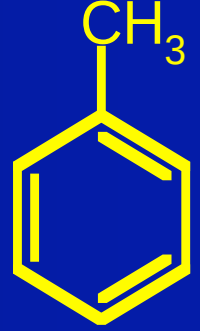
A Predictive Kinetic Model for Aerosol Formation from Toluene Oxidation



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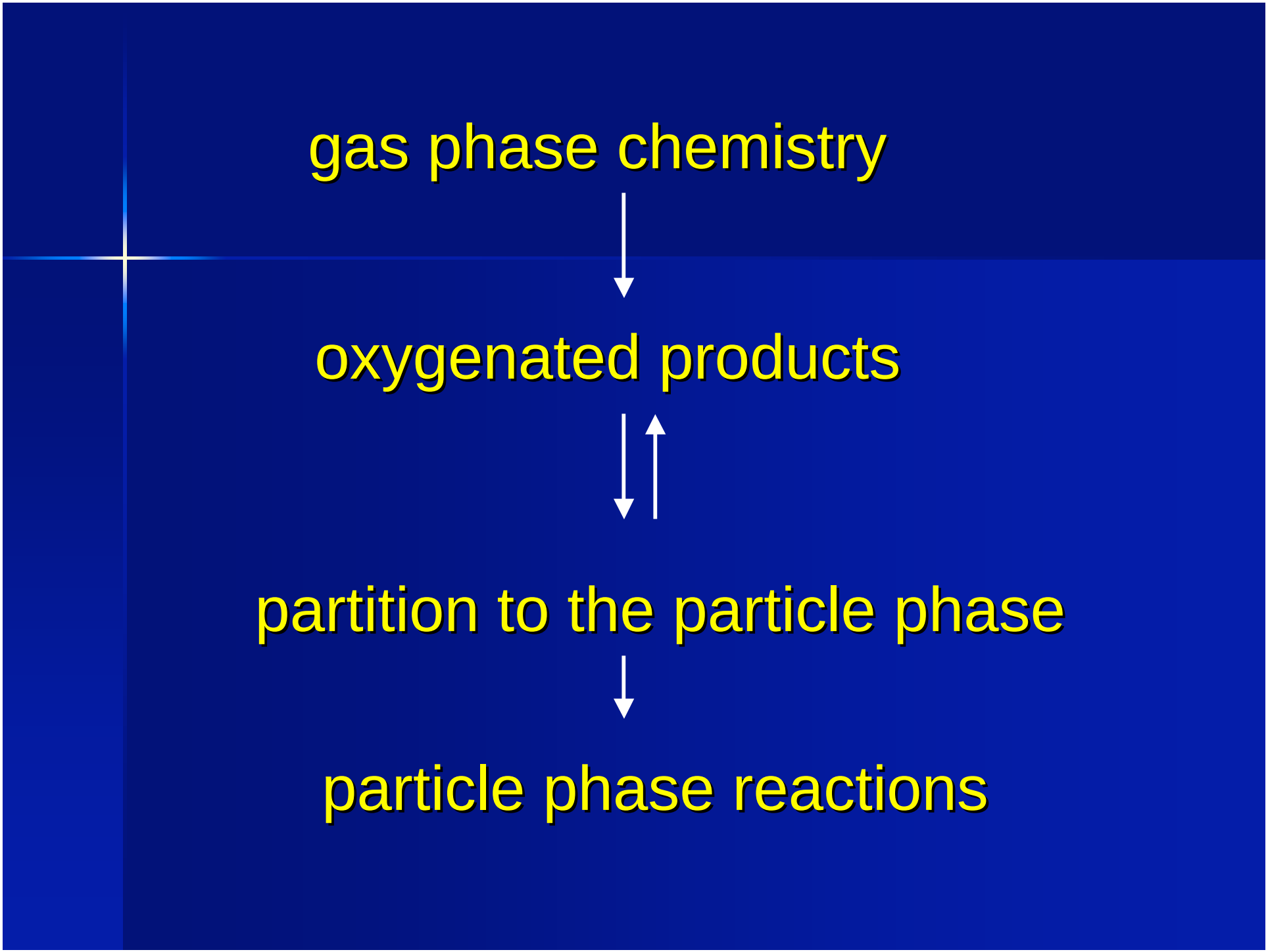
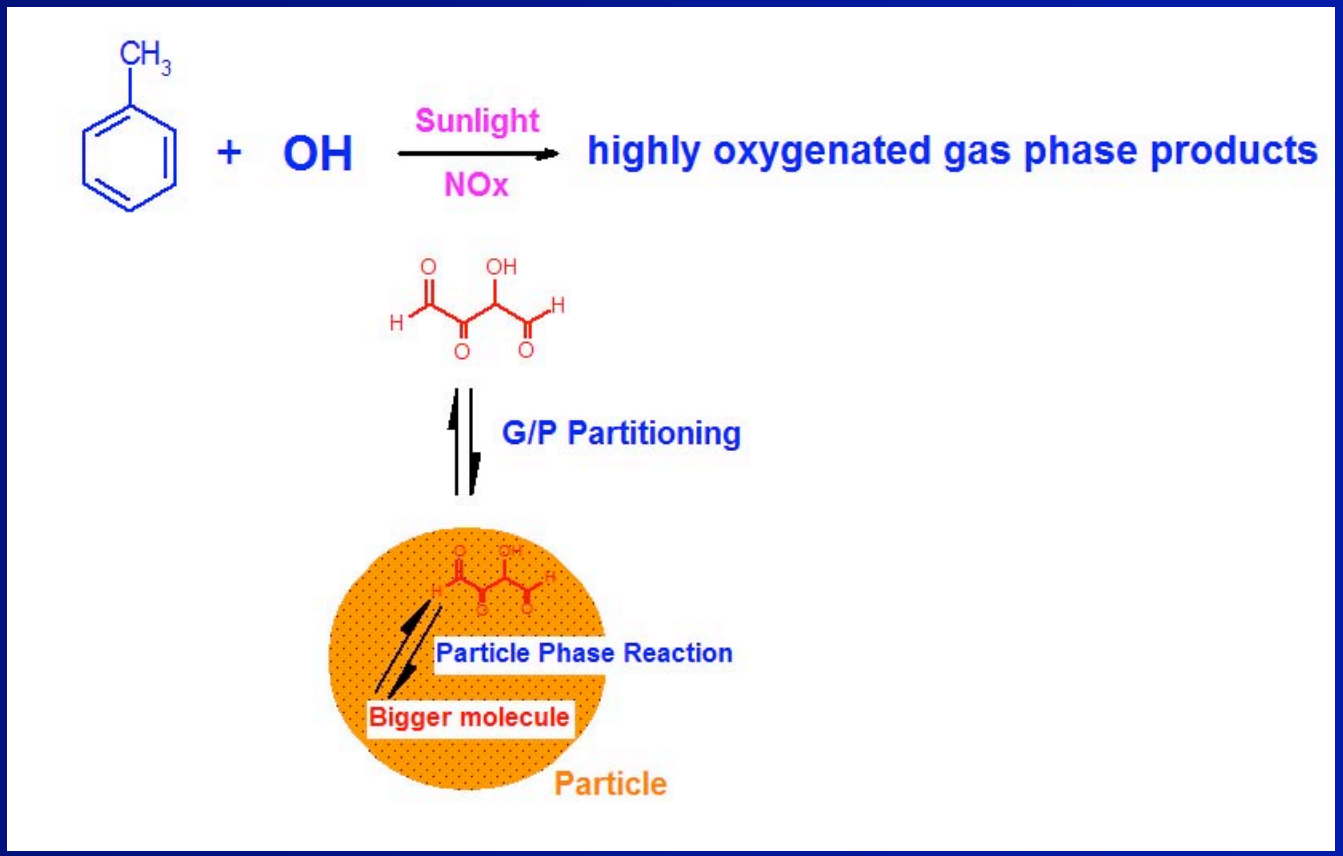
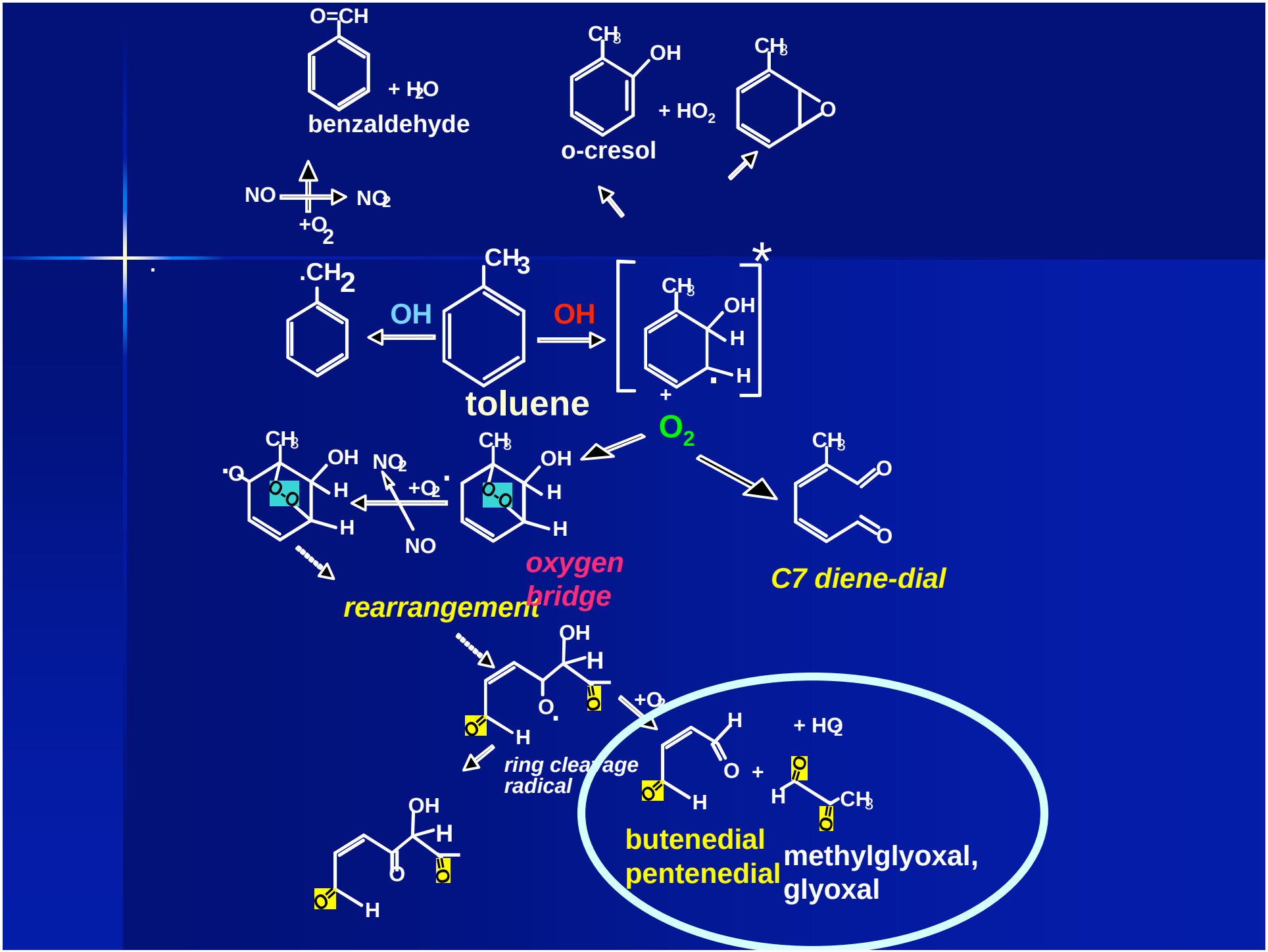
Department Environmental Sciences and Engineering, UNC Chapel Hill

