Atmospheric Chemistry Modeling and Air Quality Forecasting using Machine Learning

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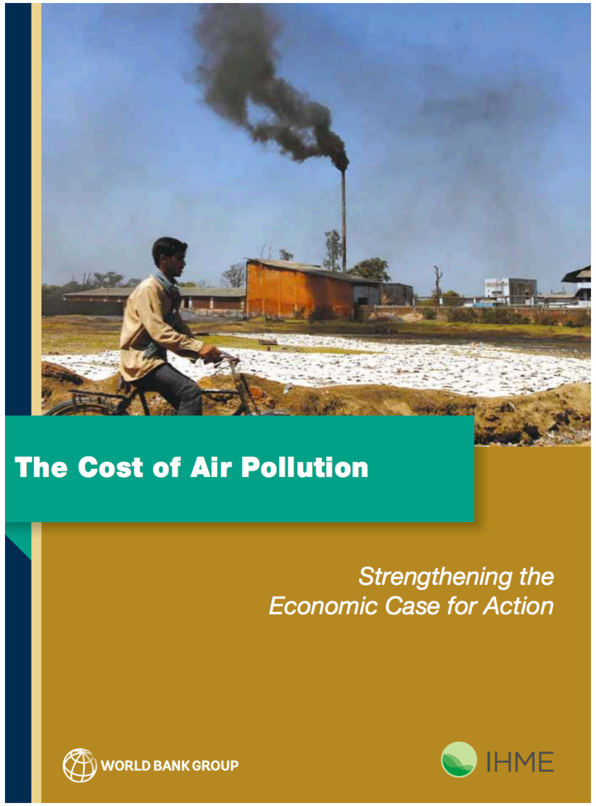
Air pollution is a global problem



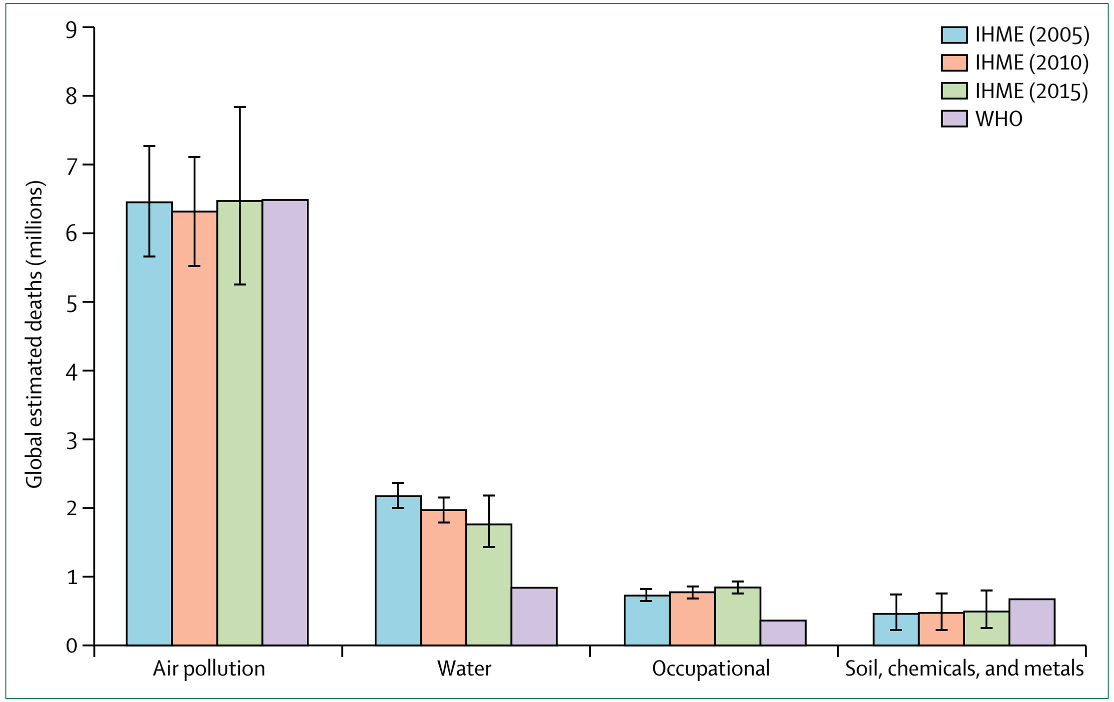
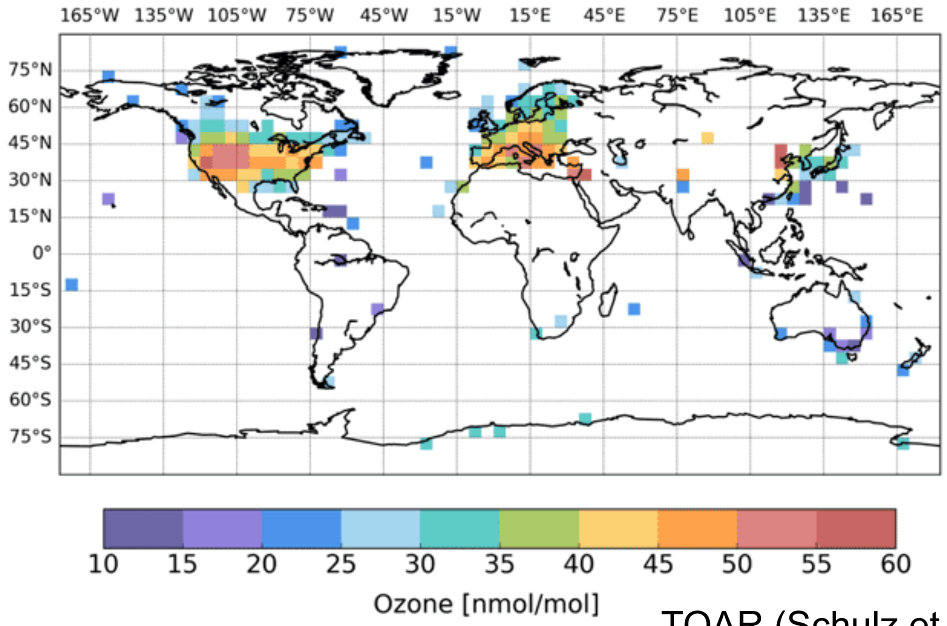


Figure 4: **Global estimated deaths (millions) by pollution risk factor, 2005–15**
Using data from the GBD study[42] and WHO.[99] IHME=Institute for Health Metrics and Evaluation.

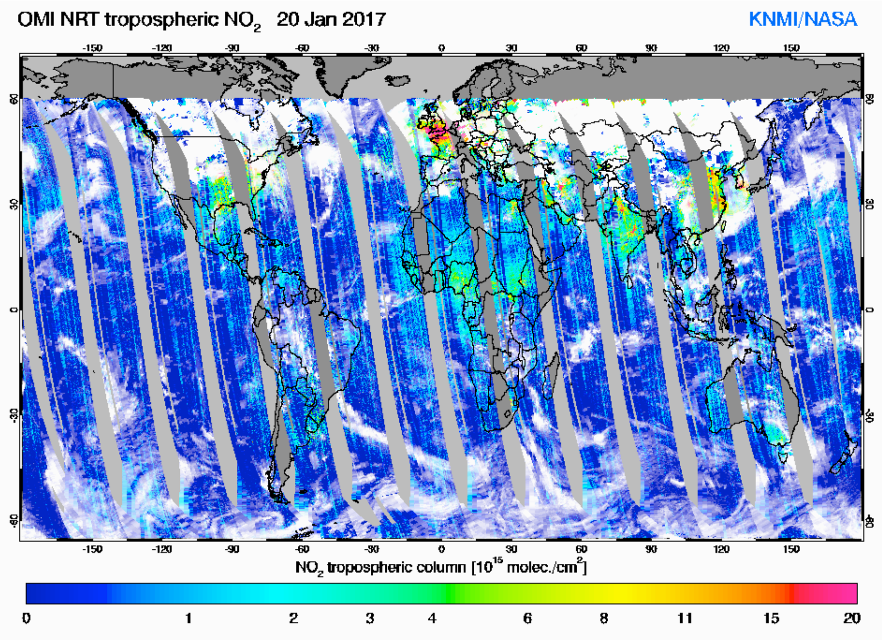
World Bank: ~$5 trillion in welfare losses in 2013

The Lancet (2017): Air pollution is responsible for 6-7 millions death / year

Need models to fill gaps in observations



TOAR (Schulz et al., 2017)



Surface observations are not global

Satellite observations are also discontinuous

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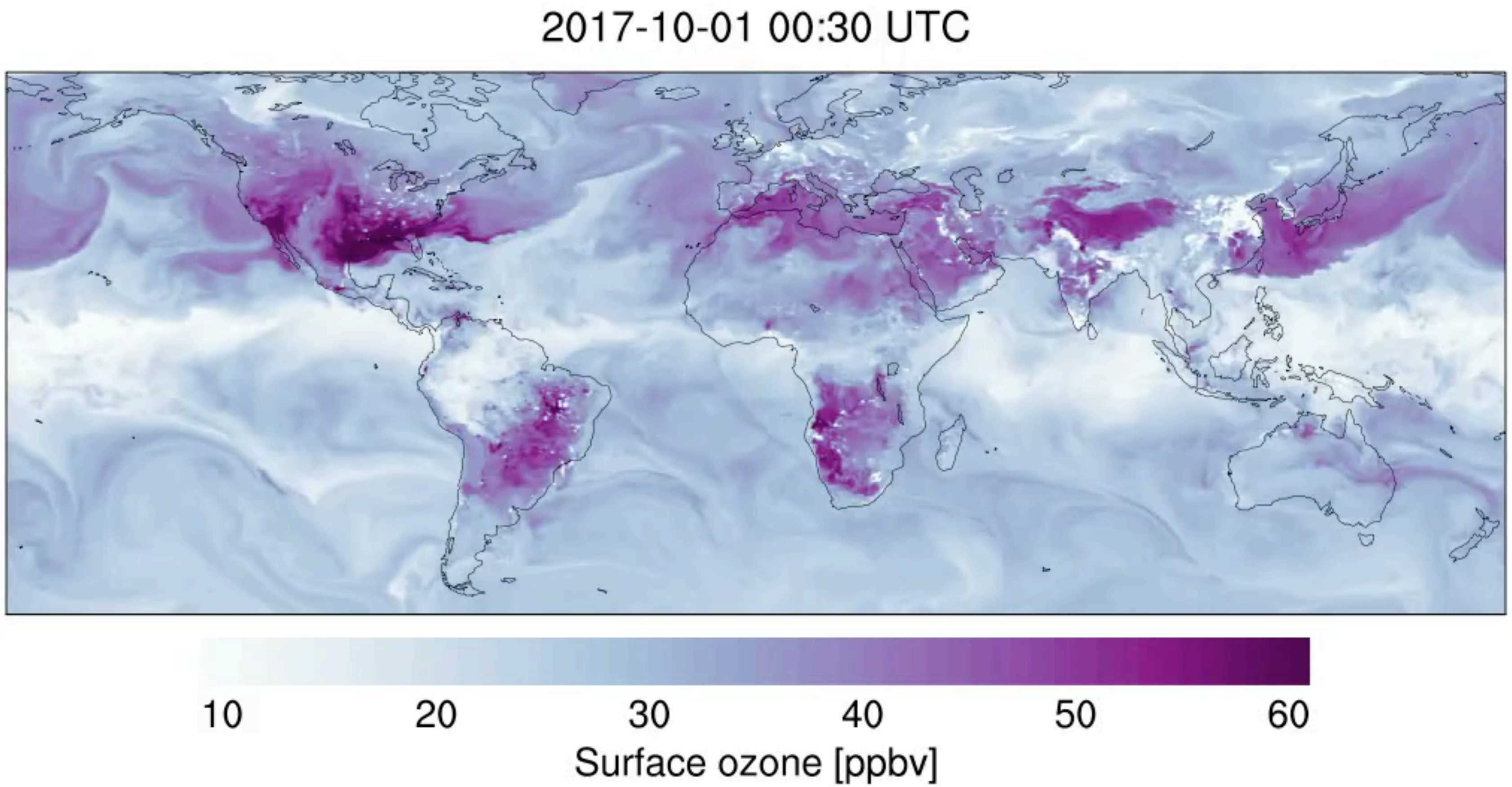
Numerical simulation of atmospheric chemistry



