The Effect of Nitrogen Oxide Emissions from Automobile Traffic on the Concentration of Tropospheric Ozone in the Great Smoky Mountains National Park

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THE PROJECT

GREAT SMOKY MOUNTAINS NATIONAL PARK

- Most visited national park in the United States of America (~9,000,000 visitors/year).
- The majority of park visitors drive through the park to various hiking, camping or sightseeing destinations, resulting in substantial emissions of nitrogen oxides (NOx) from vehicle exhaust. NOx, when combined with hydrocarbon emissions from natural vegetation can lead to ozone, a primary component of photochemical smog, which can be damaging to plants, animals and humans.
- The primary goal of our project is to initially assess how NOx emissions from visitor traffic in the park may affect concentrations of ground-level (tropospheric) ozone.

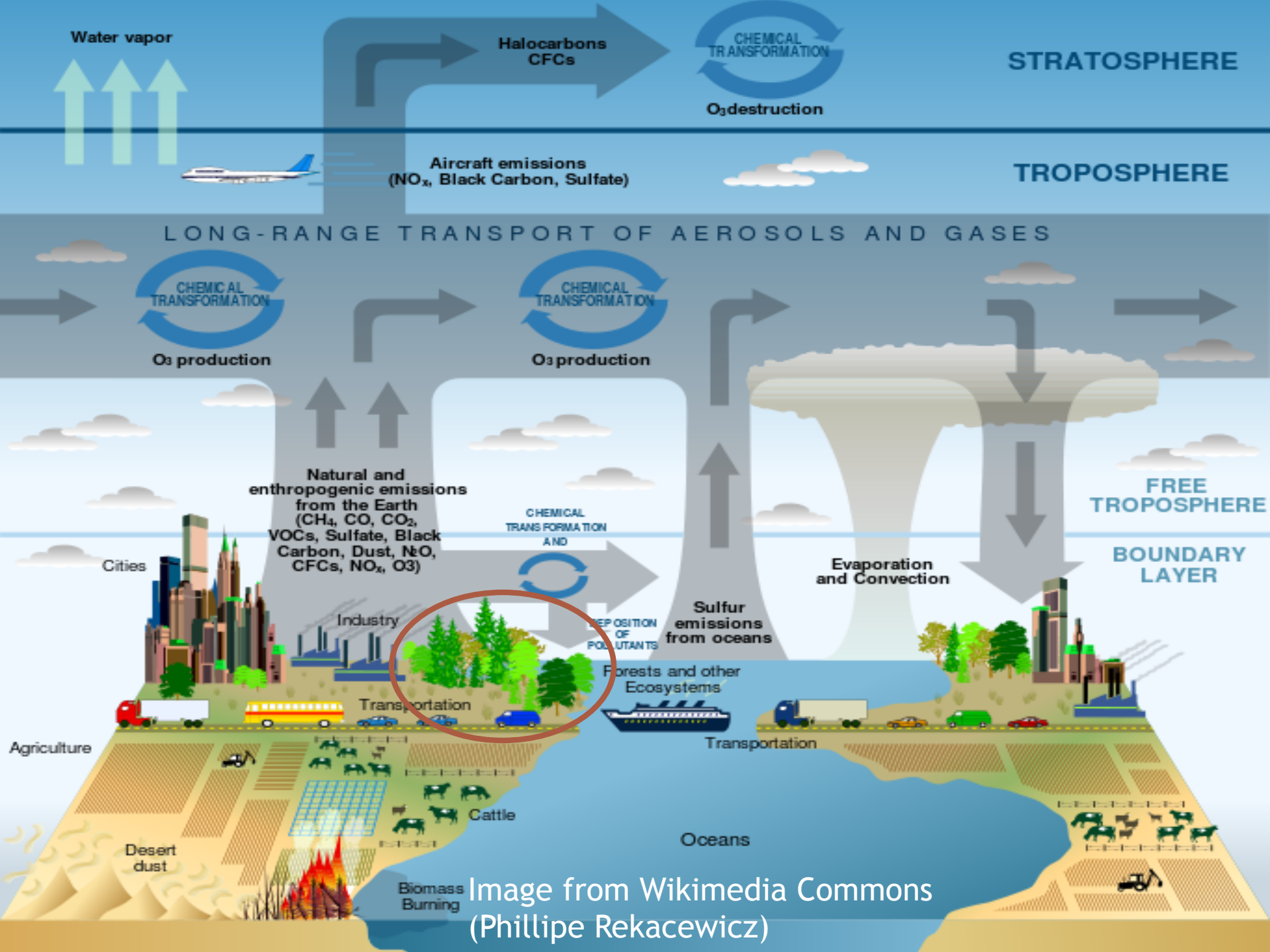
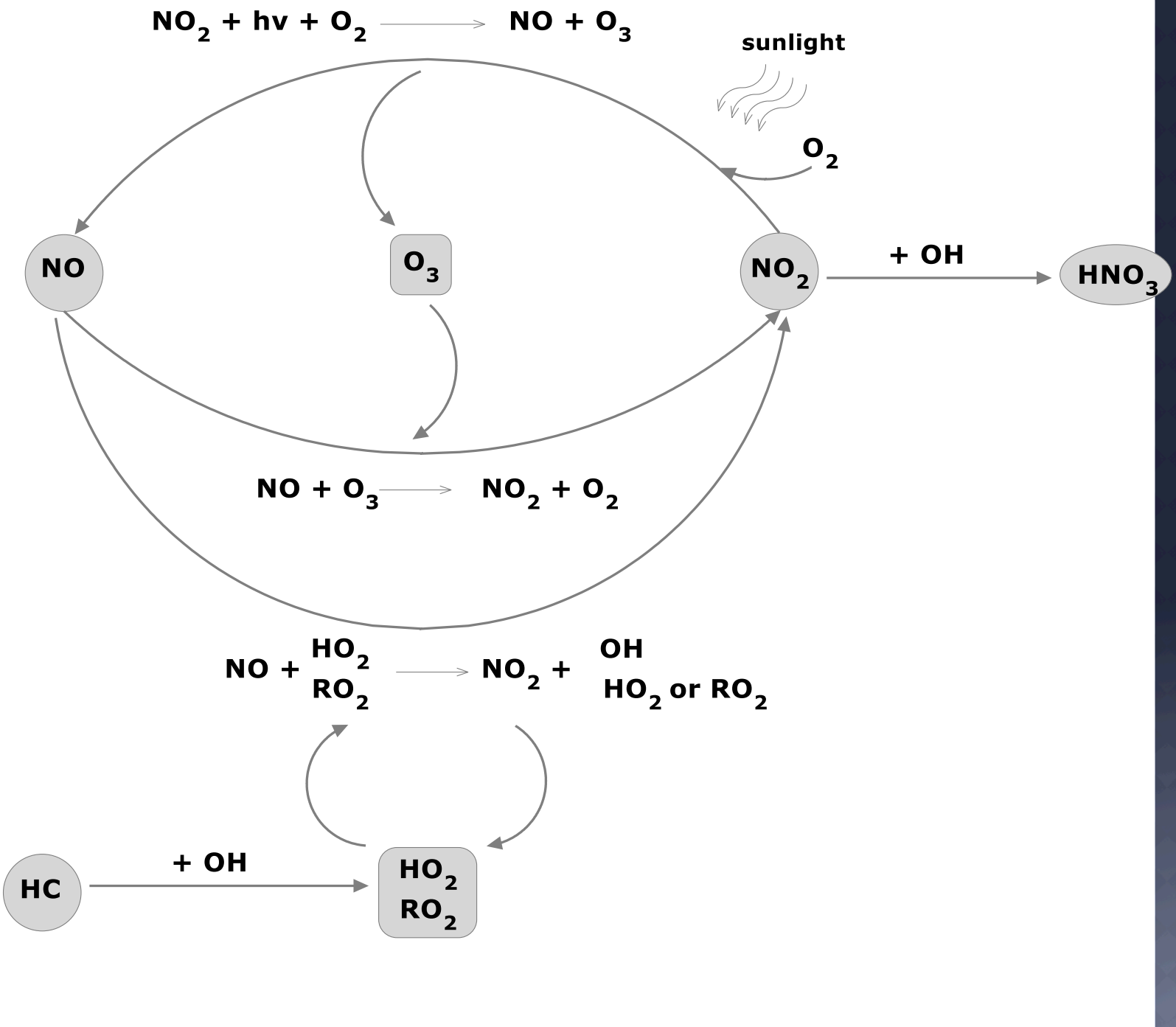


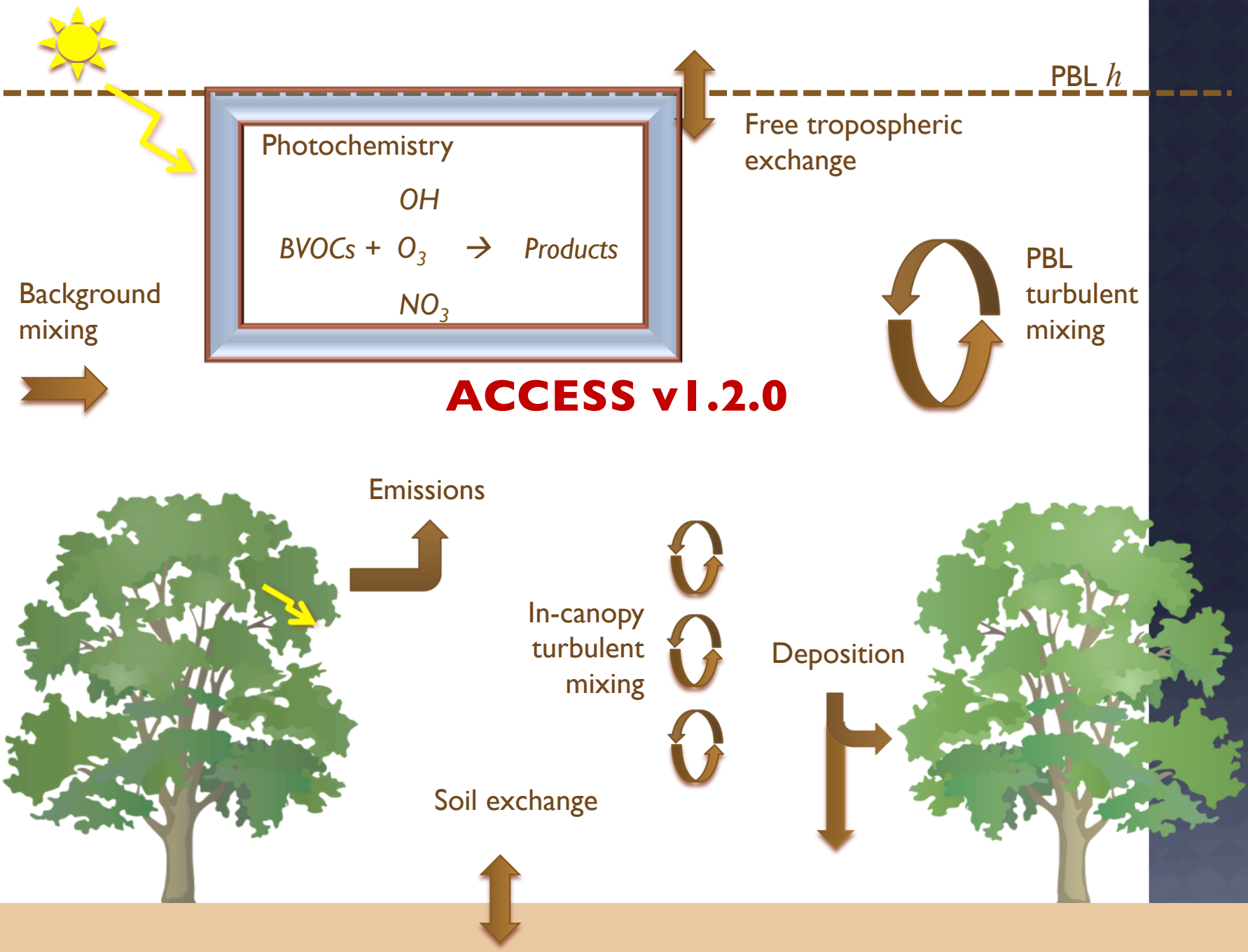
Image from Wikimedia Commons
(Phillipe Rekacewicz)


