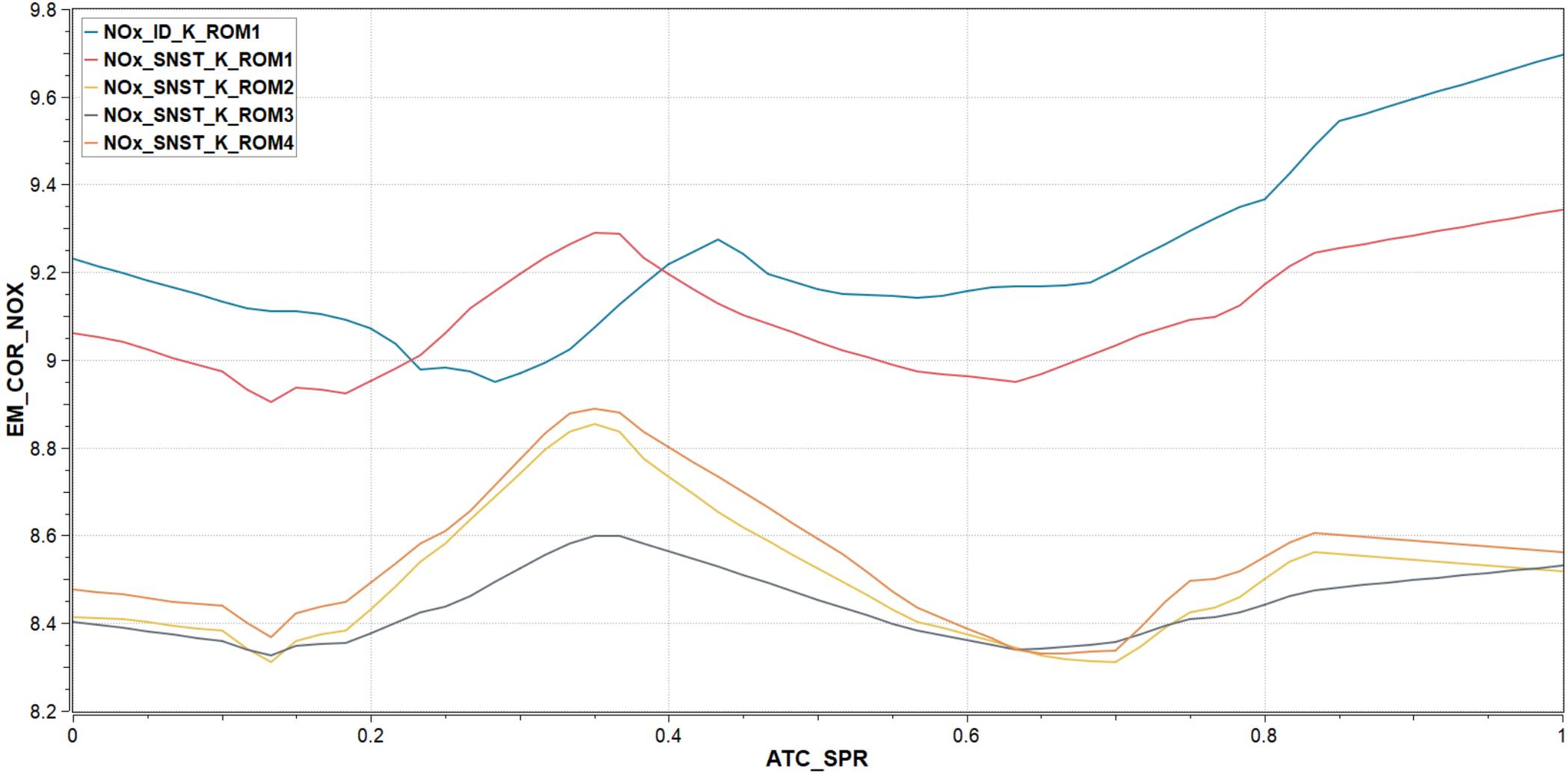
Reduced Model Shape Comparison - % Pilot