6/22/2007 EPA

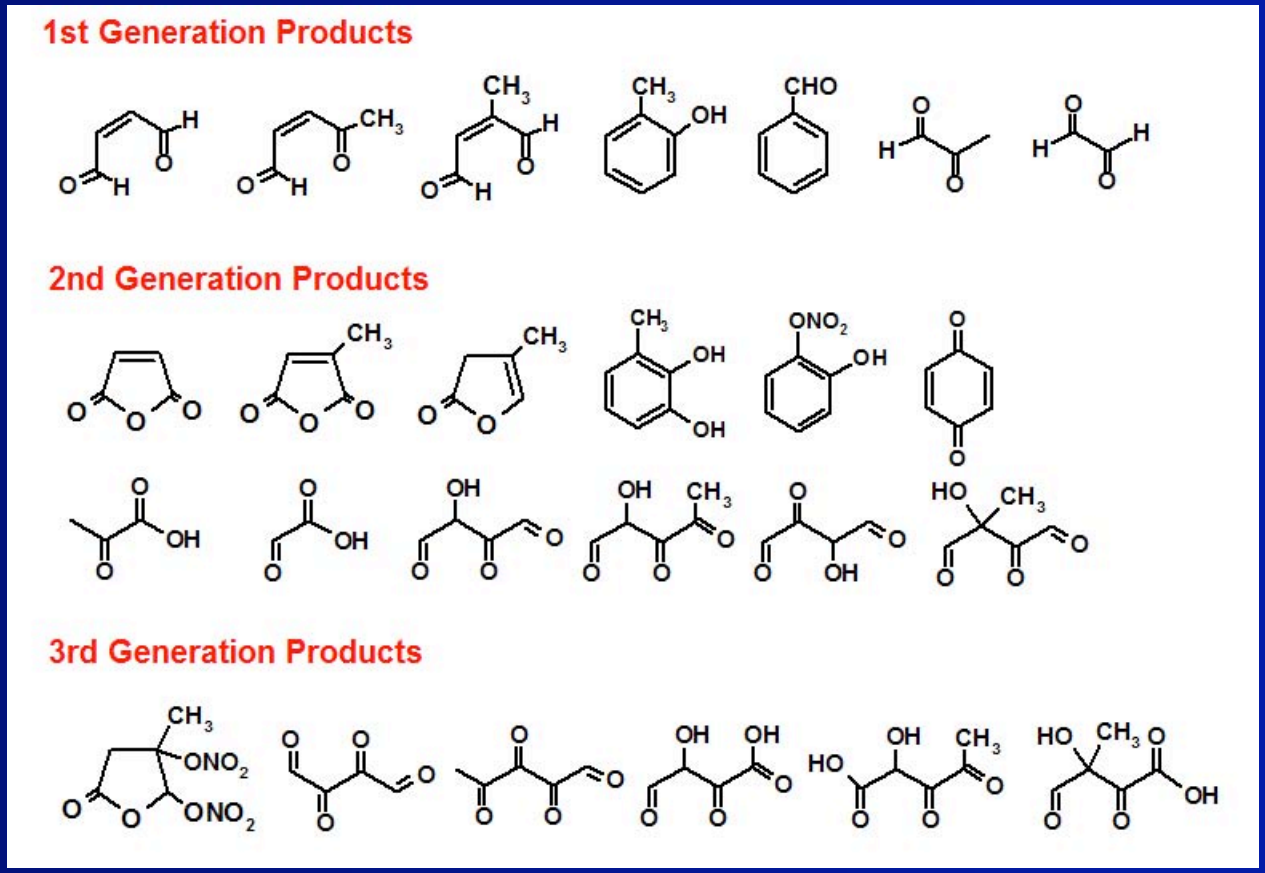


gas and particle phase reactions in Toluene system.

