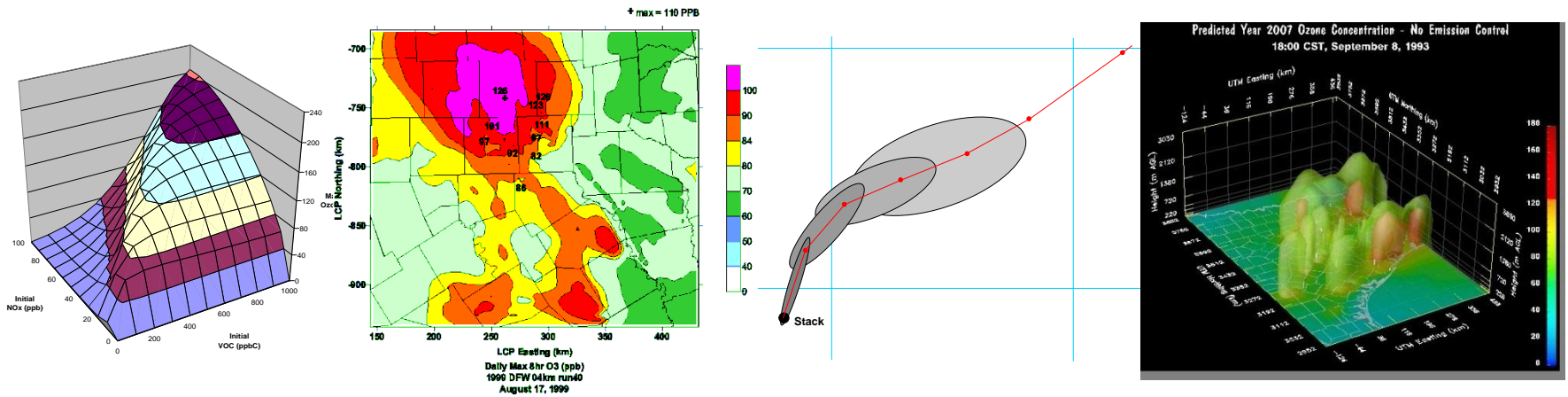
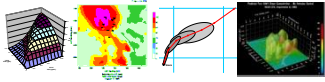


CAMx Probing Tools



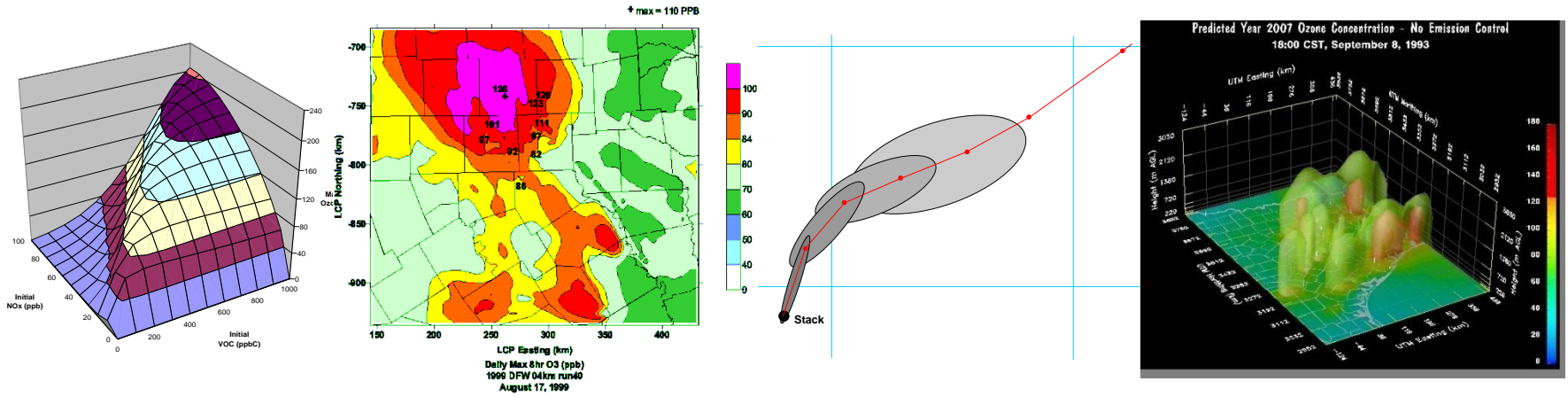
LADCO Advanced CAMx Training
Chris Emery & Greg Yarwood
August 3, 2010

