

# Atmospheric chemistry modeling using a regression forest model

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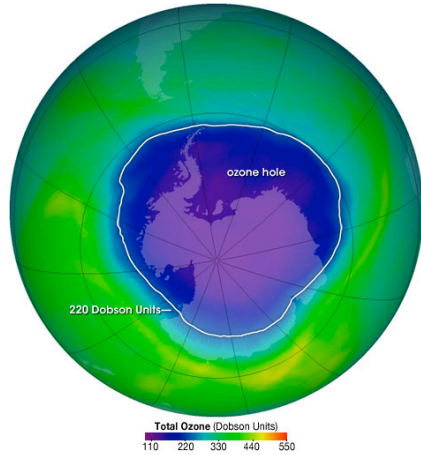
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**National Centre for  
Atmospheric Science**  
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# Why we care about atmospheric chemistry

## 1. Climate & Dynamics



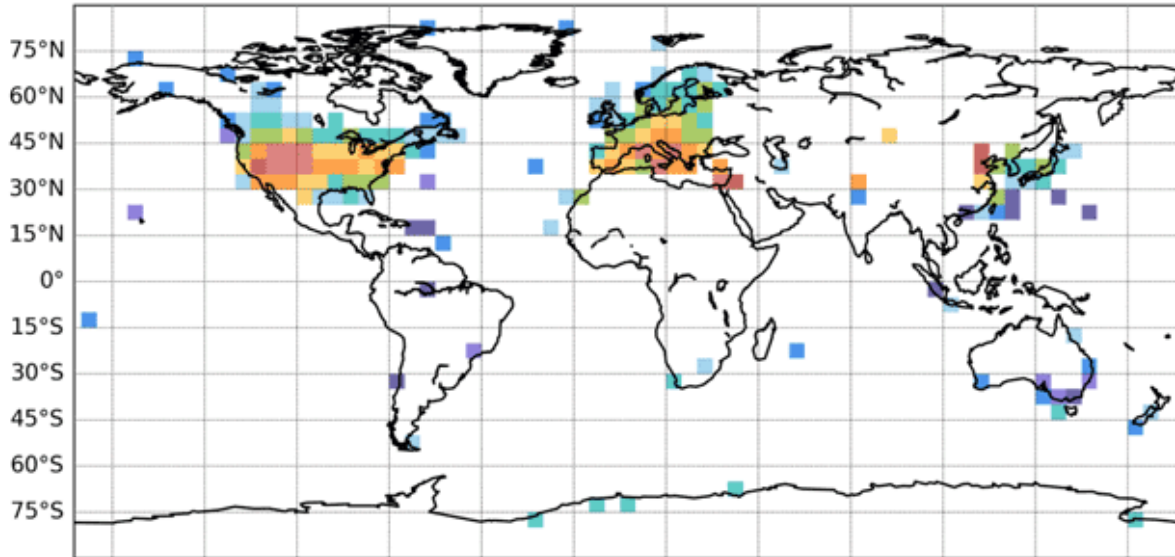
## 2. Air Quality



# Models are needed to fill gaps in observations

## Surface ozone observations

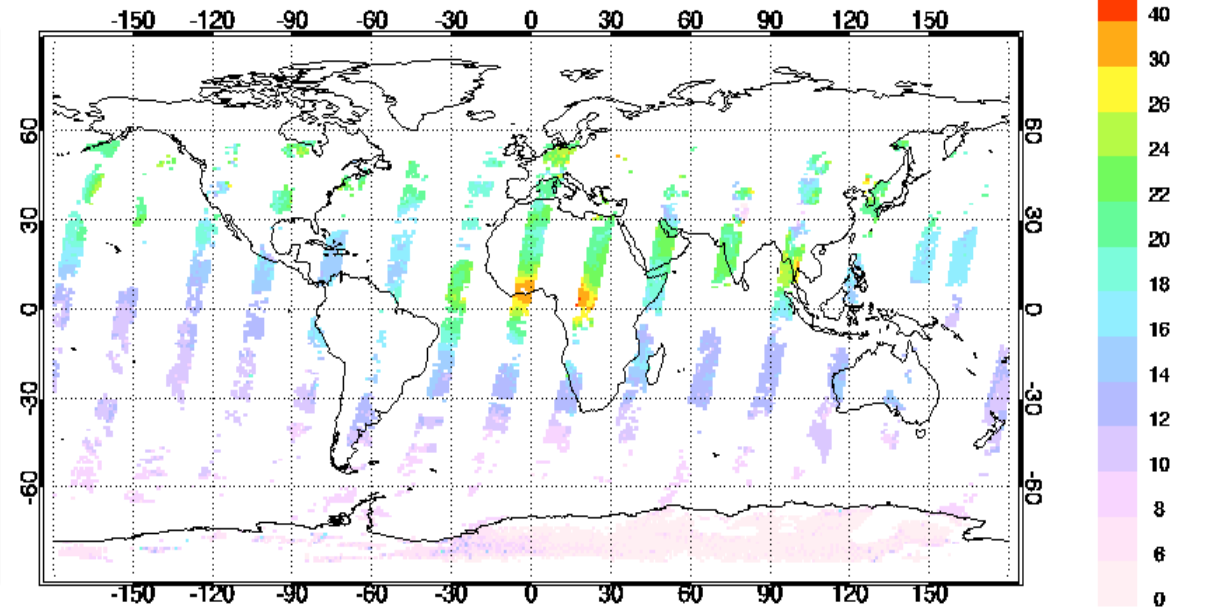
165°W 135°W 105°W 75°W 45°W 15°W 15°E 45°E 75°E 105°E 135°E 165°E



Ozone [nmol/mol] TOAR (Schulz et al., 2017)