$NO_2 + hv + O_2 \rightarrow NO + O_3$
sunlight
O_2
NO
O_3
NO_2
+ OH
HNO_3
$NO + O_3 \rightarrow NO_2 + O_2$
$NO + HO_2 / RO_2 \rightarrow NO_2 + OH / HO_2 \text{ or } RO_2$
HC
+ OH
HO_2 RO_2

THE ATMOSPHERIC CHEMISTRY AND CANOPY EXCHANGE SIMULATION SYSTEM (ACCESS)

ACCESS

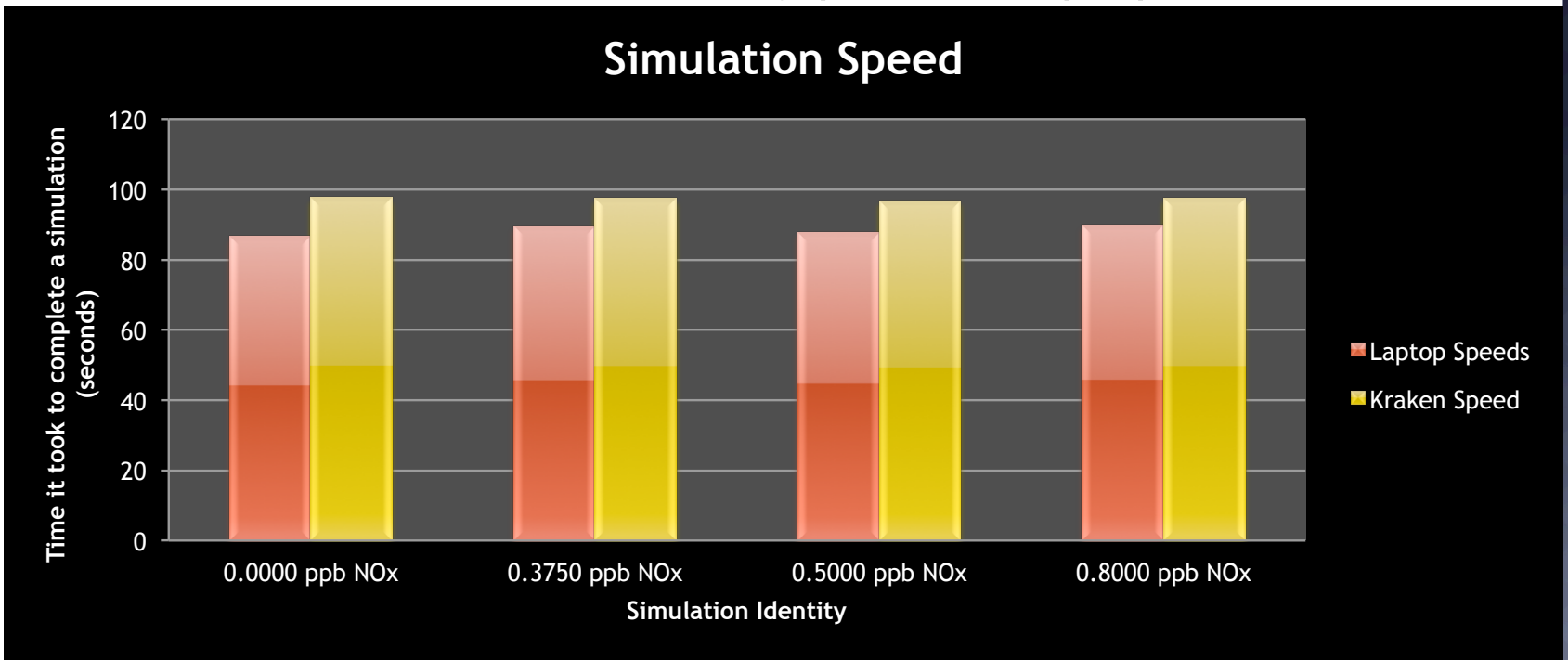
- It is a one-dimensional column model that utilizes a current state-of-the-science, near explicit atmospheric chemistry mechanism to simulate tropospheric ozone (and other compounds) from the ground level to the top of the planetary boundary layer (PBL) (~2 km above ground level).


PBL h
Free tropospheric exchange
Photochemistry
OH
$BVOCs + O_3 \rightarrow Products$
NO_3
Background mixing
PBL turbulent mixing
ACCESS v1.2.0
Emissions
In-canopy turbulent mixing
Deposition
Soil exchange

RESULTS

INITIAL TESTS

- Initially our plans were this:
  - Assess how ACCESS runs on an HPC platform and attempt to optimize it.
    - The graph below shows the results from our initial tests on Kraken versus my personal laptop.



A SLIGHT CHANGE OF PLAN…

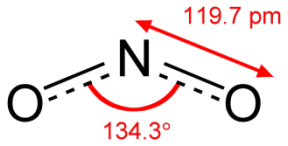
- We decided not to use Kraken because it has strict time constraints on simulations (i.e., 24 hrs maximum for a simulation for a regular user). This was not acceptable, as we needed to run the full ACCESS program soon and did not have time to parallelize the code.
  - The serial code of ACCESS itself takes around 30 CPU hours to run; this would not be possible to do on Kraken.
- Solution: Abandon the thought of using Kraken, and use Star1 (a computer at University of Tennessee), which has no time constraints.

SIMULATION RESULTS FROM STAR1

- We did two simulations on Star1:
  - 1st simulation: Neutral Atmospheric Conditions
    - With this simulation, we did not get much vertical transport, which meant that we did not get much NOx transported above the canopy, for possible reactions. Because of this, we decided to do a second simulation.
  - 2nd simulation: Unstable Atmospheric Conditions
    - More enlightening results came from this simulation. There is more transportation of NOx above the canopy. This allowed for a more accurate representation of the impact of NOx on the photochemistry above the canopy. These are the results used in the upcoming slides.

SPECIES GRAPHS

STRUCTURE OF SEVERAL OF THE SPECIES YOU WILL BE SEEING GRAPHS OF



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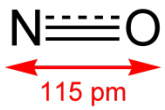
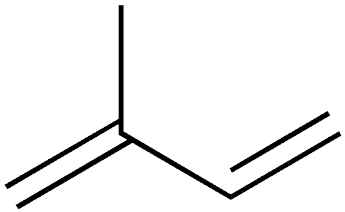
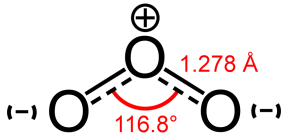
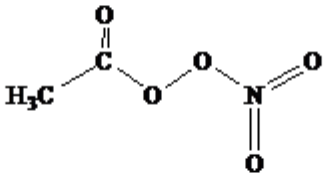


