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Investigating the Impact of Emission Reductions on Ambient PAH and Nitrated PAH Concentrations

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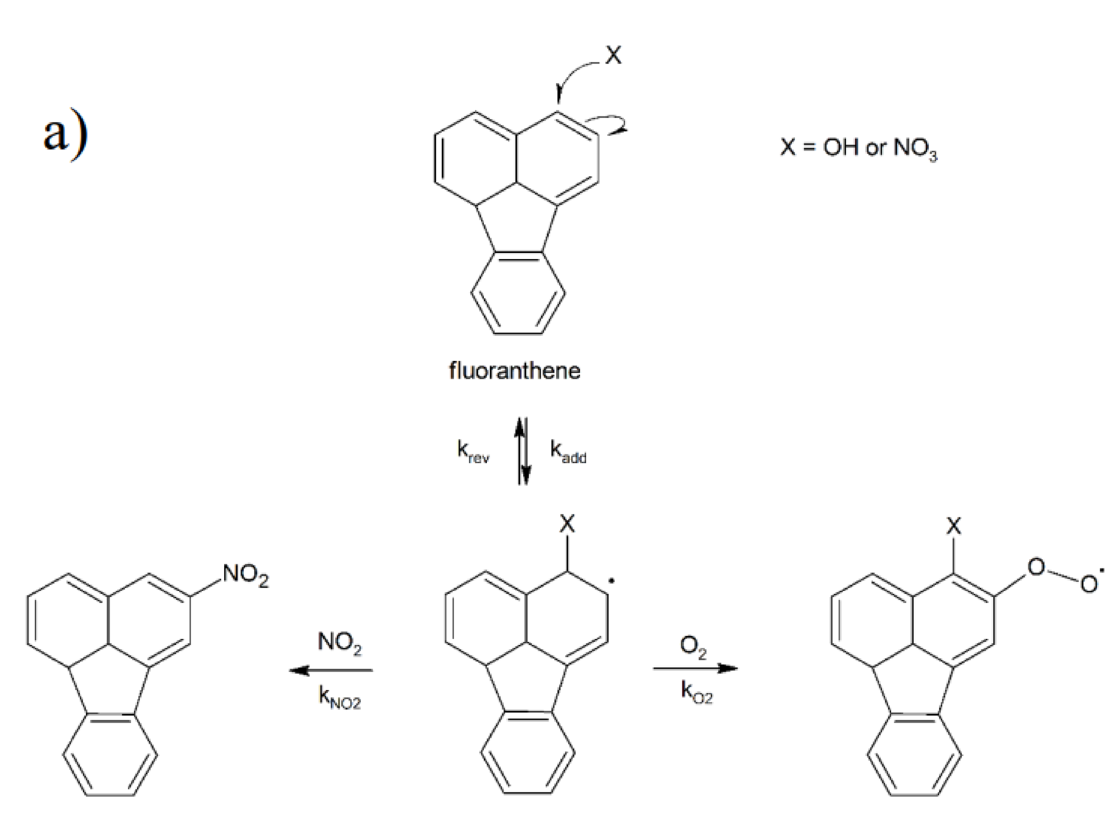
INTRODUCTION

Polycyclic aromatic hydrocarbons (PAHs) are hazardous air pollutants with potential health impacts, and nitrated PAHs (nitro-PAHs) are known to exhibit even higher toxicity. Nitro-PAHs, such as 2-nitrofluoranthene (2-NFLT), are secondary PAH species formed through atmospheric oxidant reactions with primary PAHs emitted from various anthropogenic sources. As emissions from anthropogenic sources continue to decrease, it is crucial to understand how these reductions affect the levels of primary and secondary PAHs in the atmosphere. This research proposal aims to investigate the impact of decreasing emissions on ambient PAH and nitrated PAH concentrations using a regional chemical transport model.

OBJECTIVES & METHOD

- Simulate the concentrations of key PAH species, including fluoranthene (FLT) and 2-NFLT, in the atmosphere for the years 2000, 2019, and 2036 using a regional chemical transport model.
- Assess the accuracy and reliability of the model by comparing the simulated FLT and 2NFLT concentrations with ground-based measurement data.
- Quantify the contribution of emissions from different sectors, particularly the traffic sector, to 2-NFLT concentrations through sensitivity analysis.
- Investigate the potential future levels of 2-NFLT by simulating various emission scenarios that consider the elimination of traffic sector emissions in urban areas.