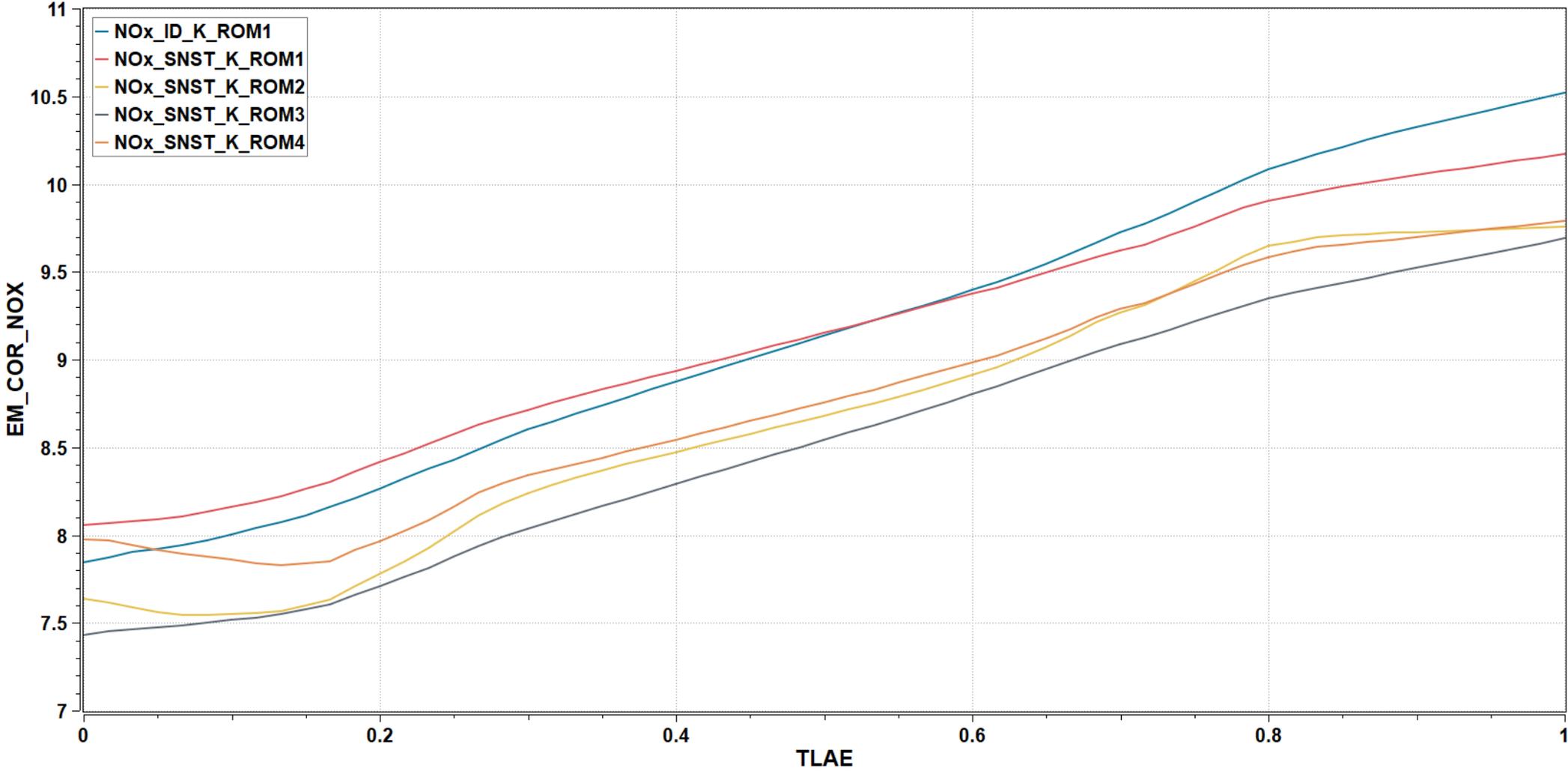
Reduced Model Shape Comparison – Inj. Eff. Area Avg.