## Terra MOPITT (CO)

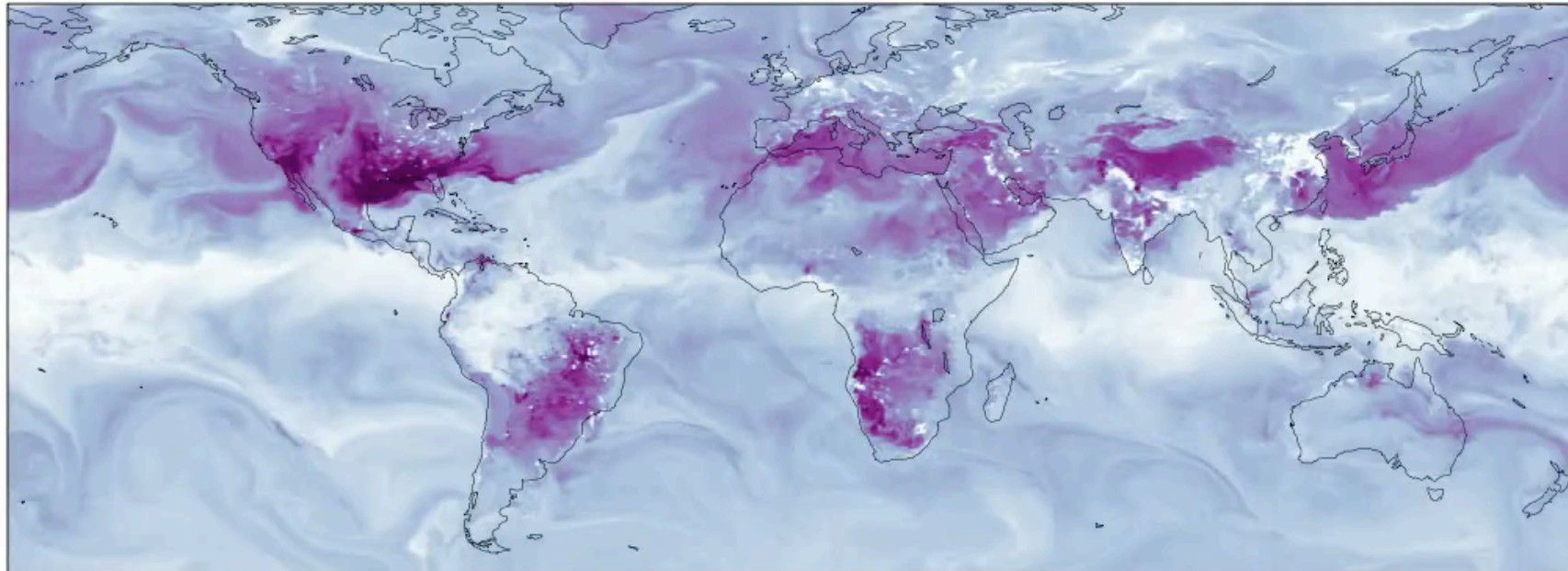
MOPITT CO Column -- 20161230



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