# Atmospheric Chemistry Modeling using Machine Learning

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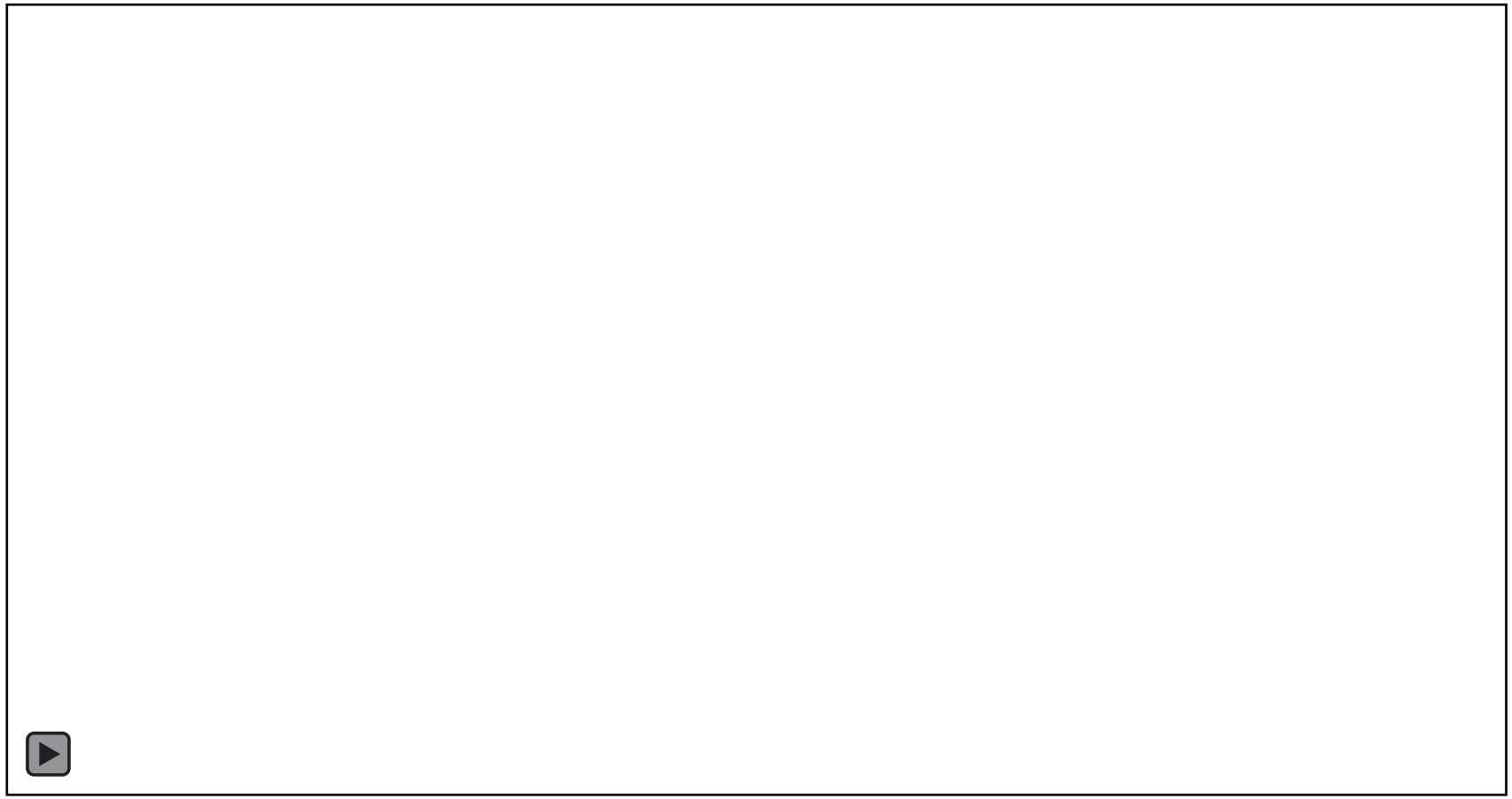
# Numerical simulation of atmospheric chemistry



- 0.25° resolution (~ 25km), 72 levels, 250 chemical species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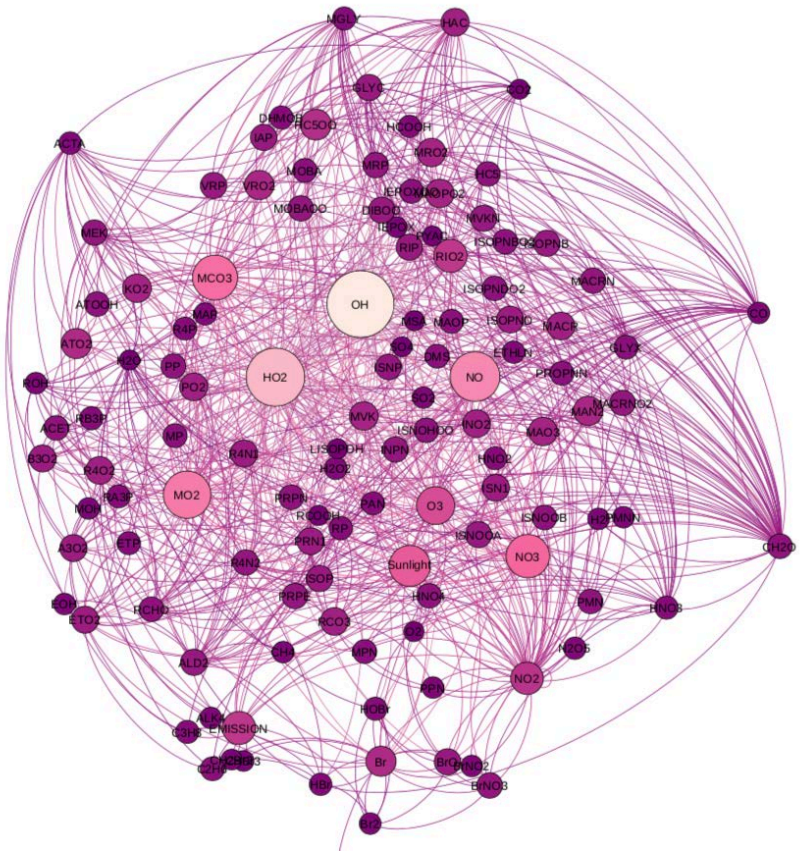
# Numerical simulation of atmospheric chemistry



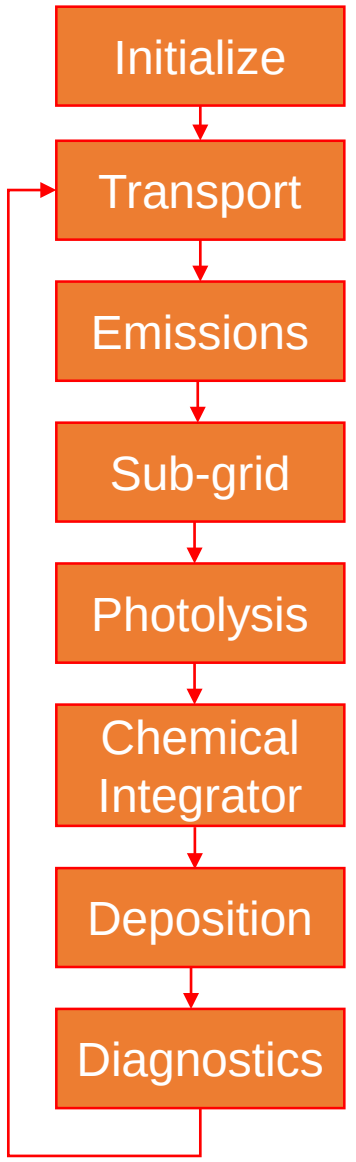

**Transport process:** Move chemicals across grid boxes

**Chemistry process:** In each grid box, solve chemical reactions, i.e. solve stiff ordinary differential equations (ODEs)

$$A + B \rightarrow C + D$$

its rate is calculated as

$$-\frac{d}{dt}[A] = -\frac{d}{dt}[B] = \frac{d}{dt}[C] = \frac{d}{dt}[D] = k[A][B]$$