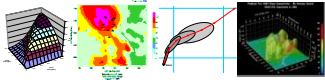


Topics

- Ozone/Particulate Source Apportionment Technology (OSAT/PSAT)
- Decoupled Direct Method (DDM) and Higher-Order DDM (HDDM) of Sensitivity Analysis
- Process Analysis (PA)
 - Integrated Process Rates (IPR)
 - Chemical Process Analysis (CPA)
- Reactive Tracer (RTRAC) and Reactive Tracer Chemical Mechanism Compiler (RTC MC)

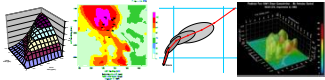
Ozone/Particulate Source Apportionment Technology





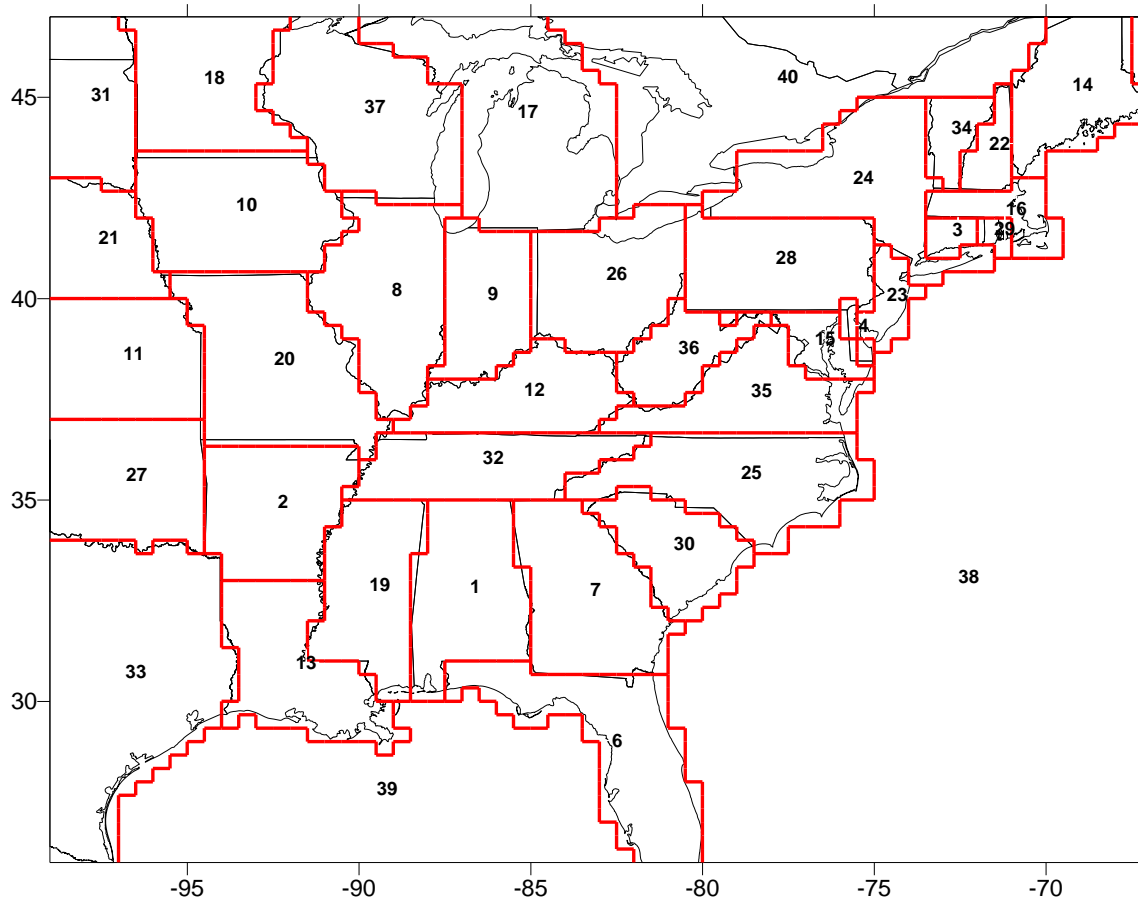
Source Apportionment

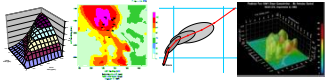
- Ozone Source Apportionment Technology (OSAT)
 - Apportions ozone to emissions and initial/boundary conditions
 - Emissions may be sub-divided by source area and/or source category
 - Ozone apportionment provided throughout the domain
 - Tracks precursor NO_x and VOC emissions
 - Associates ozone production with the precursors present when ozone is formed
 - Distinguish ozone production under NO_x and VOC sensitive conditions



Source Apportionment

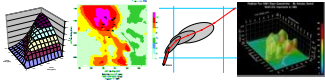
Source area map





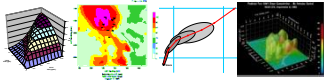
Source Apportionment

- NO_x vs. VOC sensitive chemistry defined by Sillman (1995) indicator ratio and cut-point
 - $PH_2O_2/PHNO_3 = 0.35$
 - Choice of $PH_2O_2/PHNO_3$ Indicator Ratio Cut-Point is Not Critical
 - The indicator moves rapidly through the cut-point of 0.35