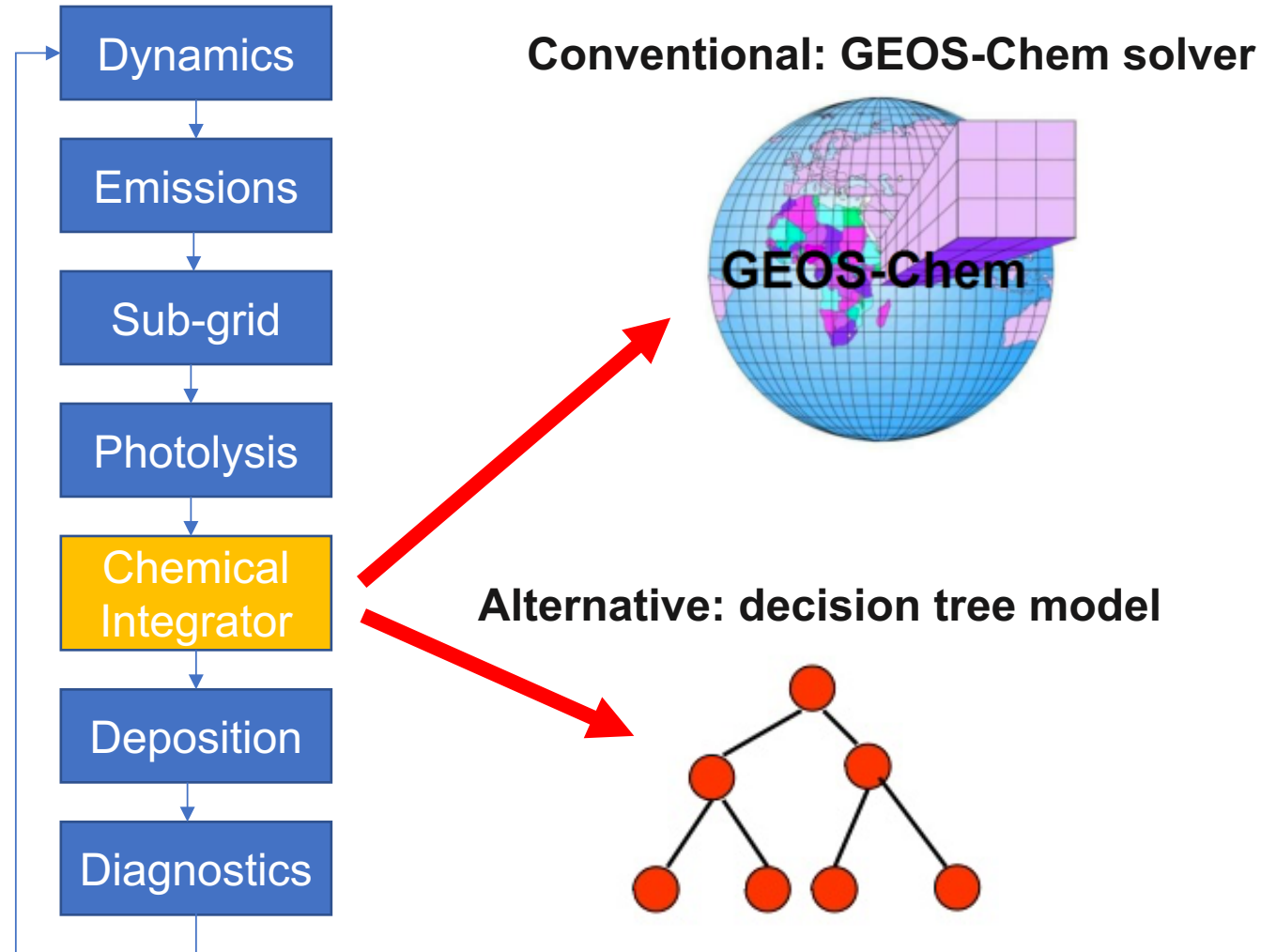
# Atmospheric chemistry is complex & computationally expensive