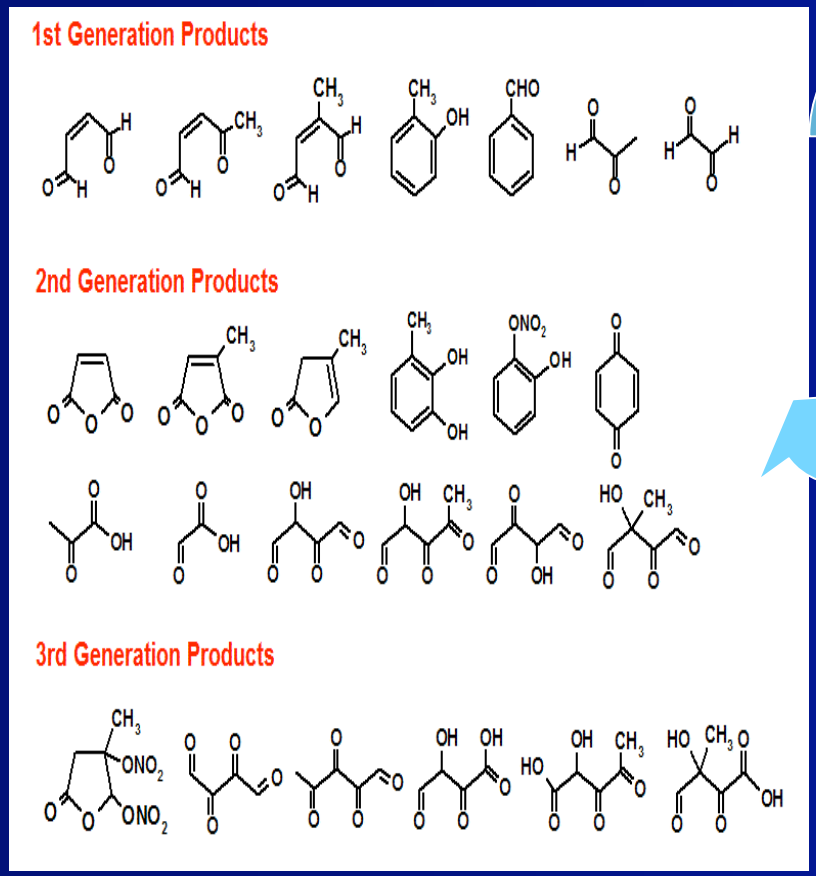




. Major products in gas and particle phases



Products Reactions



Reactions

(Semi-explicit Mechanisms)

Nucleation
Partition
Heterogeneous reactions

Current Mechanism has:

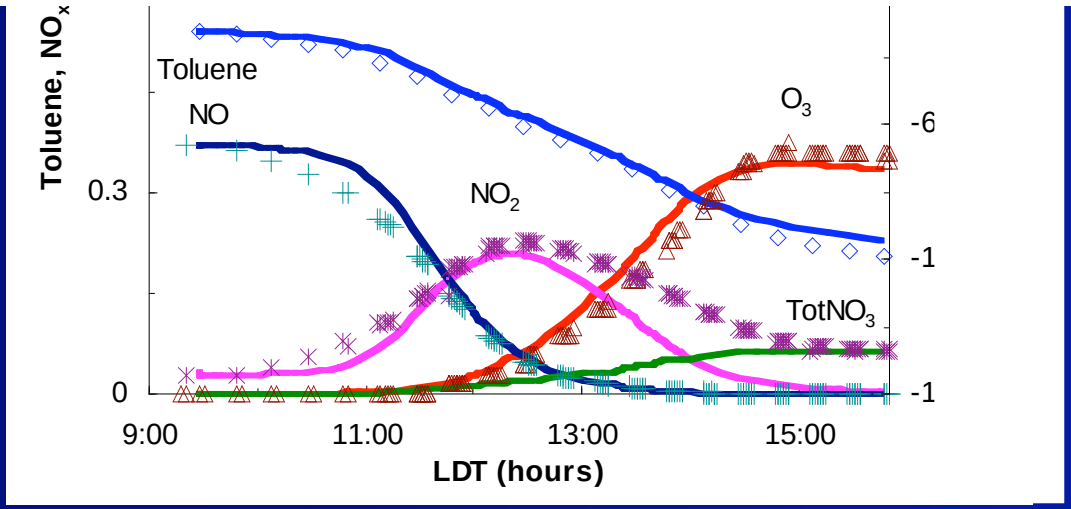
98 gas phase reactions
67 gas to particle phase species
16 "particle phase" reactions

CB4 (2002) chemistry

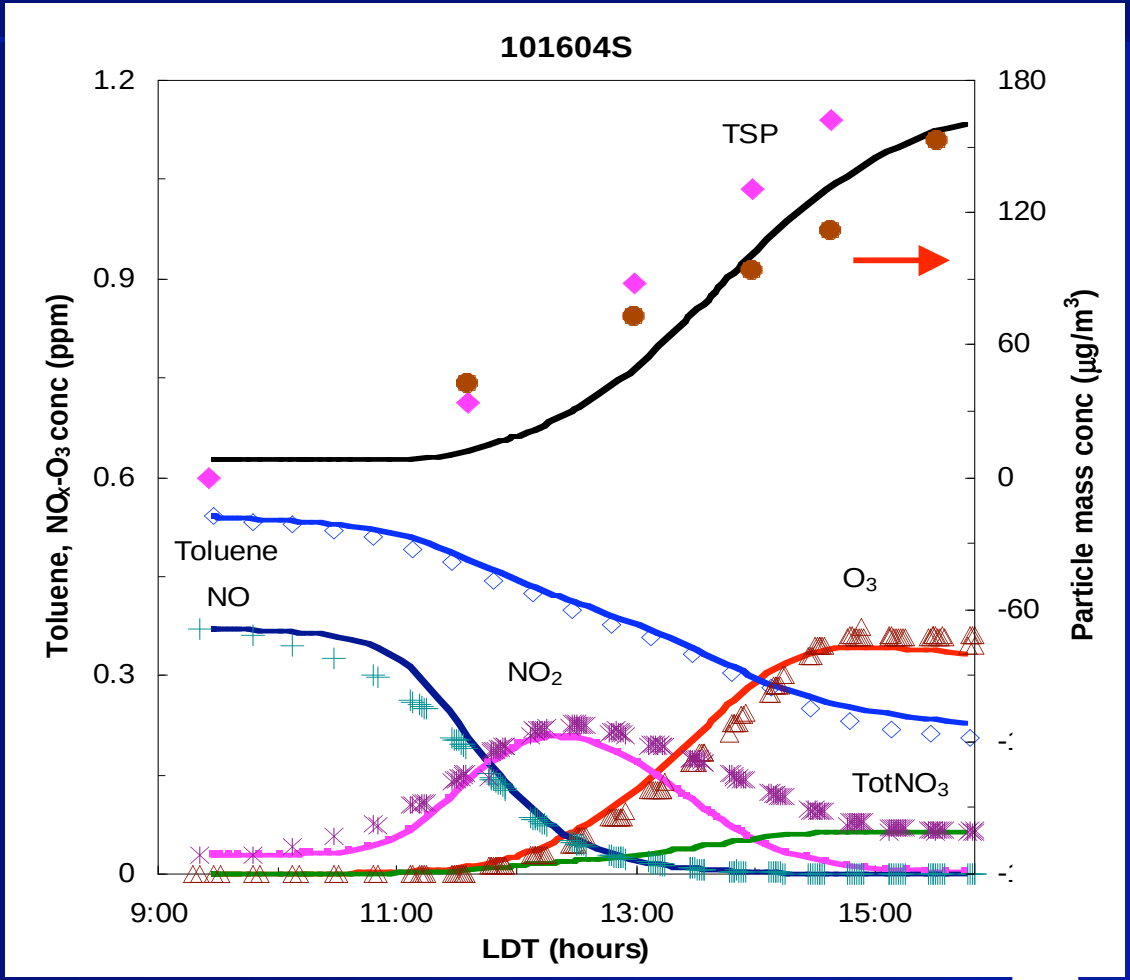
UNC Auxiliary Mechanism
(Chamber Wall reactions, dilution, et.al)