 - Above this cut-point (i.e., rapid H₂O₂ production) ozone production is considered NO_x-limited
 - OSAT uses the value for each grid cell at each time step to allocate new ozone production to tracers
 - Ozone tracers formed earlier are not changed



Source Apportionment

- Source Apportionment is NOT sensitivity
 - OSAT *can* identify what precursors participated in ozone production (culpability)
 - OSAT is *limited* for predicting ozone response to precursors controls as response becomes non-linear
- Alternate apportionment methodologies:
 - OSAT: standard approach: attributes ozone to all sources
 - APCA: attributes ozone production preferentially to anthropogenic (controllable) sources
 - For ozone attributed to biogenic VOC, change the attribution to anthropogenic NO_x that participated
 - Similar scheme for ozone attributed to biogenic NO_x, but smaller impact



Source Apportionment

OSAT tracer species names

Emission Sources

SSSeeerrr

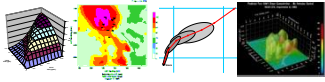
SSS	Species type, i.e., NOX, VOC, O3V or O3N
eee	Emissions group: Single group, always 000 Multiple groups, 001, 002, etc.
rrr	Region tracer released from, 001, 002, 003, etc.

Initial/Boundary

SSSeeerrr

SSS	Species type, i.e., NOX, VOC, O3V or O3N
eee	IC: always 000 non-stratified BC: always 000 stratified BC: WST, EST, STH, NTH, TOP
rrr	IC for Initial Concentrations, BC for Boundary Concentrations

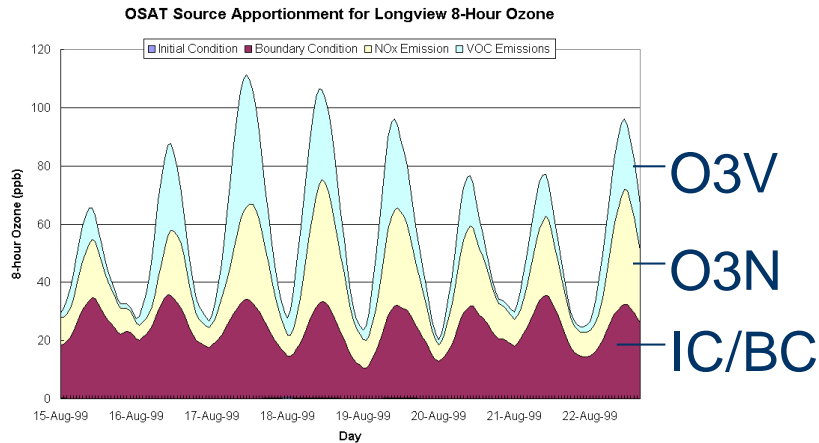
Examples: NOX000015, VOC002015, O3V000IC, O3NTOPBC