2017-10-01 00:30 UTC

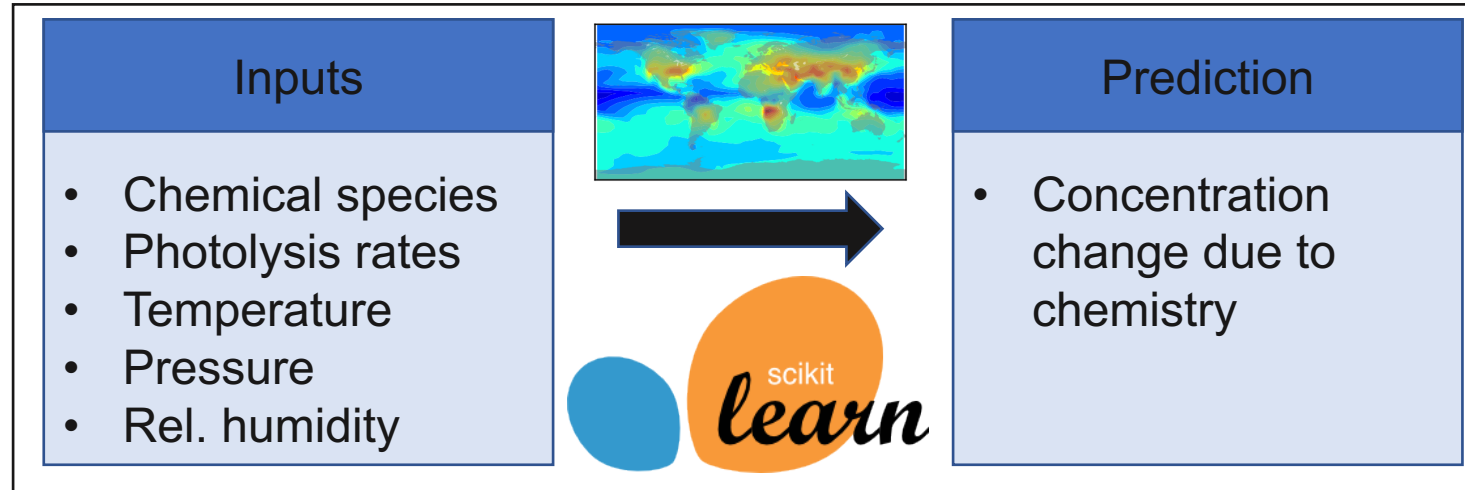


- 25km horizontal resolution, 72 vertical layers (~75M grid cells)
- 282 chemical species, 722 reactions