- 0.25° resolution (~ 25km), 72 levels, 250 chemical species

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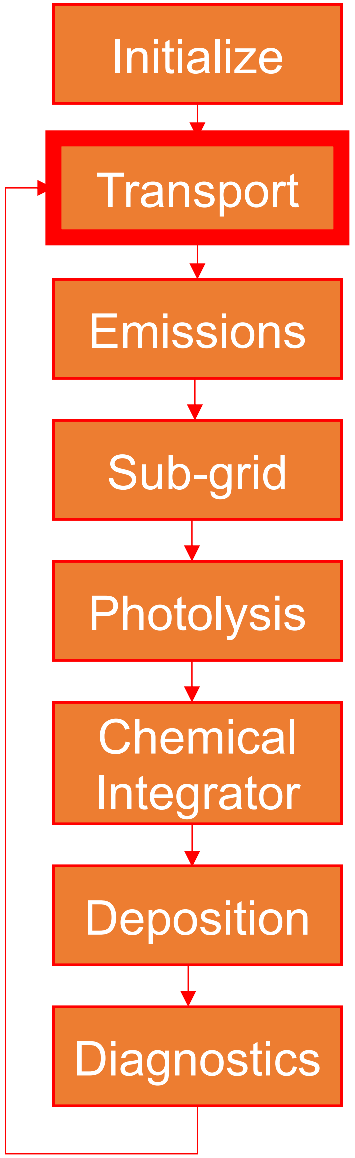
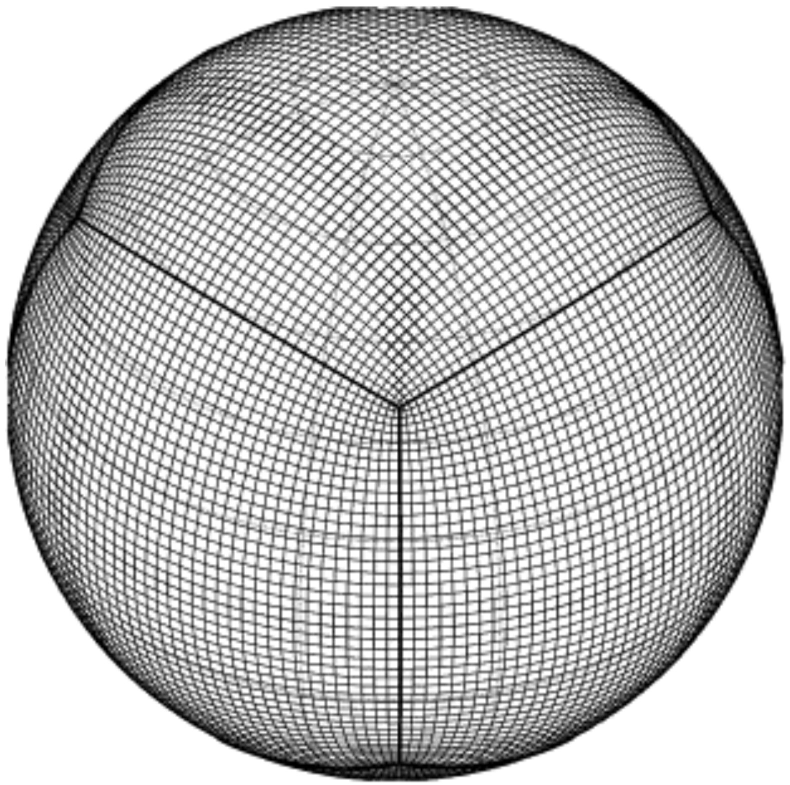
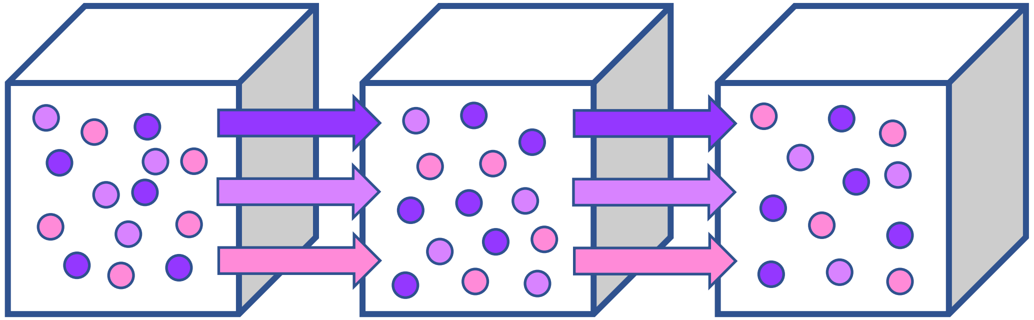


Transport process: Move chemicals across grid boxes





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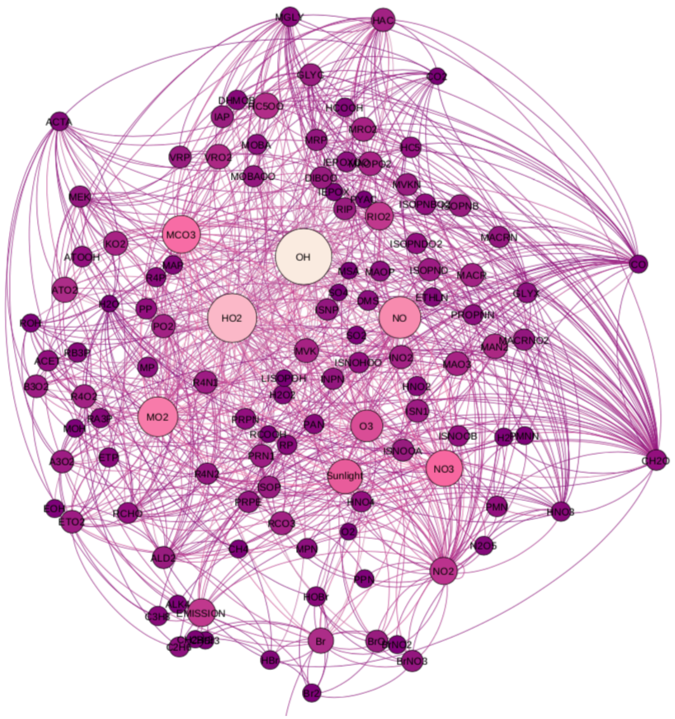


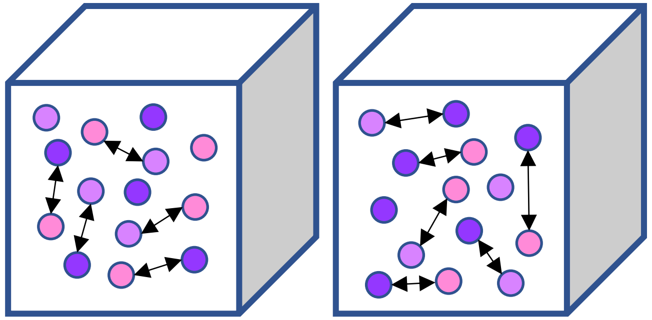
Transport process: Move chemicals across grid boxes

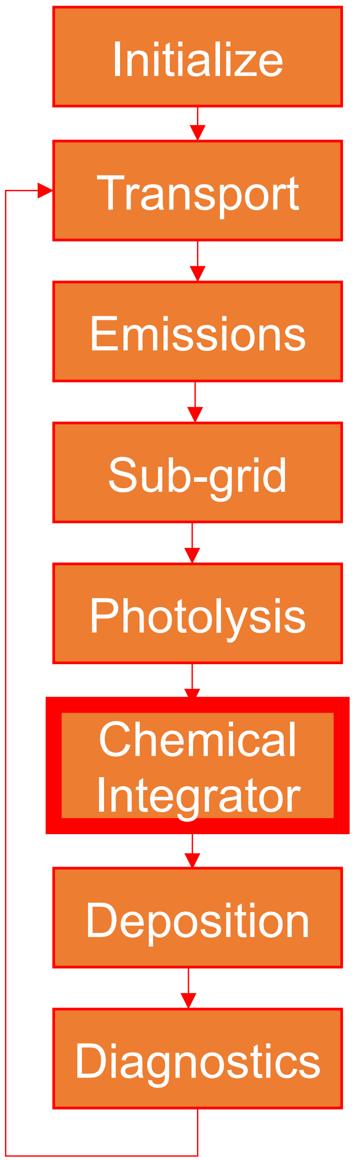
Chemistry process: In each grid box, solve chemical reactions, i.e. solve stiff ordinary differential equations (ODEs)

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

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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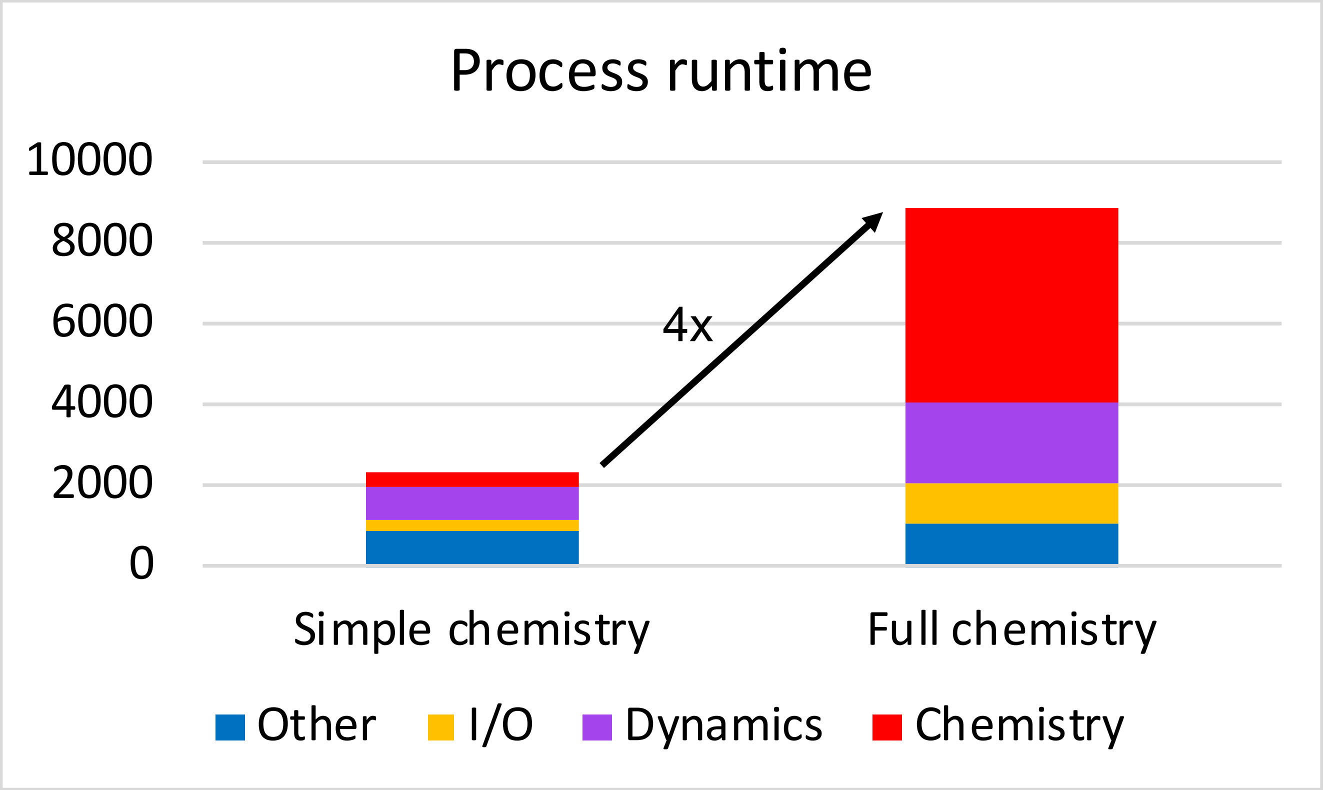
Atmospheric chemistry models are computationally expensive