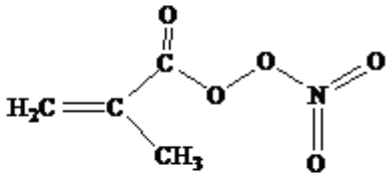
= NO_x







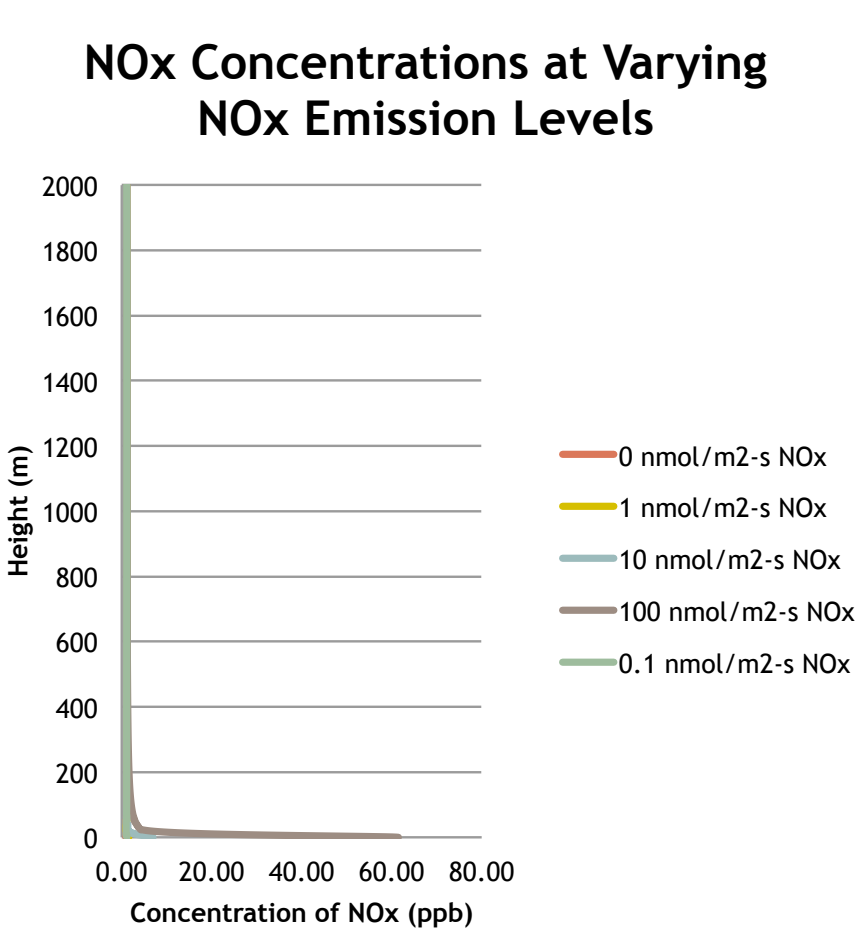
PAN

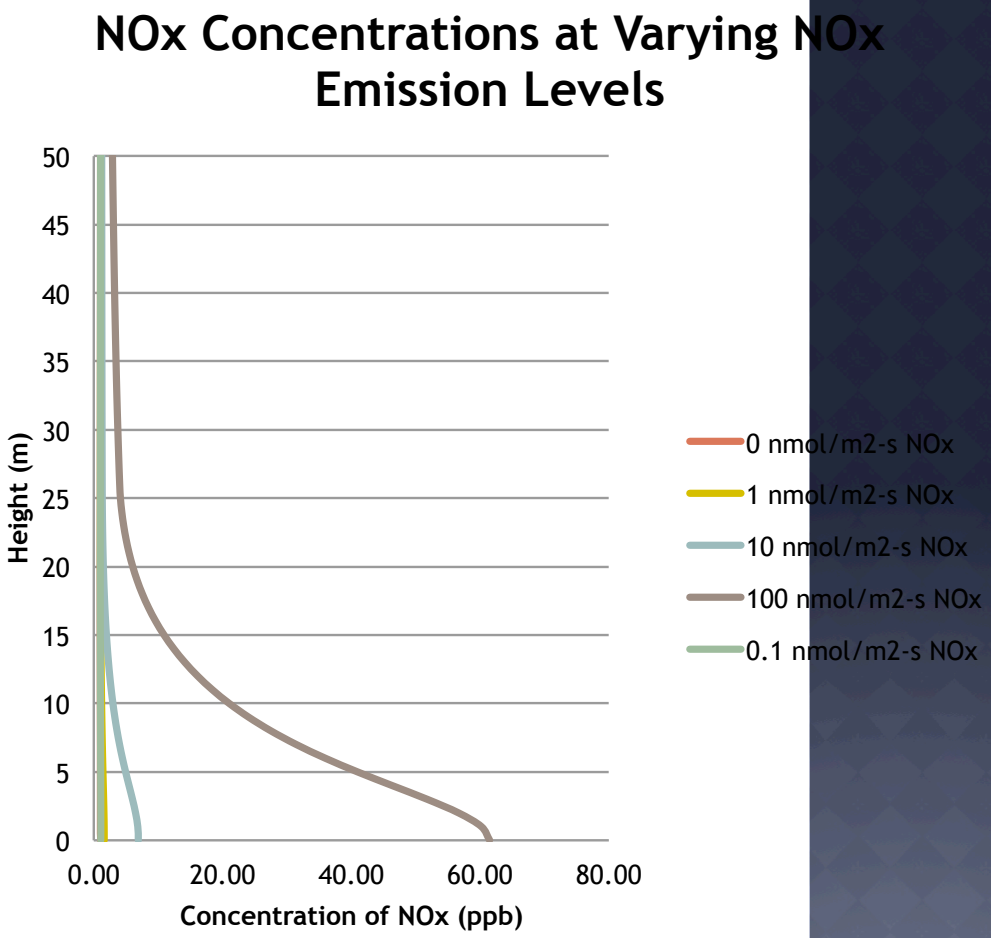


MPAN

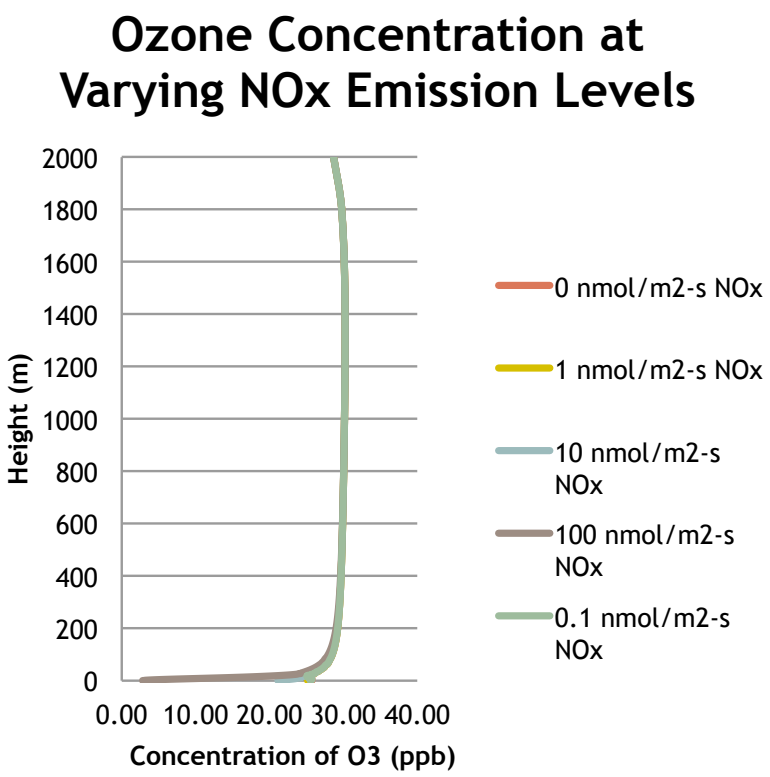
- From top-left clockwise:
  - Nitrogen dioxide (NO_2)
  - Nitric oxide (NO)
  - Nitrogen oxides (Nox)
  - Methacryloyl peroxy nitrate (MPAN)
  - Peroxyacetyl Nitrate (PAN)
  - Ozone (O_3)
  - Isoprene (C_5H_8)

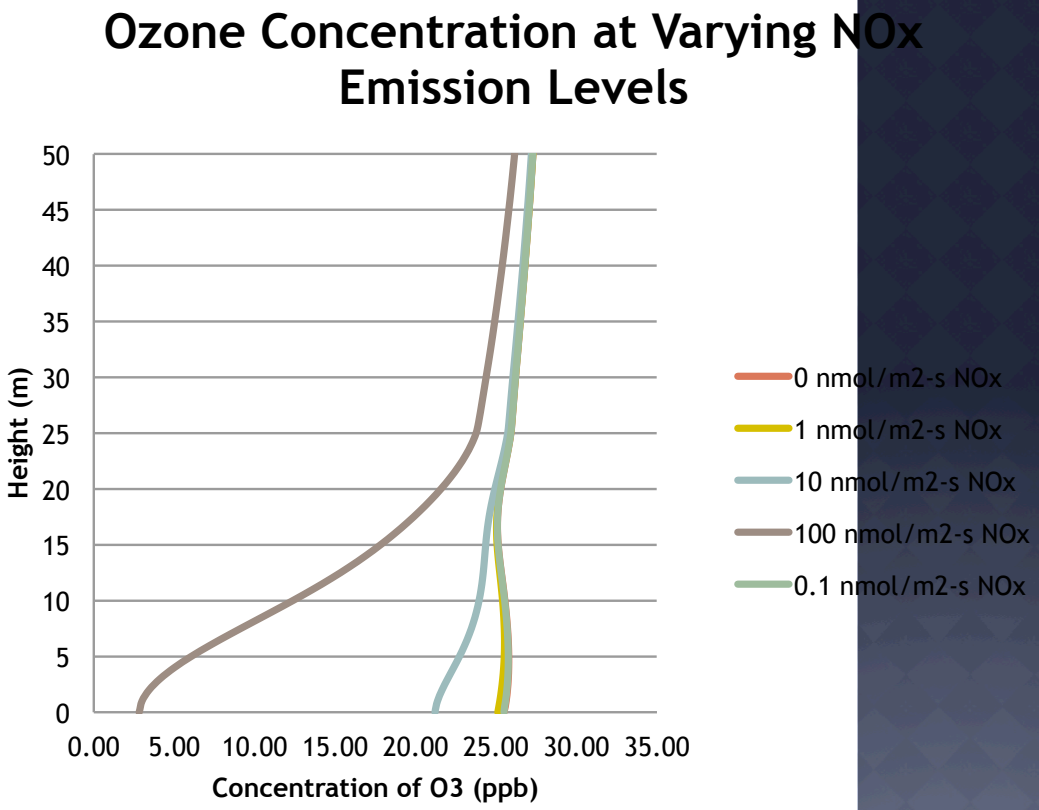
SPECIES GRAPHS (NO_x)



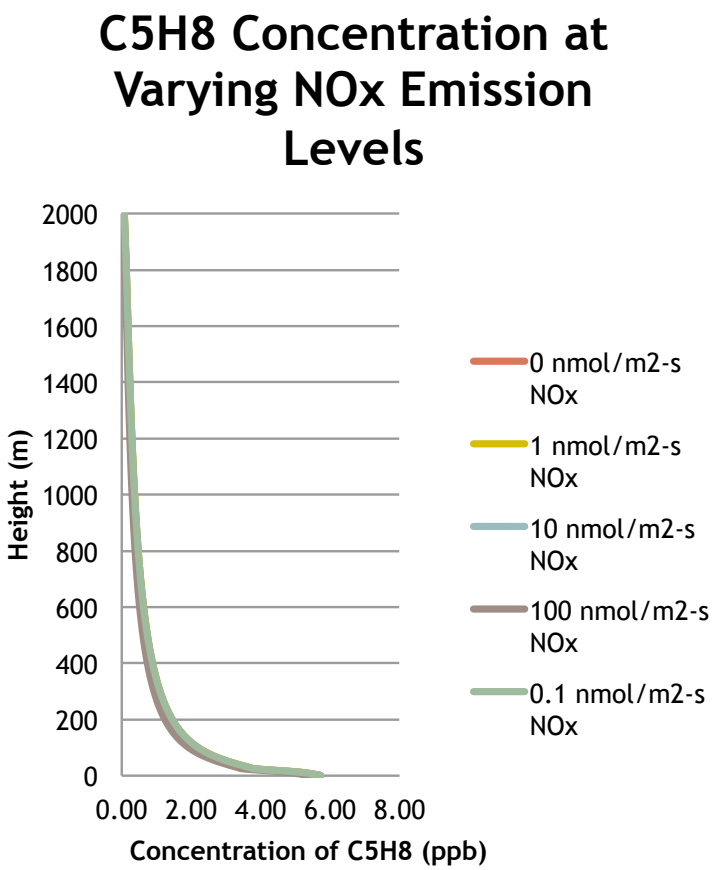


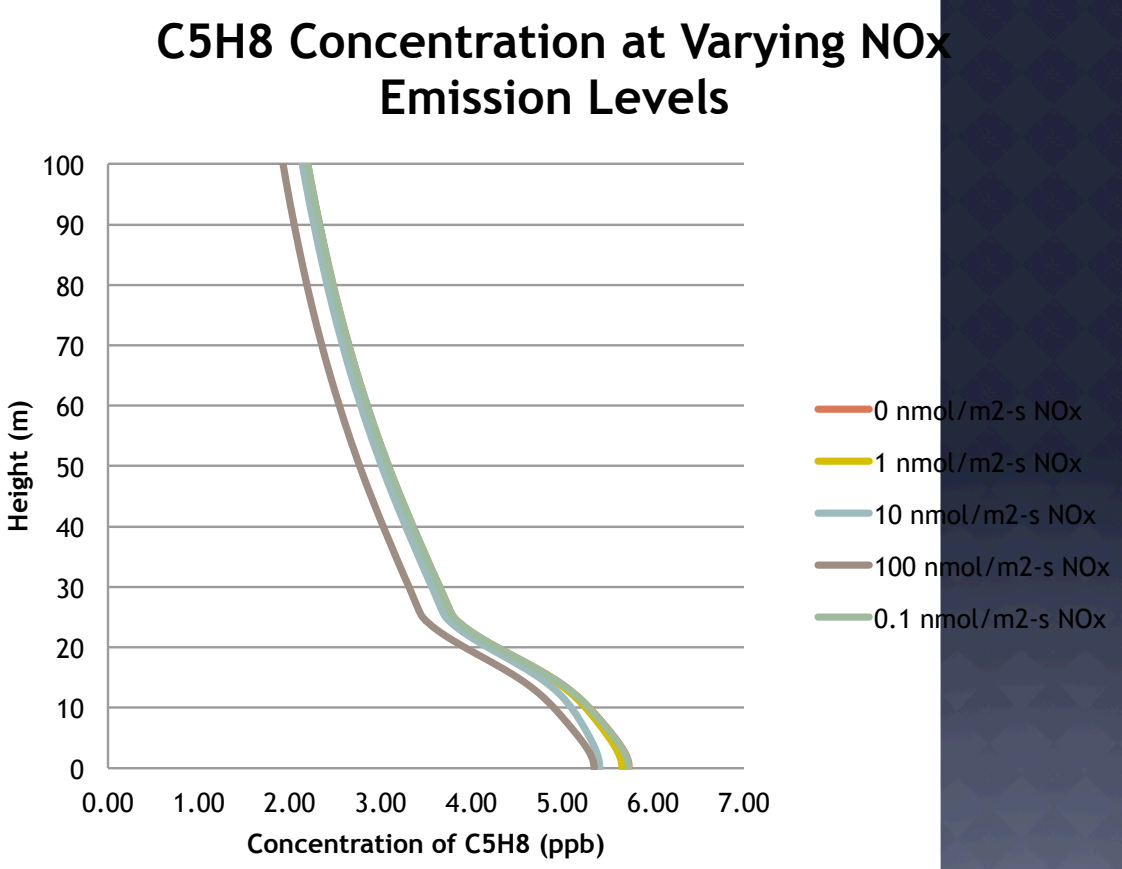
SPECIES GRAPHS (OZONE (O_3))