# Replace chemical integrator with model trained by machine learning



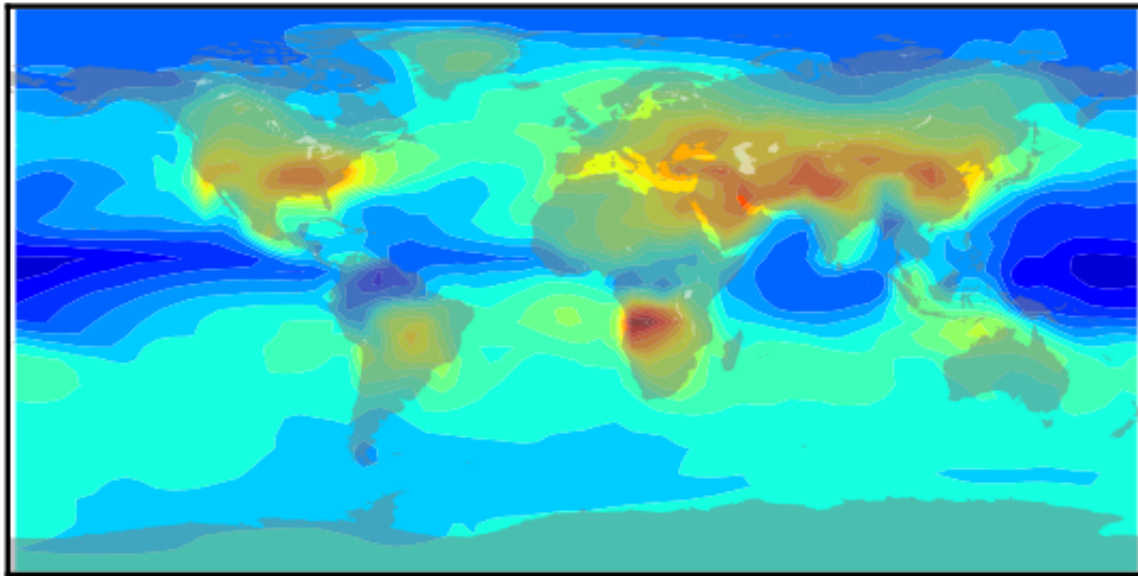
# Decision tree generation (training)



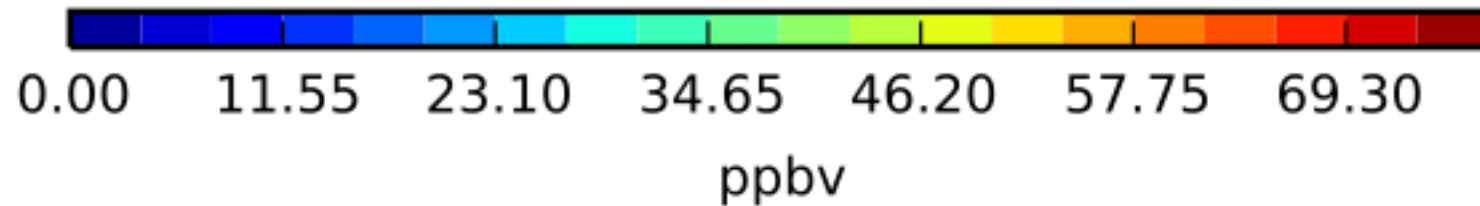
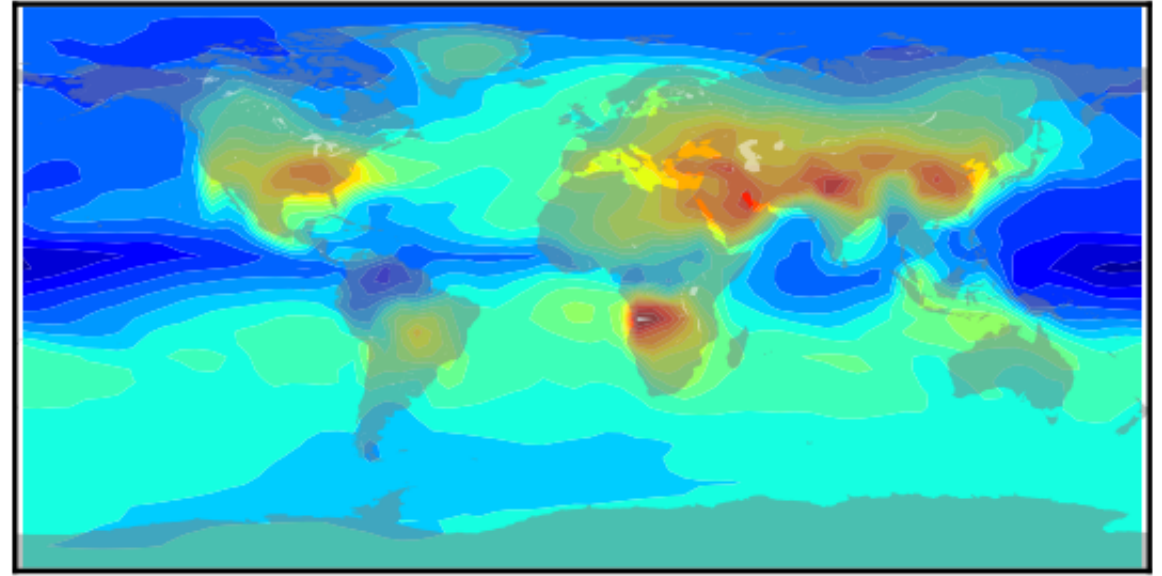
- GEOS-Chem 4x5 degrees test run, 1 year
- Randomly subsample based on deciles, ~5M points in total
- Generate decision trees with 10'000 leaves

