

A Predictive Kinetic Model for Aerosol Formation from Toluene Oxidation



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gas phase chemistry



oxygenated products

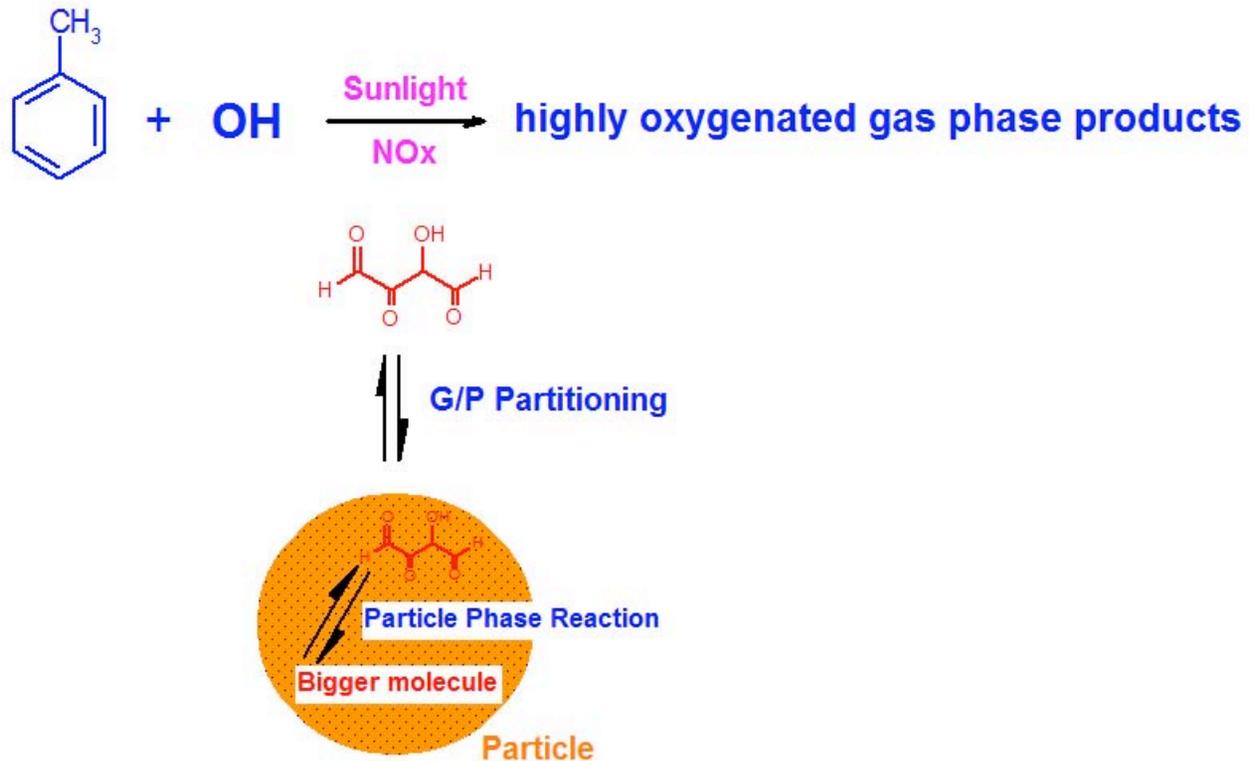


partition to the particle phase



particle phase reactions

gas and particle phase reactions in Toluene system.



Current Mechanism has:

98 gas phase reactions

67 gas to particle phase species

16 “particle phase” reactions

CB4 (2002) chemistry

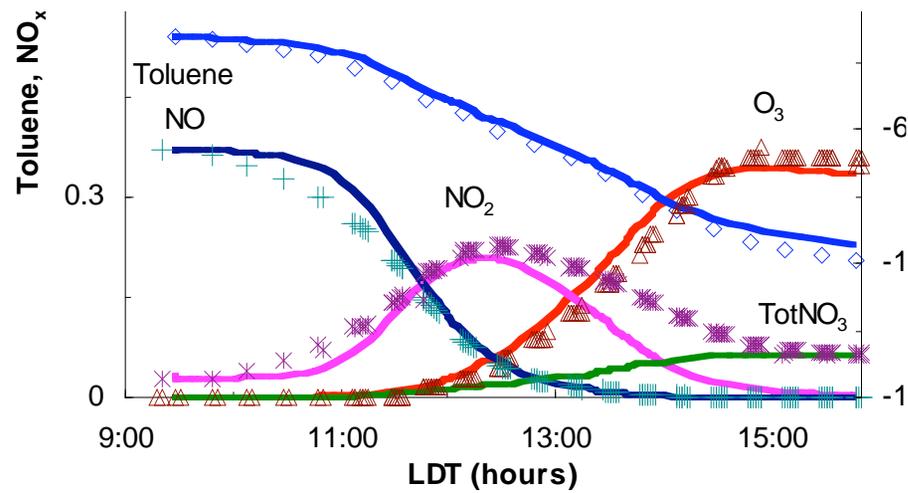
UNC Auxiliary Mechanism

(Chamber Wall reactions, dilution, et.al)