Wilson et al., 2020

Reactions

$FLT + X \rightarrow FLTX$	(k_{add})
$FLTX \rightarrow FLT + X$	(k_{rev})
$FLTX + NO_2 \rightarrow 2\text{-}NFLT$	(k_{NO2})
$FLTX + O_2 \rightarrow OFLT$	(k_{O2})

Temporal evolution of FLT and 2-NFLT

$$\frac{d[\mathrm{FLT}]}{dt} = -k_{\mathrm{add}}[\mathrm{FLT}][\mathrm{X}] + k_{\mathrm{rev}}[\mathrm{FLTX}],$$

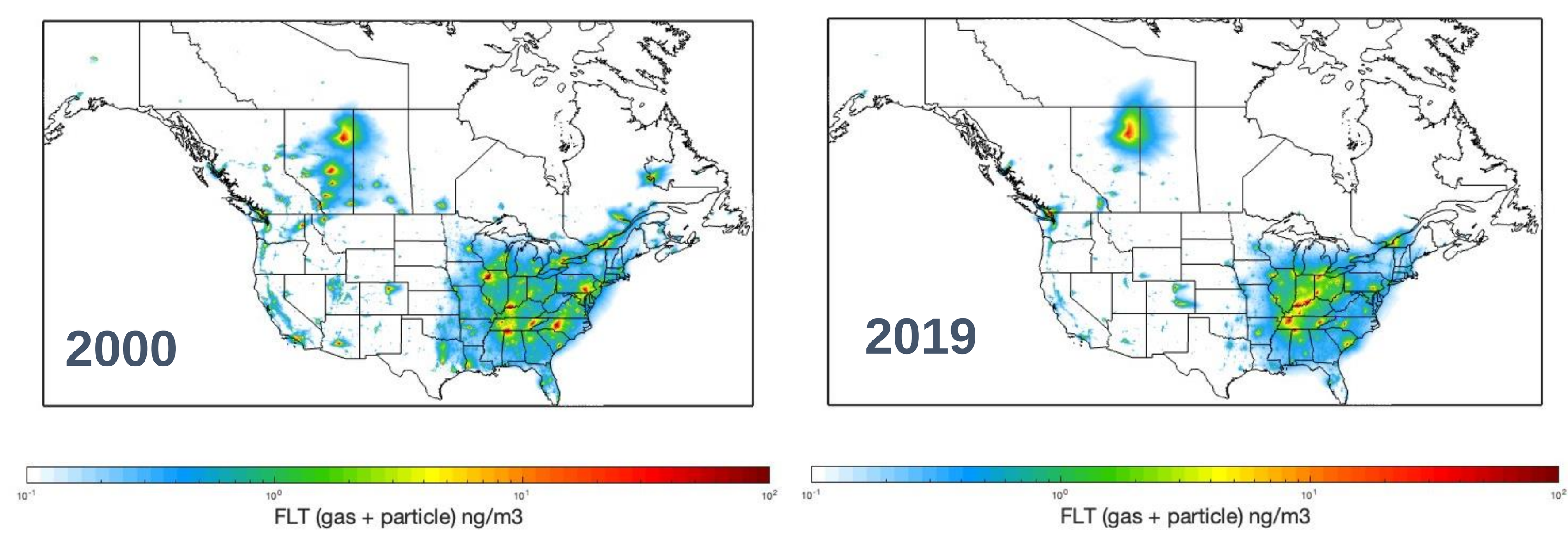
$$\frac{d[\mathrm{FLTX}]}{dt} = k_{\mathrm{add}}[\mathrm{FLT}][\mathrm{X}] - (k_{\mathrm{rev}} + k_{\mathrm{NO2}}[\mathrm{NO_2}] + k_{\mathrm{O2}}[\mathrm{O_2}])[\mathrm{FLTX}],$$