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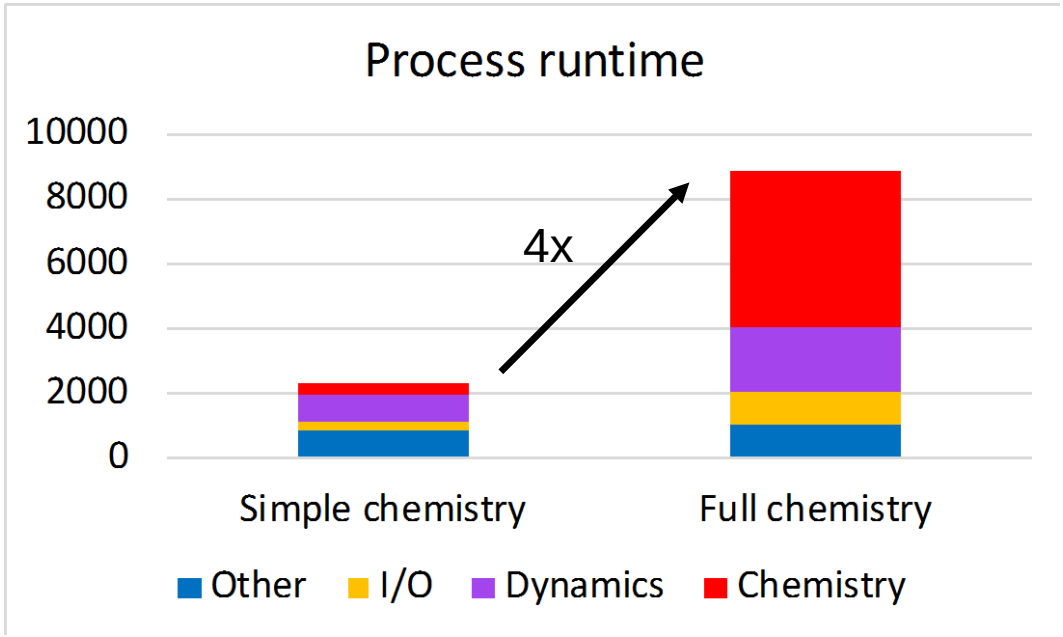
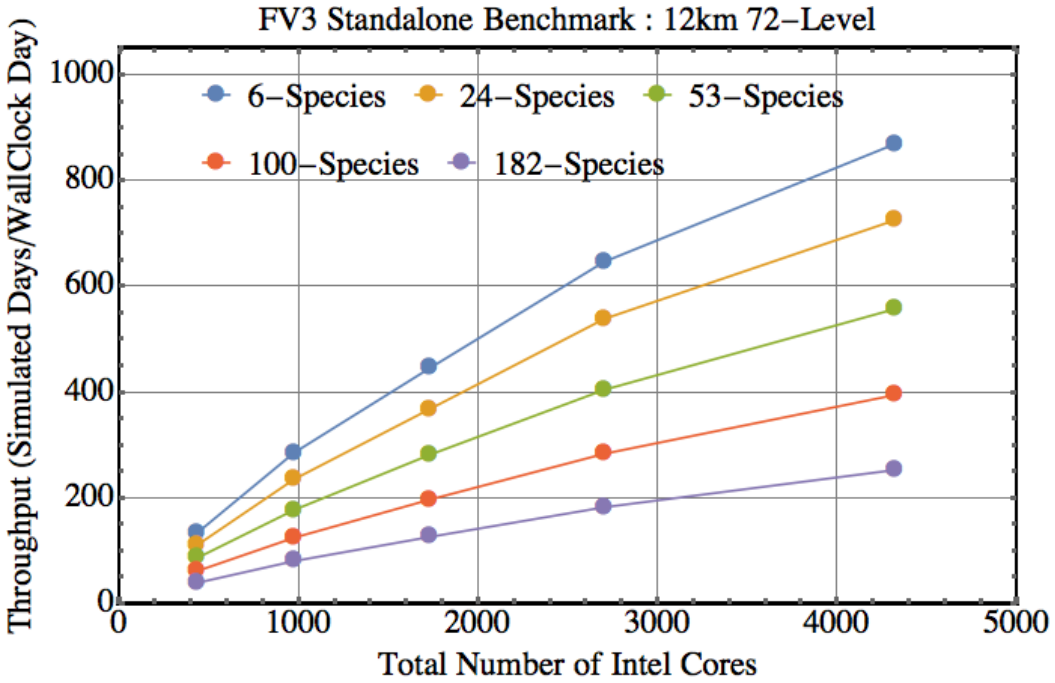
# The current solution: wait, wait, wait




Courtesy of W. Putman, NASA GMAO

- High-resolution chemistry simulation requires 3416 CPU's
- Can simulate approx. 20 days in 24 hours
- Outputting the full chemical state is 1.5 TB / simulation day



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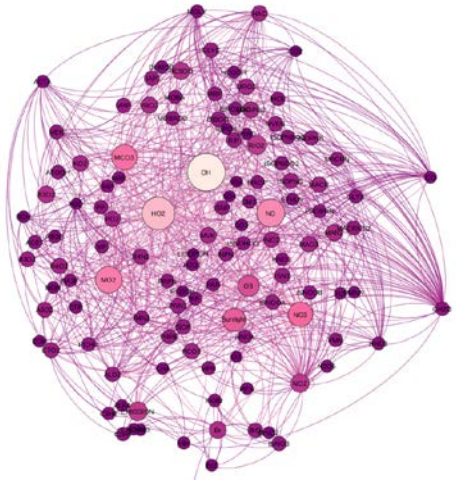
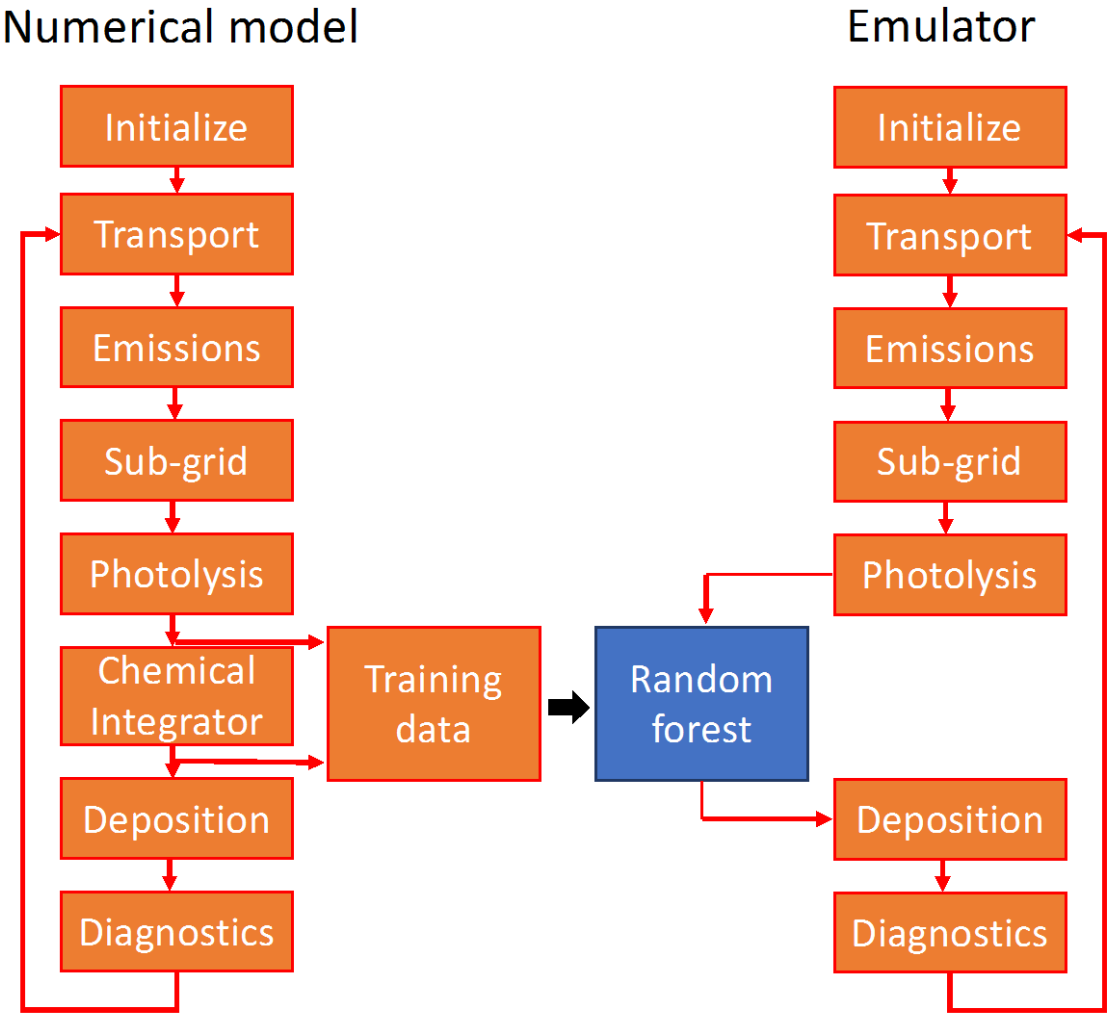
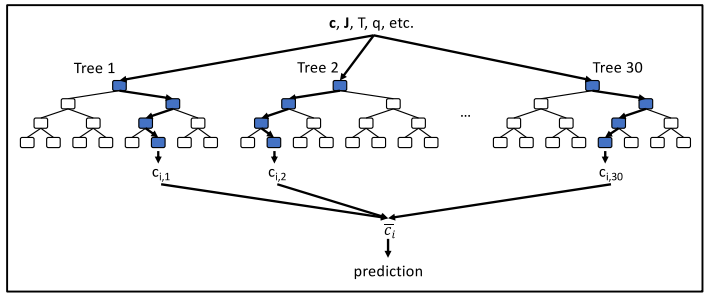
# Replace chemical integrator with machine learning model