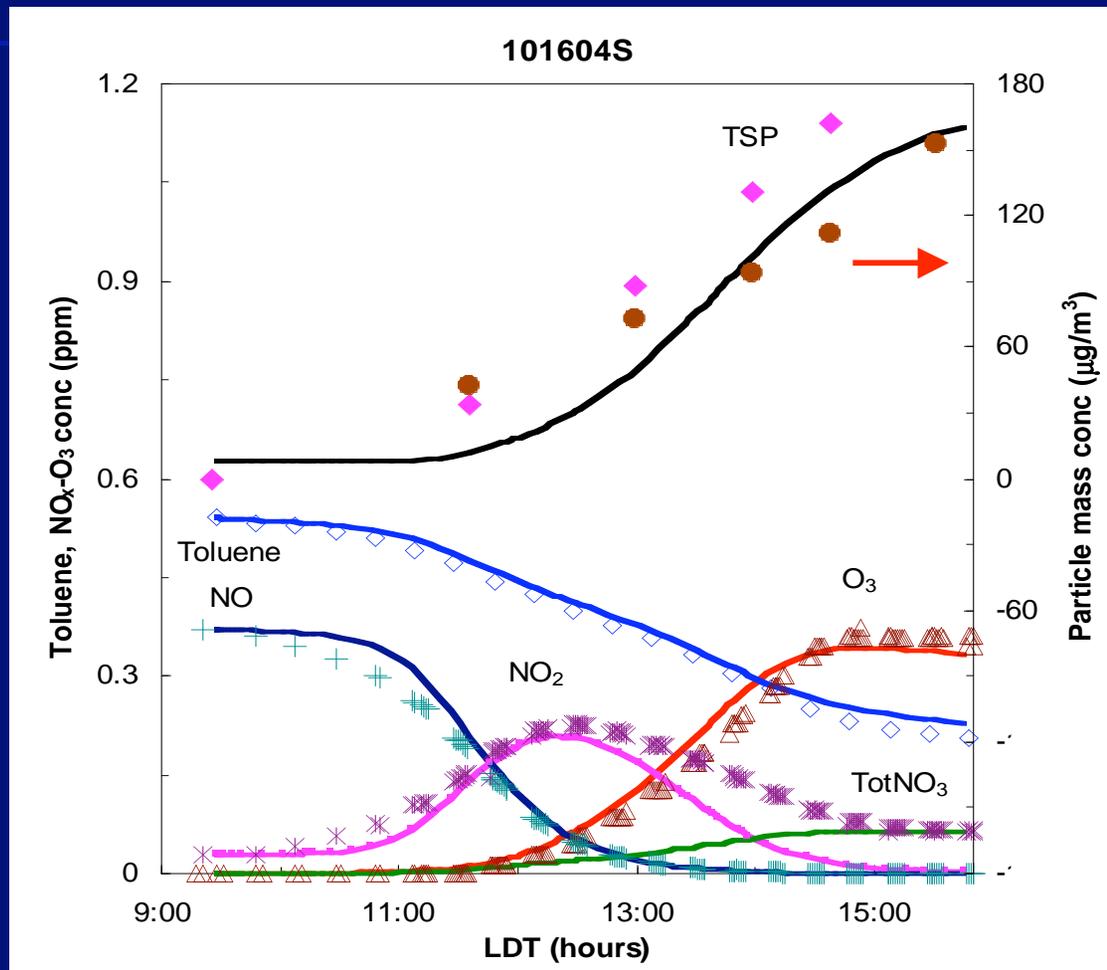
Model Simulations of UNC outdoor Toluene/NO_x Experiments