- High-resolution chemistry simulation requires >1000 CPU’s
- Throughput: approx. 20 days in 24 hours

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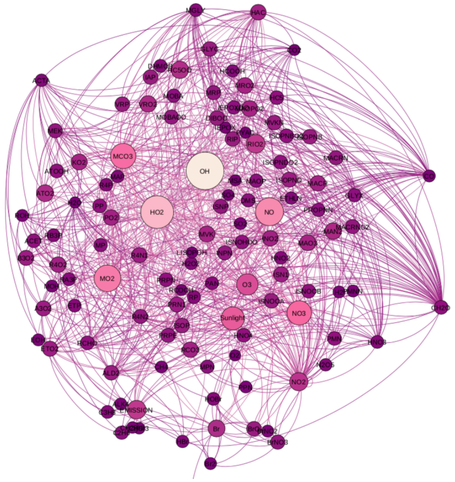
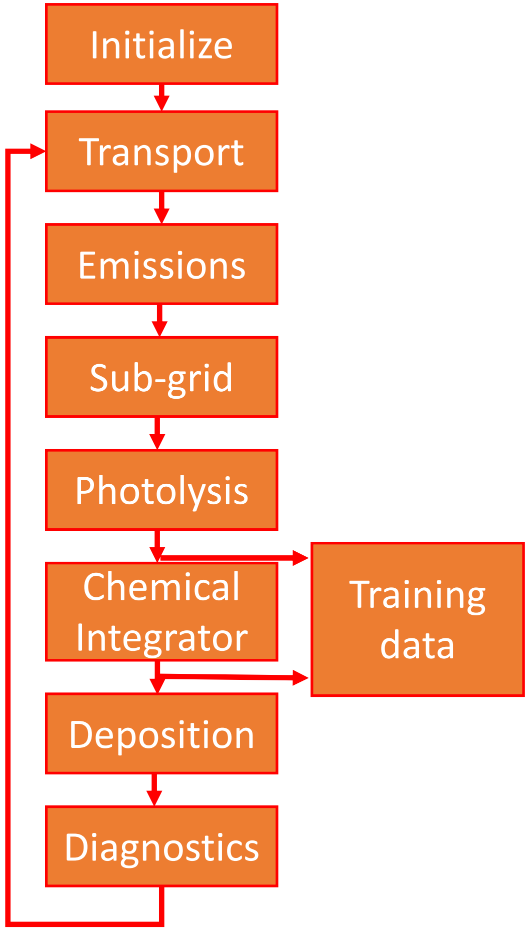
Replace chemical integrator with machine learning model



Numerical model



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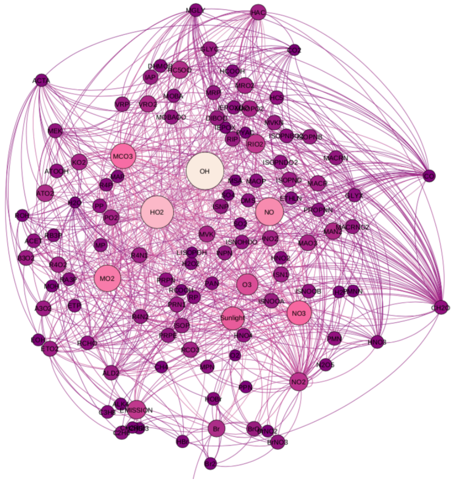

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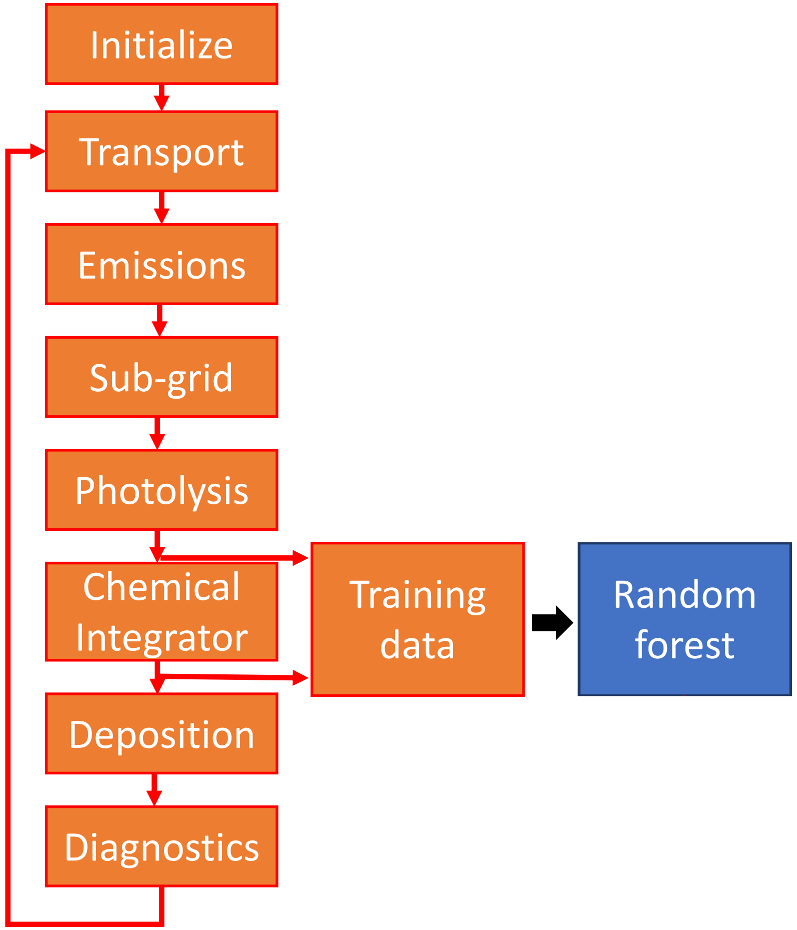

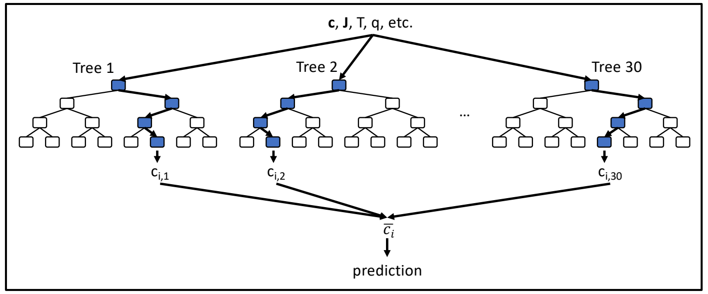

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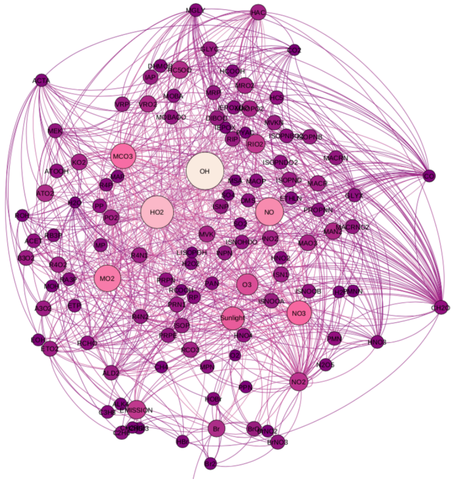