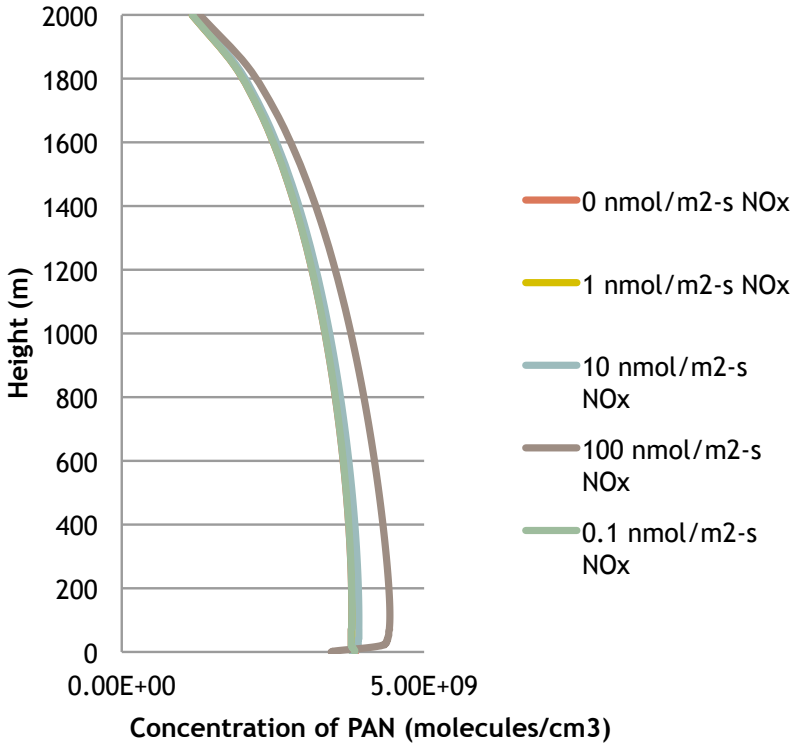
SPECIES (ISOPRENE (C_5H_8))



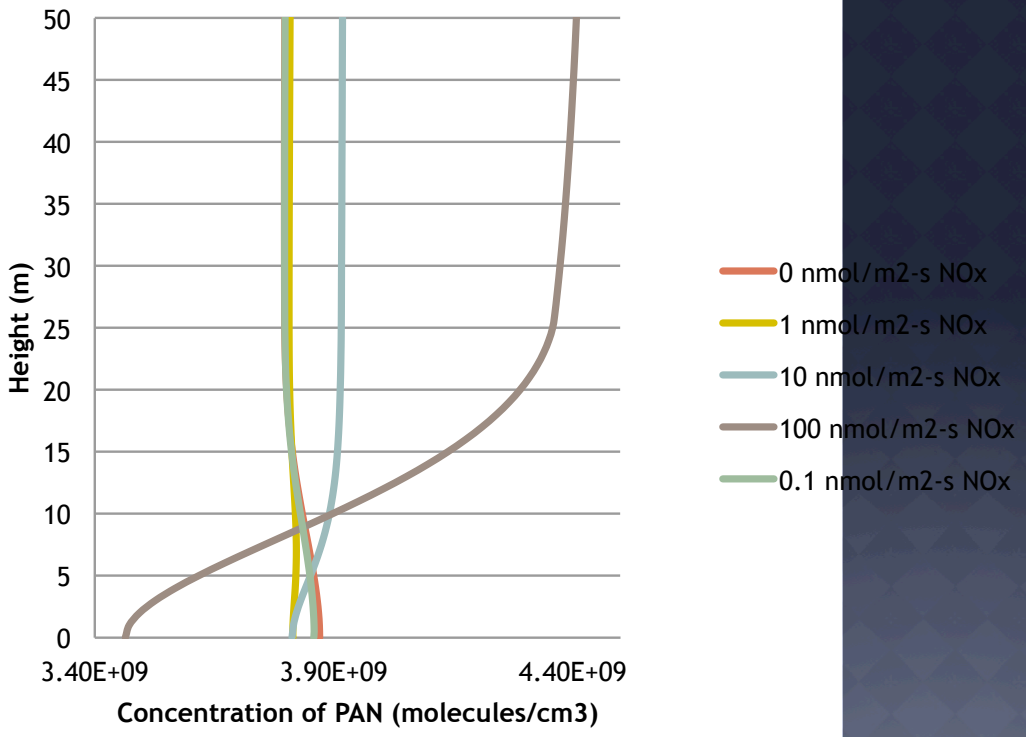


SPECIES (PEROXYACETYL NITRATE (PAN))

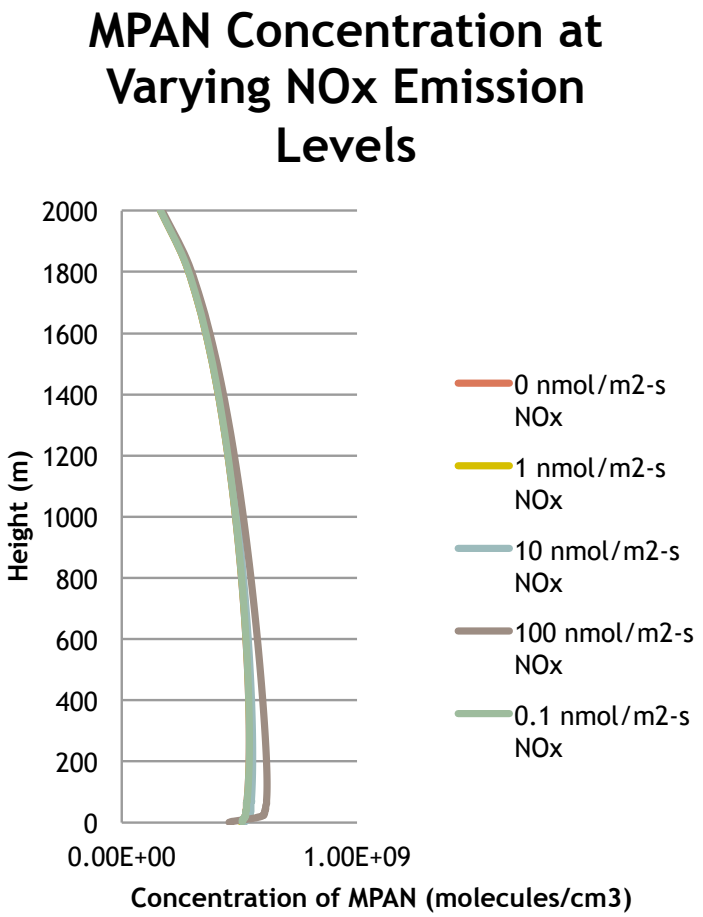
PAN Concentration at Varying NOx Emission Levels

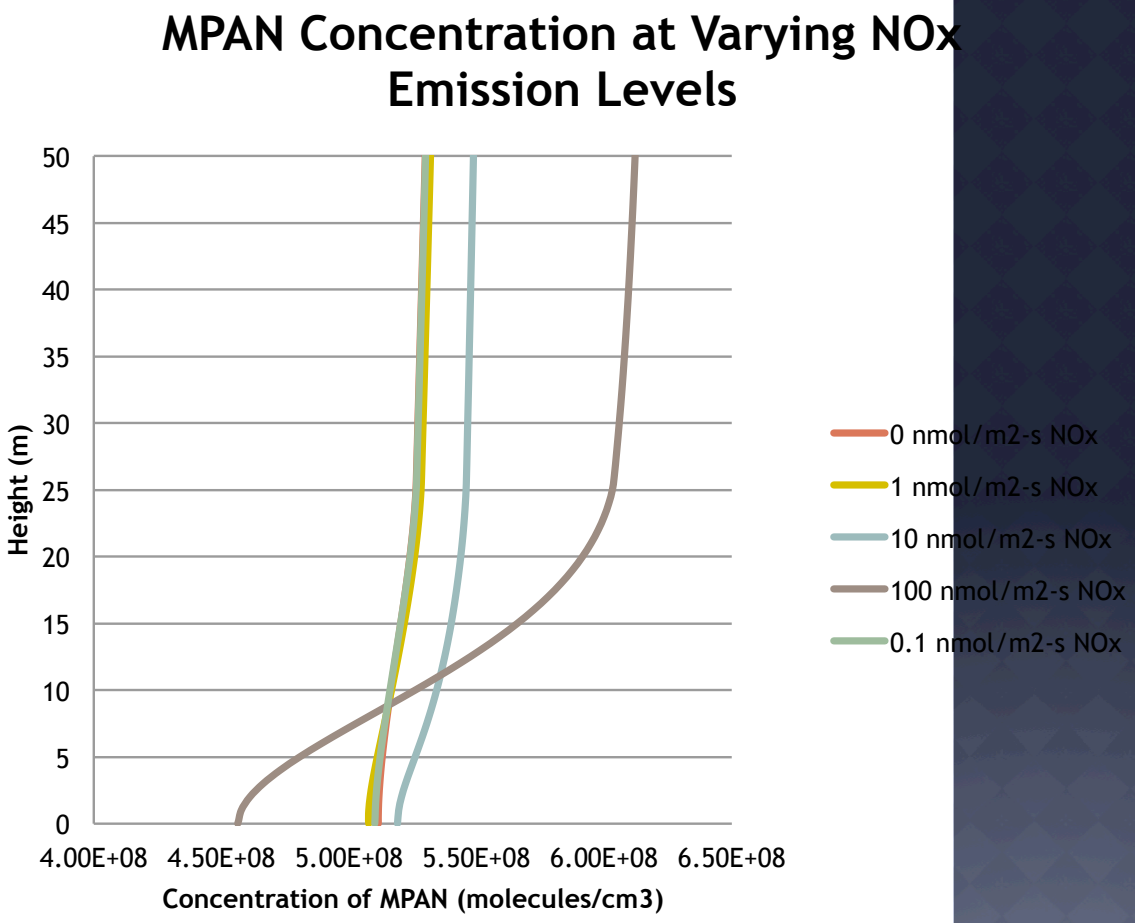


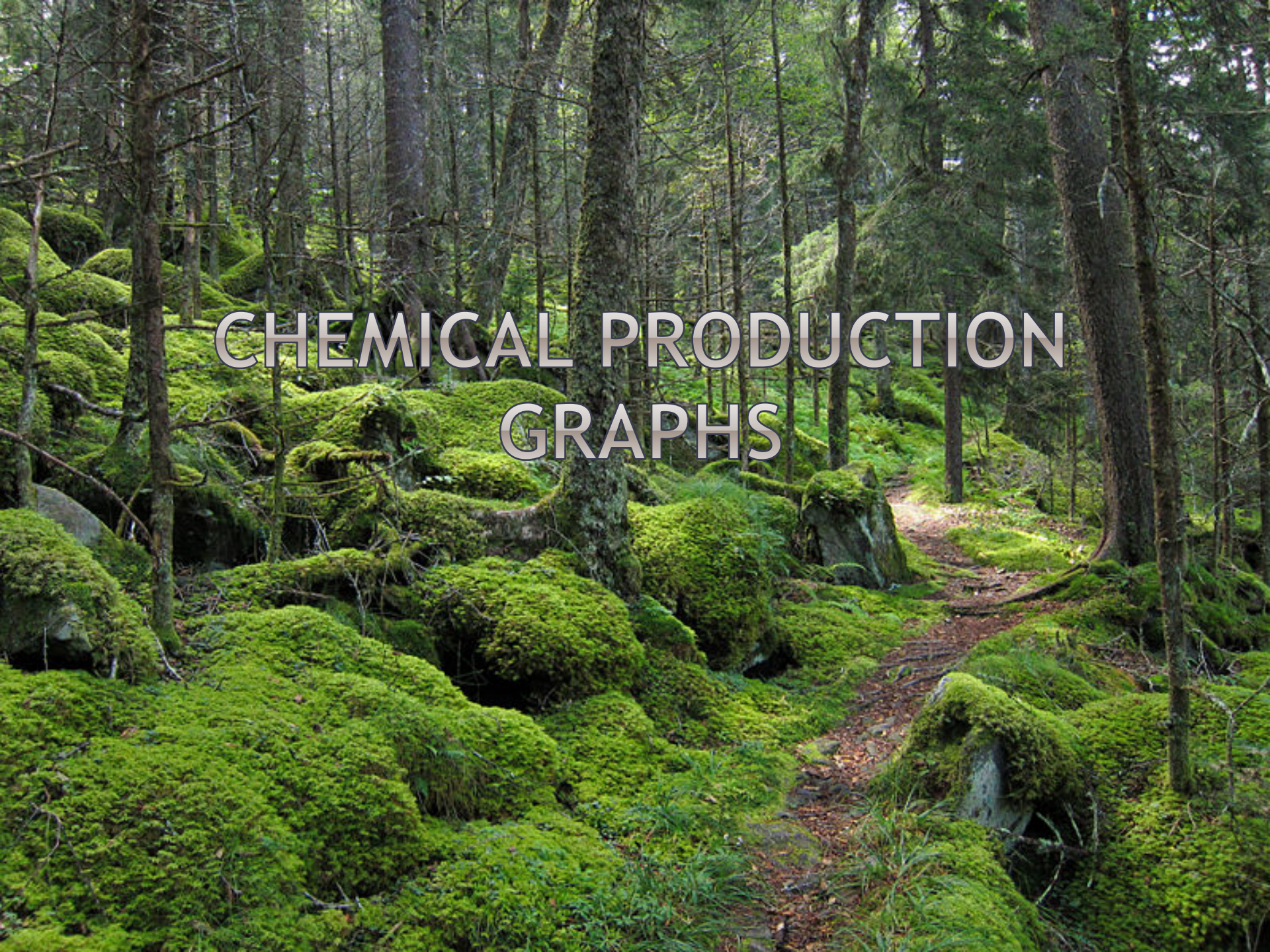
PAN Concentration at Varying NOx Emission Levels