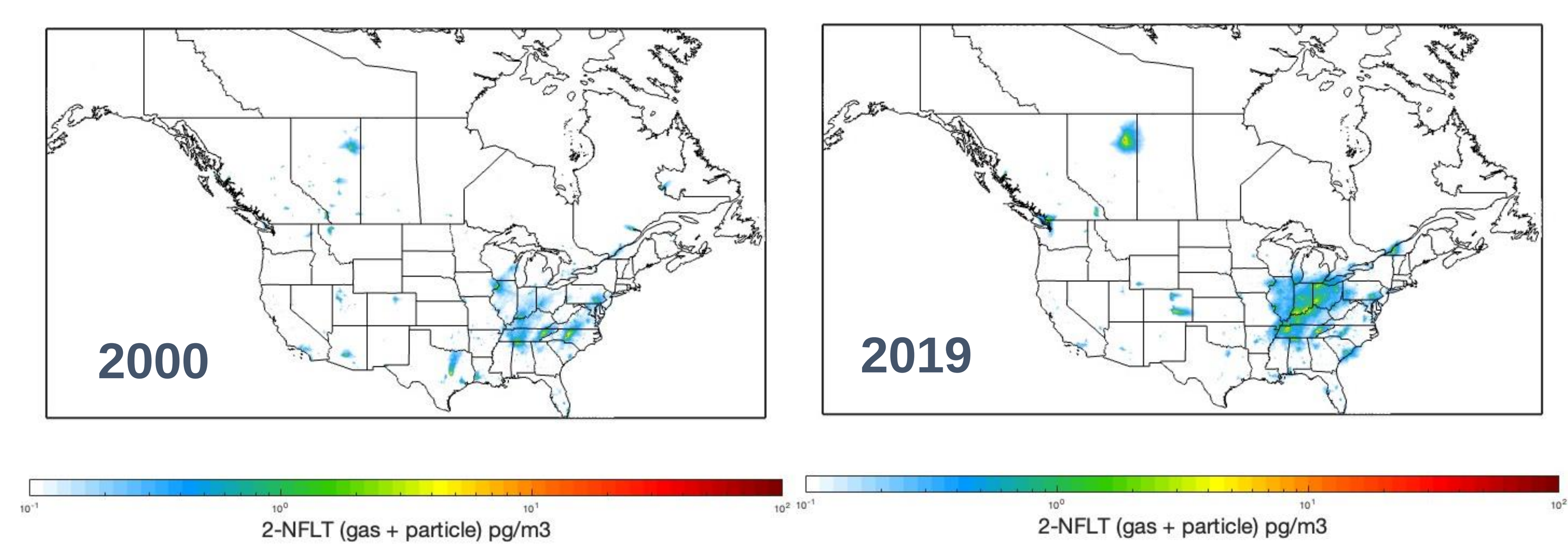
$$\frac{d[\mathrm{2\text{-}NFLT}]}{dt} = k_{\mathrm{NO2}}[\mathrm{NO_2}][\mathrm{FLTX}],$$