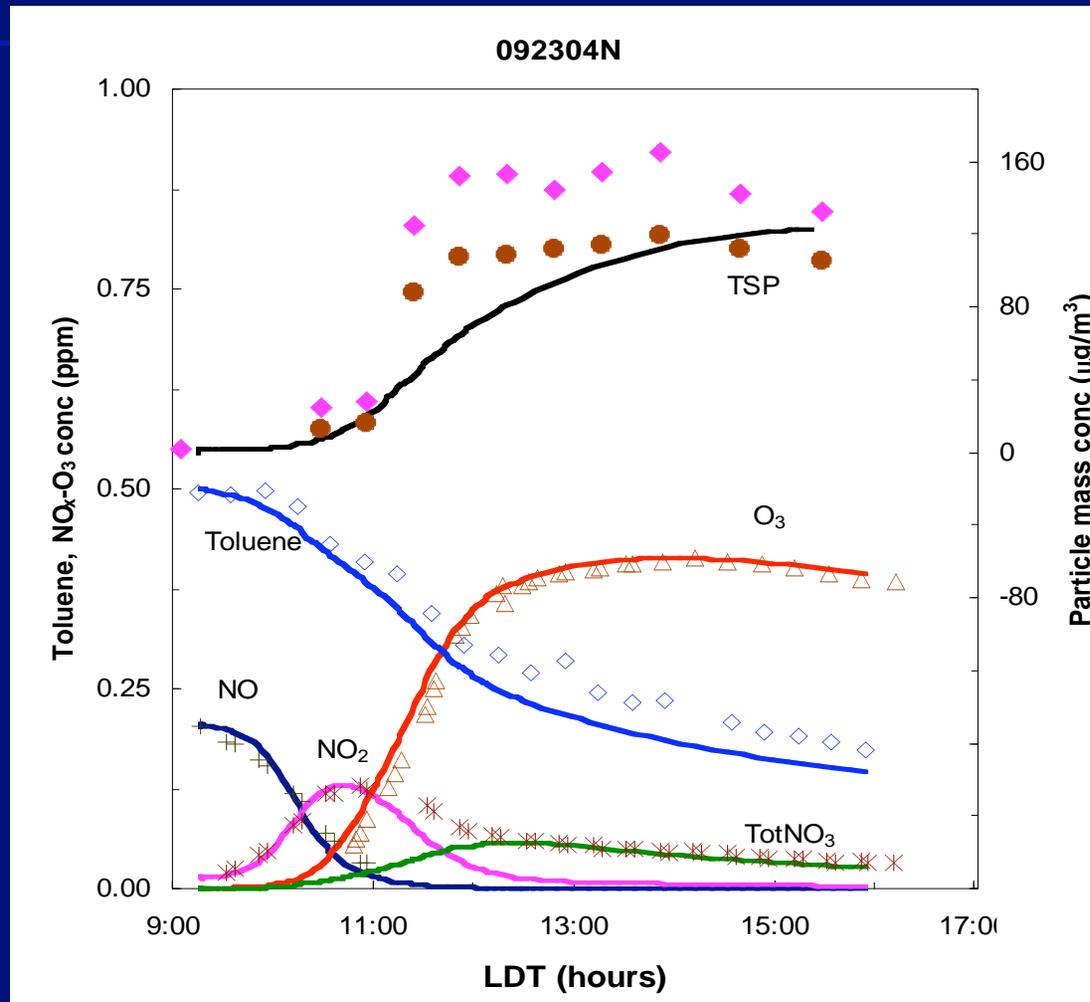
0.54 ppmV TOL + 0.37 ppm NOx



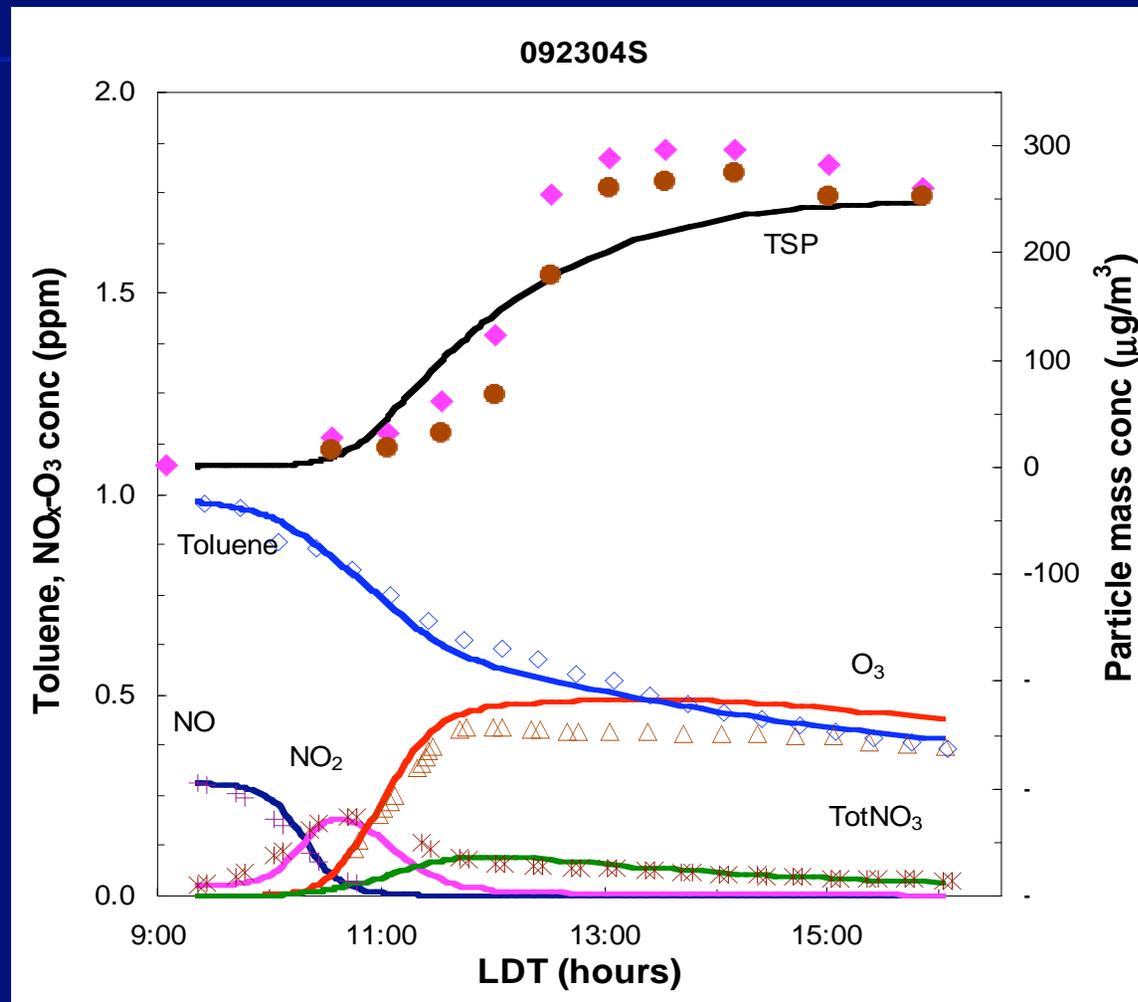
0.54 ppmV TOL + 0.37 ppm NOx



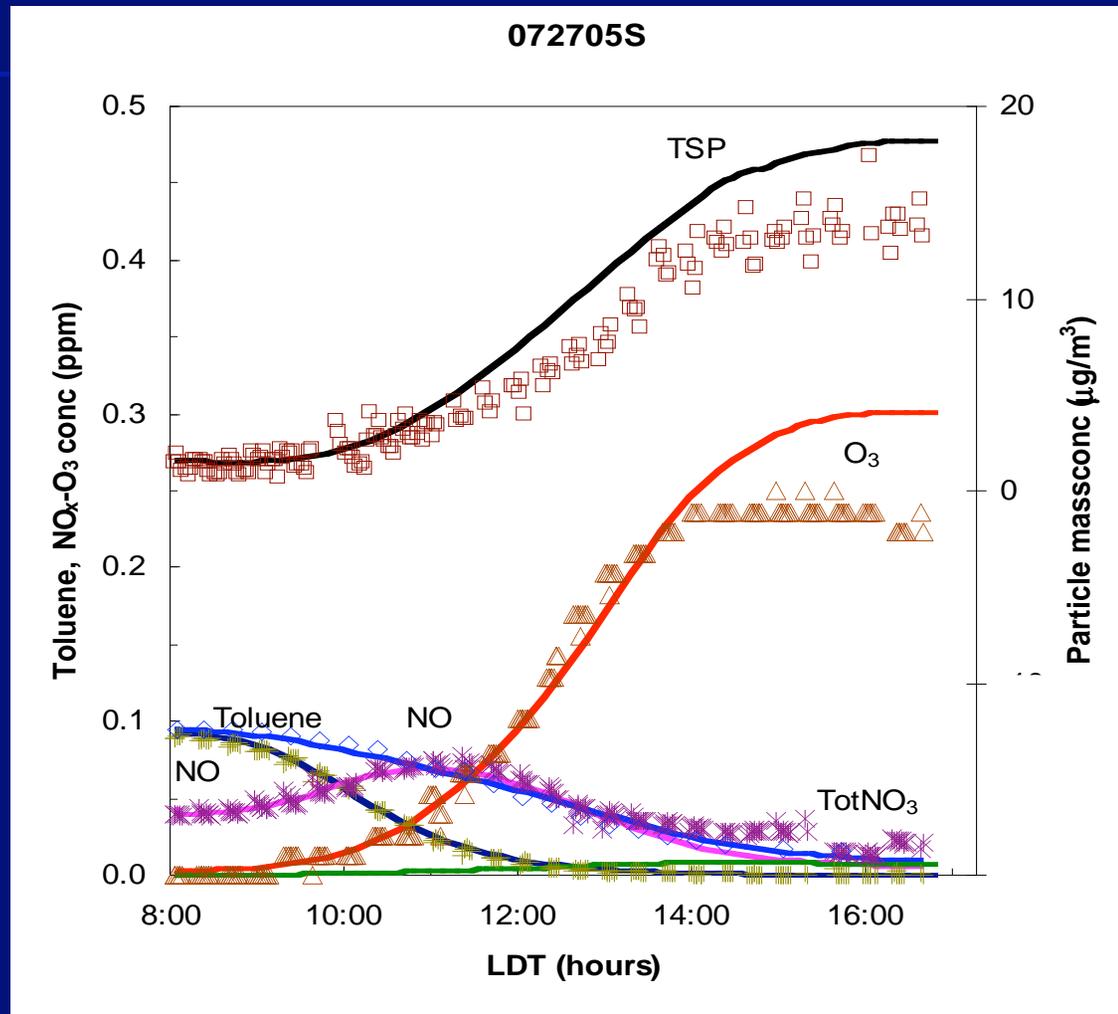