SPECIES (METHACRYLOYL PEROXY NITRATE (MPAN))

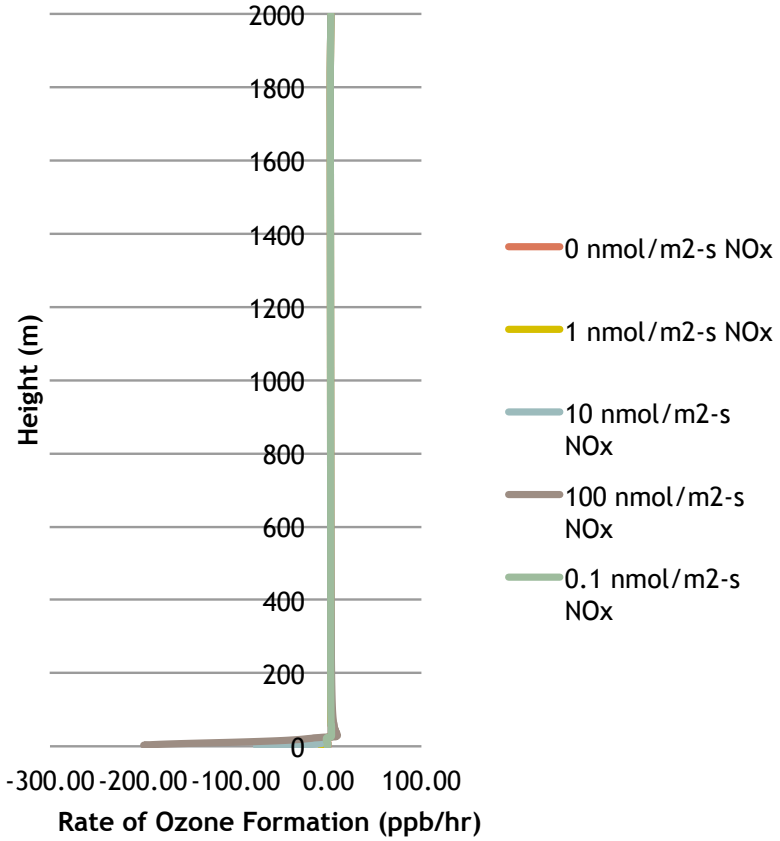




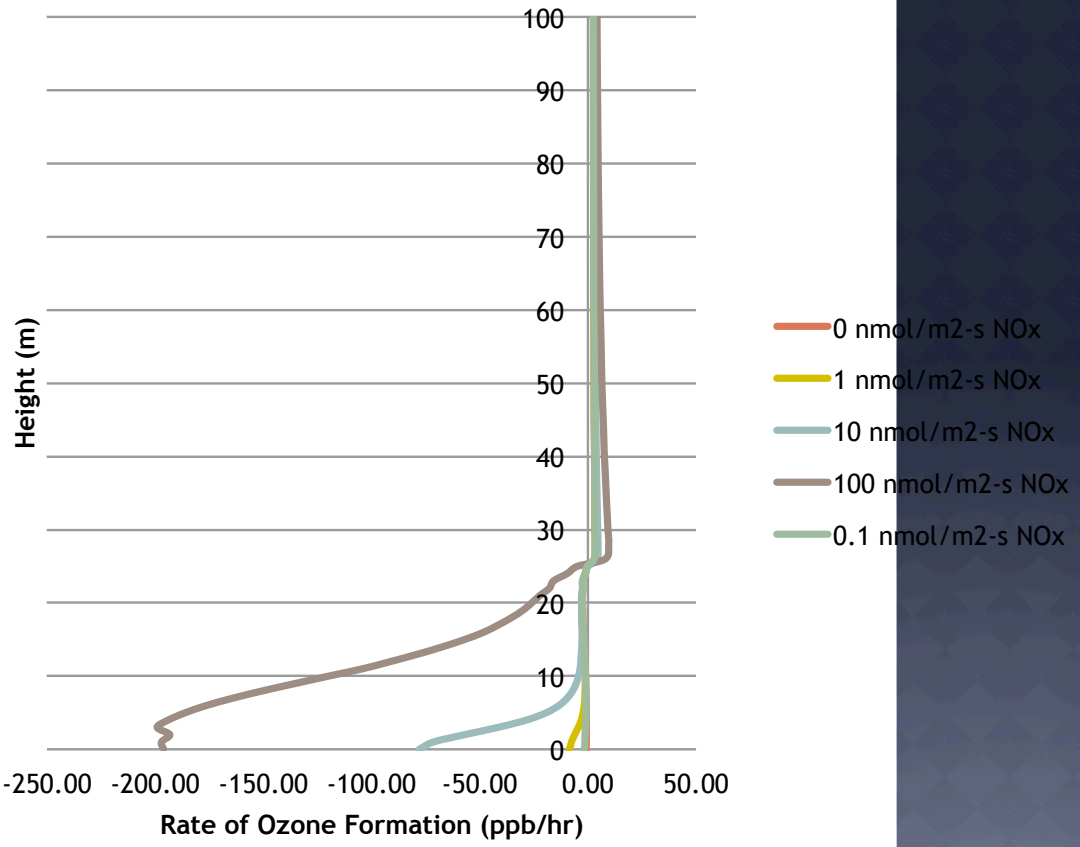

CHEMICAL PRODUCTION
GRAPHS

CHEMICAL PRODUCTION (OZONE)

Ozone Budget at Varying NOx Emission Levels

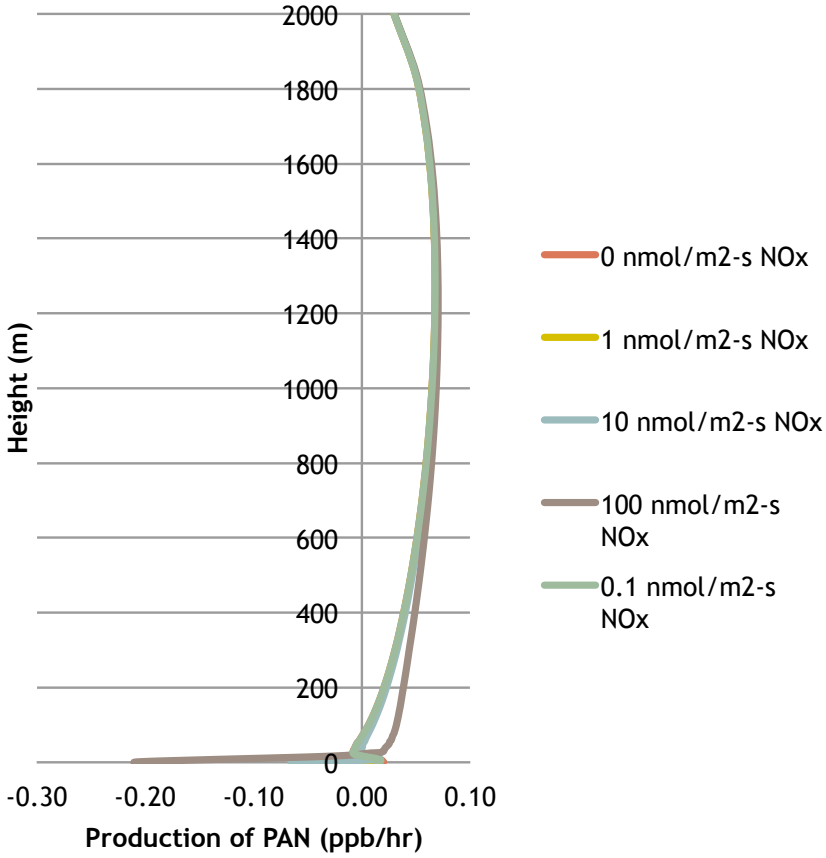


Ozone Budget at Varying NOx Emission Levels

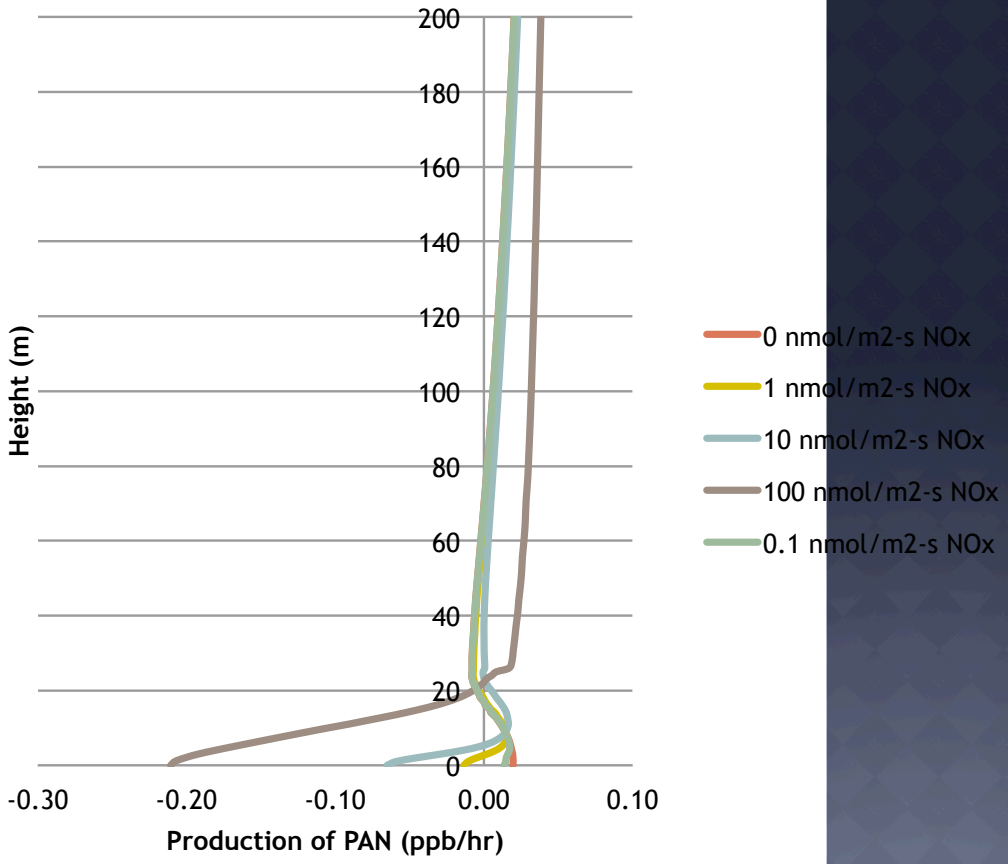


CHEMICAL PRODUCTION (PAN)