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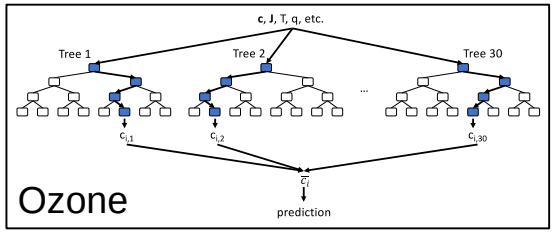
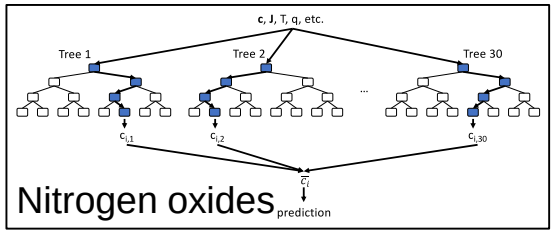
# Machine learning for atmospheric chemistry modeling

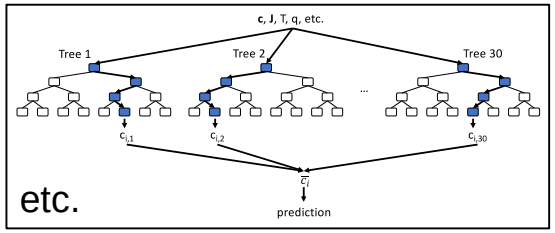
- 143 chemical species
- 91 photolysis rates
- Temperature
- Pressure
- Rel. humidity
- Solar zenith angle

Concentrations after chemistry

Separate model for each species




- Training data set has 2.7 billion data points (44 GB)
- Tested: (neural network), random forest and XGBoost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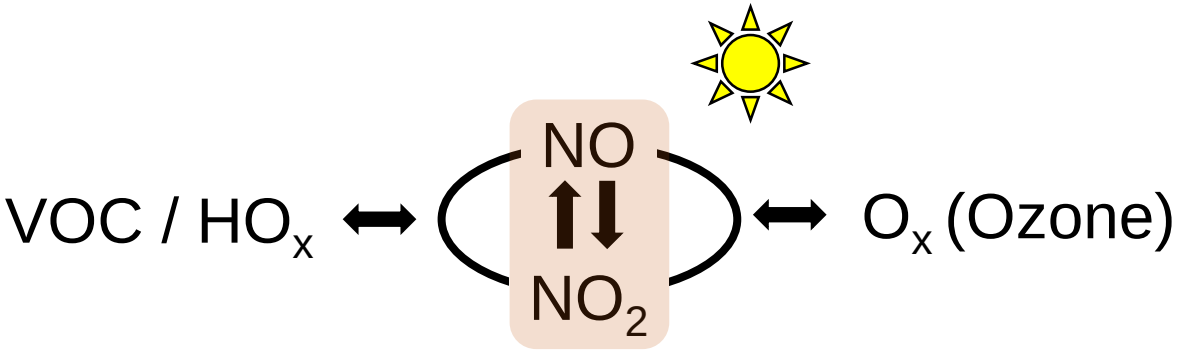
# Impose chemical constraints on ML model to improve (long-term) accuracy

## 1. Distinguish between short-term vs. long-term species

Long-lived (tendencies): $[X_i]_{T+\Delta T} = [X_i]_T + f(\mathbf{k, J, [X]})$

Short-lived (steady state): $[X_i]_{T+\Delta T} = f(\mathbf{k, J, [X]})$

## 2. Predict NO + $NO_2$ combined (NOx family approach)





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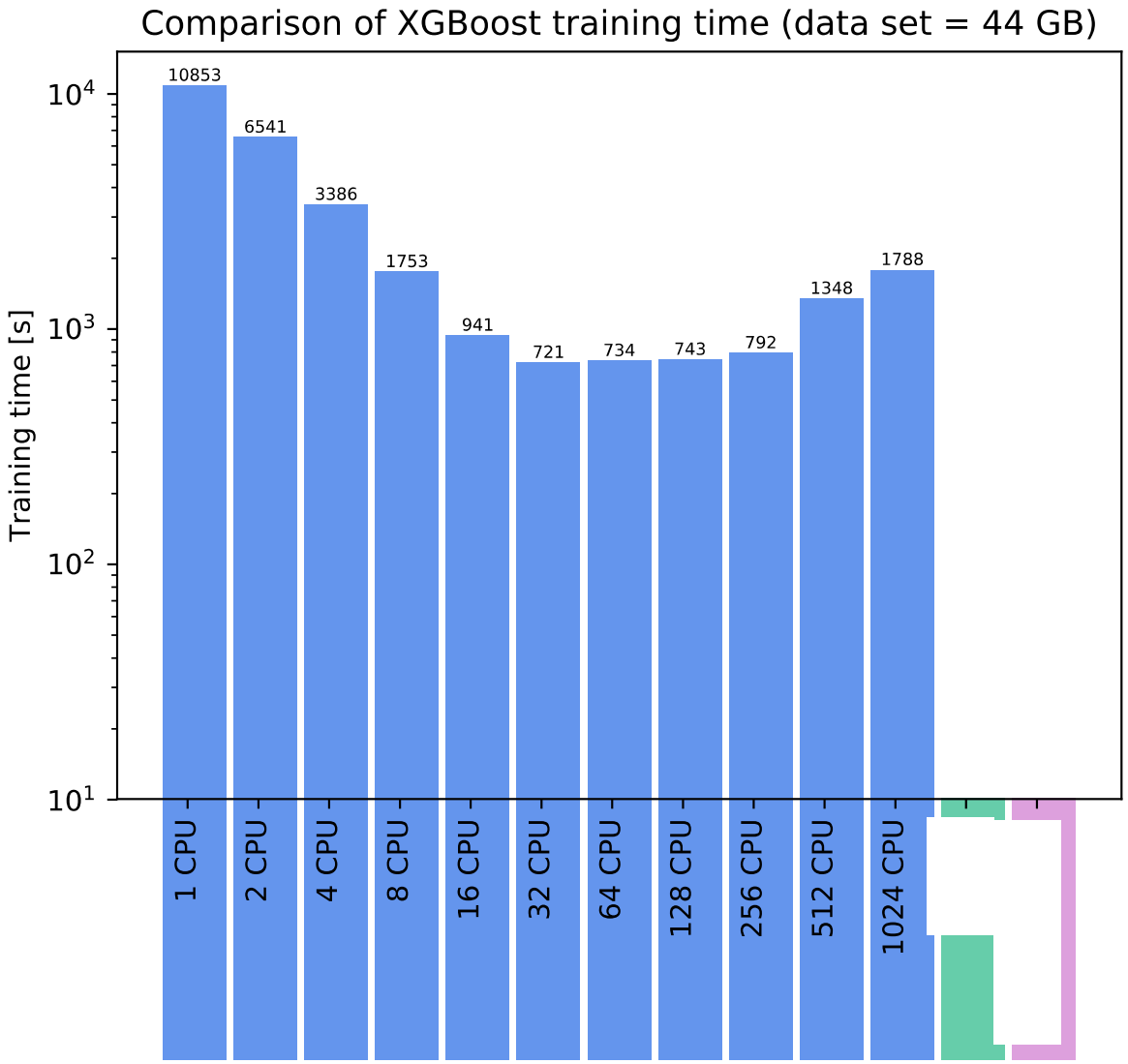
# Random forest / XGBoost training benchmarks