Model Simulations of UNC outdoor Toluene/NOx Experiments

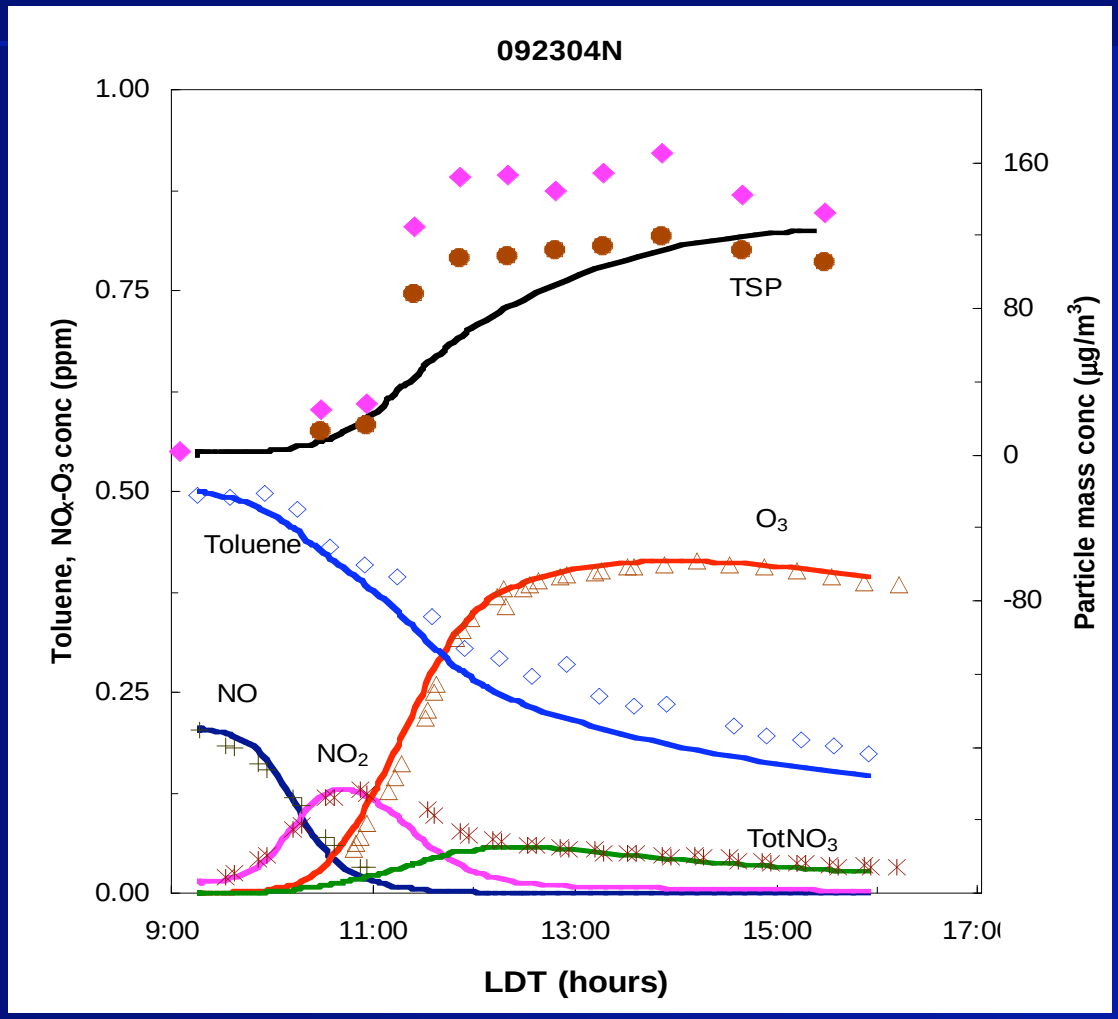
0.54 ppmV TOL + 0.37 ppm NOx



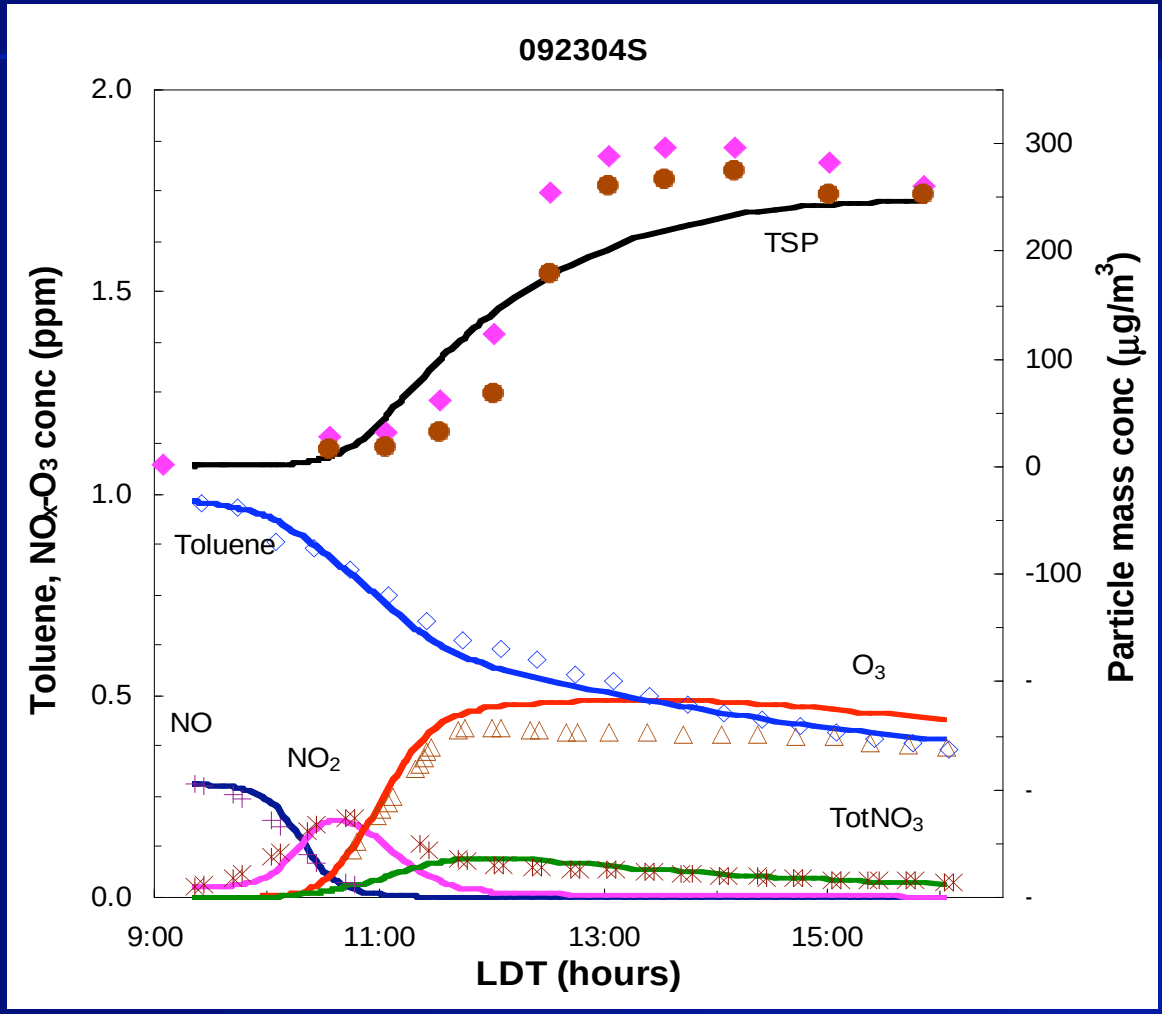
0.54 ppmV TOL + 0.37 ppm NOx



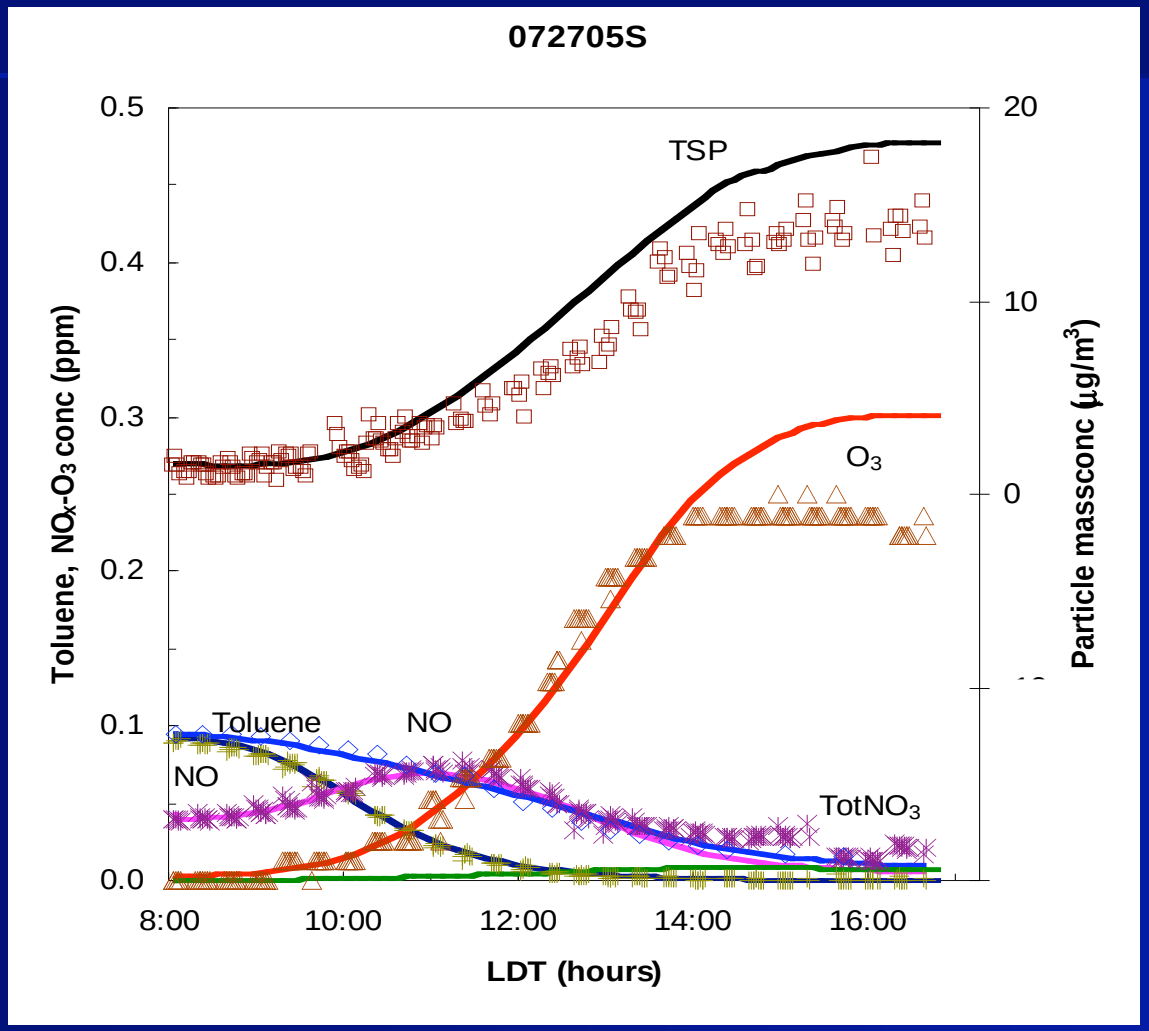
0.5 ppmV TOL + 0.2 ppm NOx



1 ppmV TOL + 0.3 ppm NOx