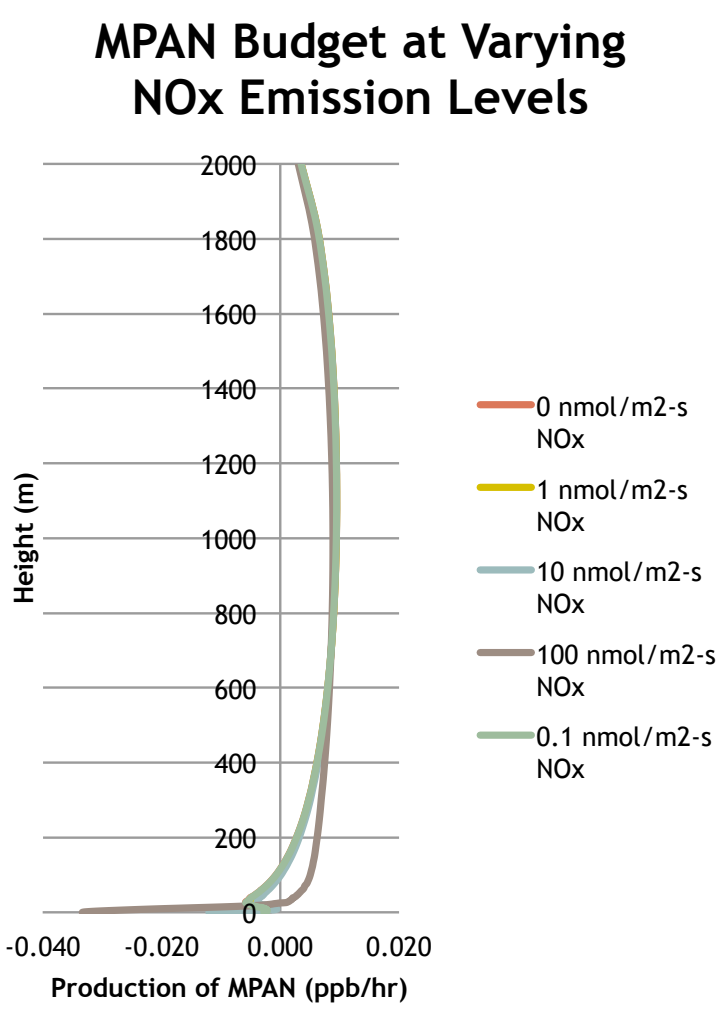
PAN Budget at Varying NOx Emission Levels

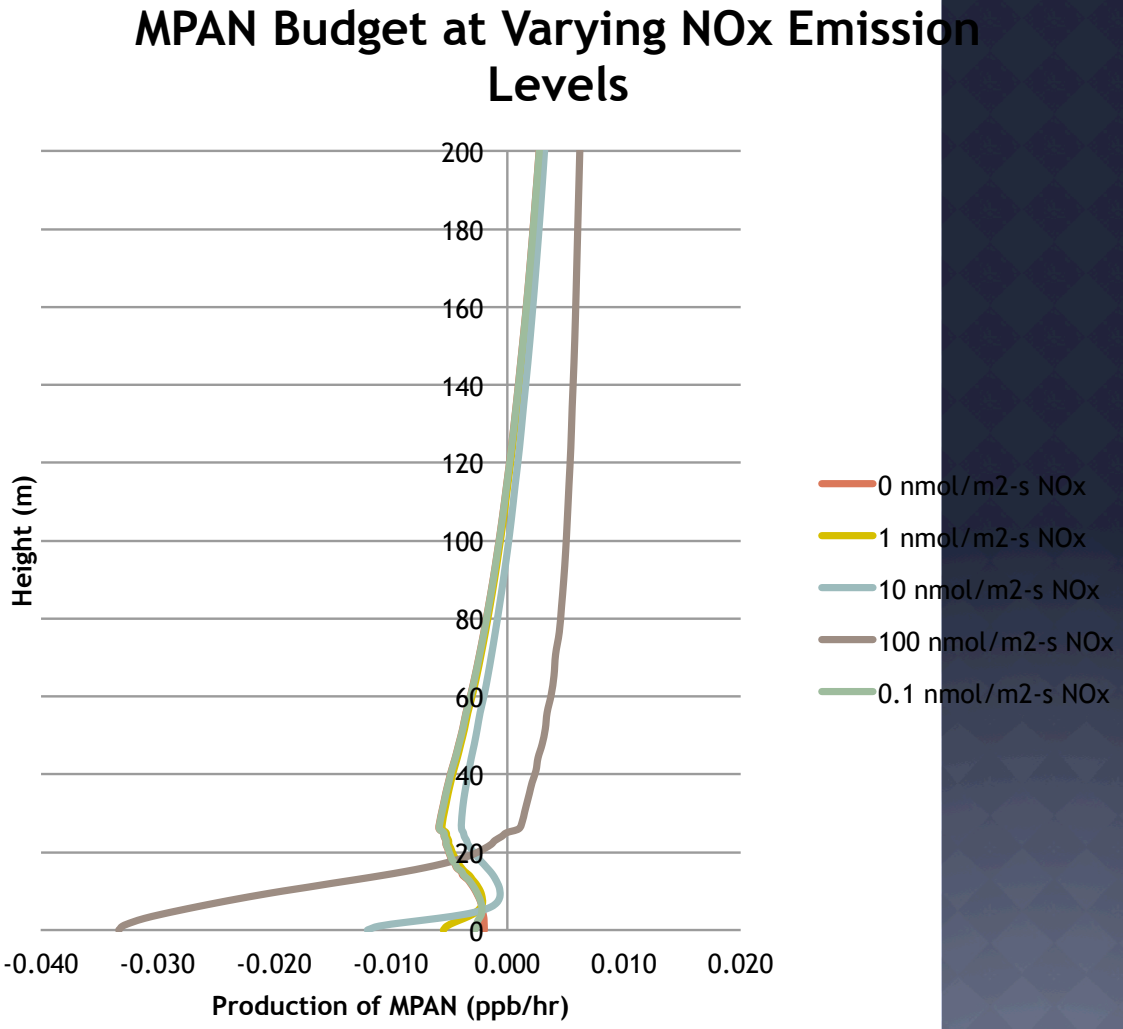


PAN Budget at Varying NOx Emission Levels



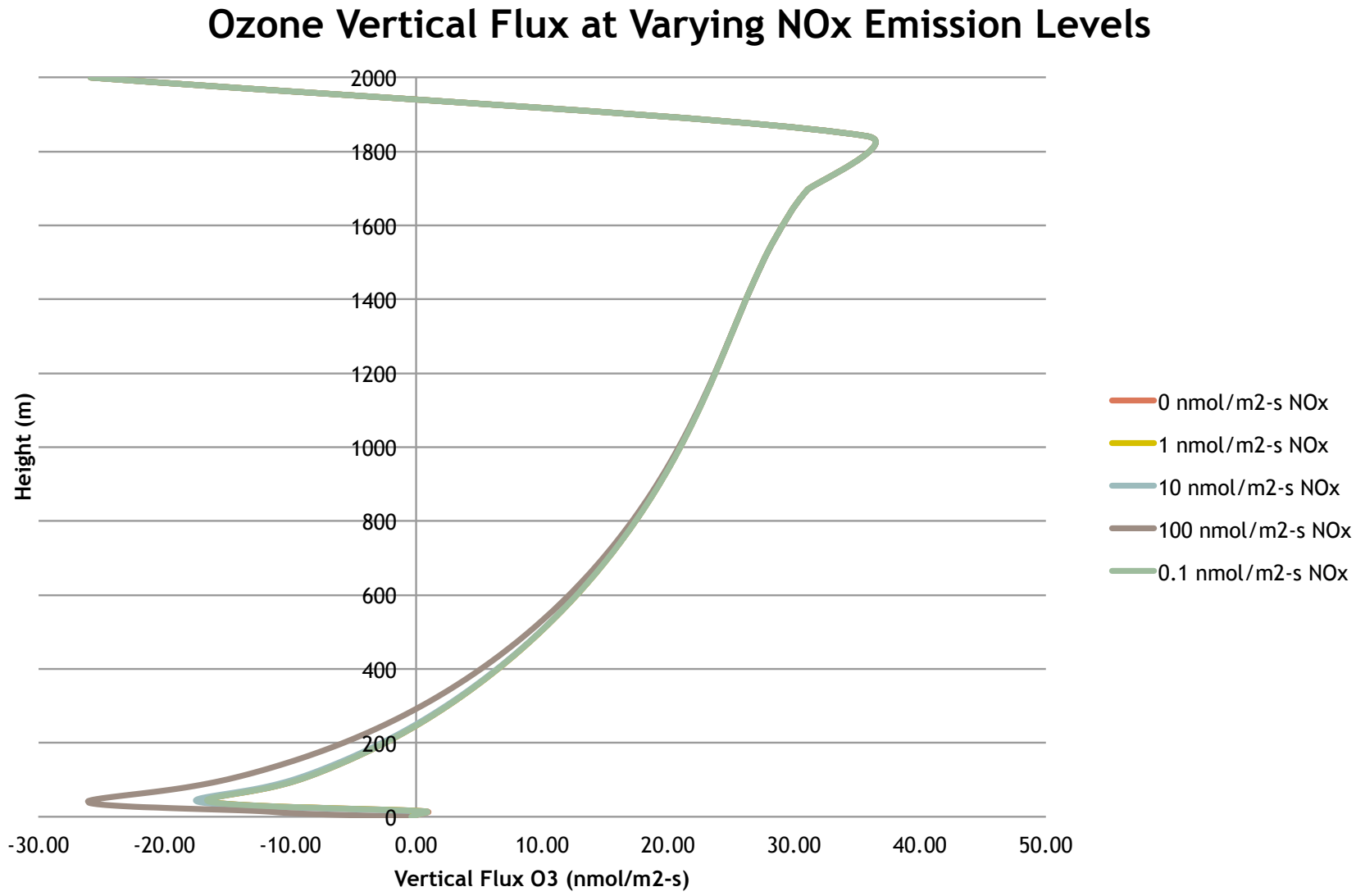
CHEMICAL PRODUCTION (MPAN)





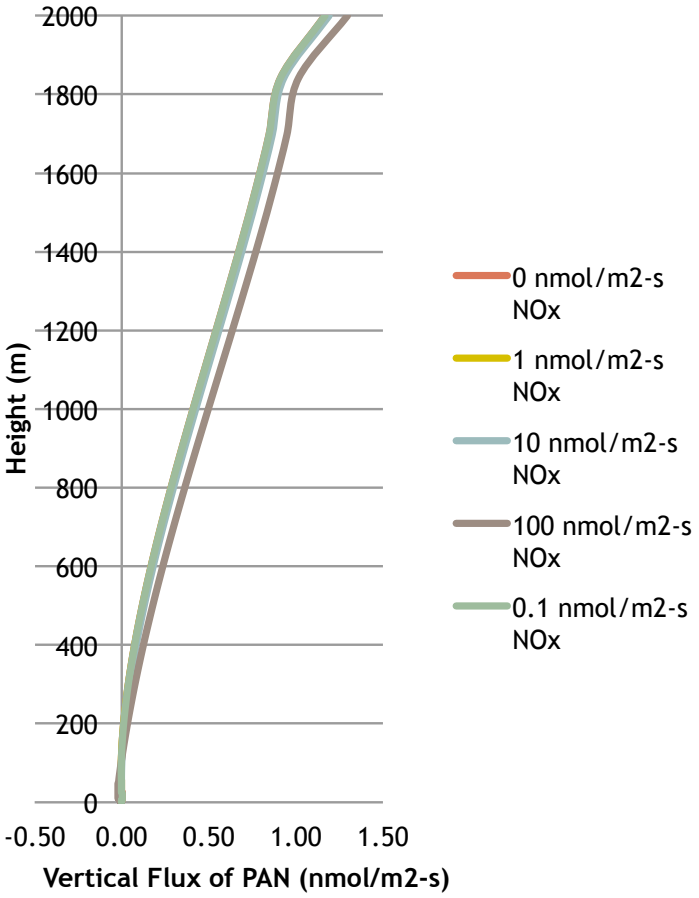
VERTICAL FLUX GRAPHS

VERTICAL FLUX (OZONE)