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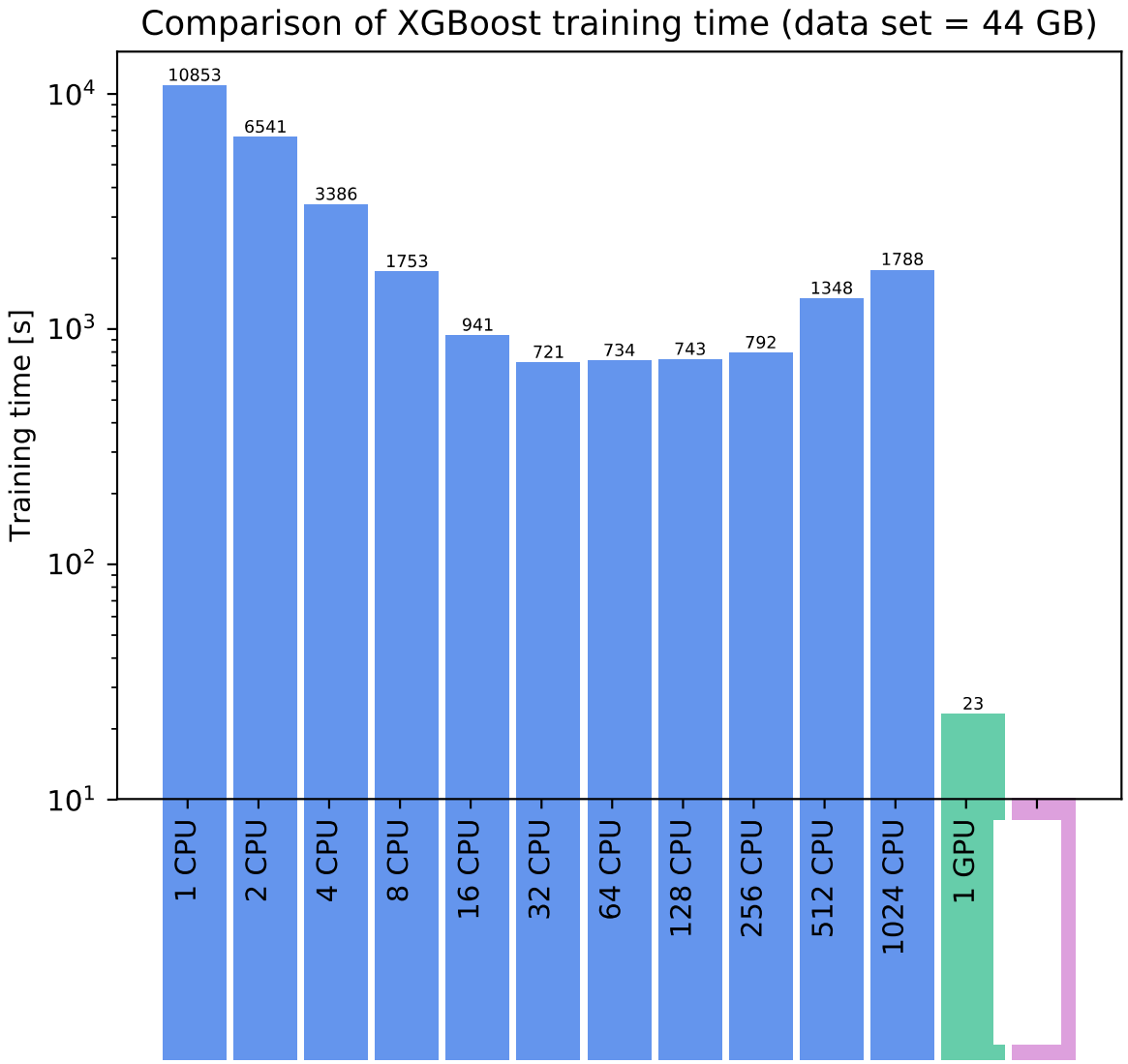



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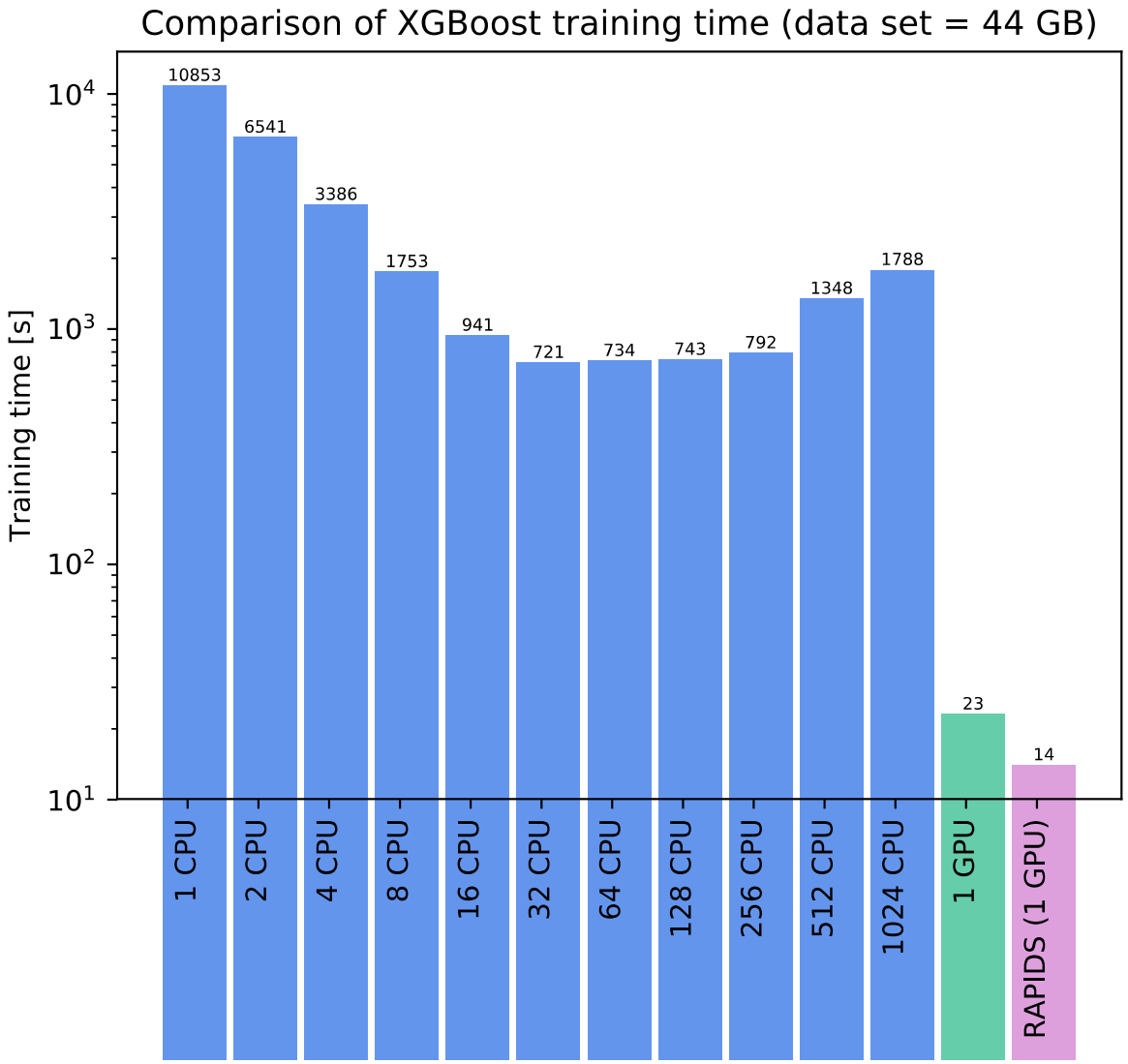



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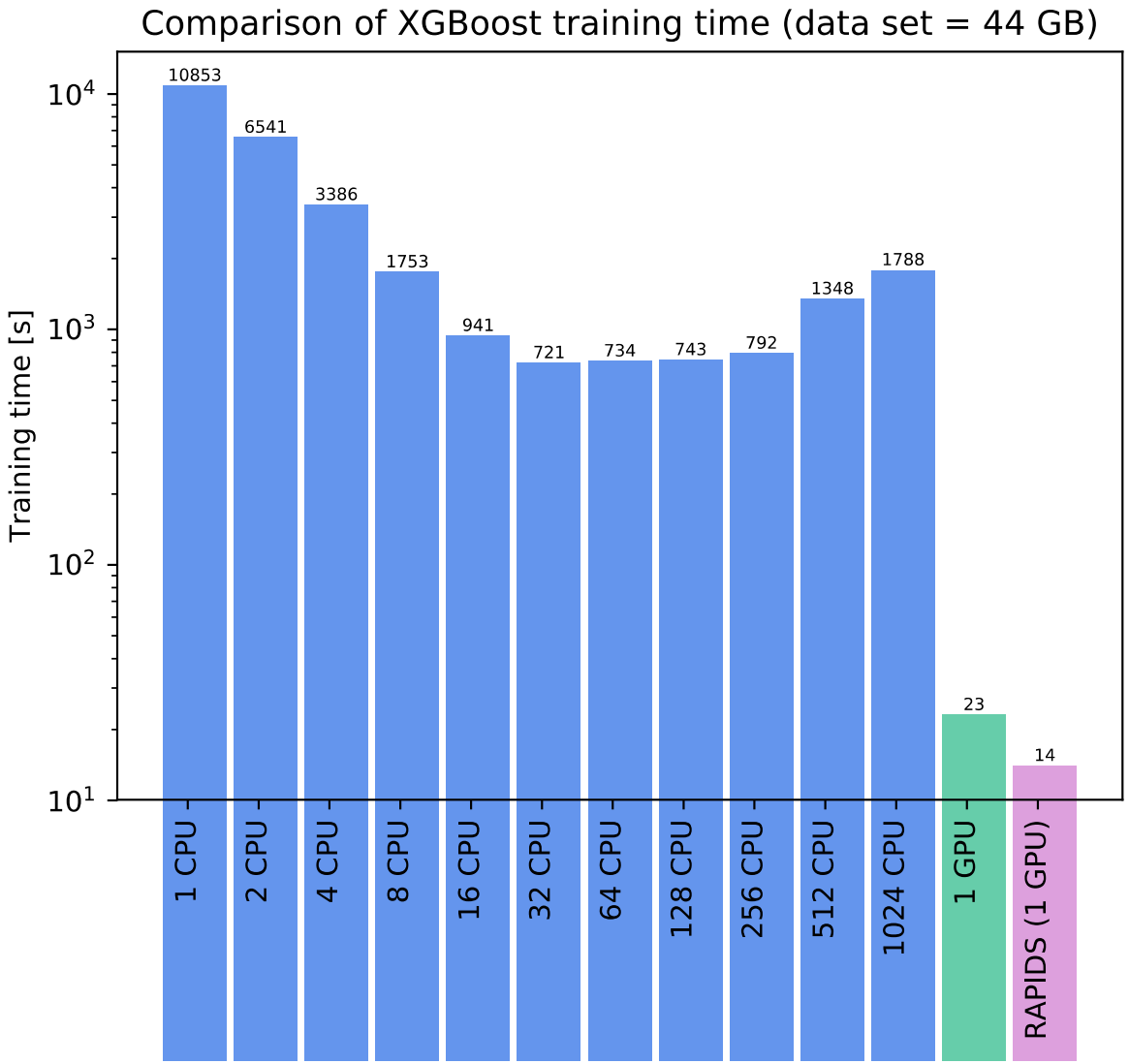