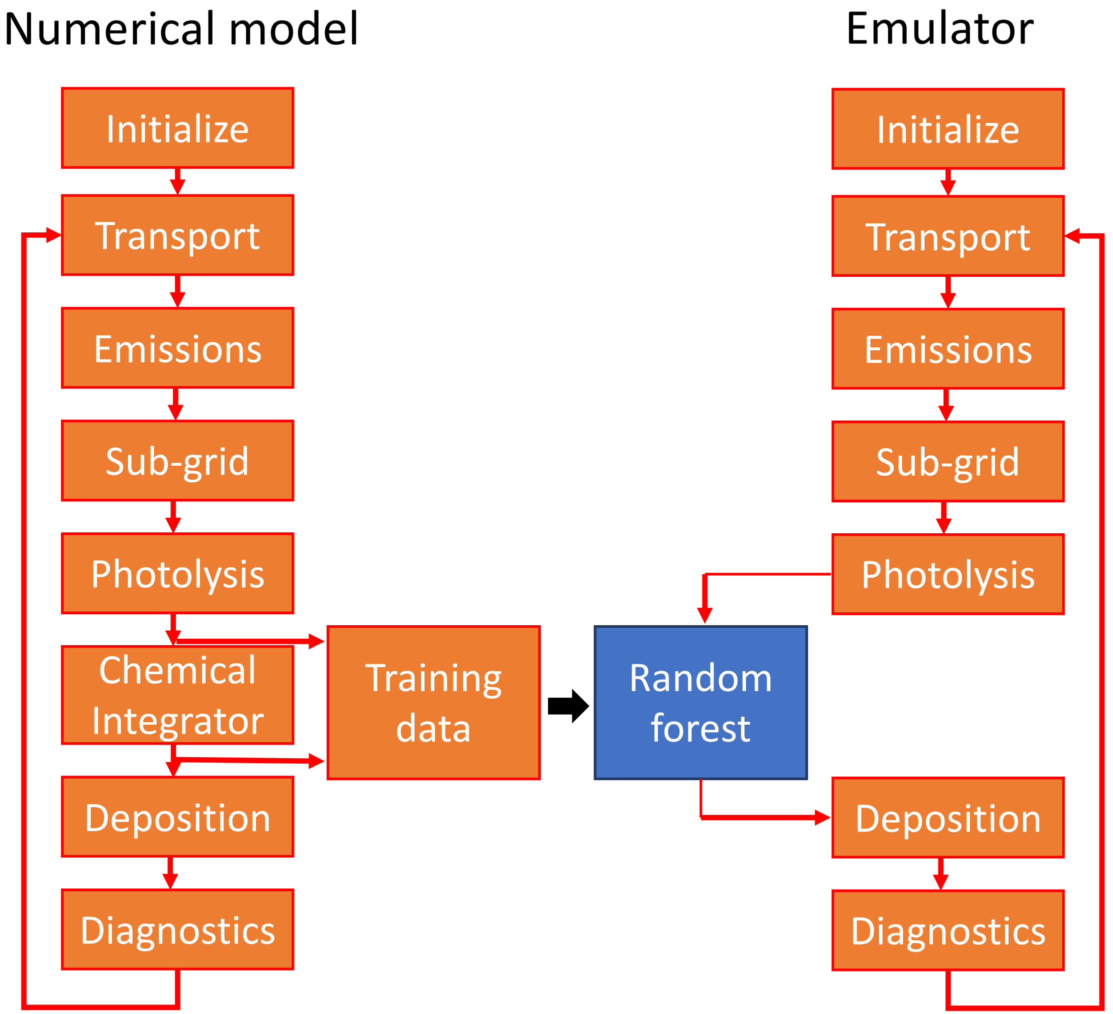

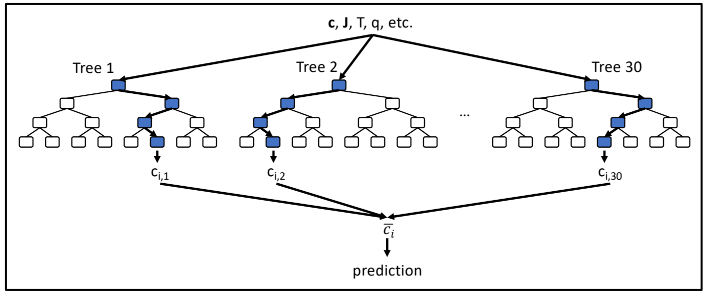

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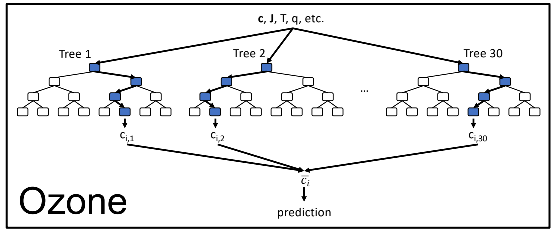
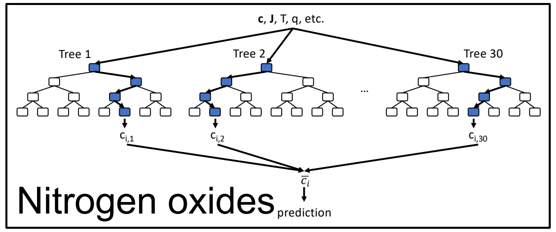
Machine learning for atmospheric chemistry modeling

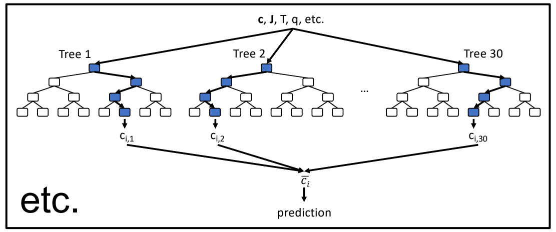
- 143 chemical species
- 91 photolysis rates
- Temperature
- Pressure
- Rel. humidity
- Solar zenith angle

Concentrations after chemistry

Separate model for each species







- ➢ Training data set: 2.7 billion data points (44 GB)
- ➢ Tested: (neural network), random forest and XGBoost

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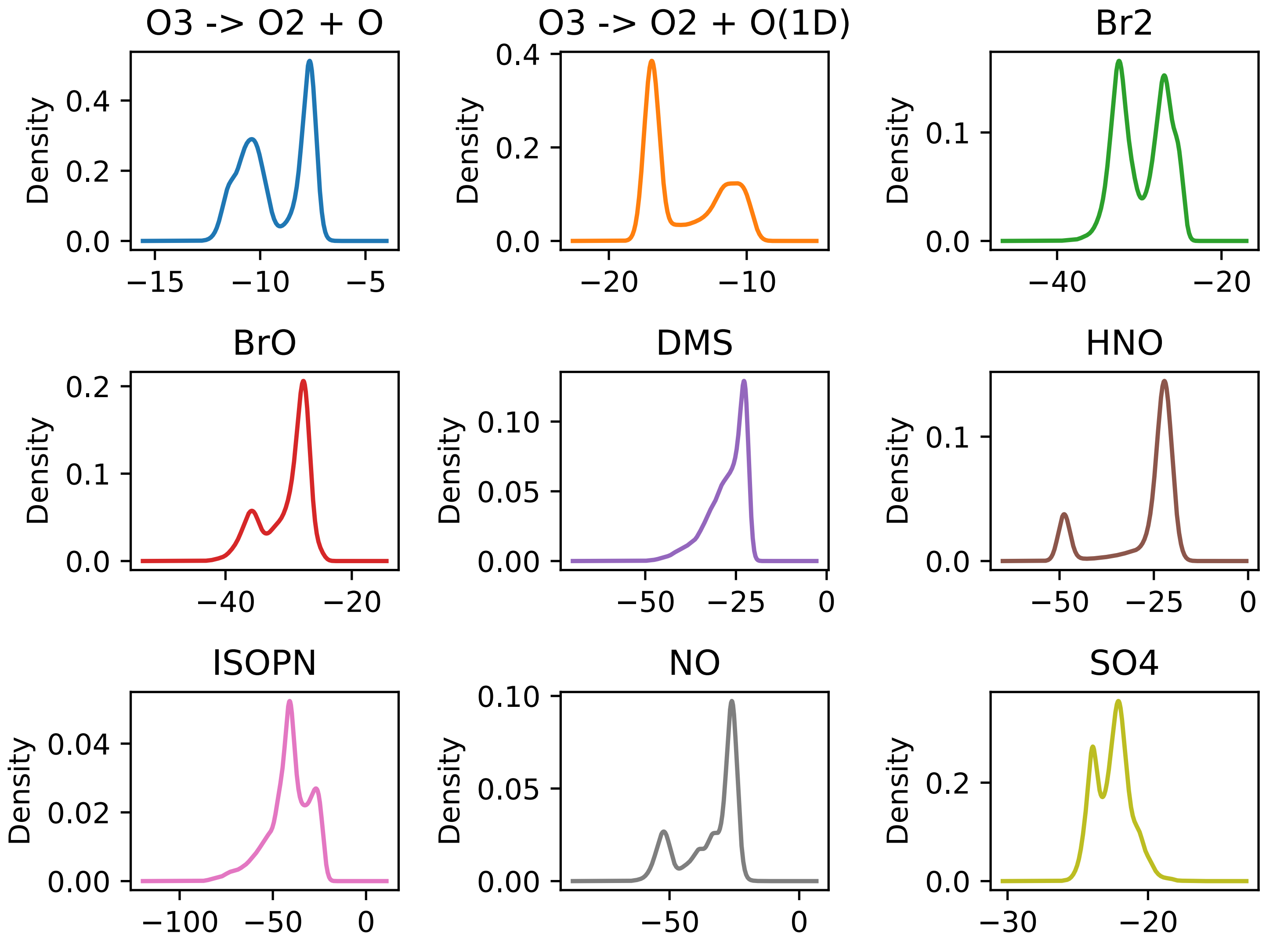
Many input features have multiple modes



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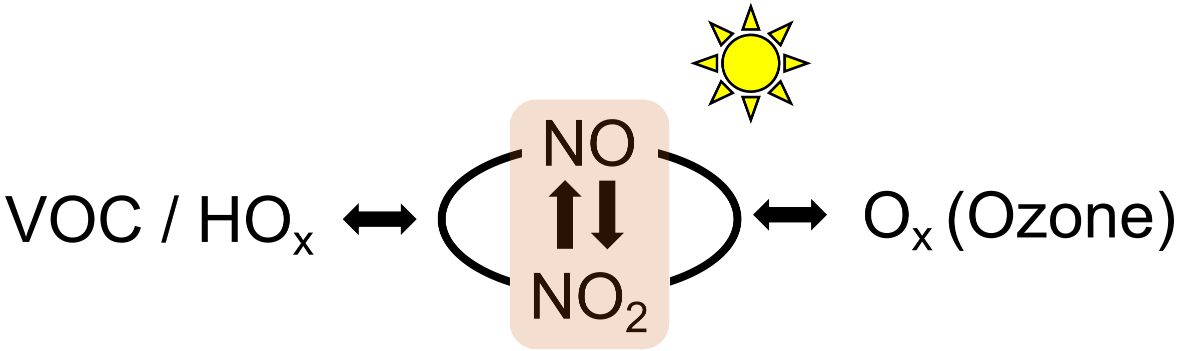
Impose chemical constraints on ML model to improve (long-term) accuracy

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

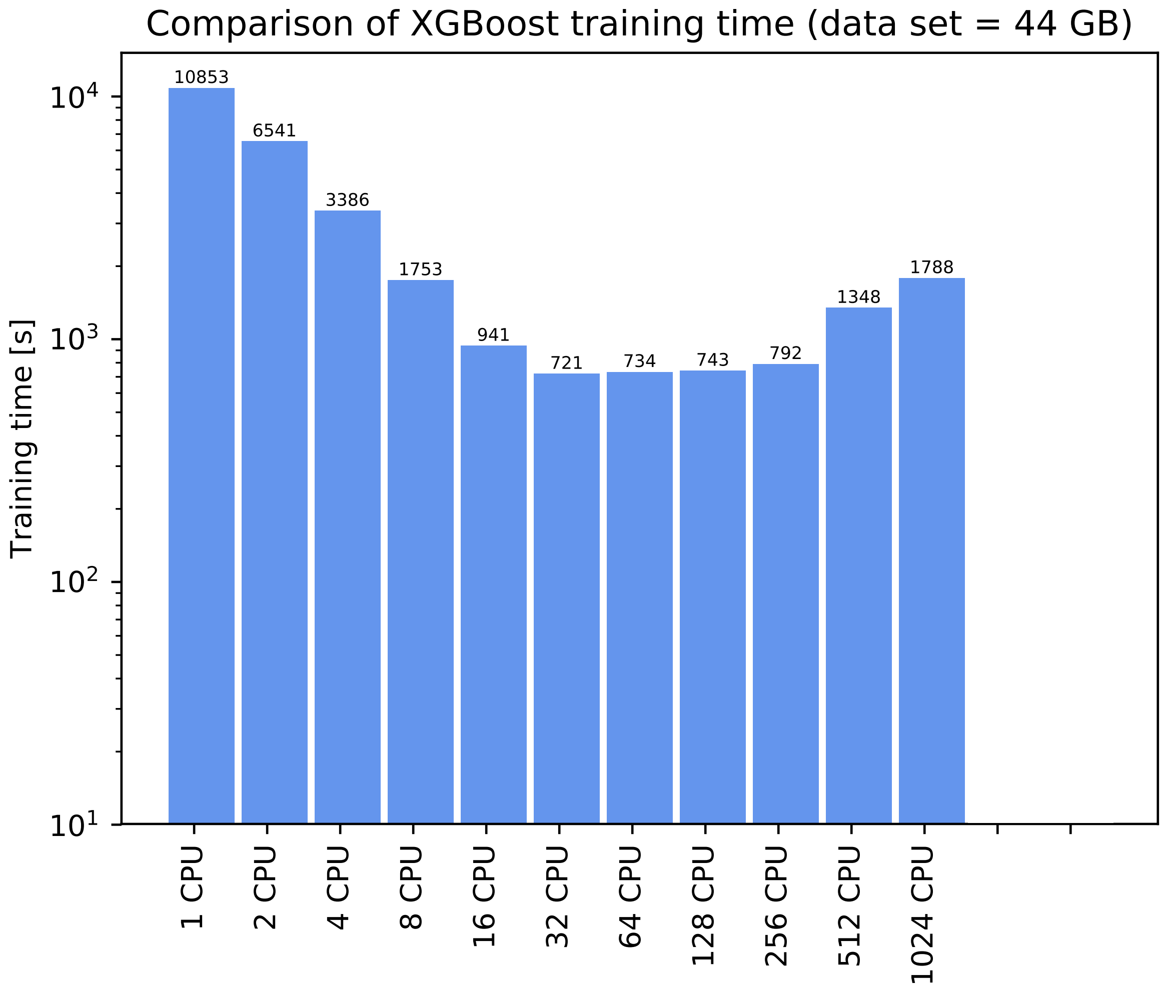
Long-lived (tendencies): $[X_i]_{T+\Delta T} = [X_i]_T + f(\,\mathbf{k}, \mathbf{J}, [\mathbf{X}]\,)$