# Decision tree model successfully reproduces surface ozone (monthly mean)

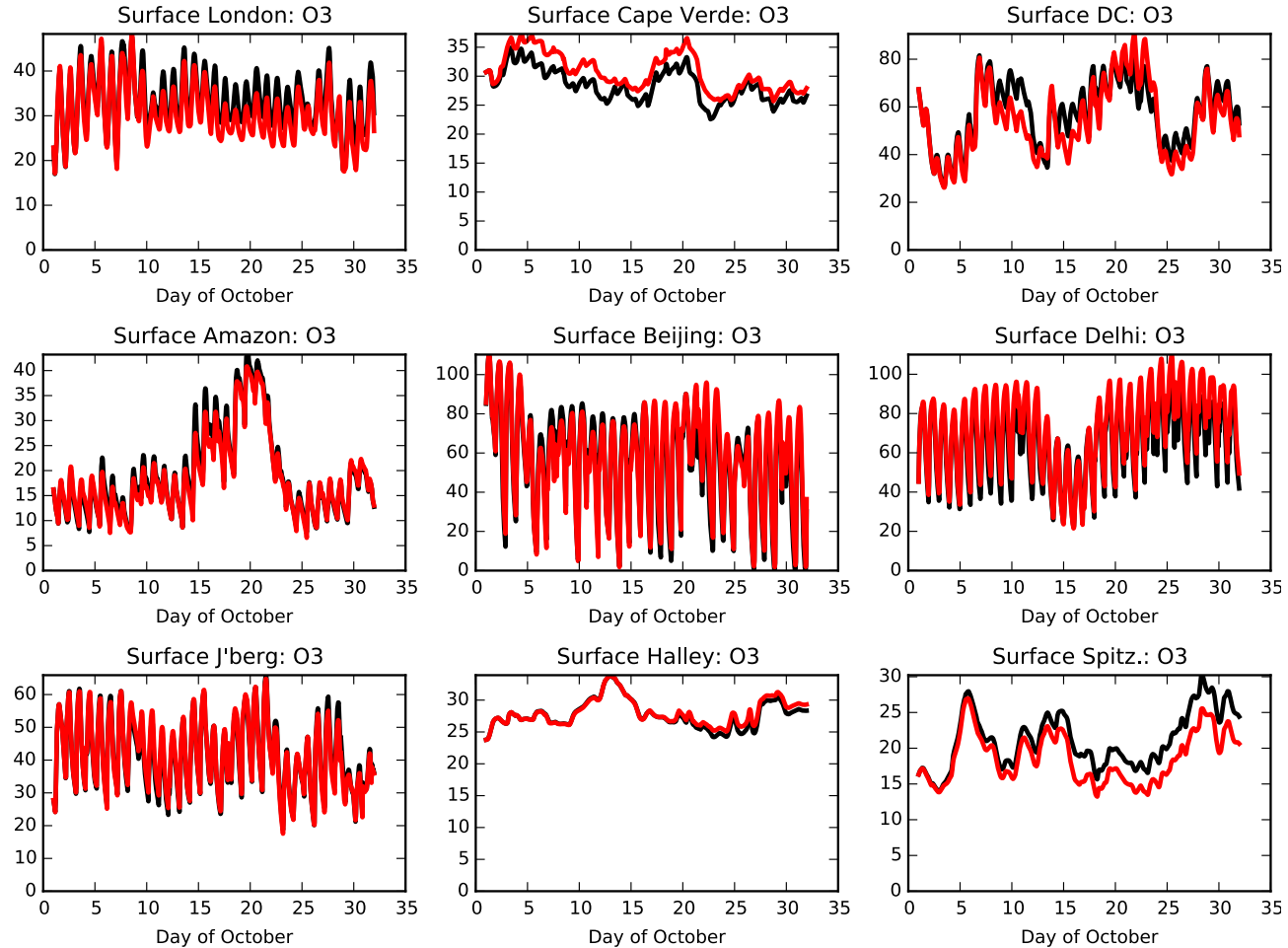
Full chemistry