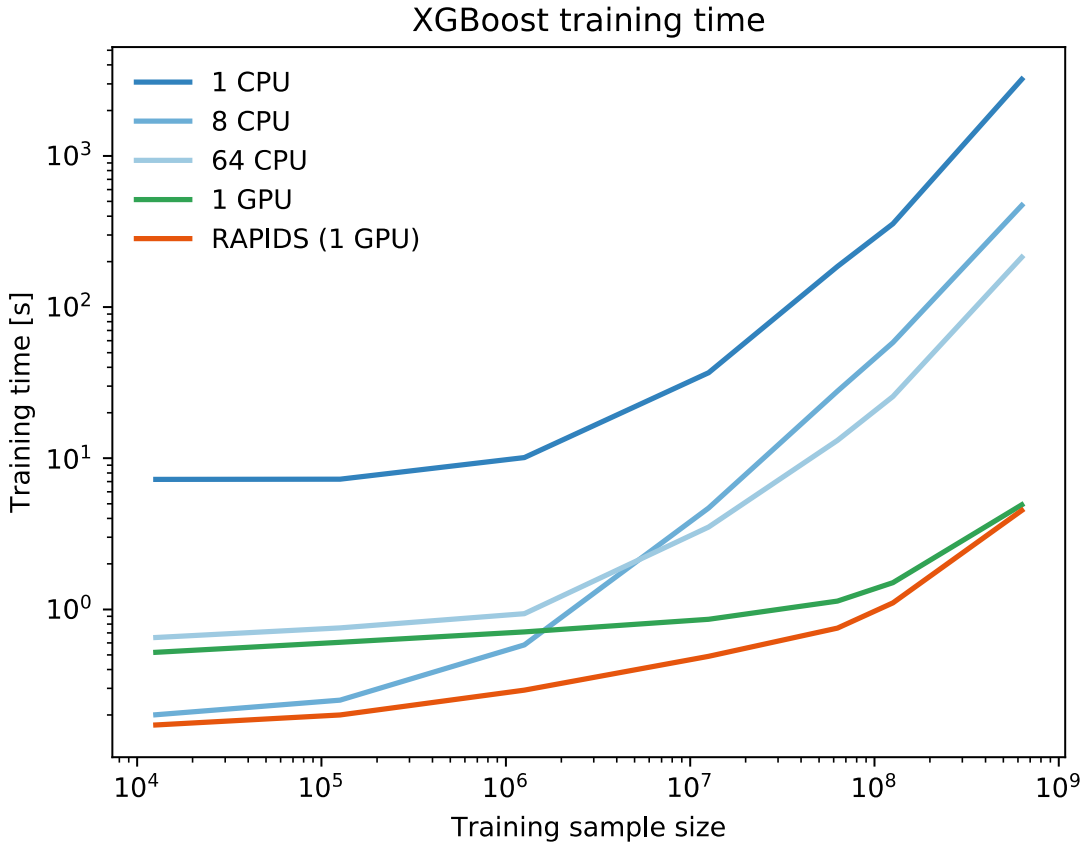



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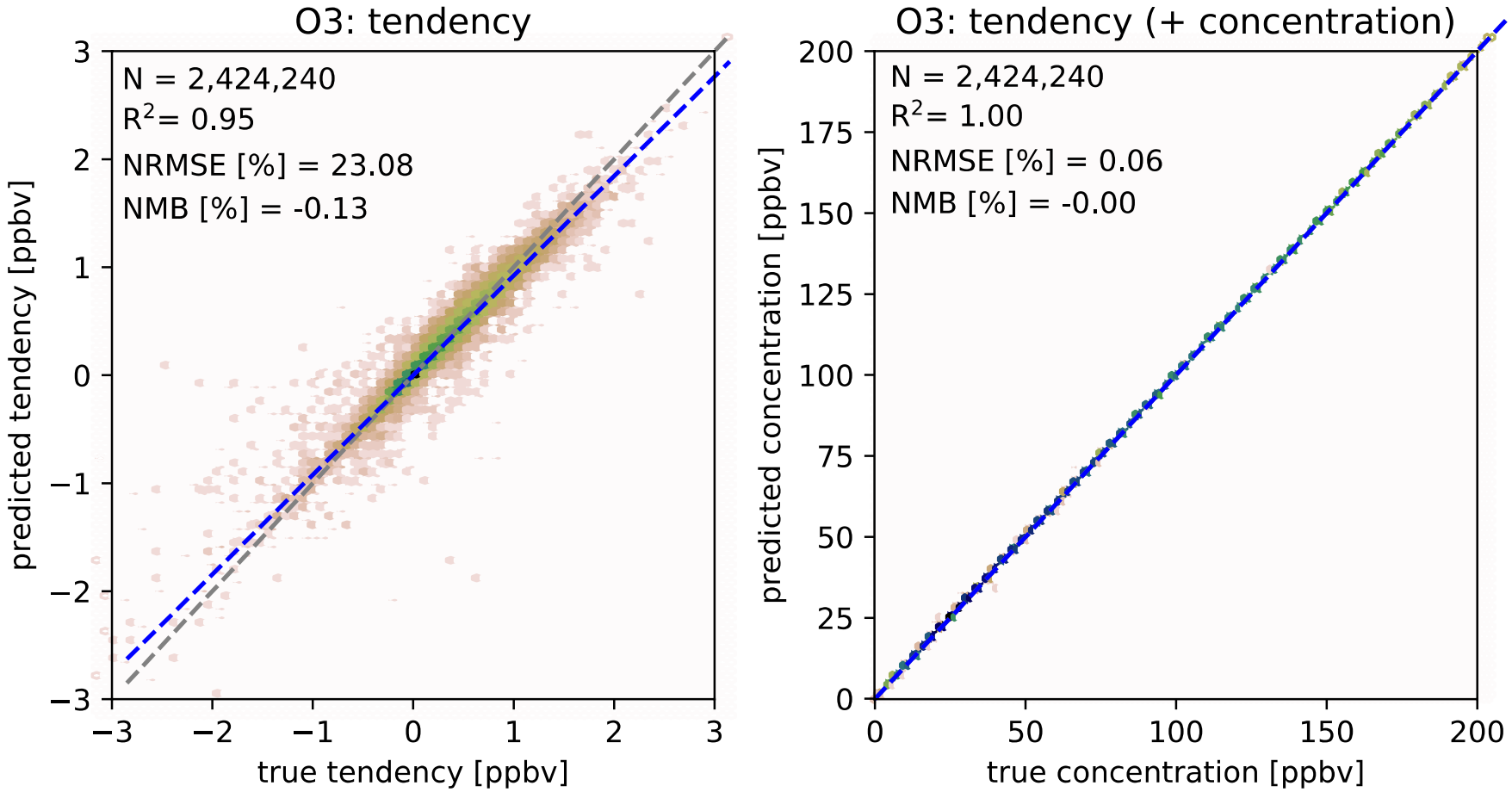
# Random forest / XGBoost can reproduce target concentrations almost perfectly (single-step prediction)