0.5 ppmV TOL + 0.2 ppm NOx



1 ppmV TOL + 0.3 ppm NOx



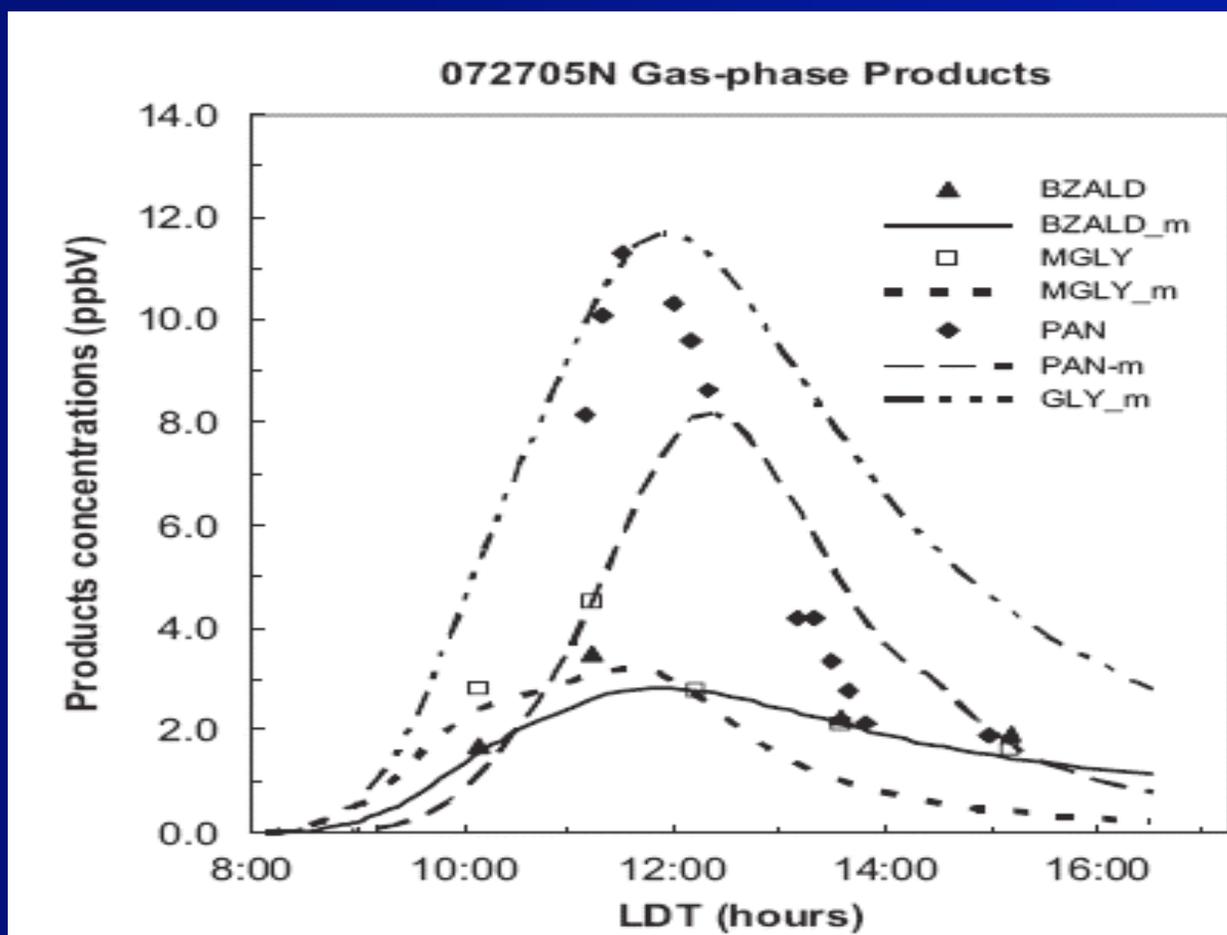
0.1 ppmV TOL + 0.13 ppm NOx



Major Products and Percentage

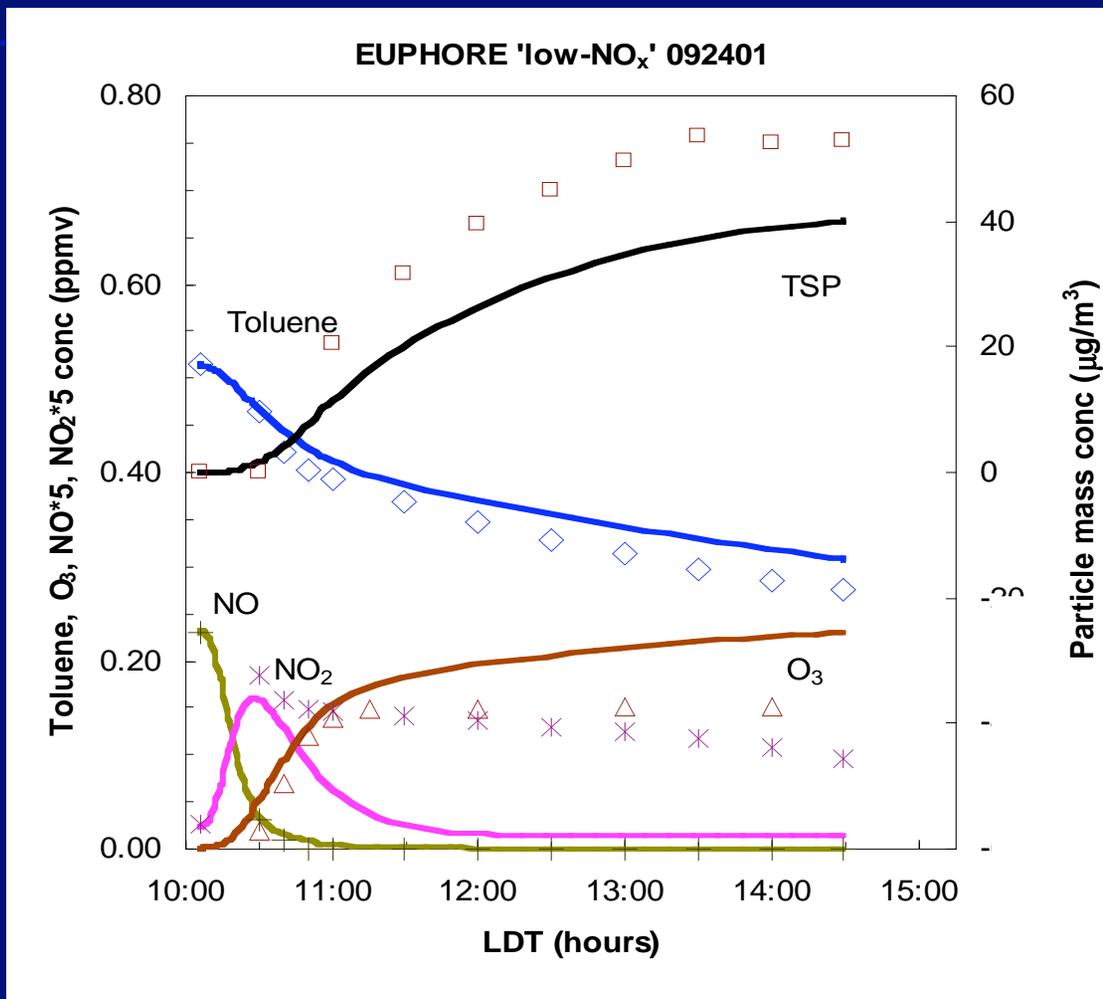
	250 $\mu\text{g}/\text{m}^3$	13 $\mu\text{g}/\text{m}^3$
GLYPOLY	60	17
MGLYPOLY	5	1
SEED1	10	20
Organic nitrates	7	26
CH3N02phenols	11	13
organic peroxides	4	5
C6OHNO2ACID	1	13
others	2	5