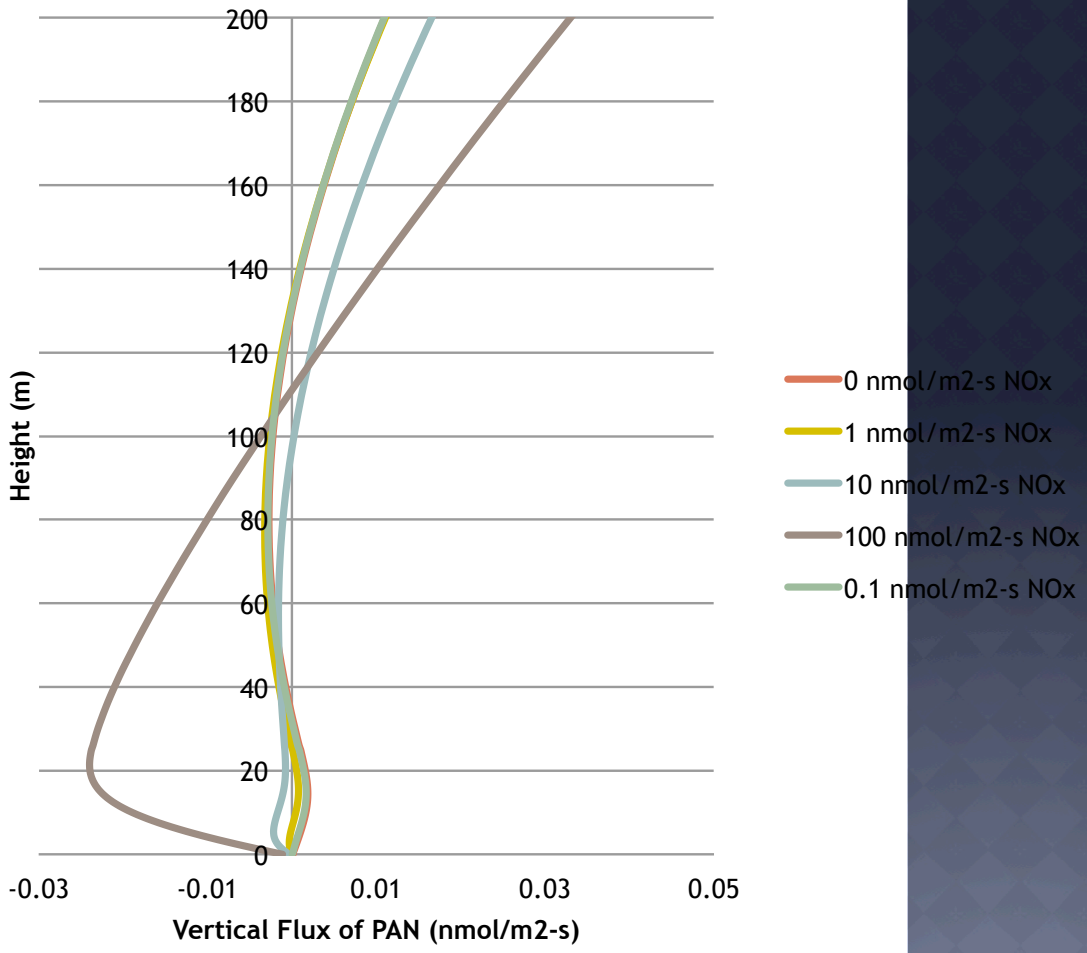


VERTICAL FLUX (PAN)

PAN Vertical Flux Data at Varying NOx Emission Levels

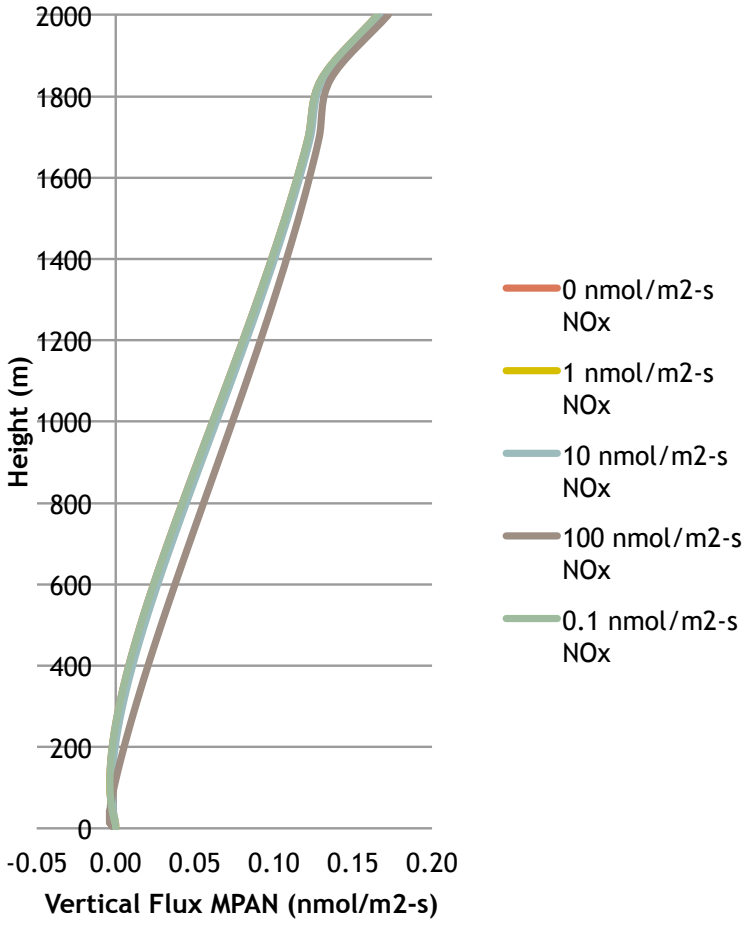


PAN Vertical Flux Data at Varying NOx Emission Levels

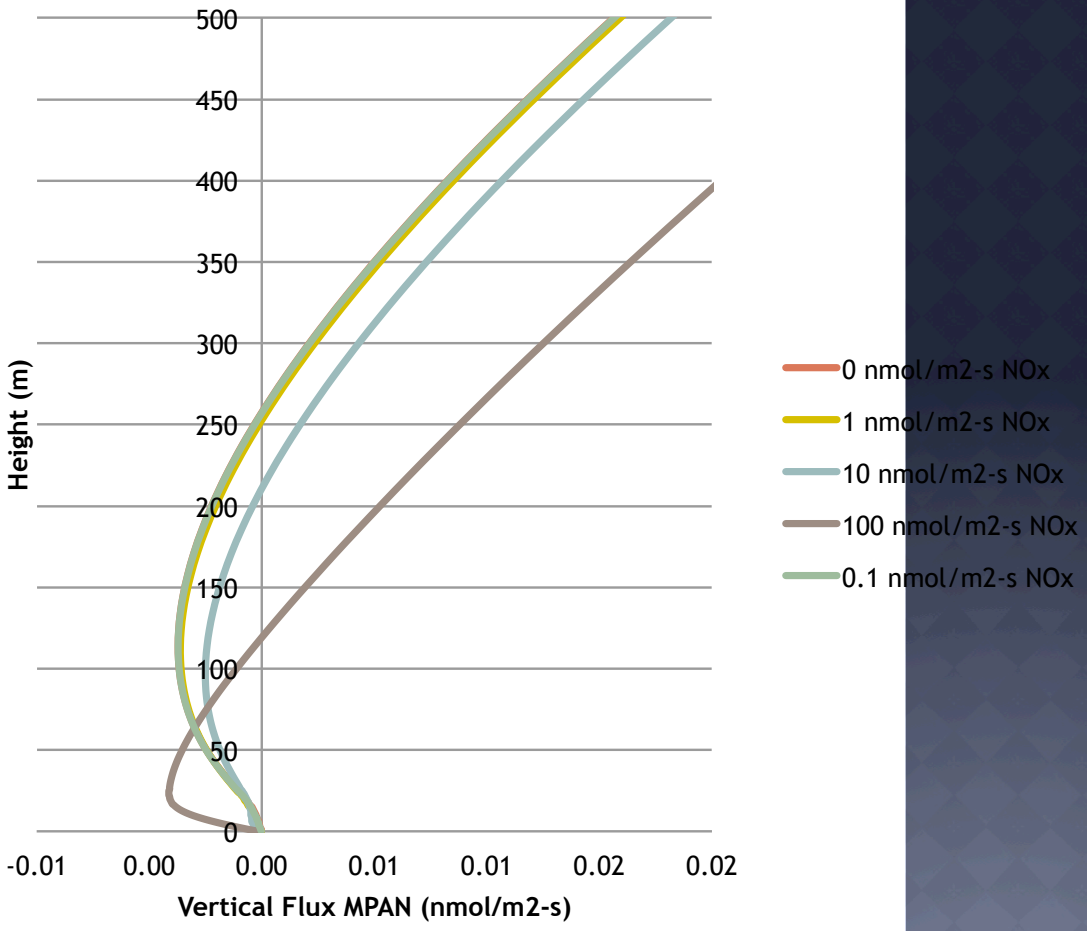


VERTICAL FLUX (MPAN)

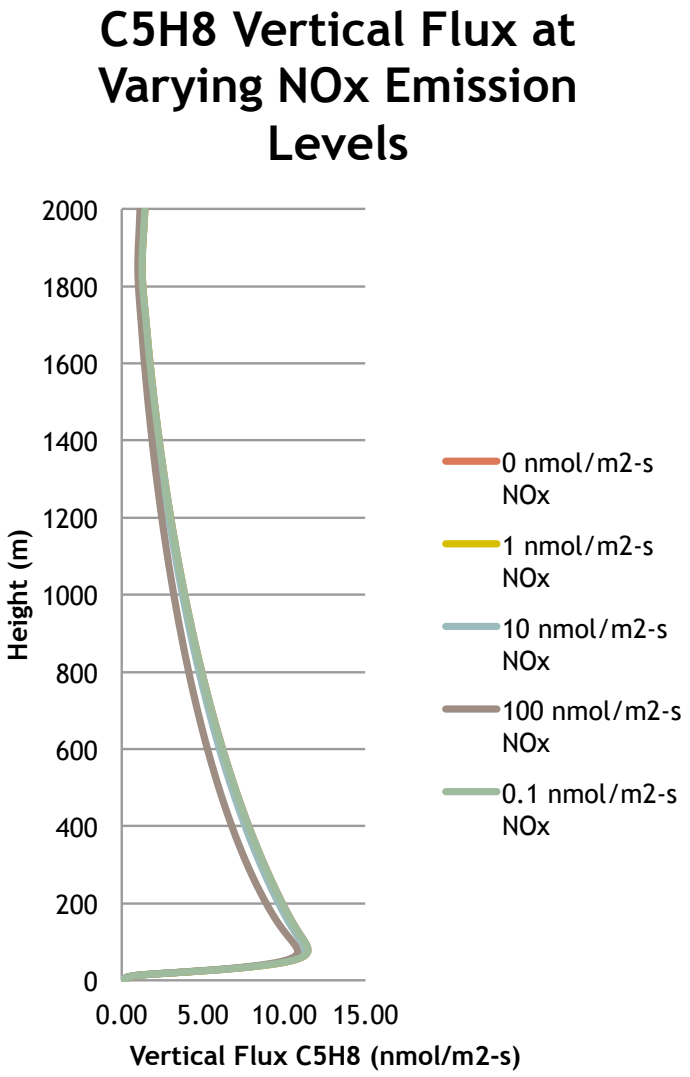
MPAN Vertical Flux at Varying NOx Emission Levels