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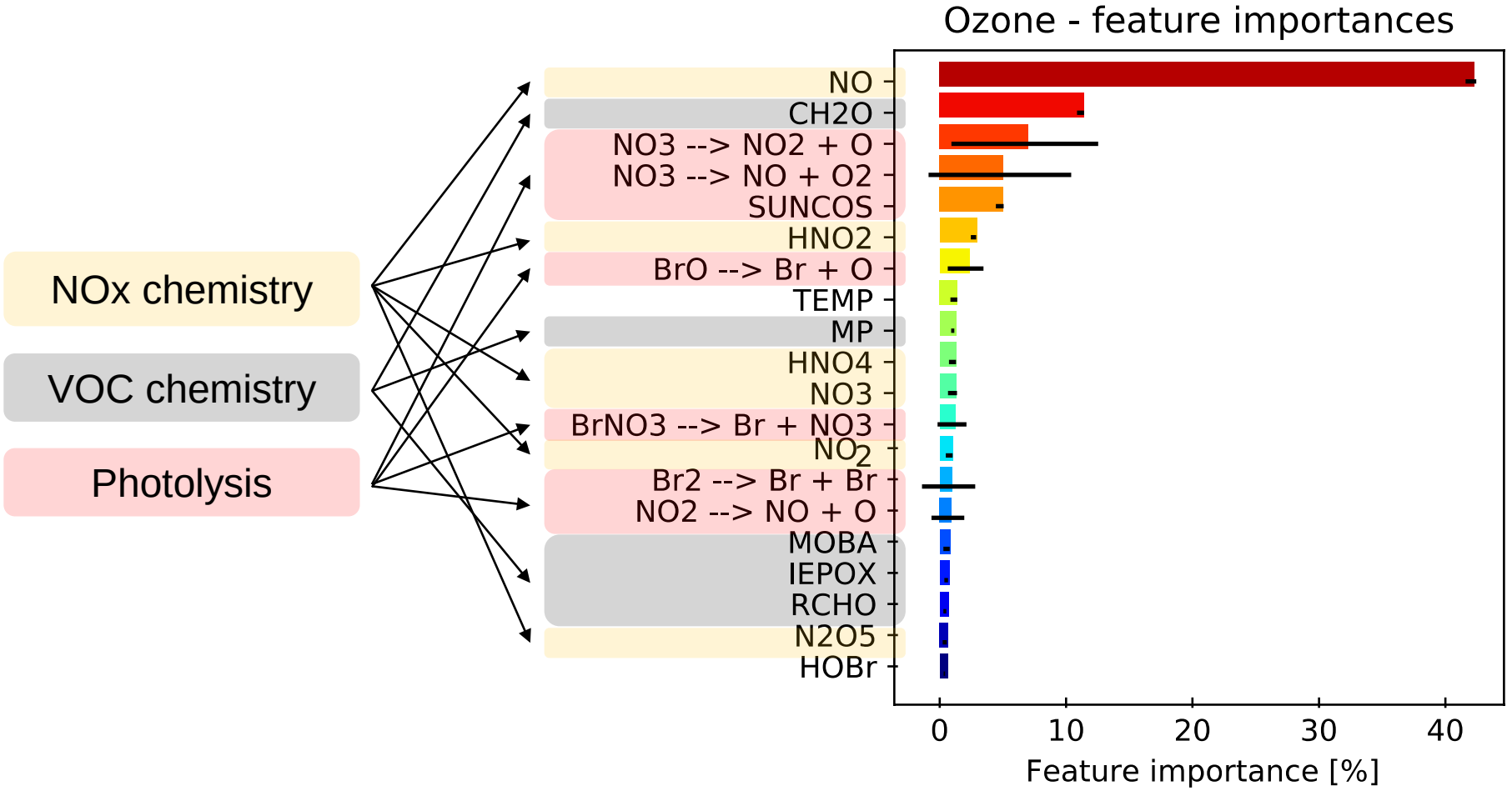
# Random forest / XGBoost solutions reflect known features of chemical kinetics





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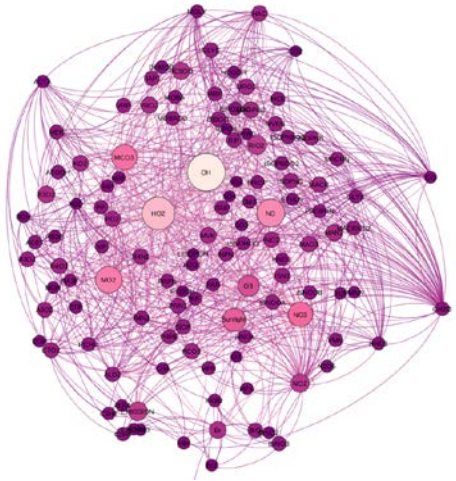
# 1-month simulation with random forest emulator



Numerical model

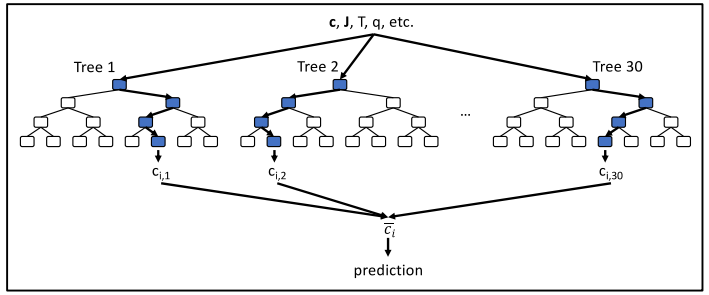
Initialize
Transport
Emissions
Sub-grid
Photolysis
Chemical Integrator
Deposition
Diagnostics

Training data

Random forest

Emulator

Initialize
Transport
Emissions
Sub-grid
Photolysis
Deposition
Diagnostics





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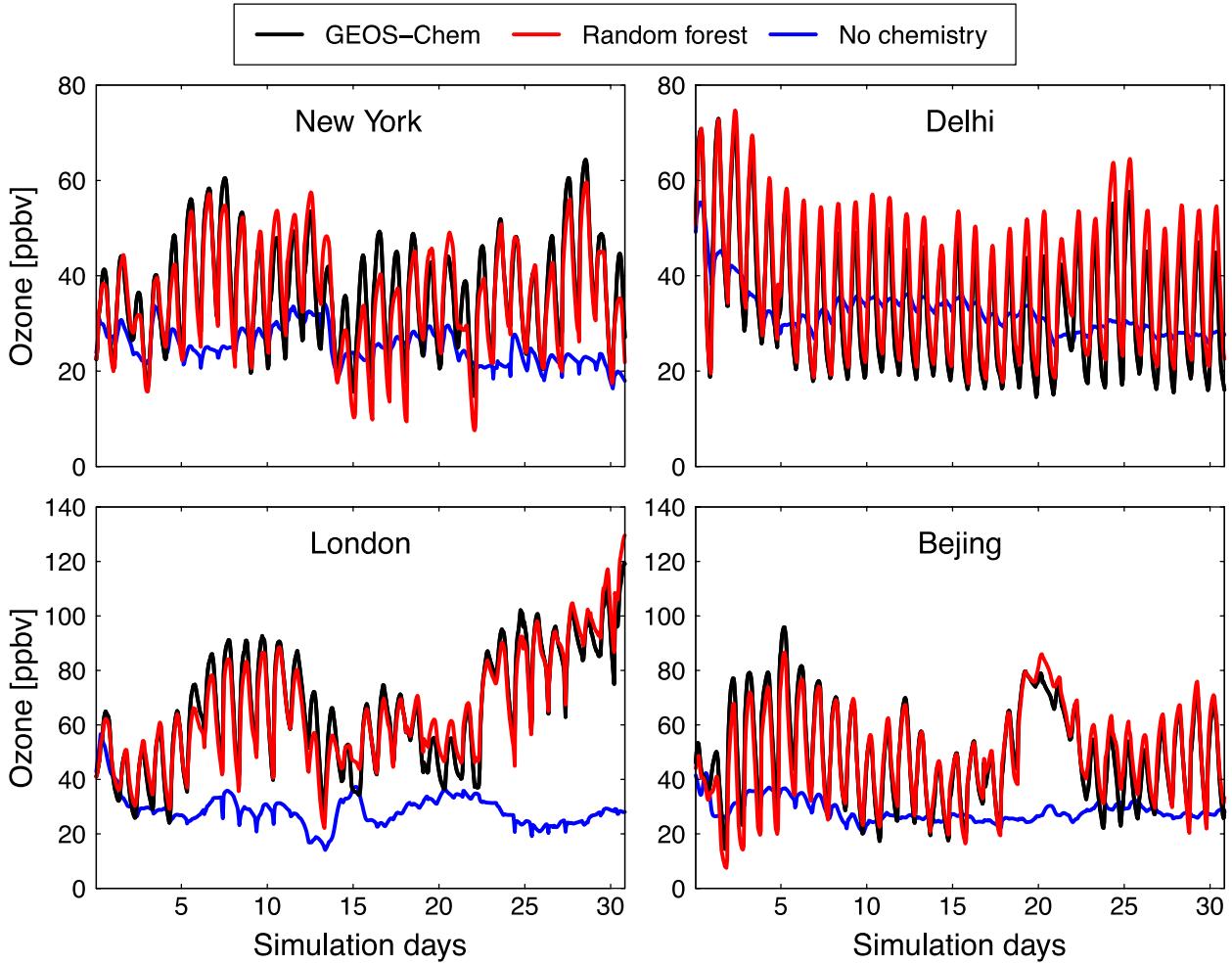
# Surface concentrations over polluted regions are well reproduced by ML model