Products Simulation

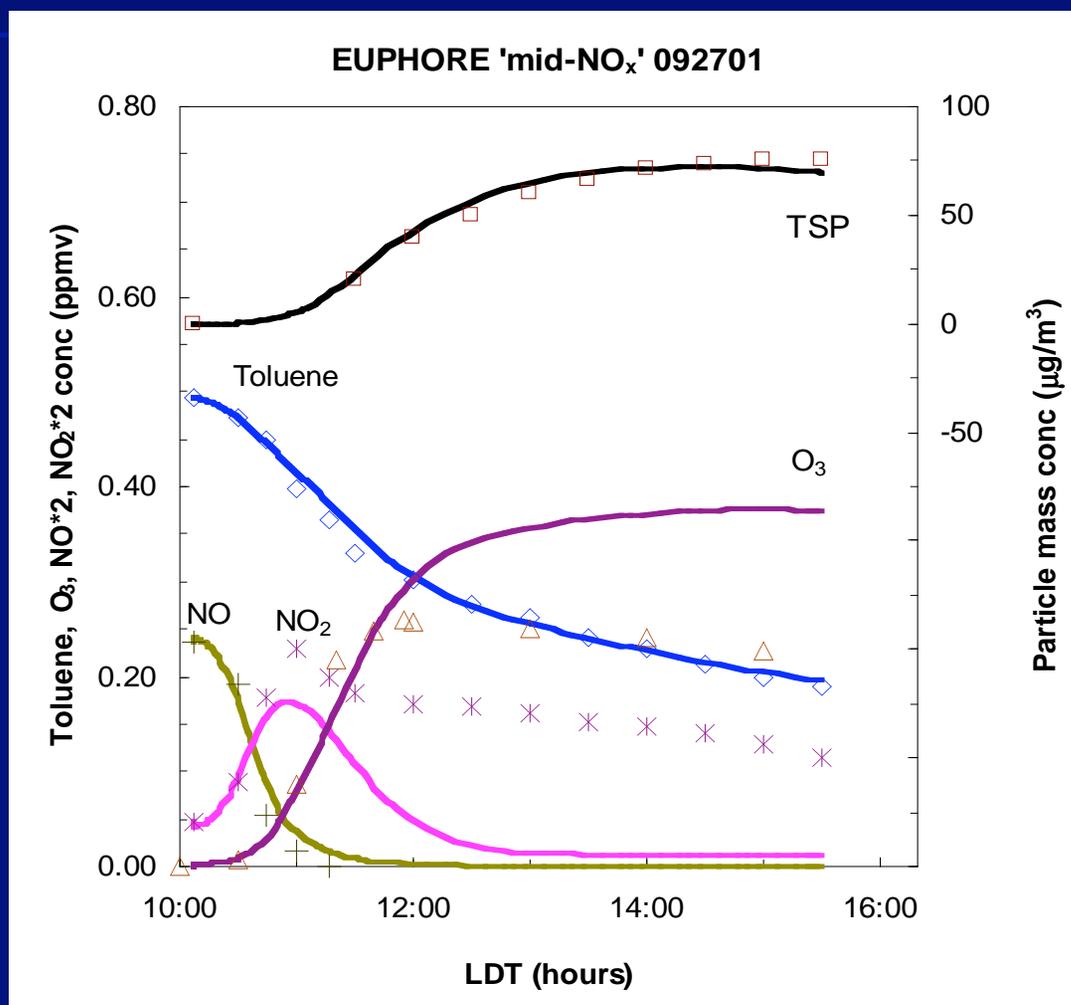


Model Simulations of the EUPHORE Chamber Data

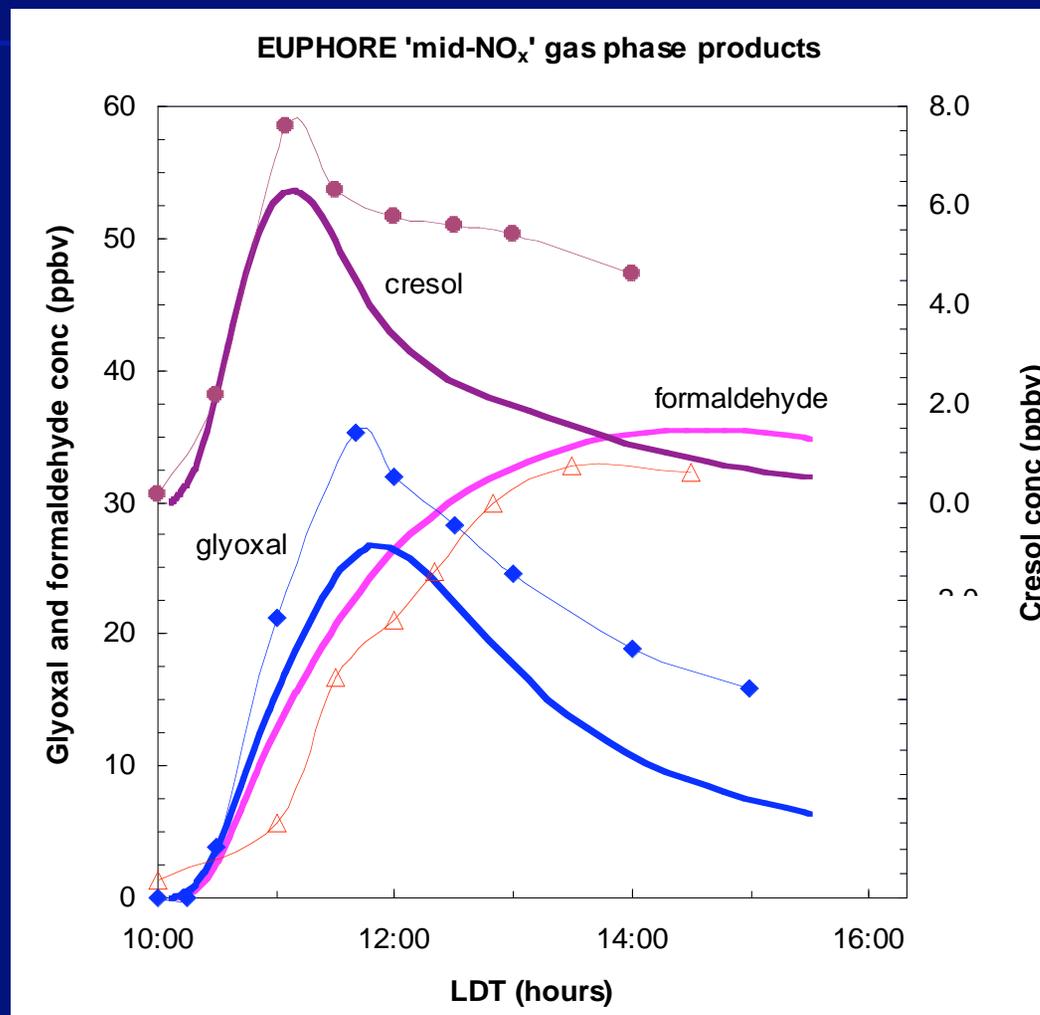
0.5ppmv TOL + 0.05 ppm NOx