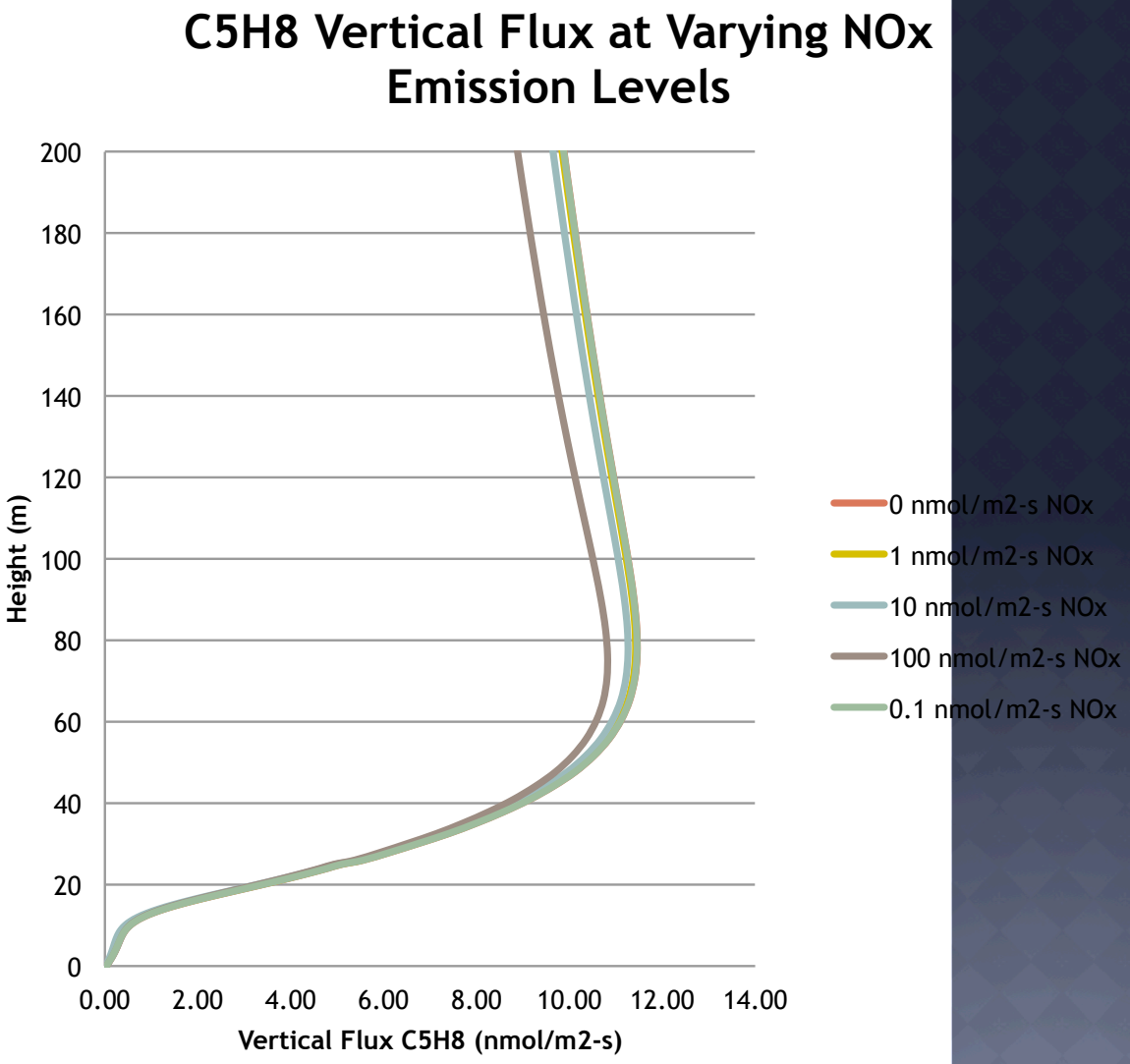


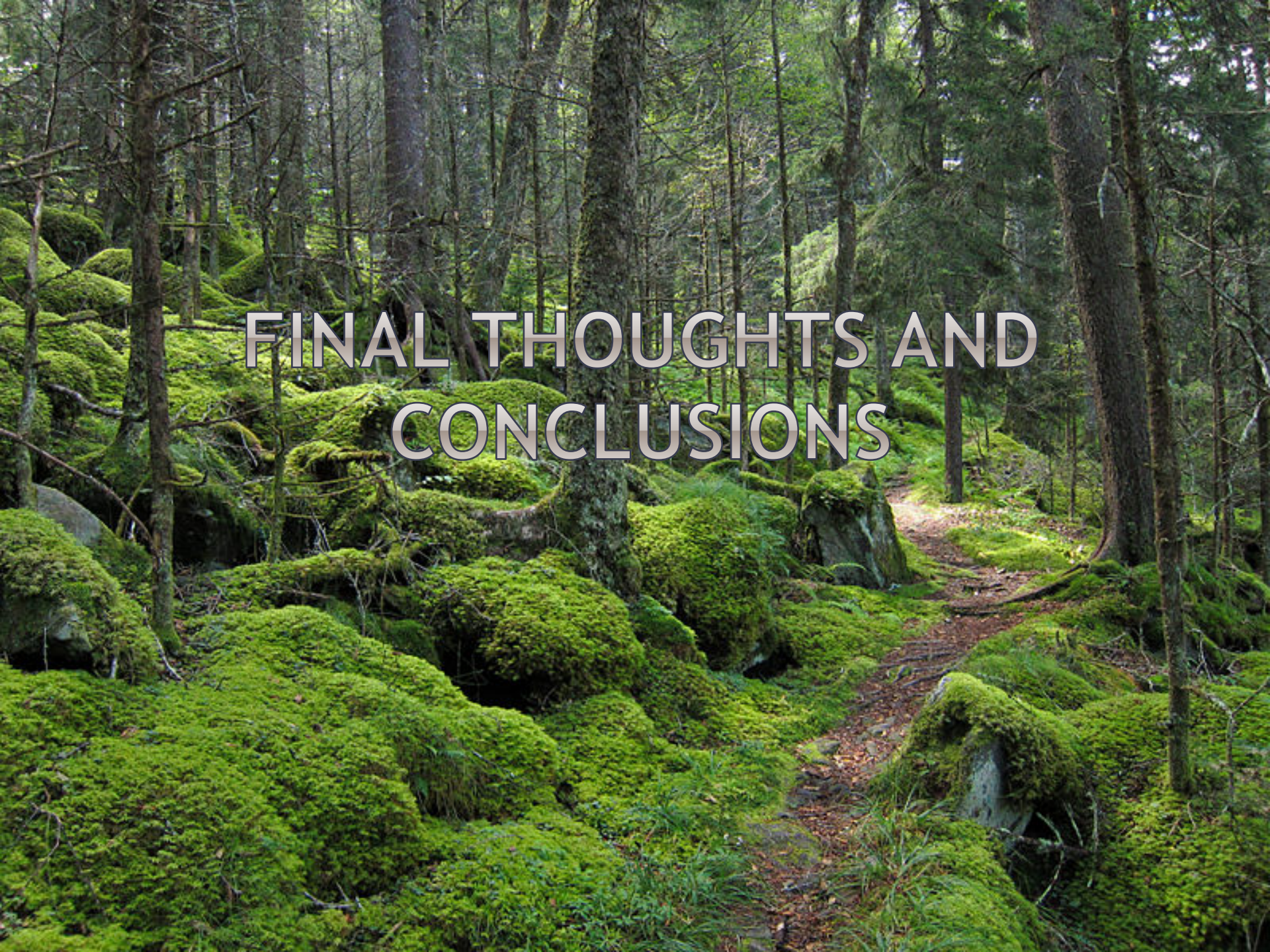
MPAN Vertical Flux at Varying NOx Emission Levels



VERTICAL FLUX (ISOPRENE)






FINAL THOUGHTS AND
CONCLUSIONS

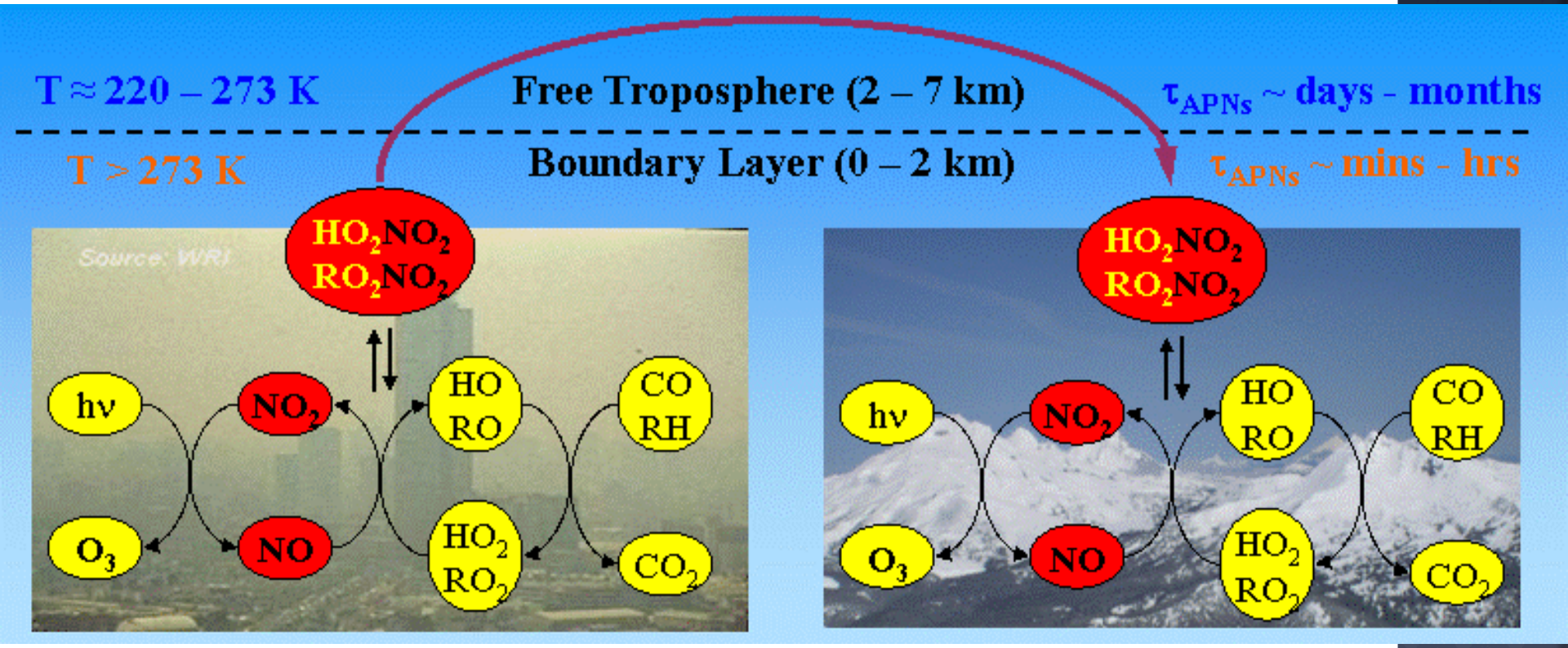
THOUGHTS ON WHAT THE GRAPHS SAY ABOUT OZONE

- With increasing traffic within the canopy the direct effect is a reduction of ozone concentrations within the canopy because of the direct reaction with NO and ozone.
  - REACTION: $NO + O_3 \rightarrow NO_2 + O_2$
- We are only seeing minor enhancements in ozone concentration above the canopy.

CONCLUSIONS

- Even though we are not seeing direct increases in ozone from NOx emissions, we are seeing enhanced production of PAN and MPAN above the canopy, which, when transported downwind, can contribute to enhanced ozone formation in areas with little or no NOx emissions.

PHOTOCHEMICAL CONVERSION OF PAN (OR MPAN) BACK TO NO_X



- Image Credit: Department of Atmospheric Sciences, University of Washington; Seattle, WA.
- URL: http://www.atmos.washington.edu/~thornton/PANs.html

CONCLUSIONS (CONT.)

- Under the environmental conditions studied so far in our simulations, only minor amounts of local ozone production above the canopy are predicted. However, the simulation results suggest that the enhancements in PAN and MPAN formation from visitor traffic in the park may lead to increased ozone concentrations downwind from major highways within the park. Ozone data within and downwind of the park will be further analyzed to test the model prediction.
- Results and further analysis of this work will be published in a journal article at a later date.

CREDITS

- Image on section introduction slides is from Wikimedia Commons and is an image of Baxter Creek Trail in Great Smoky Mountains National Park.
- The ACCESS diagram (Slide 8) and the graphical representation of reactions that produce ozone (Slide 5) were both done by Dr. Rick D. Saylor.
- Molecules on Slide 14 all come from Wikimedia commons with the exception of PAN and MPAN, which come from the University of Washington website (URL given on slide 32).
- All other photos and/or diagrams are credited on their slide.