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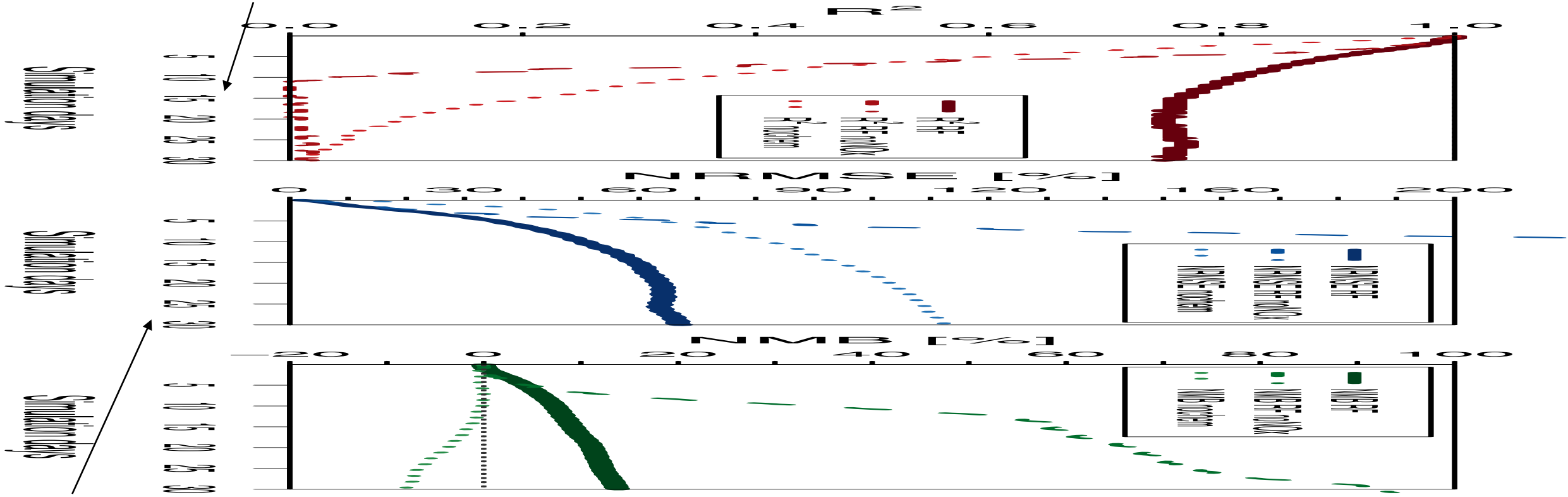
# Machine learning model remains stable over the long-term (but only if NOx is predicted as a family)

Model with NOx family prediction




Model without NOx family prediction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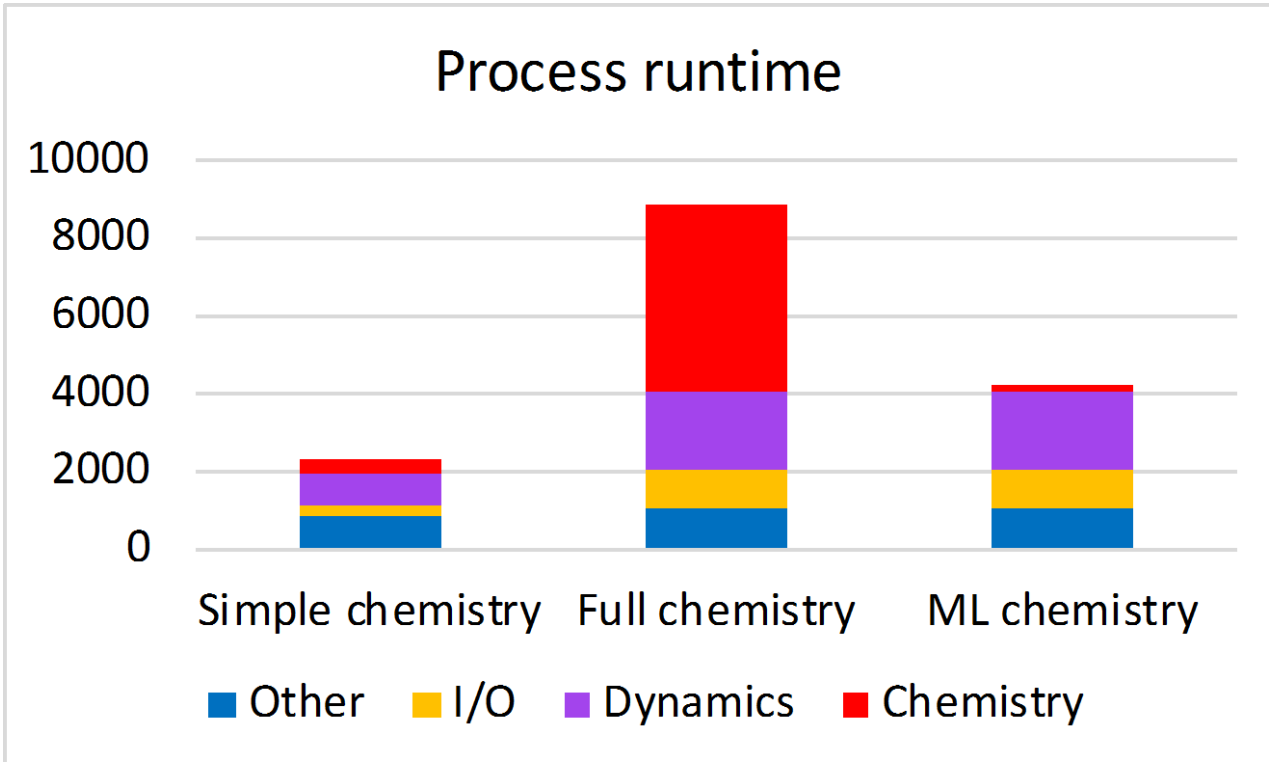
# Speedup potential




- Offline evaluation of one forest is 1000x faster than numerical integration
- Current implementation is very inefficient (2x slower than full chemistry)
- Currently working on seamless integration of XGBoost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# Summary

- Tree models do a good job at simulating atmospheric chemistry
- Adding constraints (e.g., chemical families) to the machine learning model is critical
- Potential applications:
  - Chemical data assimilation
  - Air quality forecasting
- Issues:
  - Train on very large data sets (>1 TB)
  - Dynamics for >200 chemical species is still slow

Keller and Evans: Application of random forest regression to the calculation of gas-phase chemistry within the GEOS-Chem chemistry model v10, GMD, 2019.