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

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



Random forest / XGBoost training benchmarks



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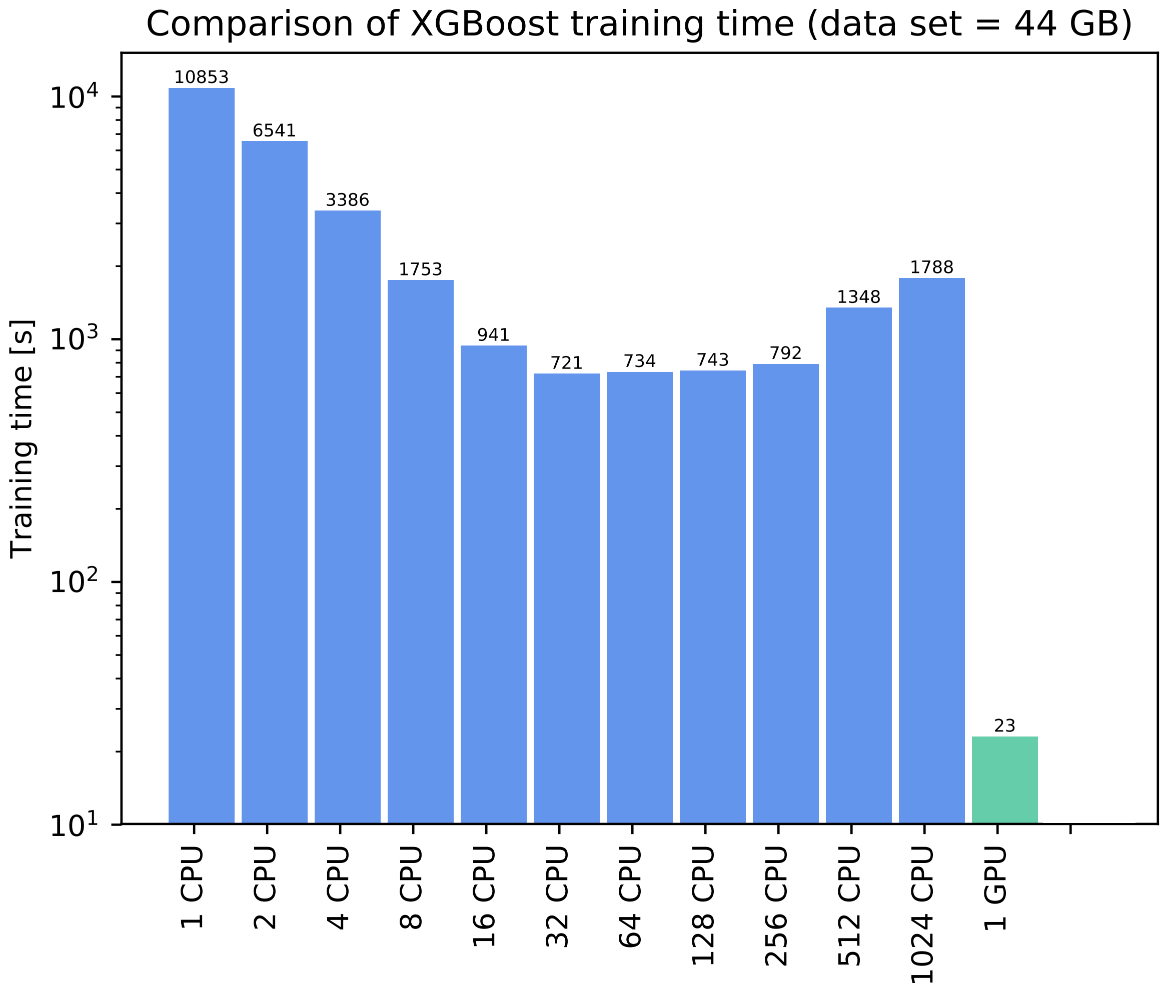

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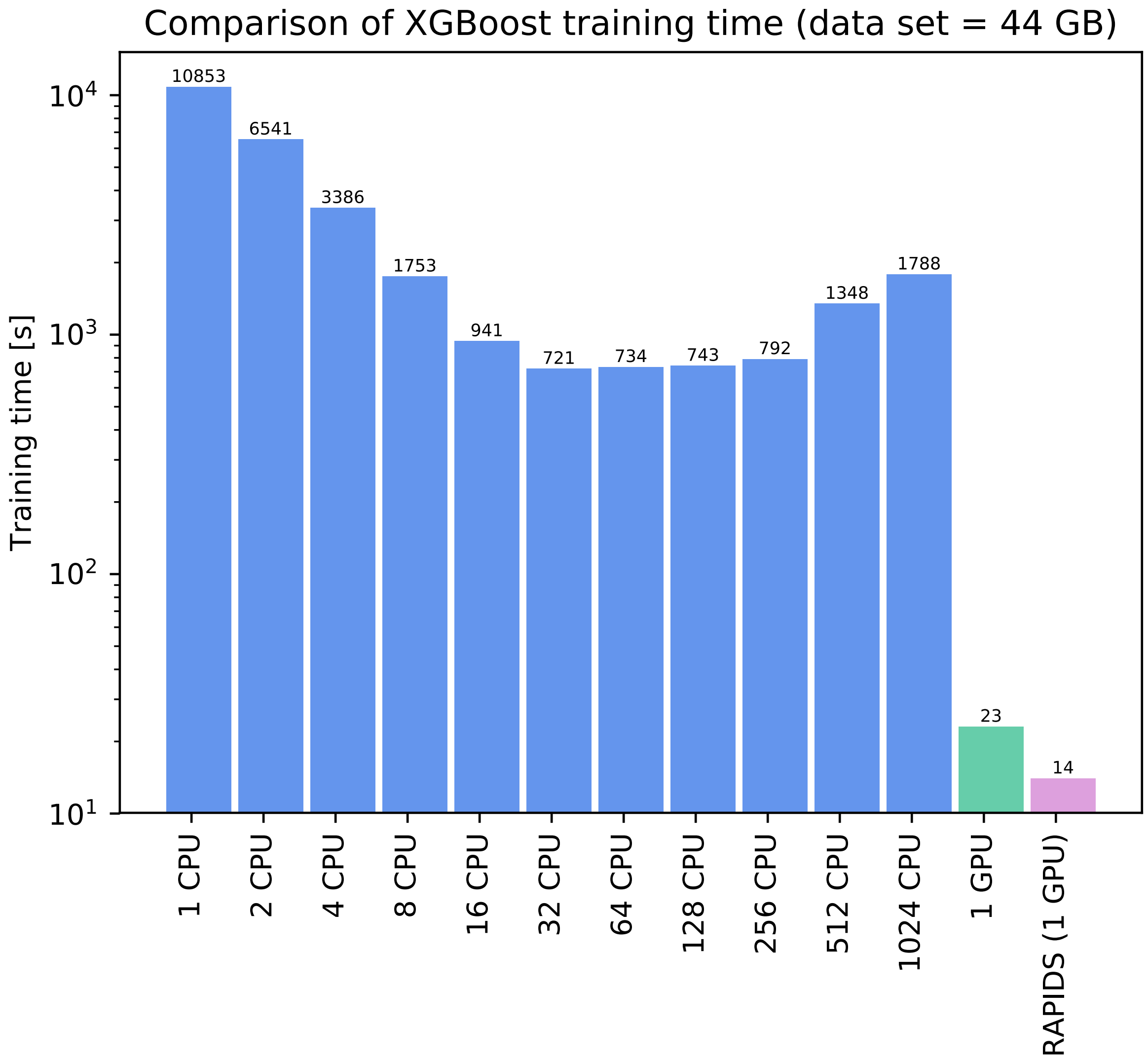

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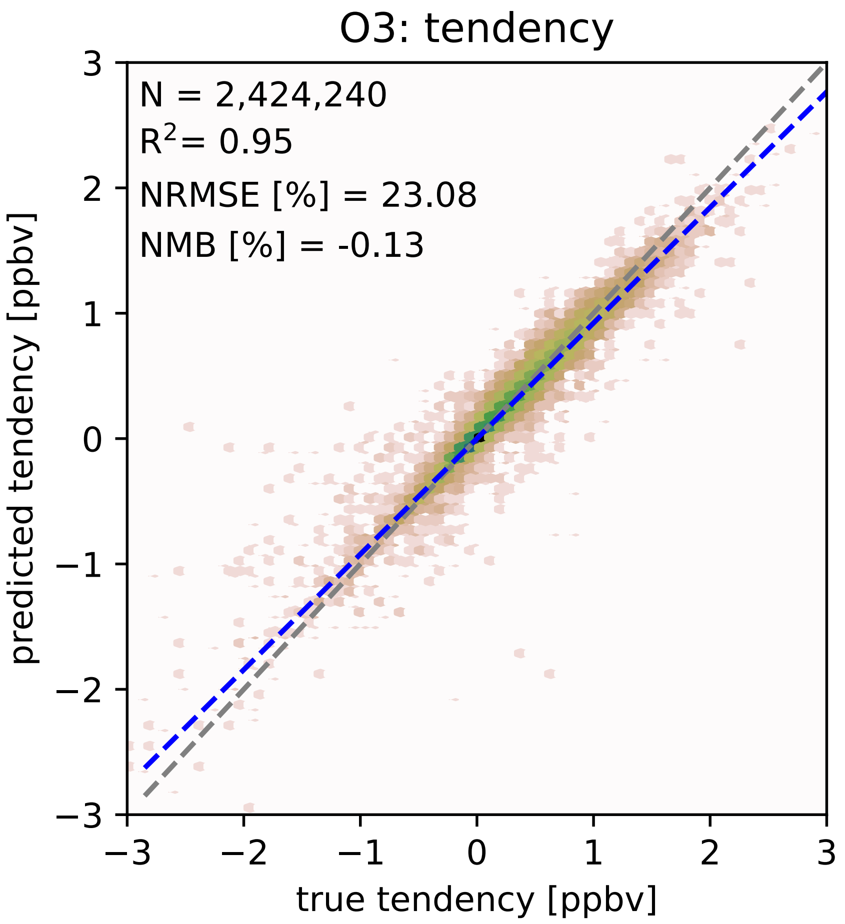
Random forest / XGBoost reproduce target concentrations well (single-step prediction)