Decision tree



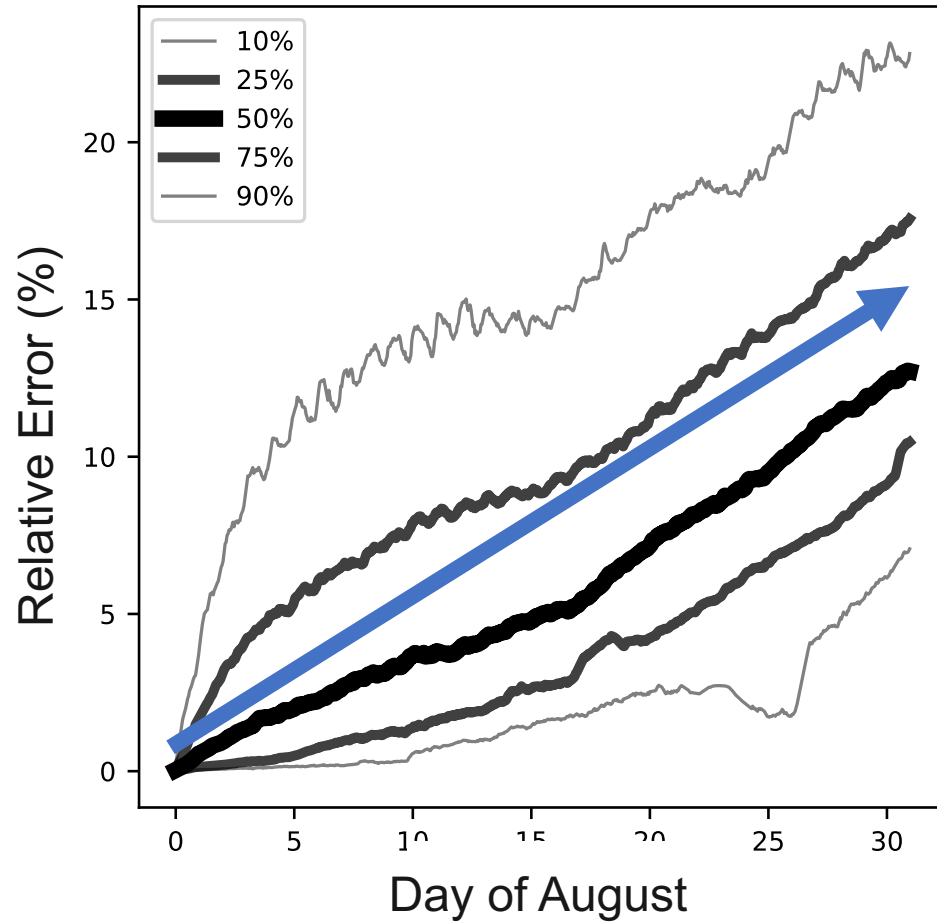
# Decision tree model successfully reproduces surface ozone (cont.)