0.5 ppmV TOL + 0.13 ppm NOx

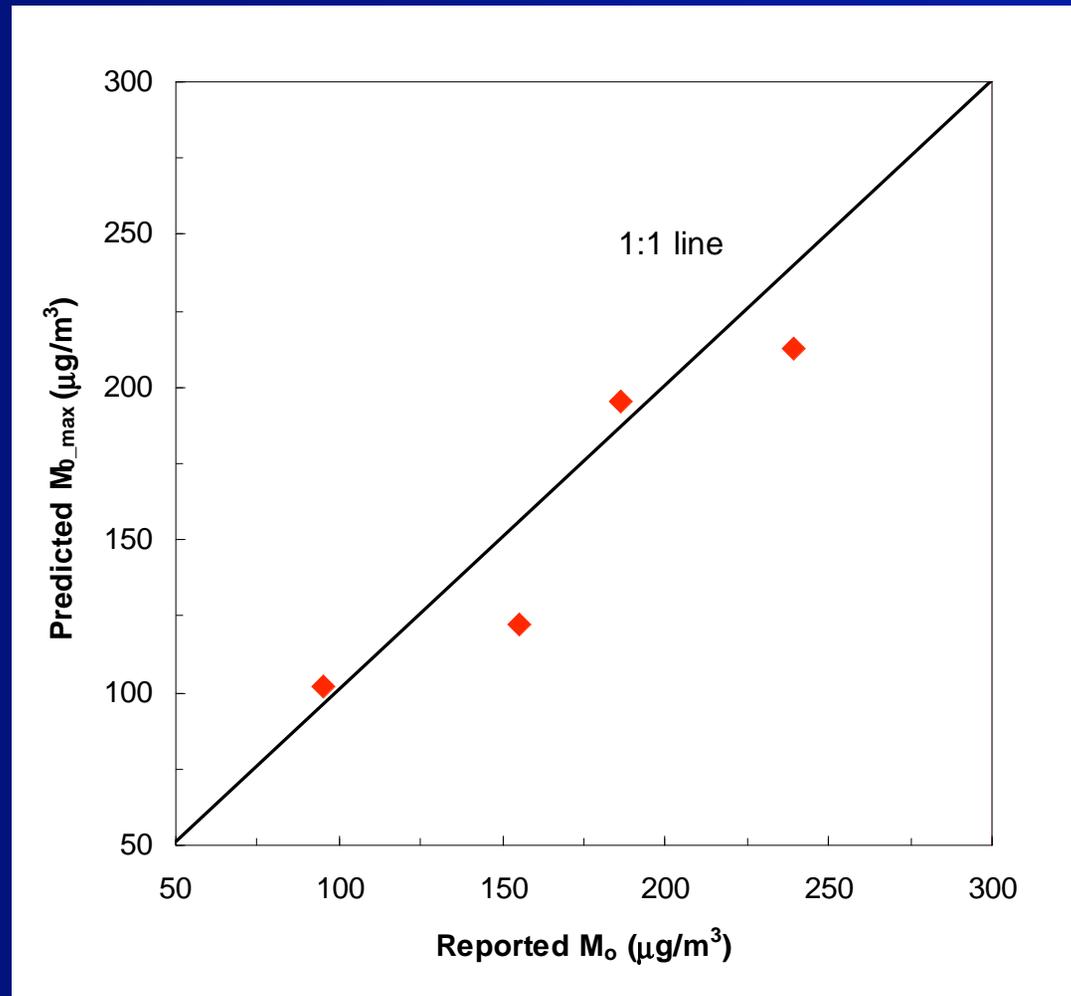


0.5 ppmv TOL + 0.13ppmv NOx



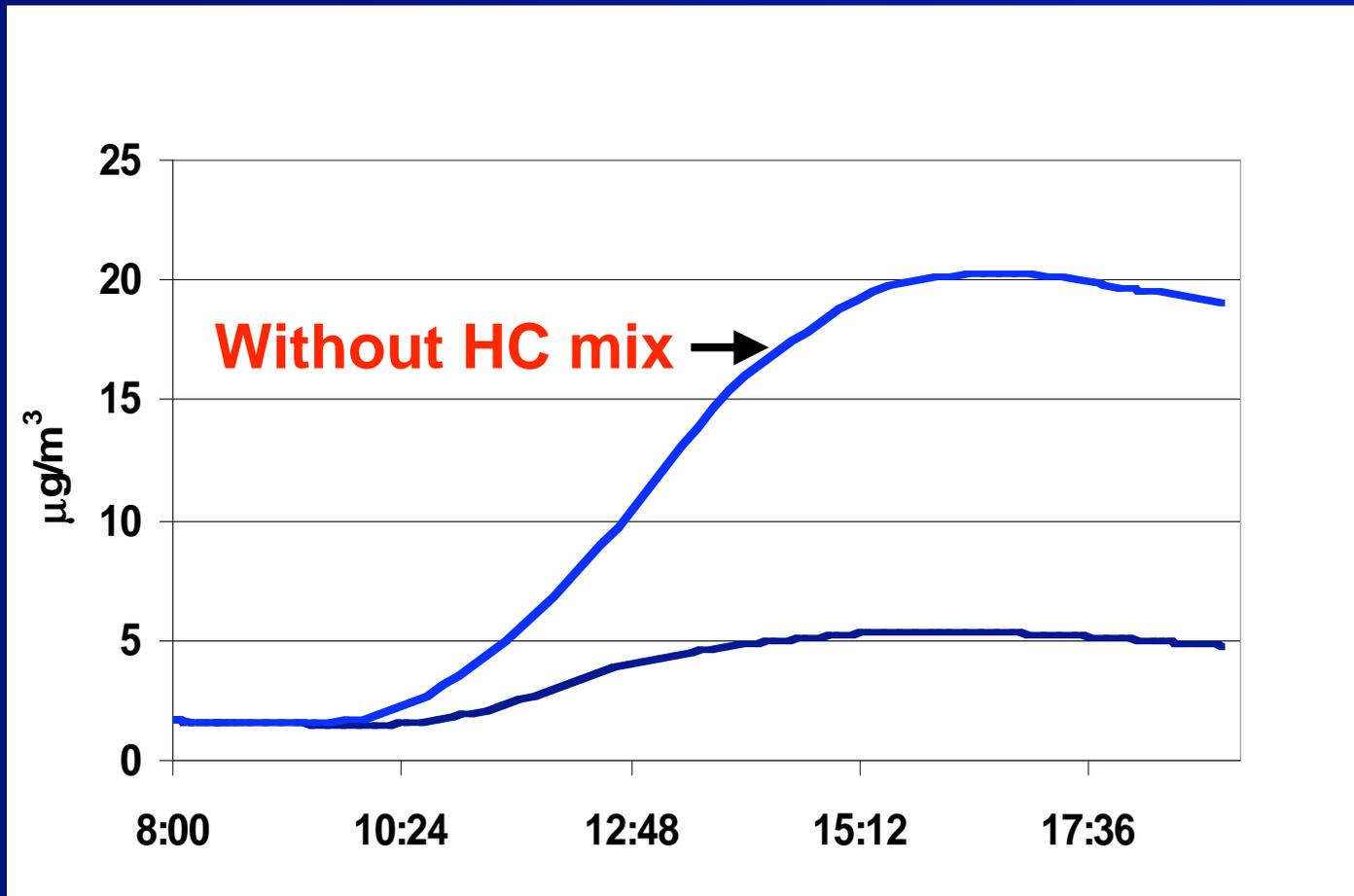
Model Simulations of the Caltech Chamber Data