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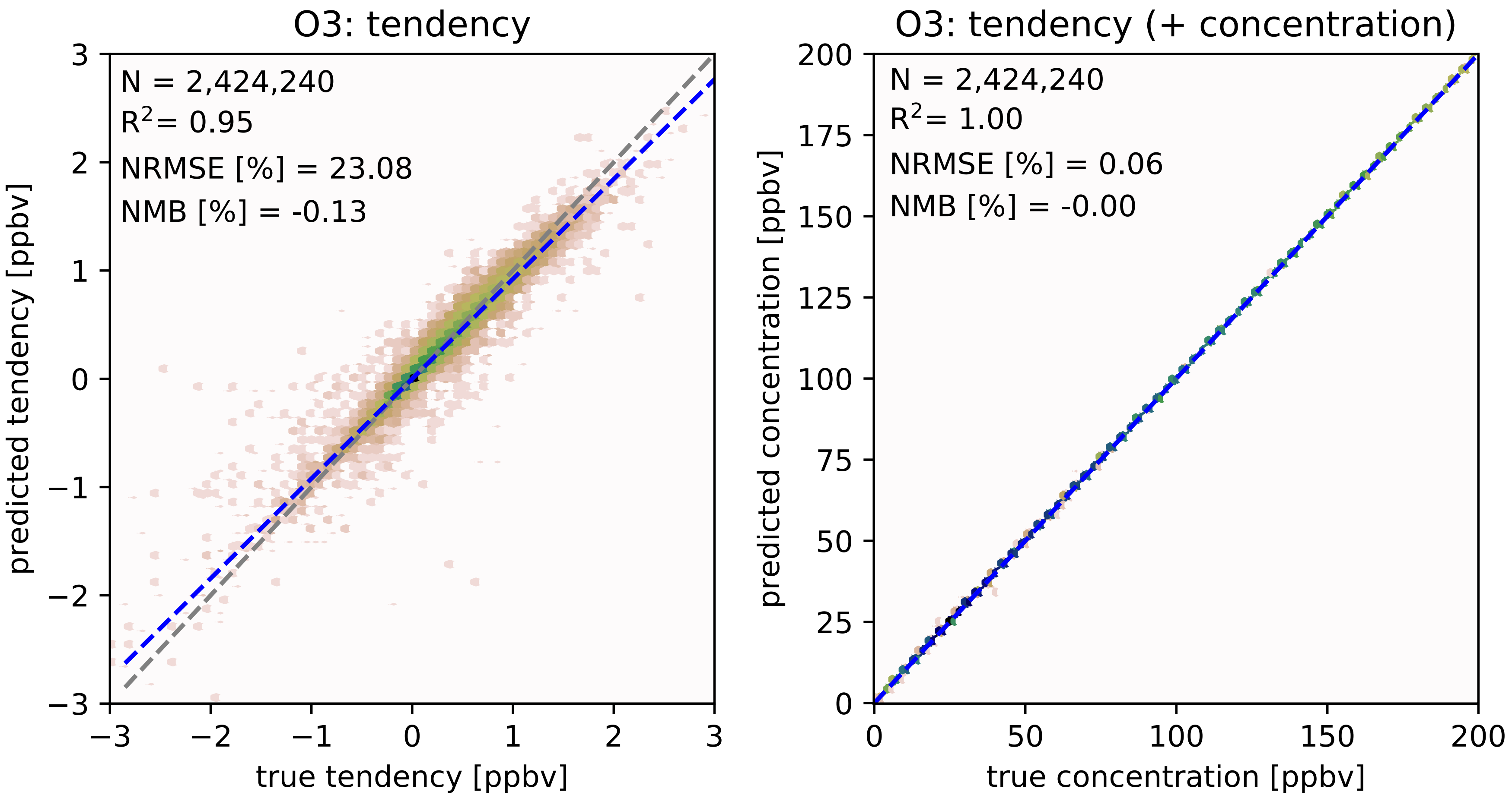

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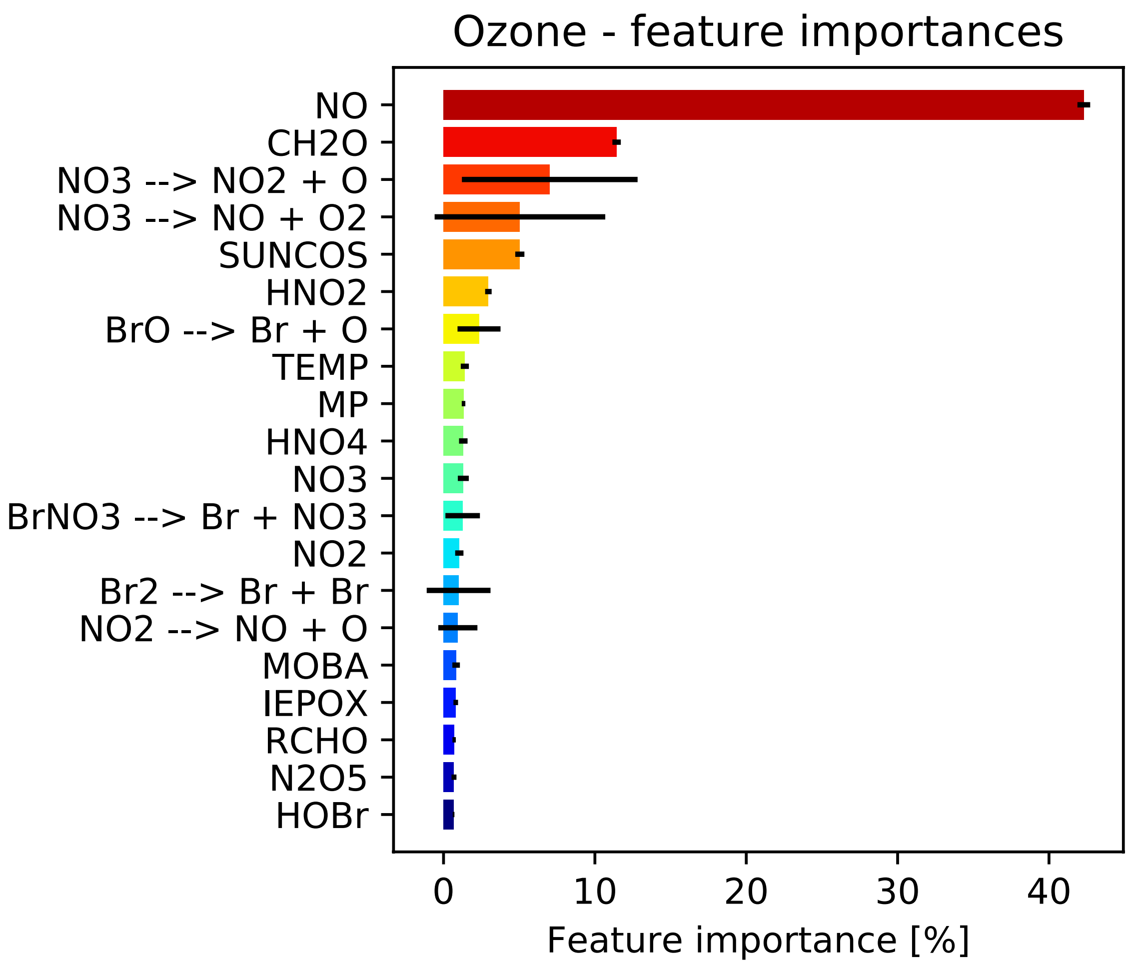
Random forest / XGBoost solutions reflect known features of chemical kinetics



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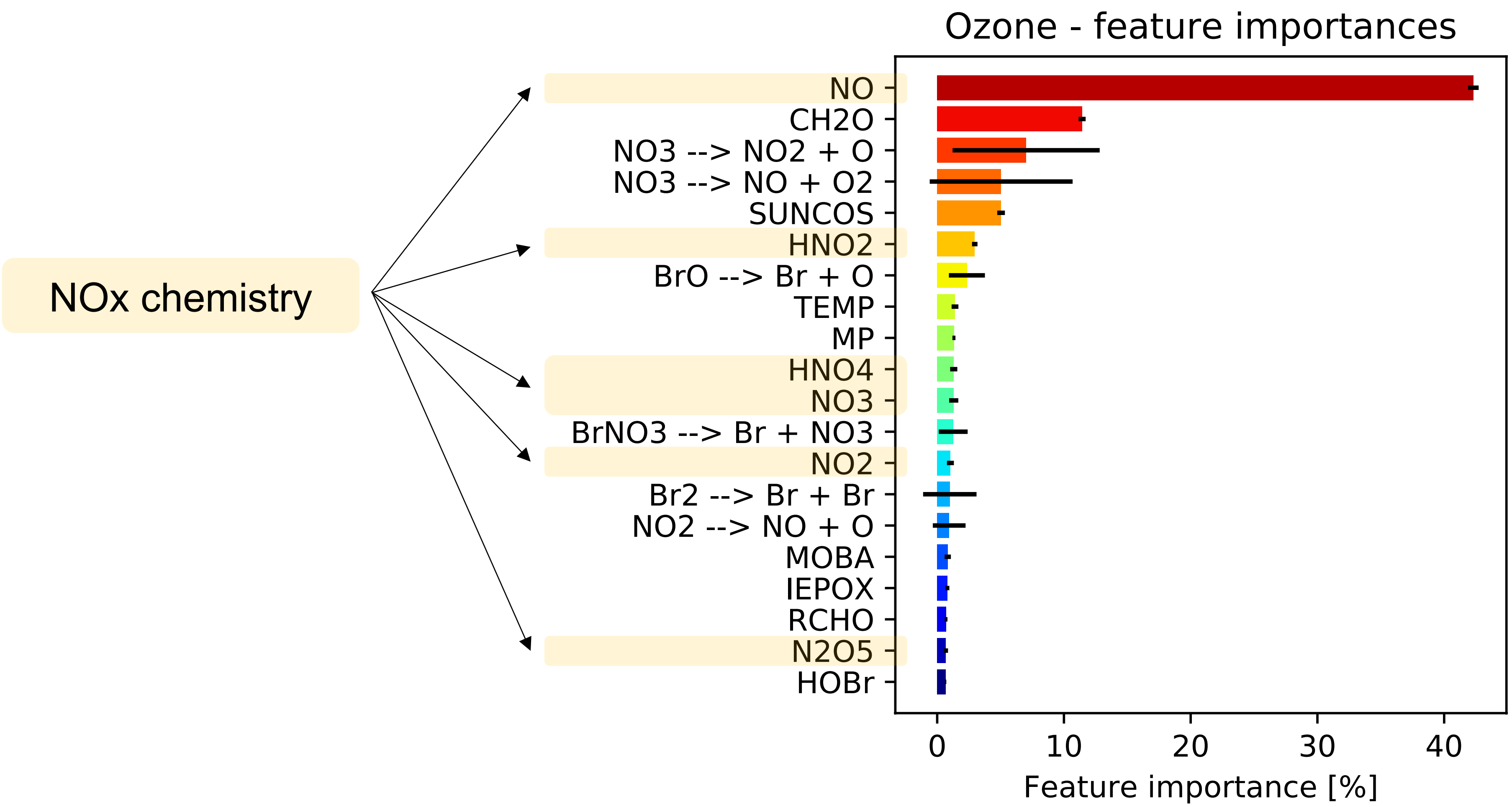