Source Apportionment

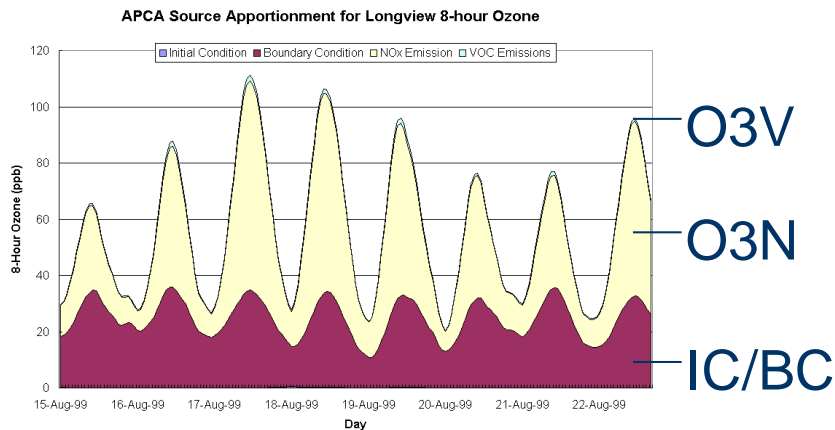
OSAT vs. APCA

OSAT

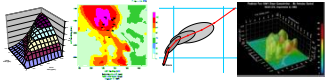


- Northeast Texas has high biogenic VOCs and major NO_x point sources
- OSAT finds significant biogenic VOC contribution to ozone (dominates the O3V)

APCA

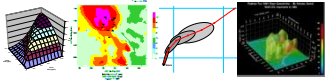


- APCA minimizes the biogenic contribution and shifts contributions to anthropogenic NO_x (O3N)
- IC/BC contribution unchanged



Source Apportionment

- PM Source Apportionment Technology (PSAT)
 - Similar concept to OSAT
 - Apportion PM components to emissions and initial/boundary conditions
 - PM components are sulfate, nitrate, ammonium, secondary organic aerosol and primary PM
 - Precursors are SO₂, NO_x, NH₃, organics and primary PM
 - Can choose which “family” of tracers to track
 - Sulfate, nitrate, SOA, Primary PM, Ozone, Hg



Source Apportionment

PSAT “family” tracer species names

Sulfur

SO2	Primary SO ₂ emissions
PS4	Primary/secondary particulate sulfate

Nitrogen

RGN	Reactive gaseous nitrogen (NO _x , NO ₃ , HONO, N ₂ O ₅)
TPN	Gaseous PAN + PNA
NTR	Organic nitrates (RNO ₃)
HN3	Gaseous nitric acid (HNO ₃)
PN3	Primary/secondary particulate nitrate
NH3	Gaseous ammonia (NH ₃)
PN4	Particulate ammonium (NH ₄)

Mercury

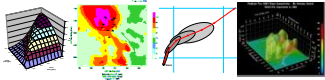
HG0	Elemental Mercury vapor
HG2	Reactive gaseous Mercury vapor
PHG	Particulate Mercury

Primary Particulate

PEC	Primary Elemental Carbon
POA	Primary Organic Aerosol
PFC	Fine Crustal PM
PFN	Other Fine Particulate
PCC	Coarse Crustal PM
PCS	Other Coarse Particulate