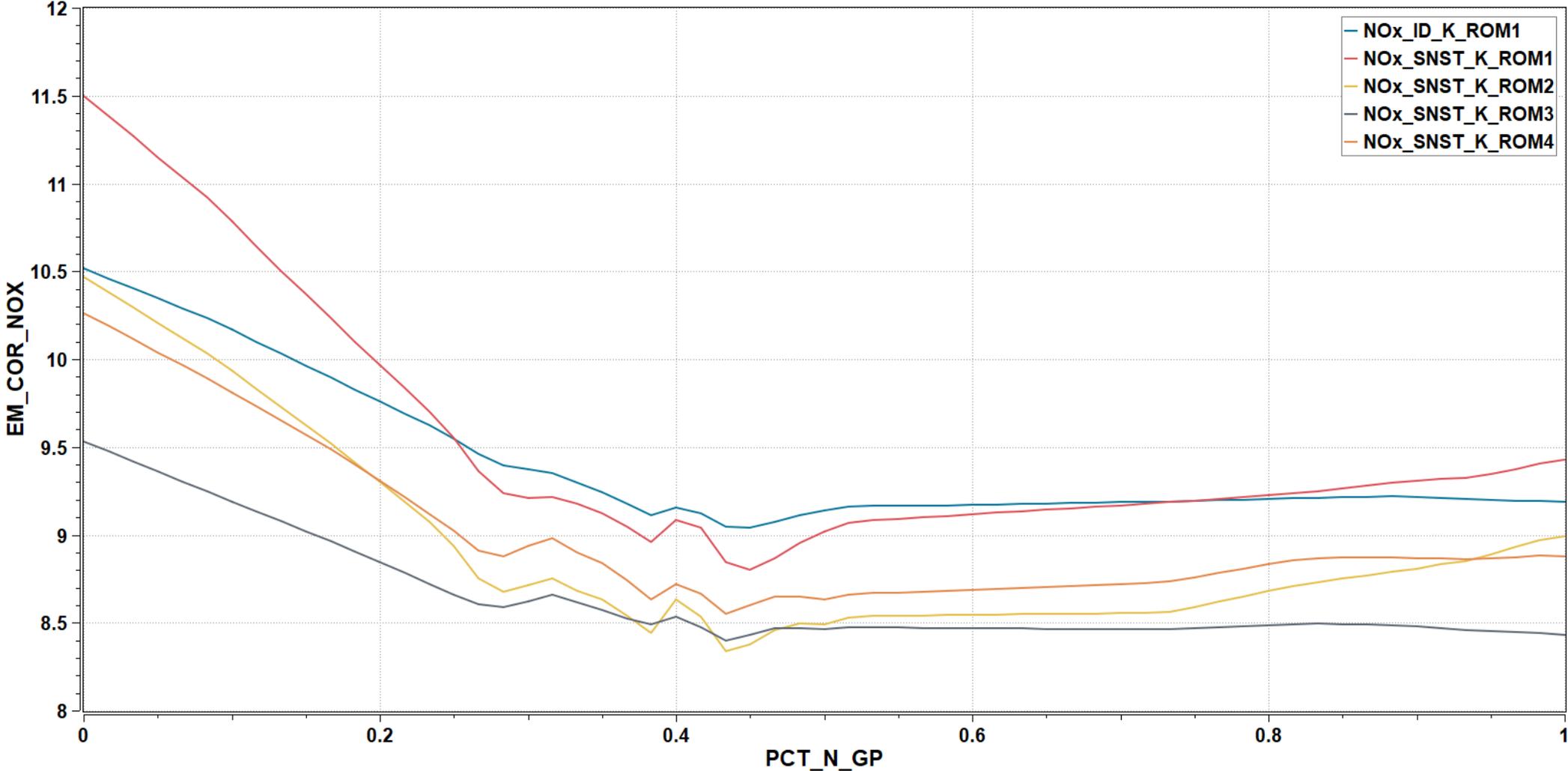
Reduced Model Shape Comparison – Inj. Eff. Area Spread