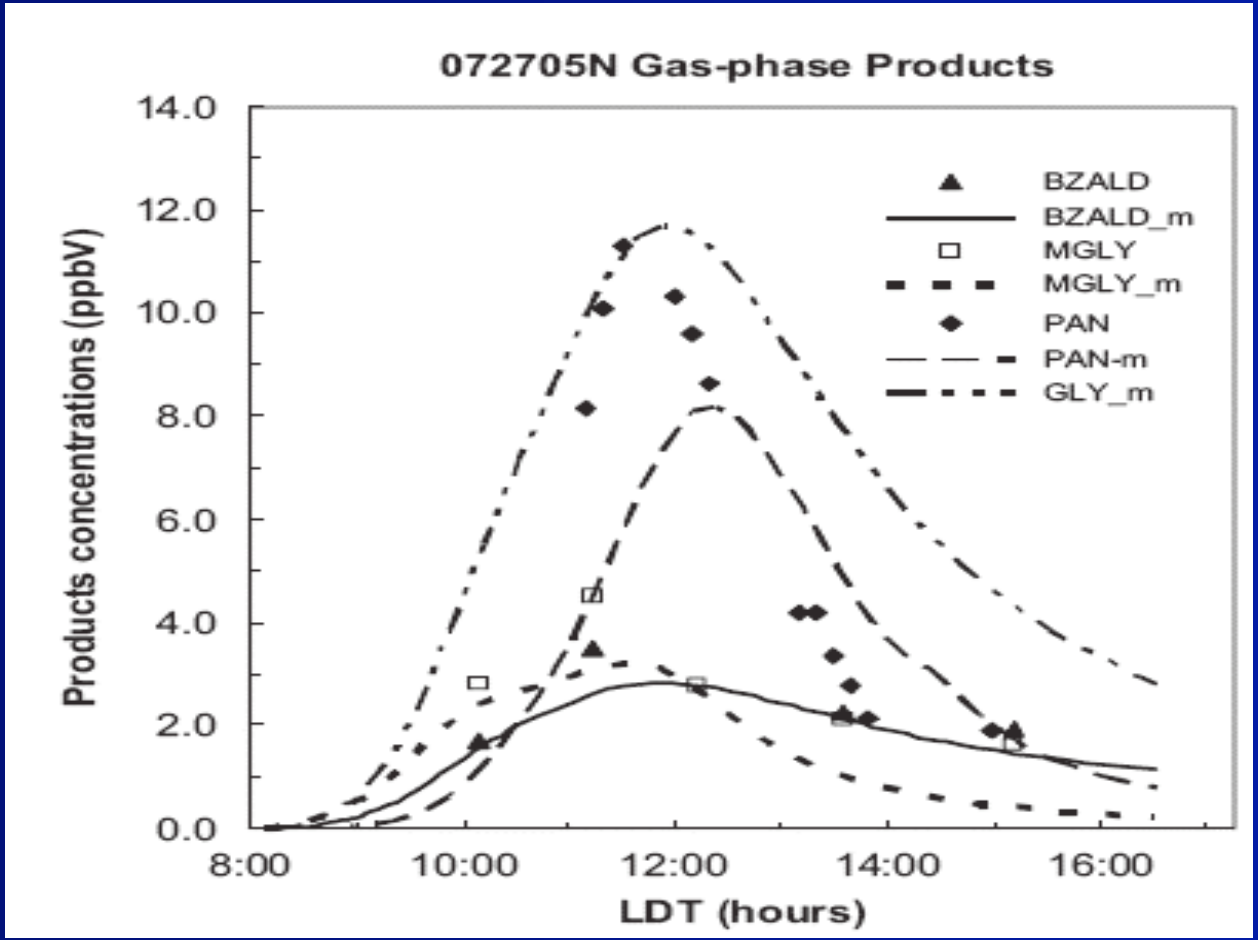
0.1 ppmV TOL + 0.13 ppm NOx



Major Products and Percentage

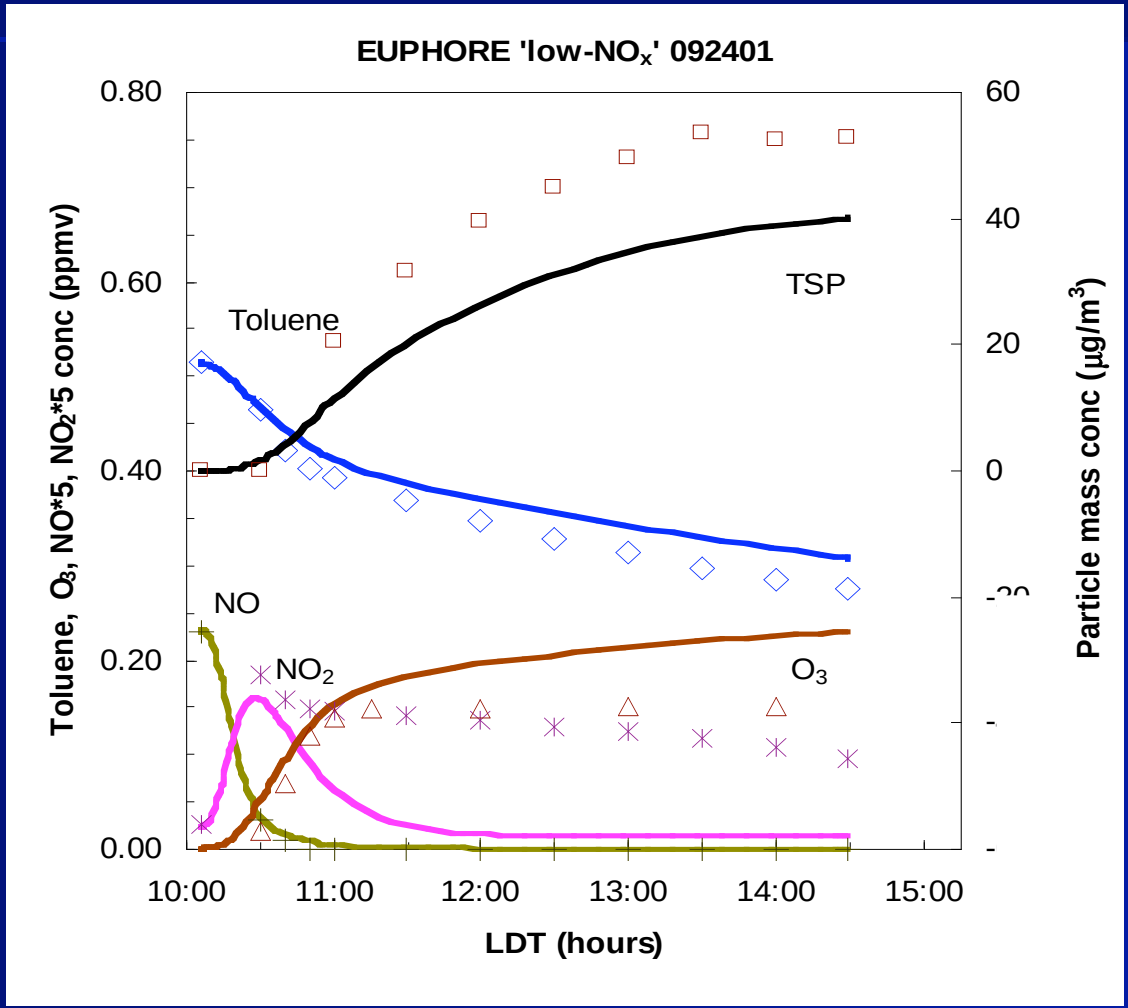
	250μg/m^3	13 μg/m^3
GLYPOLY	60	17
MGLYPOLY	5	1
SEED1	10	20
Organic nitrates	7	26
CH3N02phenols	11	13
organic peroxides	4	5
C6OHNO2ACID	1	13
others	2	5