Secondary Organic

ARO	Aromatic (toluene and xylene) precursors
ISP	Isoprene precursors
TRP	Terpene precursors
SQT	Sesquiterpene precursors
CG1	Condensable gases from aromatics (low volatility)
CG2	Condensable gases from aromatics (high volatility)
CG3	Condensable gases from isoprene (low volatility)
CG4	Condensable gases from isoprene (high volatility)
CG5	Condensable gases from terpenes (low volatility)
CG6	Condensable gases from terpenes (high volatility)
CG7	Condensable gases from sesquiterpenes
PO1	Particulate organic aerosol associated with CG1
PO2	Particulate organic aerosol associated with CG2
PO3	Particulate organic aerosol associated with CG3
PO4	Particulate organic aerosol associated with CG4
PO5	Particulate organic aerosol associated with CG5
PO6	Particulate organic aerosol associated with CG6
PO7	Particulate organic aerosol associated with CG7

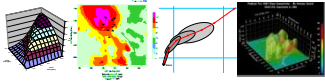


Source Apportionment

- PSAT computational efficiency
 - Measure efficiency relative to zero-out
 - PSAT is very efficient
 - 30x for sulfate
 - 20x for nitrate/ammonium
 - 10x for SOA
 - Number of tracer families governs efficiency
 - May be computer system dependant
 - Ensure adequate memory and rapid disk I/O access

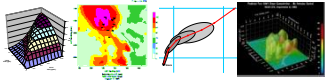
Table 5-1. Computational efficiency of PSAT compared to zero-out analysis for 80 source groups.

Type of Analysis	PSAT Run-Time (hours/day)	Zero-out Run-Time (hours/day)	PSAT Efficiency Gain
Base run	1.15	N/A	N/A
Sulfate contributions	3	93	31
SOA contributions	10	93	9
Nitrate and Ammonium contributions	5.5	93	17



Source Apportionment

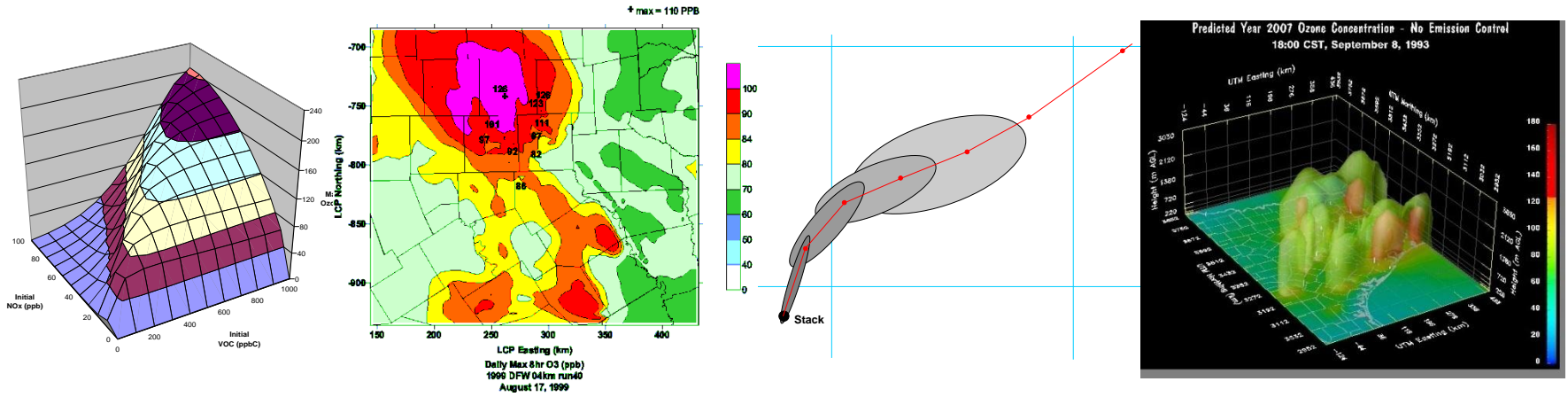
- Design features for maximum efficiency
 - Independent species apportionment
 - Select just the species you need
 - Summary output
 - Restrict output to PM species (e.g., PNO₃ without RGN, TPN, NTR, HN₃)
 - Save disk space, minimize I/O delays
 - Surface concentrations only
 - No 3-D average concentrations for PSAT tracers (can use aloft receptors)
 - Save memory, minimize disk space and I/O