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

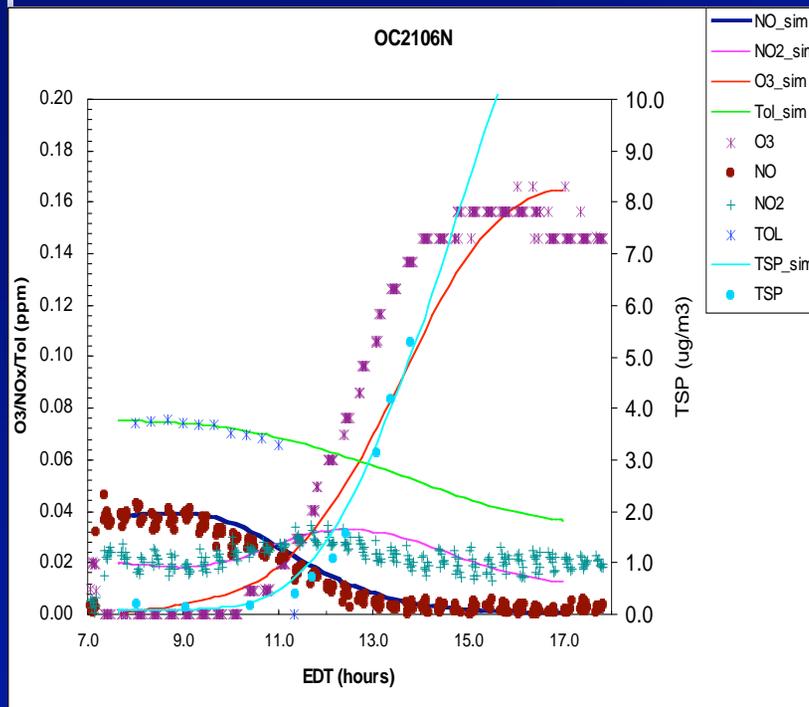


Toluene SOA behavior with in an atmospheric HC mixture

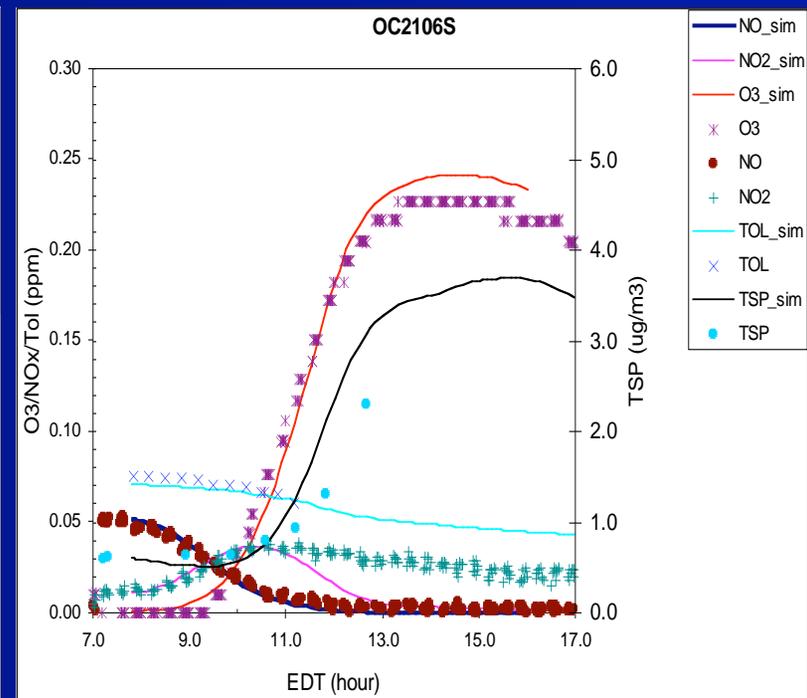
SOA from 0.1 ppmV toluene+0.1ppm NOx w/wo 3ppmC HC mixture



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