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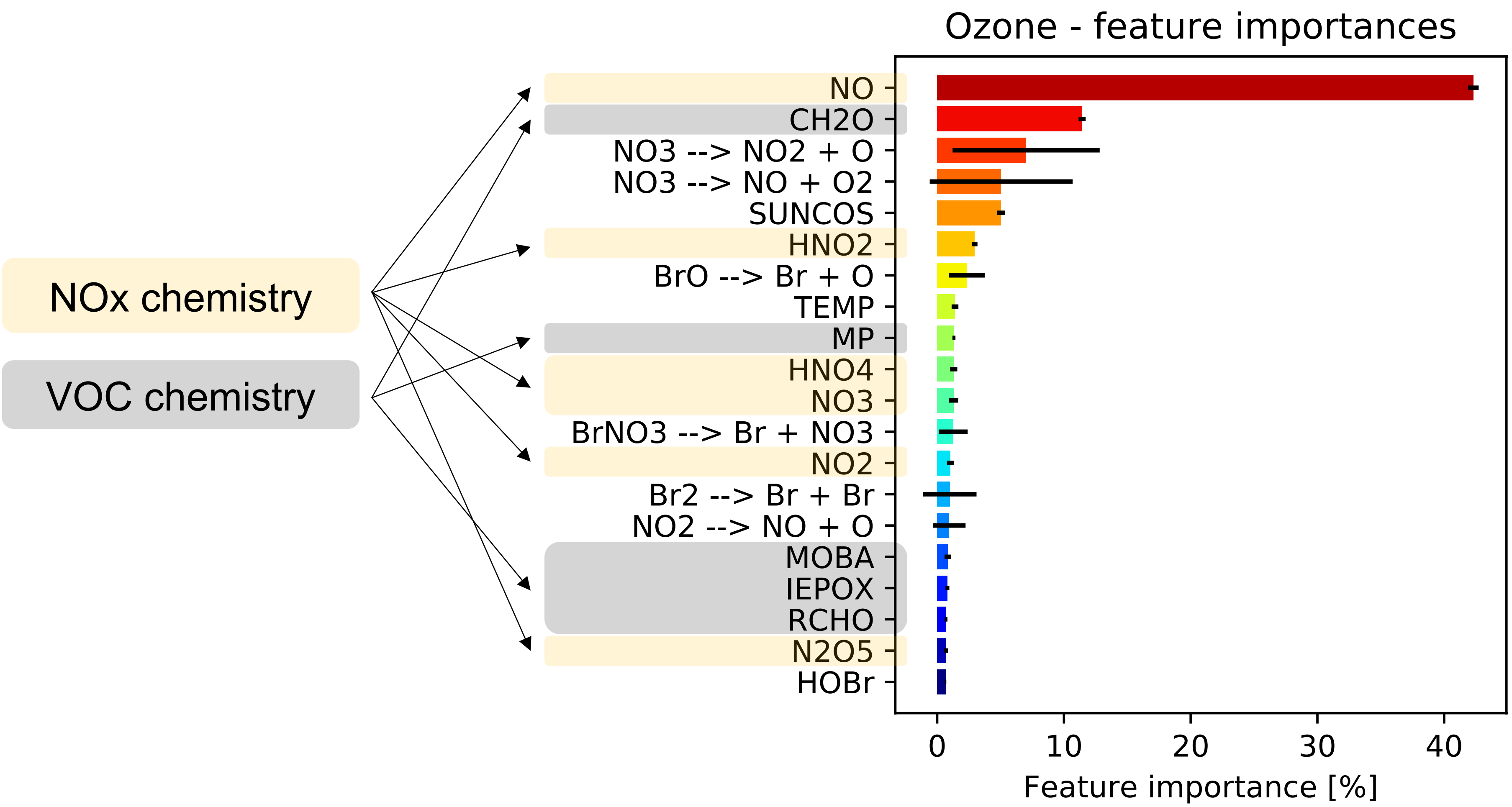

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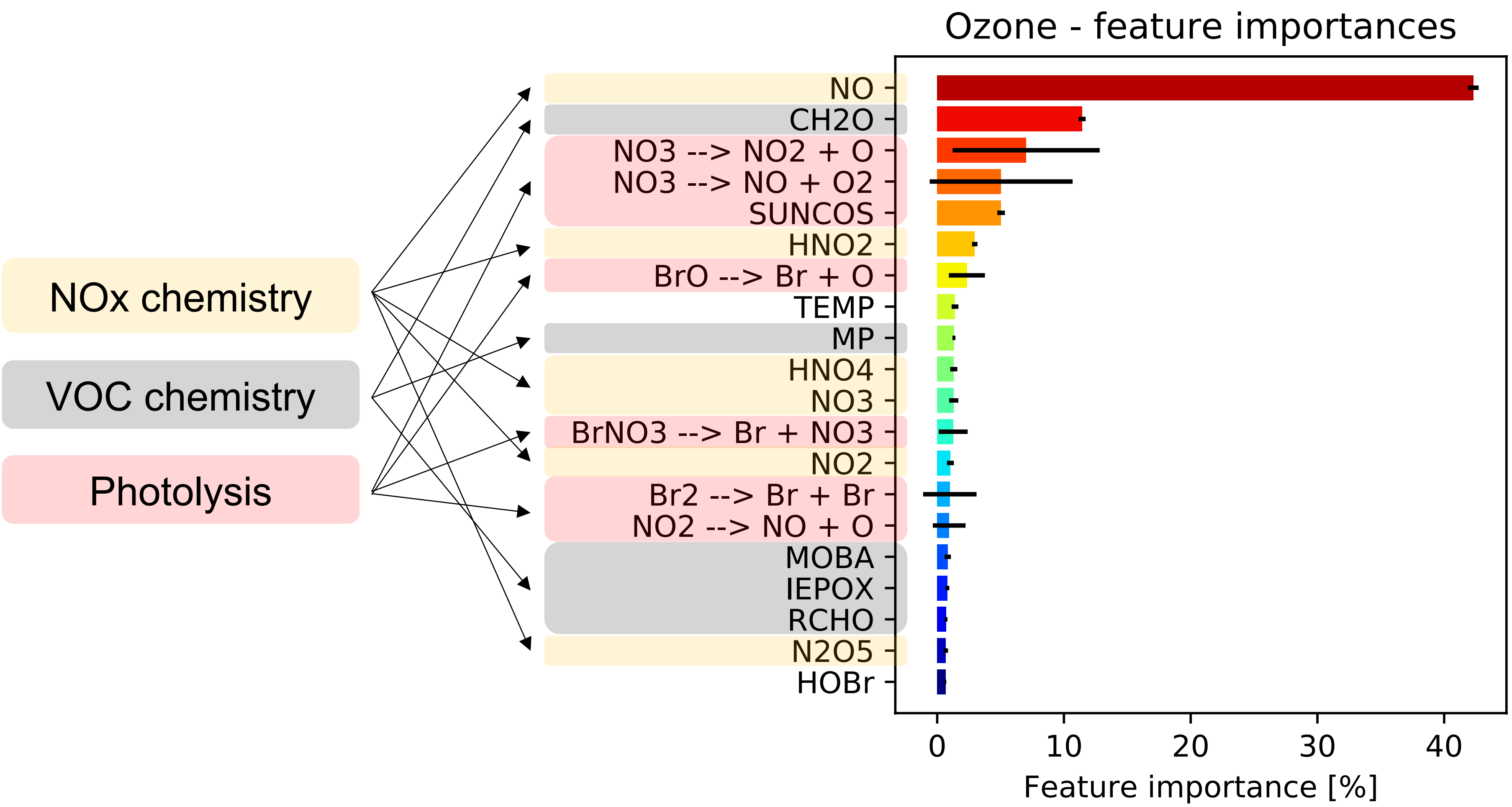

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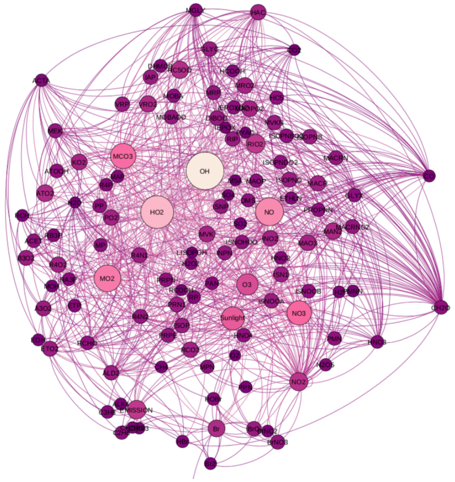
1-month simulation with random forest emulator



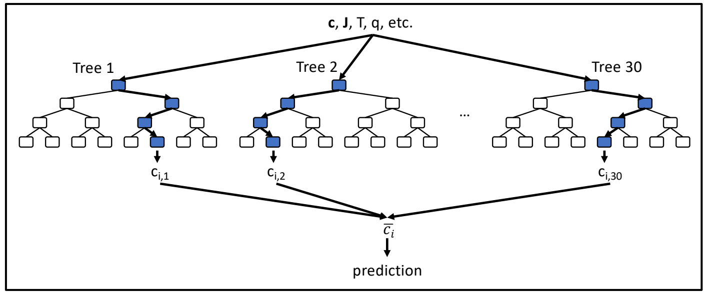
Numerical model

Initialize → Transport → Emissions → Sub-grid → Photolysis → Chemical Integrator → Deposition → Diagnostics