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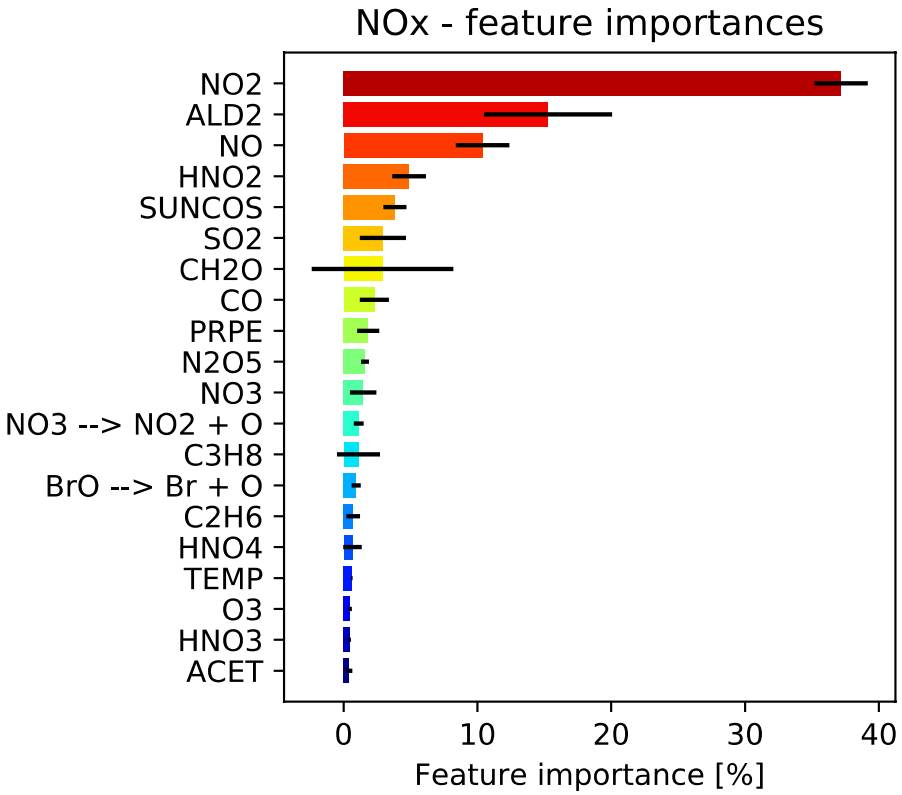
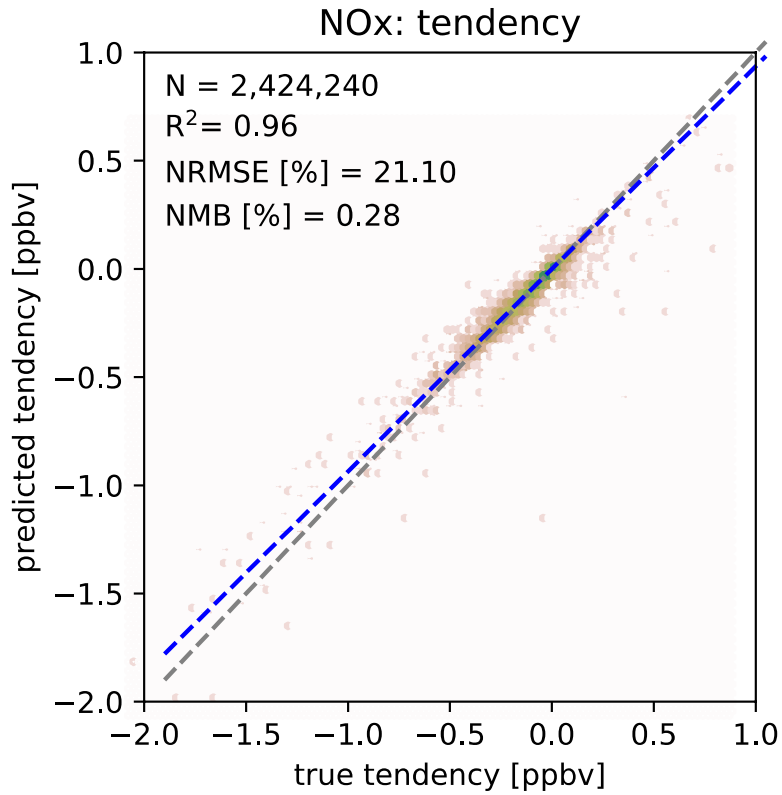
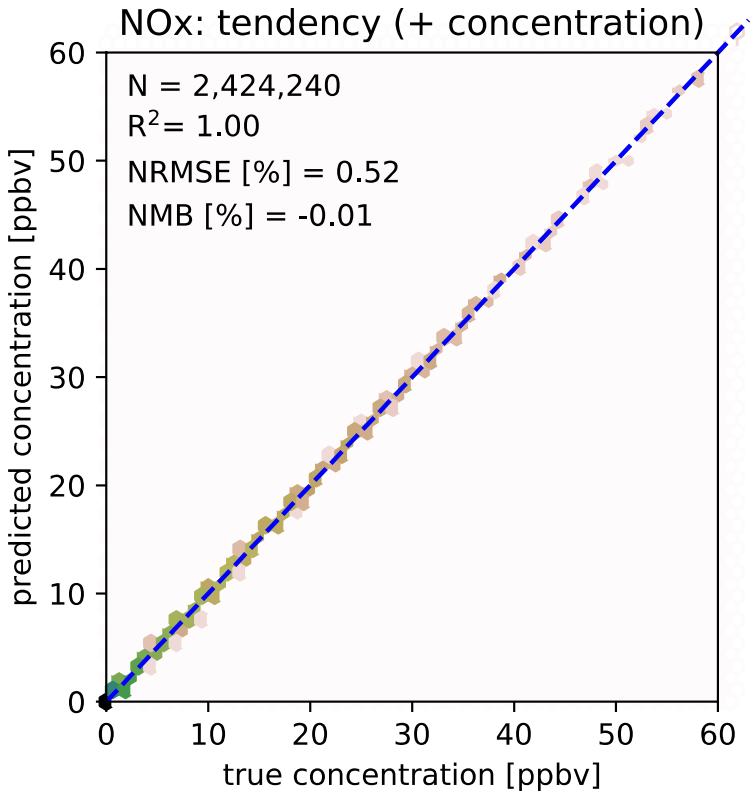
# Prediction of NOx





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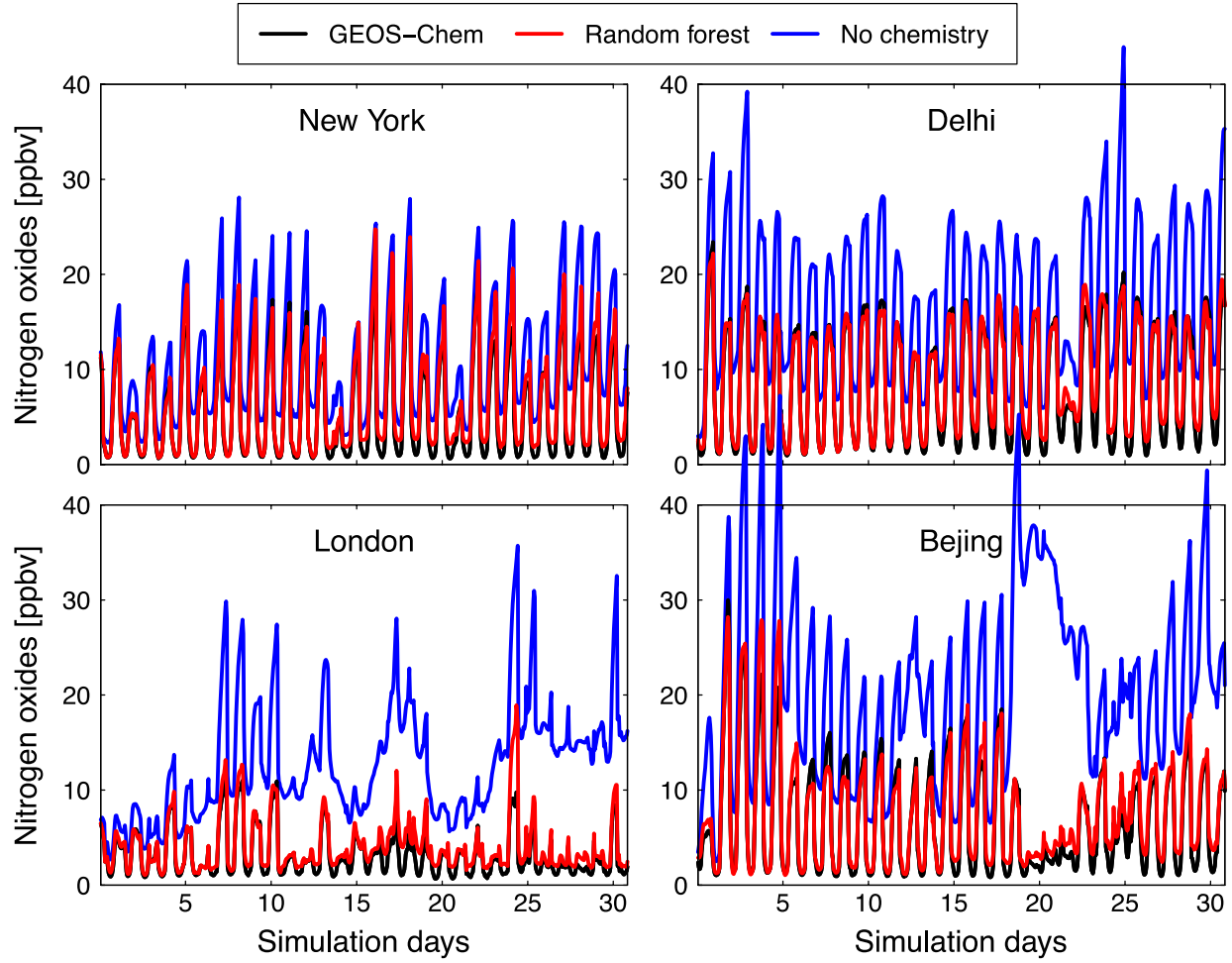



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