Products Simulation

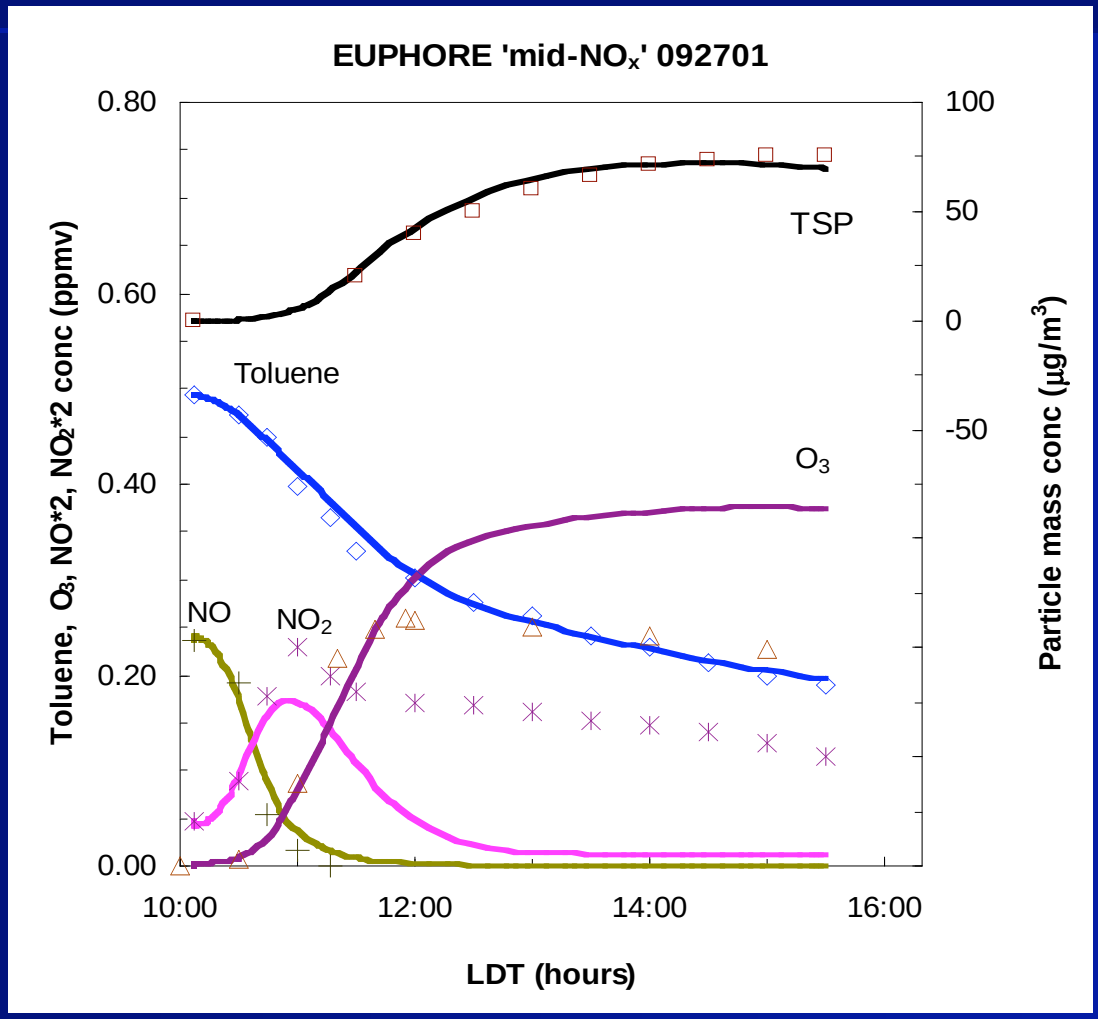


Model Simulations of the EUPHORE Chamber Data

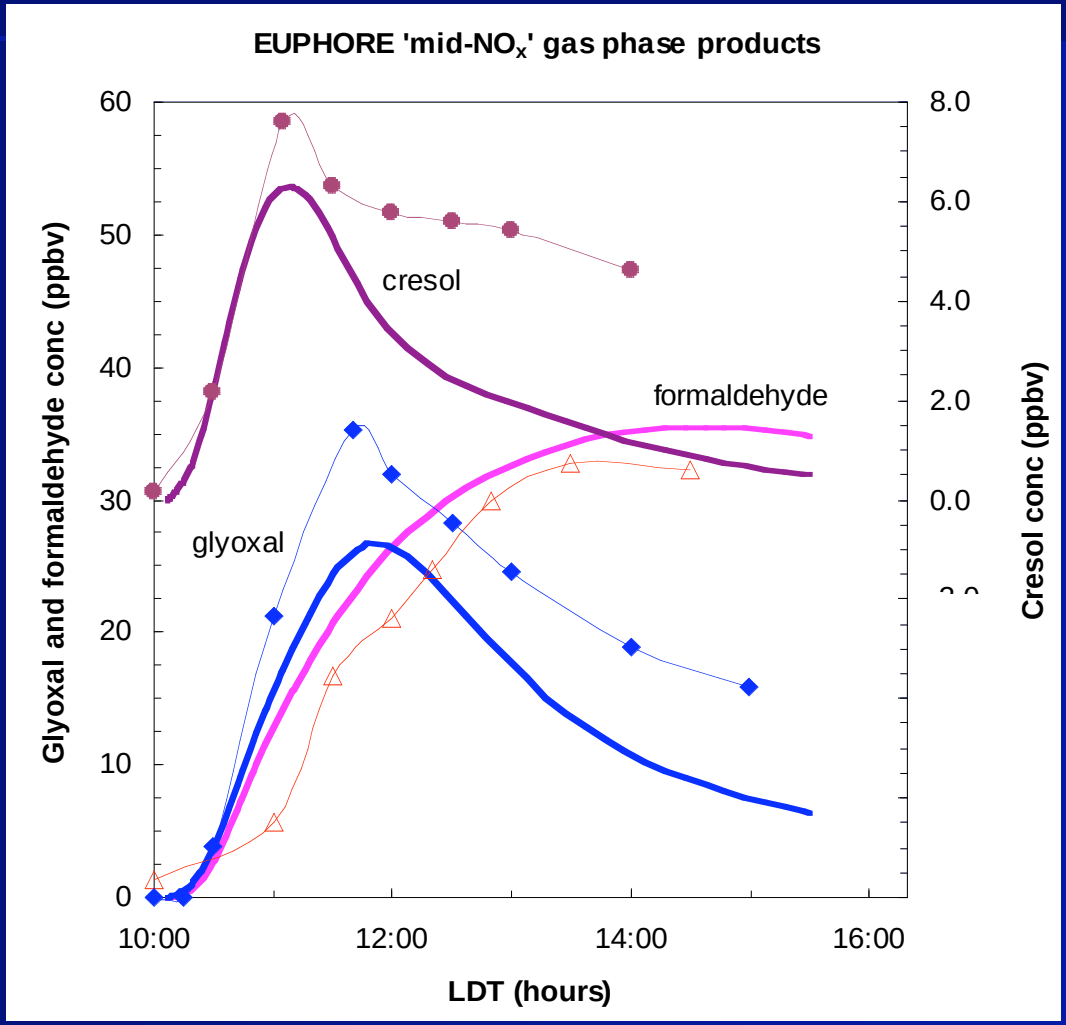
0.5ppmv TOL + 0.05 ppm NOx



0.5 ppmV TOL + 0.13 ppm NOx

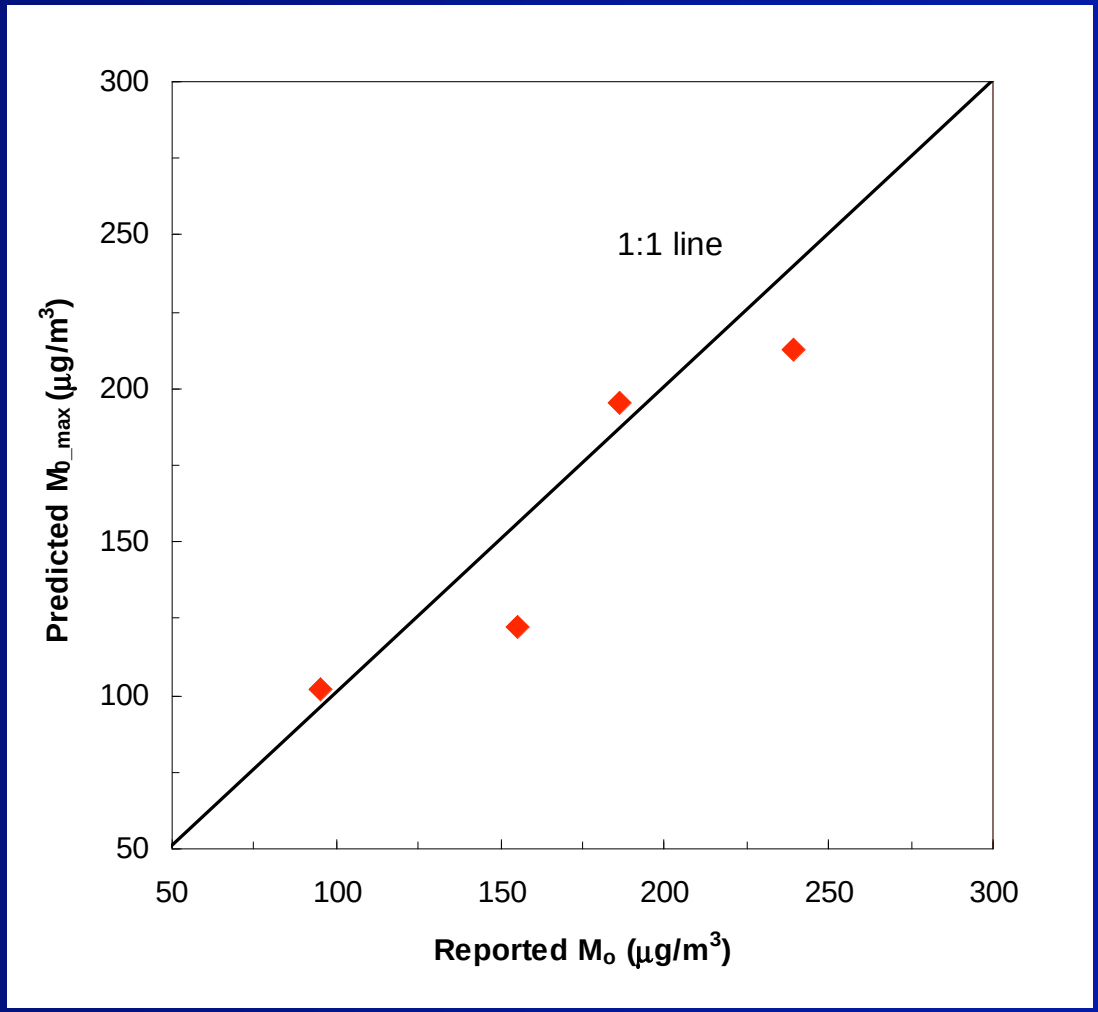


0.5 ppmv TOL + 0.13ppmv NOx



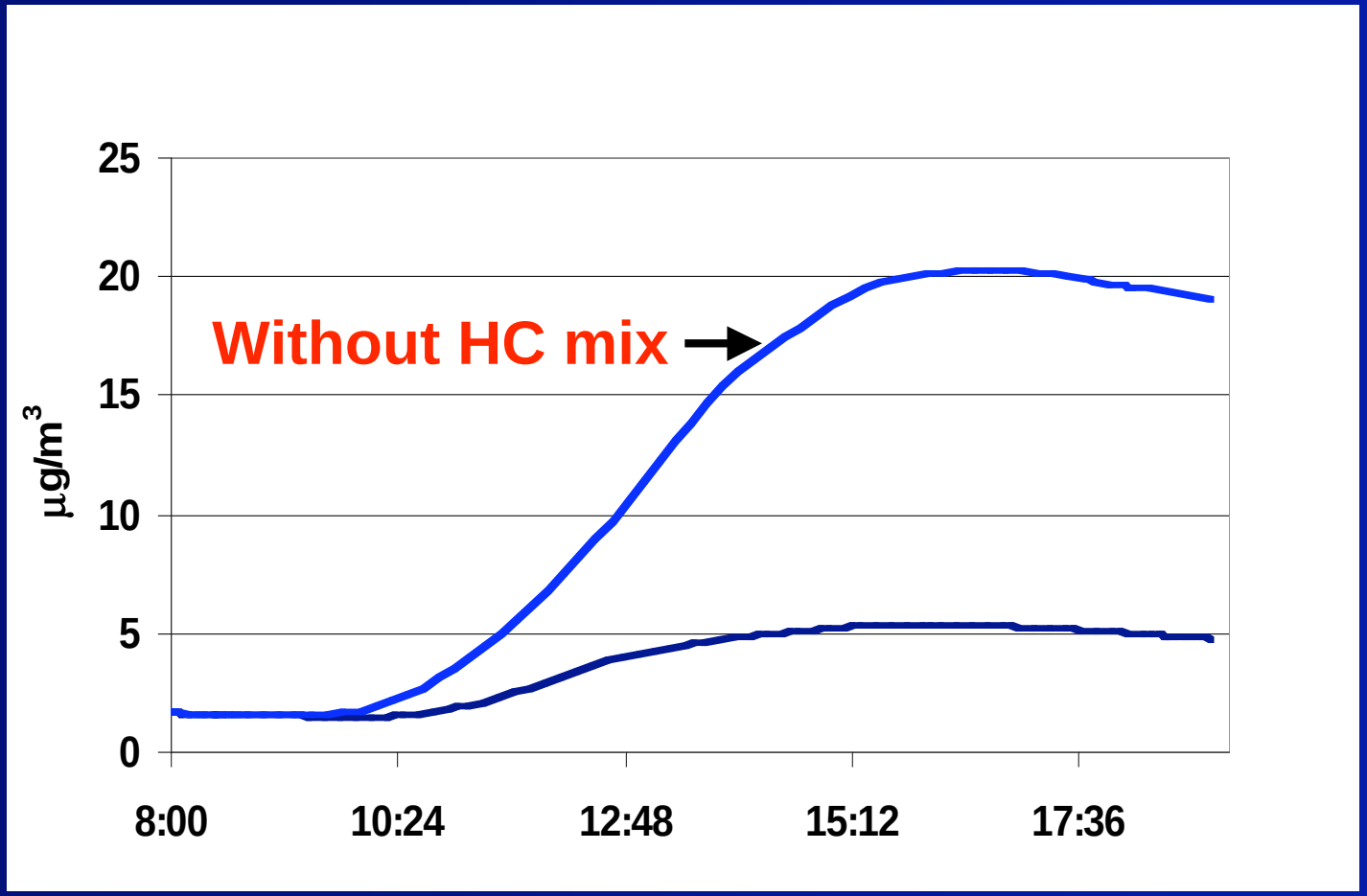
Model Simulations of the Caltech Chamber Data

Predicted aerosol mass conc. vs. Caltech reported mass conc.

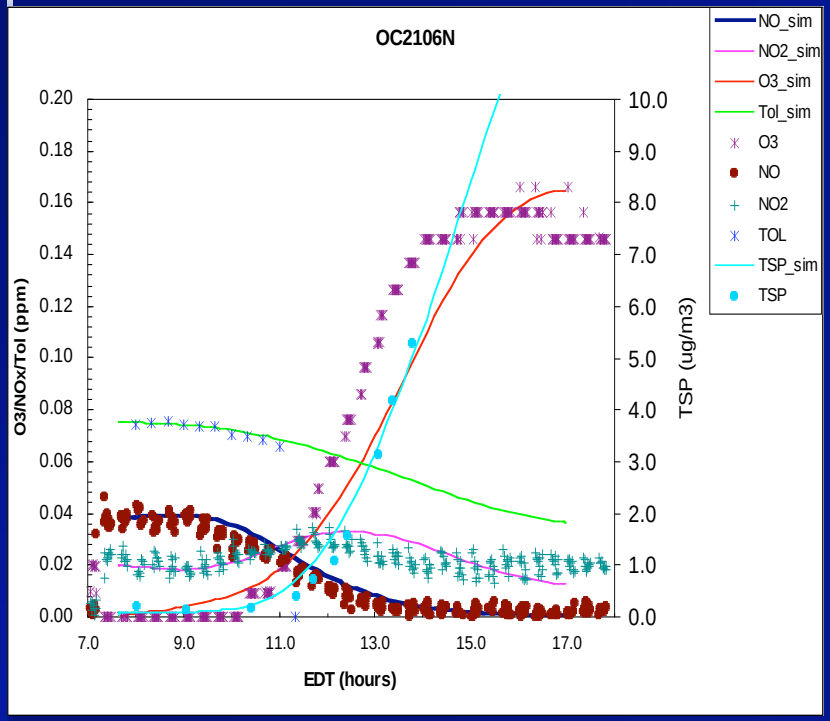


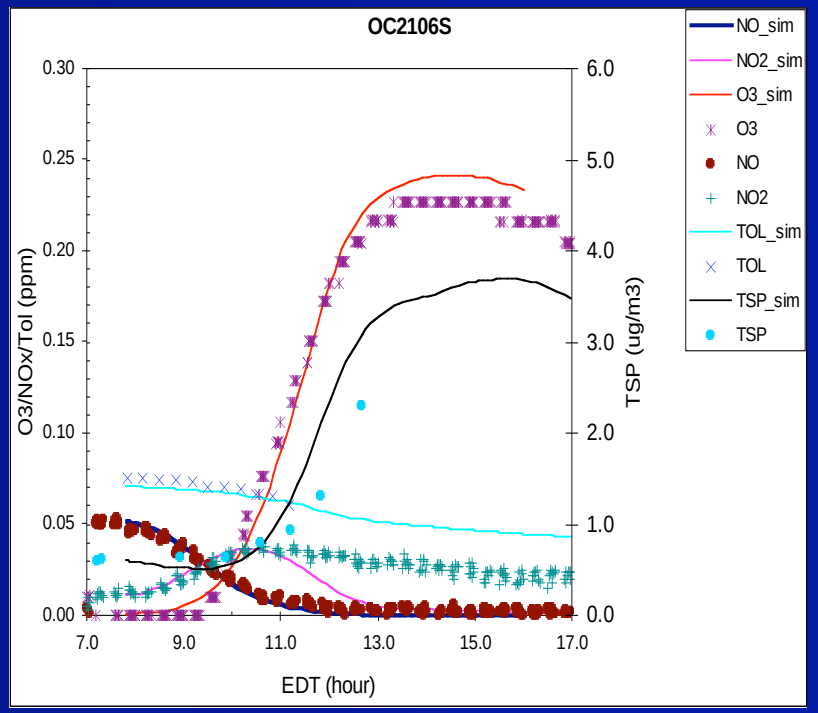
Toluene SOA behavior with in an atmospheric HC mixture

SOA from 0.1 ppmV toluene+0.1ppm NOx w/wo 3ppmC HC mixture



0.07 ppmV toluene+0.06ppm NOx W/O or W/ 3ppmC HCx mixture





Without HC_X **With HC_X**

Summary statements

- Did not use any acidity reactions
- tends to simulate toluene
- many products
- concentration levels
- Toluene with Mixture HCx
- Particle Phase Reactions (Lots of unknown)
- Chamber to real atmosphere

Thanks!

- Thanks to the EPA STAR program
- And to Harvey Jeffries for providing the Morpho kinetics solver program