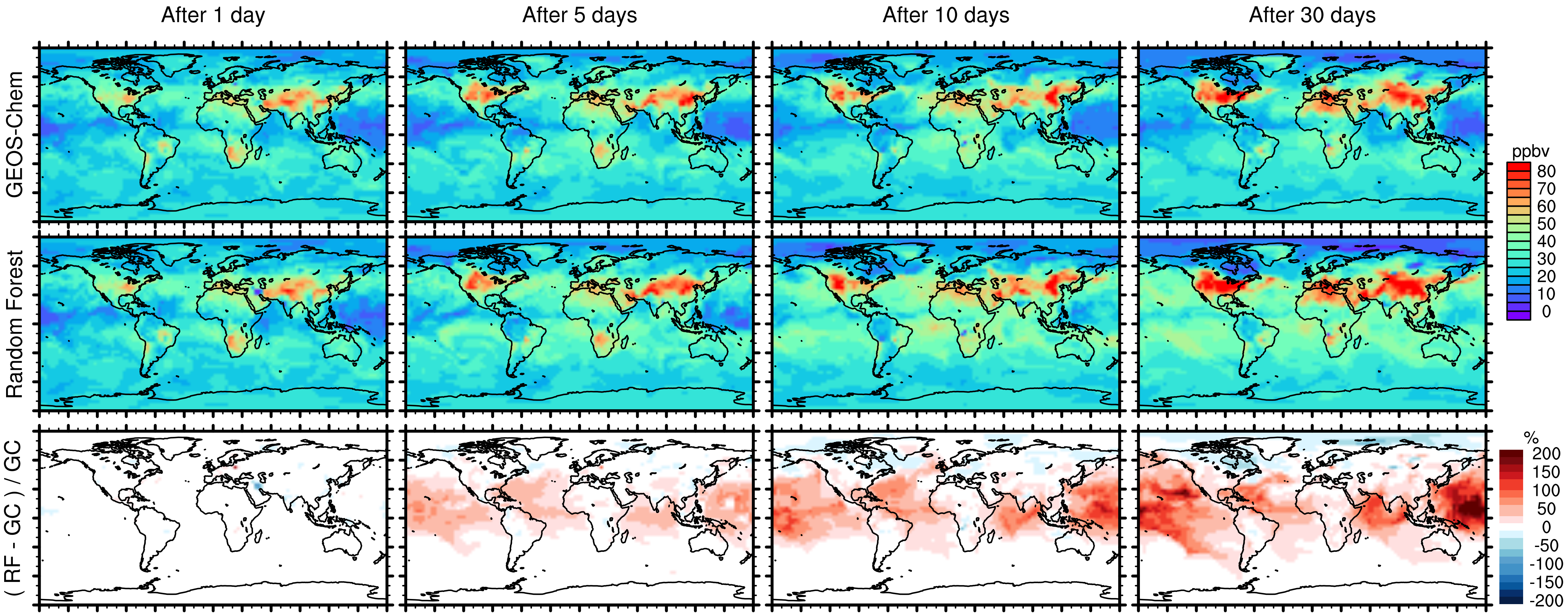
Training data → Random forest

Emulator

Initialize → Transport → Emissions → Sub-grid → Photolysis → Random forest → Deposition → Diagnostics



Random forest overestimates ozone surface concentrations over remote regions



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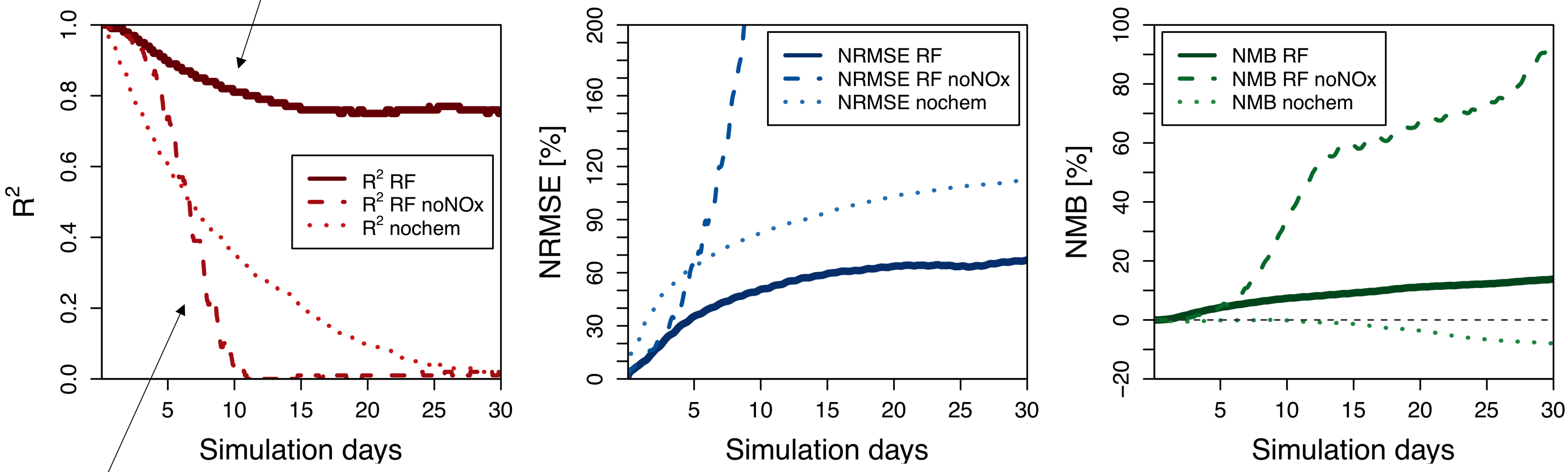
Machine learning model remains stable over the long-term (but only if NOx is predicted as a family)

Model with NOx family prediction



Model without NOx family prediction

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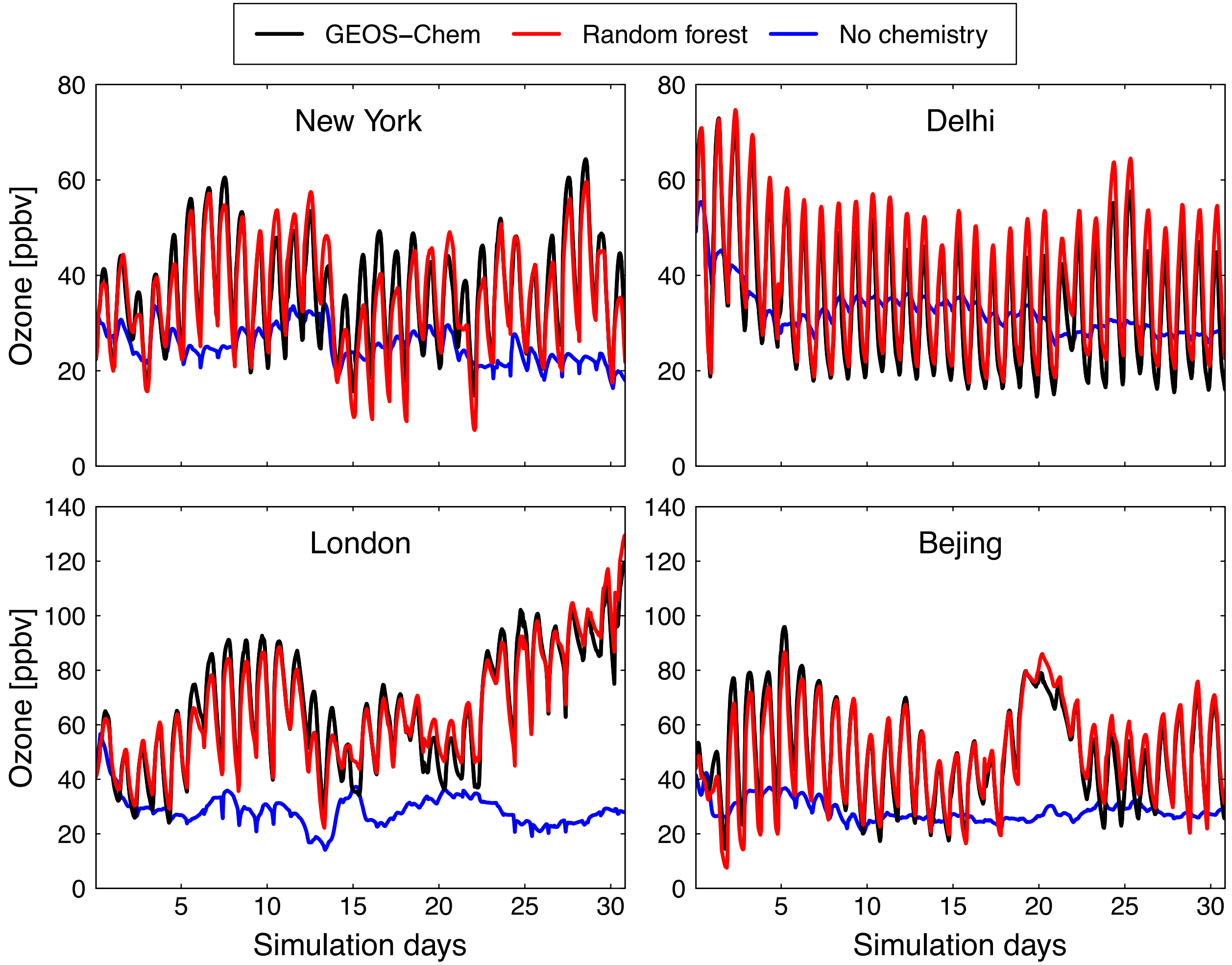
Surface concentrations over polluted regions are well reproduced by ML model



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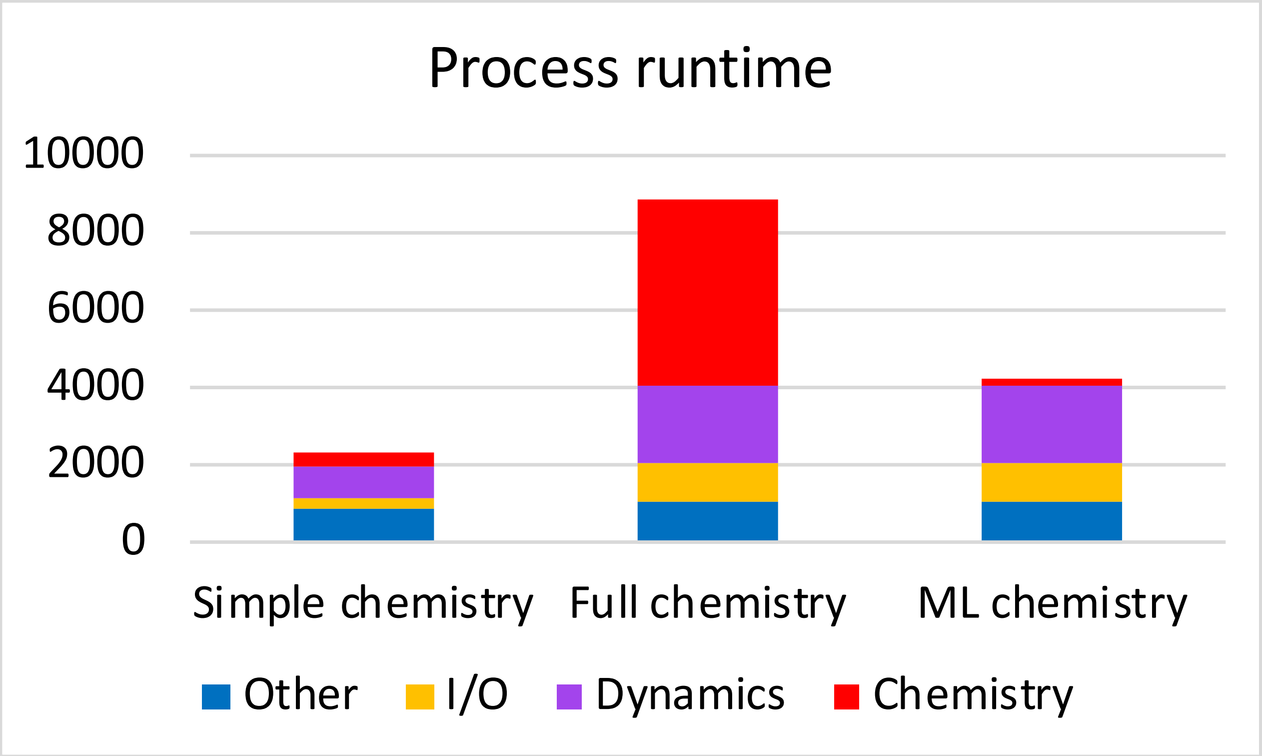
Speedup potential



- Offline evaluation of single 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 decent job at simulating atmospheric chemistry
- Adding constraints (e.g., chemical families) to the machine learning model is critical
- Potential applications:
  - Chemical data assimilation
  - (Short-term) 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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