Assume chemical steady state for FLTX $\frac{d[\mathrm{FLTX}]}{dt} = 0:$

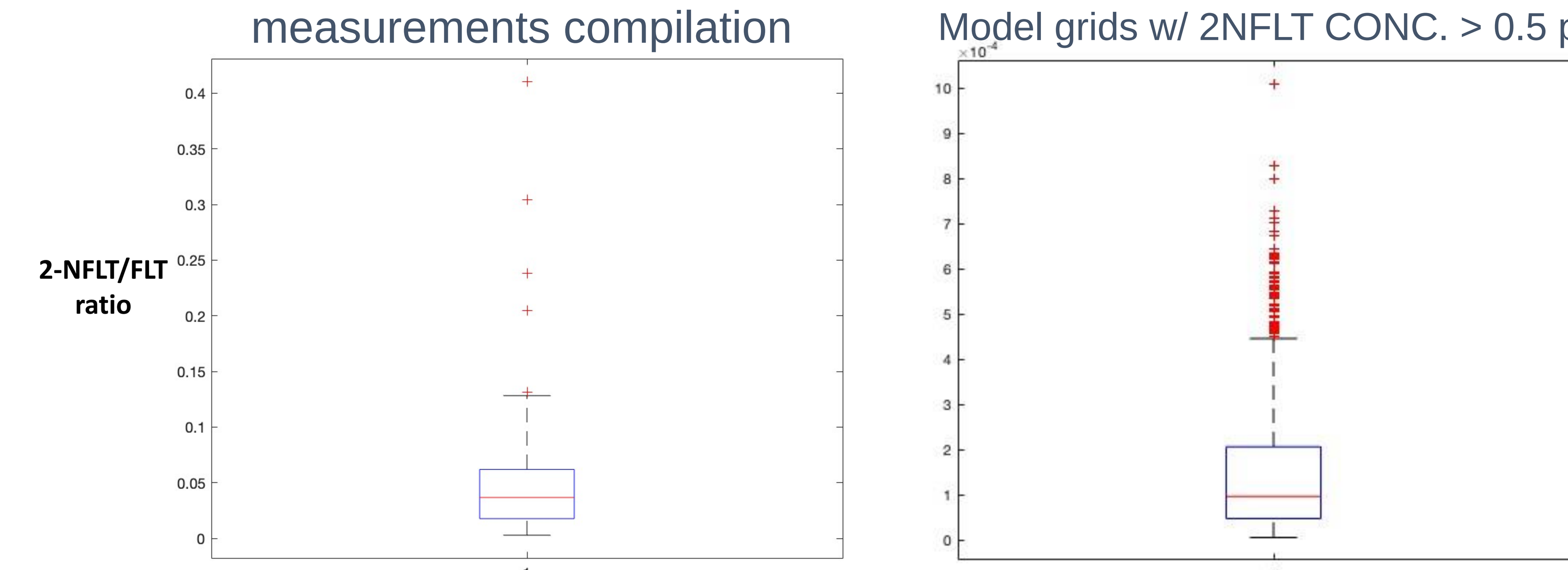
RESULTS & DISCUSSION

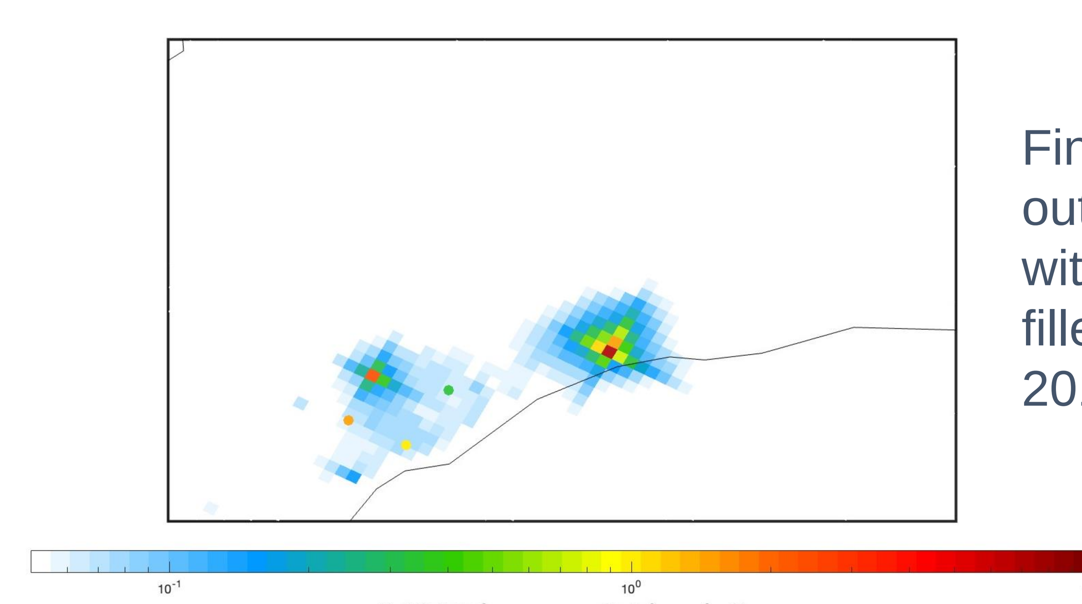
- Simulated Annual Average PAH Spatial Distribution





- Model Evaluation





Fine resolution (2.5km) model output for Greater Toronto Area with measurements shown in filled dots (Jariyasopit et al., 2019)

Take home: model simulation seems to be underestimating 2-NFLT conc.

- Moving forward

- Adjust model parameterization parameters, such as reaction rate constant, to represent more realistic PAH conc. spatial distribution (Atkinson et al., 1990)
- Conduct sensitivity simulations with traffic-free emissions to investigate the contribution from traffic sector

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