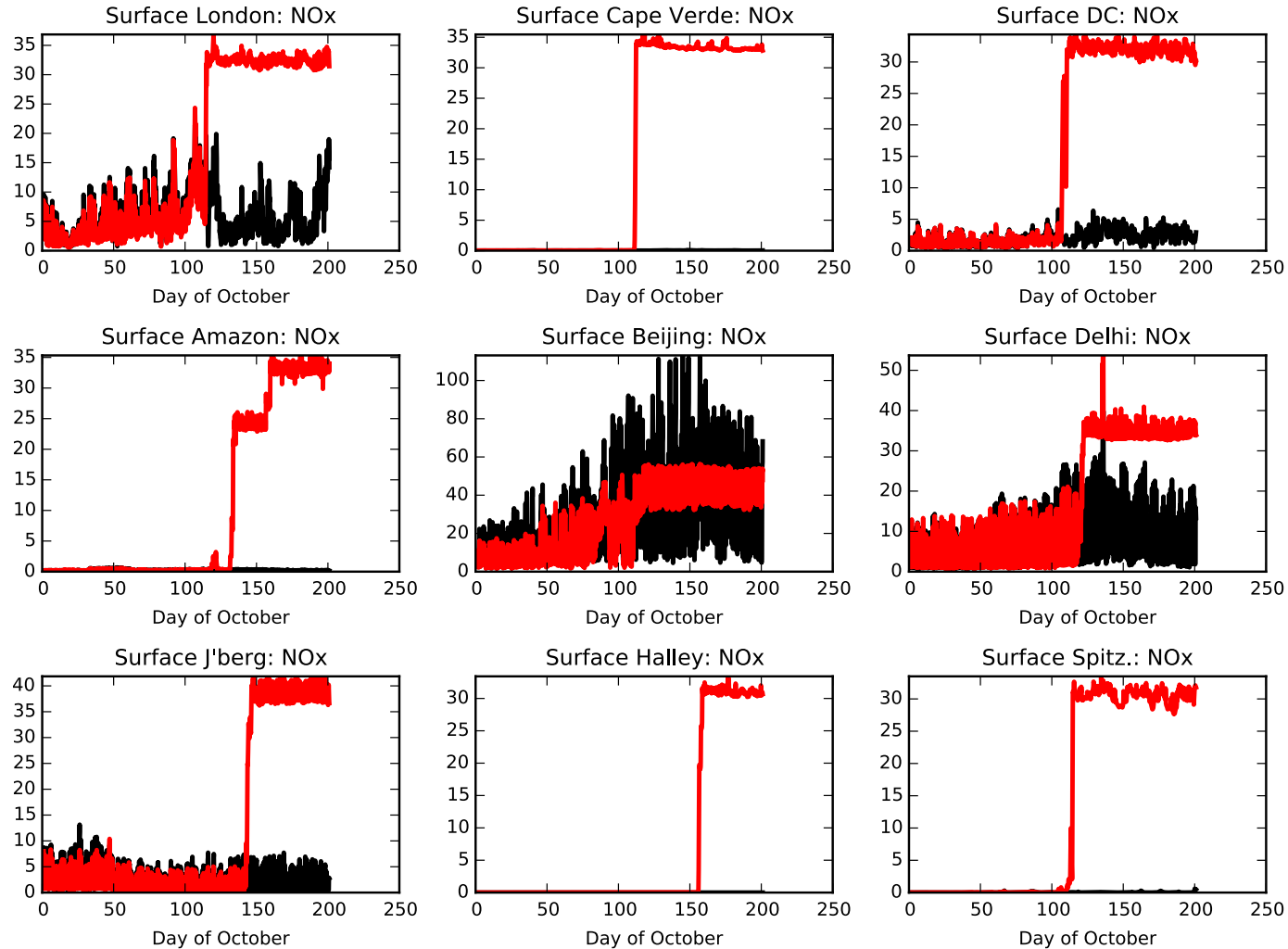
**GEOS-Chem**  
**Decision tree**



# Decision tree model error increases over time...



# ... and eventually becomes unstable



**GEOS-Chem**  
**Decision tree**

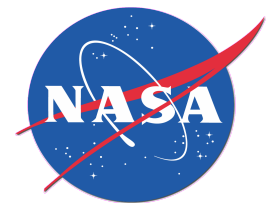


# CHemistry of the Atmosphere through MachinE LEarning for Optimizing Numerics.

## Summary

- Decision tree model does a good job at simulating model chemistry
- Potential applications:
  - Chemical data assimilation
  - Air quality forecasting
- Issues:
  - Unstable long-term (>100 days)
  - Dynamics for >200 chemical species is still slow

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