Reduced Model Shape Comparison – Total Liner Eff. Area



Reduced Model Shape Comparison – % GP Speed

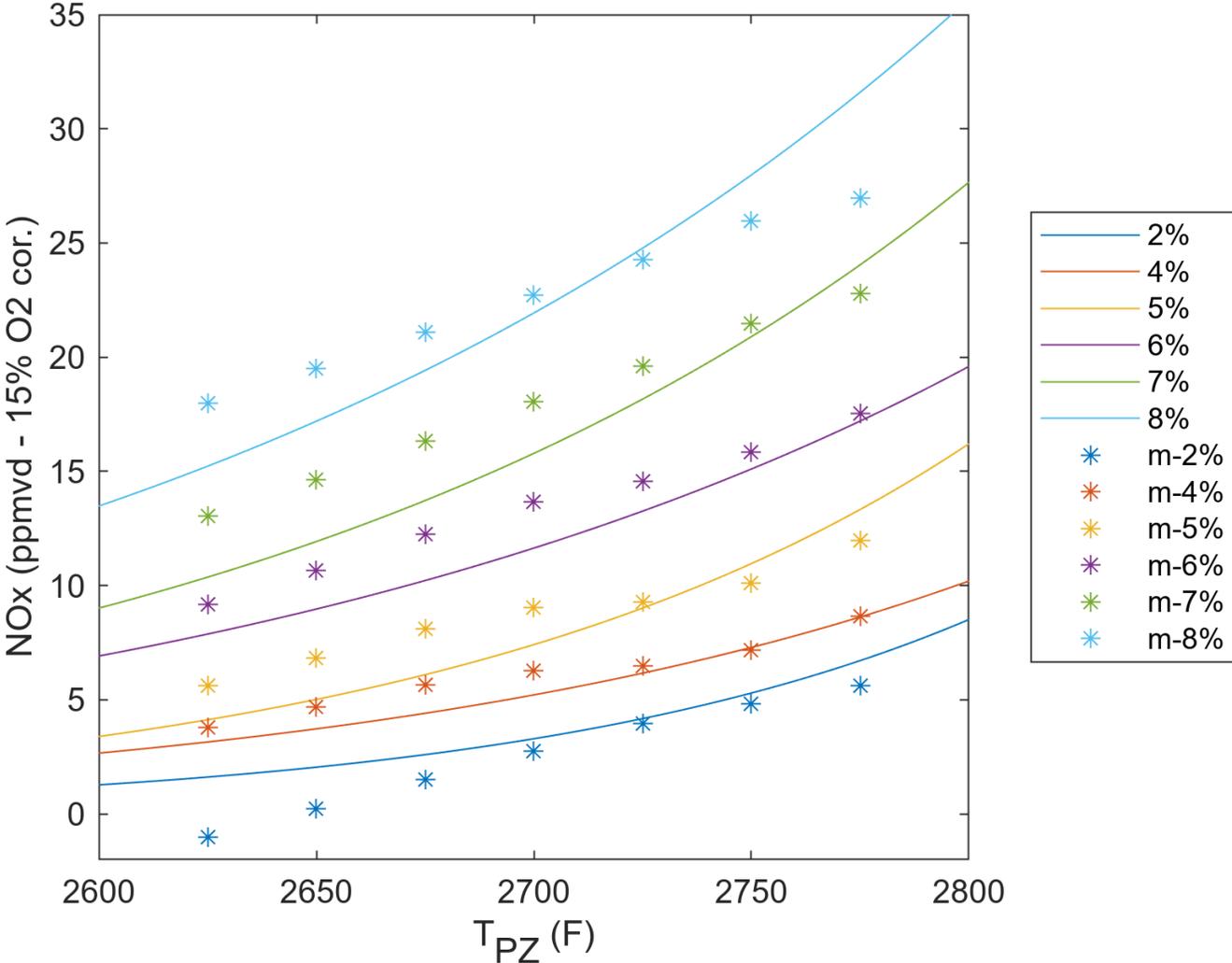


Reduced Model Performance Comparison

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

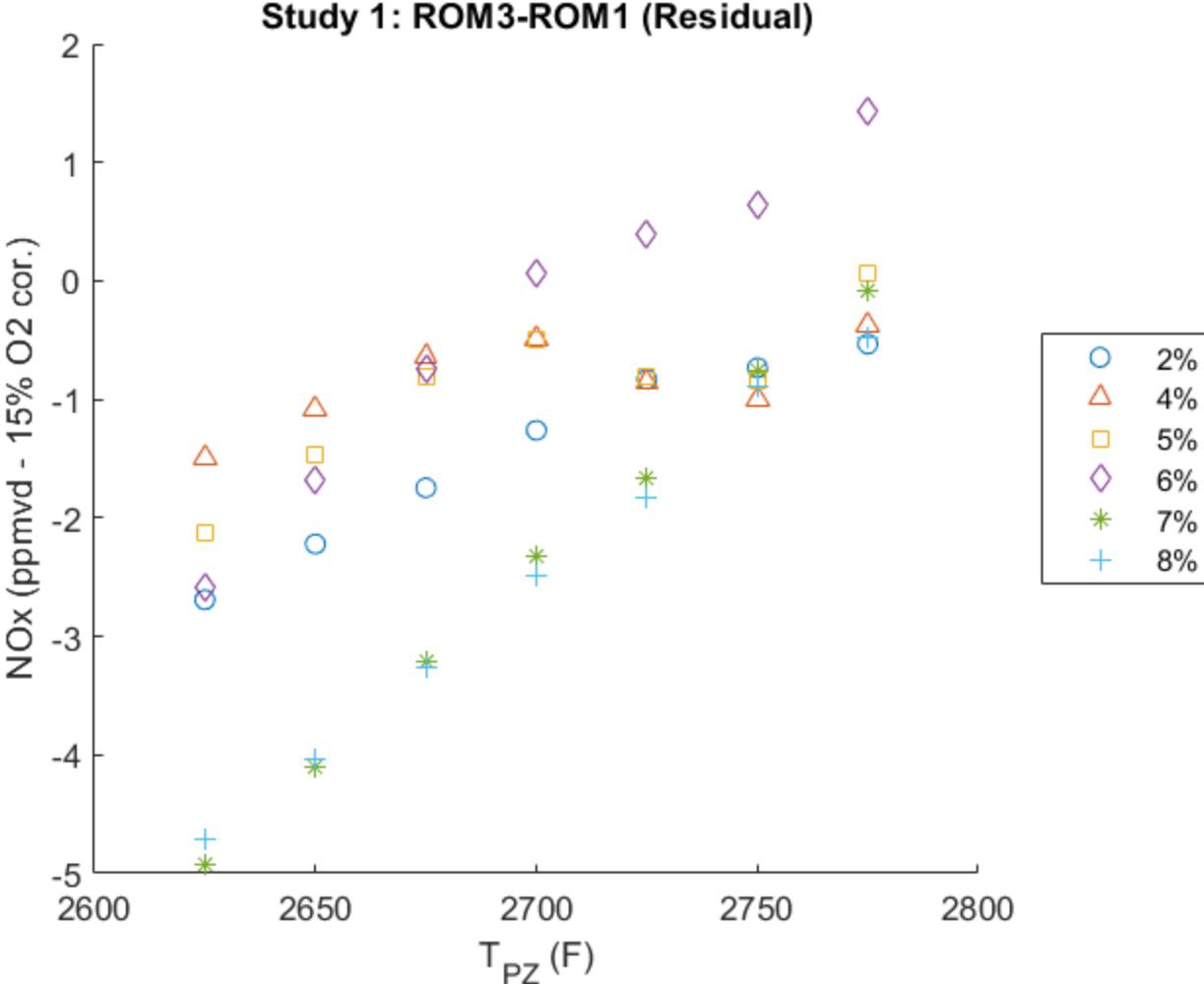
23001S Combustion Map Comparison

- 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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Outline

- Background
- NOx Modeling
- **Conclusions**
- **Acknowledgments**

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

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THANK YOU

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