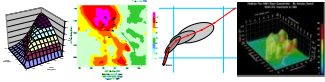


Source Apportionment

- OSAT/PSAT input
 - Namelist control parameters (CAMx.in)
 - Source area map (text)
 - Receptor definition file (text)
 - Restart files (CAMx binary)
 - Point/gridded source category files (CAMx binary)
- OSAT/PSAT output
 - Master/fine grid instantaneous tracer files (CAMx binary)
 - Grid-specific average tracer files (CAMx binary)
 - Grid-specific deposition tracer files (CAMx binary)
 - Receptor output file (text)

Decoupled Direct Method of Sensitivity Analysis





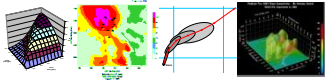
Sensitivity Analysis

- Decoupled Direct Method (DDM)

- Calculate 1st-order (DDM) and 2nd-order (HDDM) derivatives, or sensitivities:

$$\begin{aligned}
 c(\underline{x}, t; \underline{\lambda}) &= c(\underline{x}, t; \underline{\lambda}_0) + \sum_{i=1}^n \left. \frac{\partial c}{\partial \lambda_i} \right|_{\underline{\lambda}_0} (\lambda_i - \lambda_{i0}) \\
 &+ \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \left. \frac{\partial^2 c}{\partial \lambda_i \partial \lambda_j} \right|_{\underline{\lambda}_0} (\lambda_i - \lambda_{i0}) (\lambda_j - \lambda_{j0}) \\
 &+ \dots
 \end{aligned}$$

- Sensitivity of a concentration output to an emissions or IC/BC input
 - Calculate many sensitivities at once
 - Emissions may be specified by region and/or category



Sensitivity Analysis

– Applications

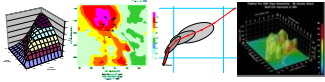
- Estimate effects of emission changes
- Rank relative importance of source region/categories to ozone formation, or other species

– Sensitivity is NOT Source Apportionment

- It *can* predict ozone response to precursor controls:
 - DDM: small-moderate (near-linear) changes, highly accurate
 - HDDM: large (non-linear) changes, less accurate
- It is *limited* for source attribution (culpability) because some sensitivities are *negative*

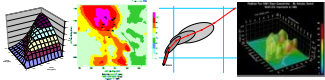
– DDM is slower than OSAT, but:

- Provides information for all species (not just ozone)
- More flexible in selecting which parameters to track



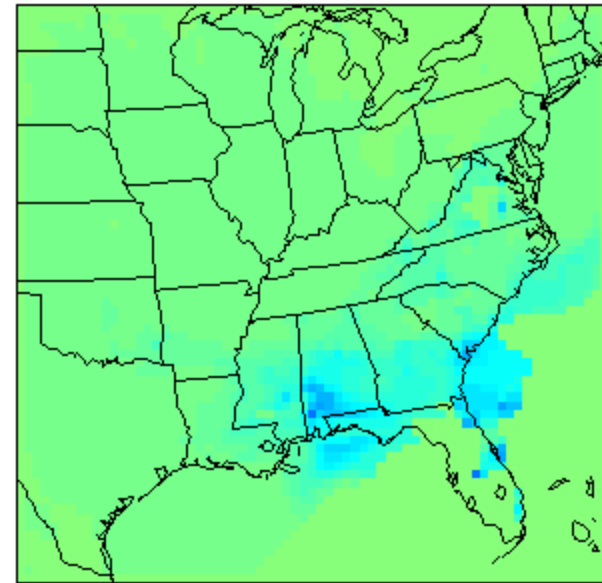
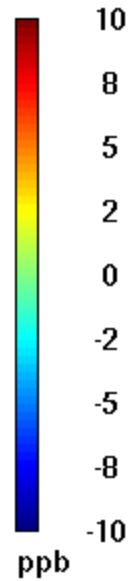
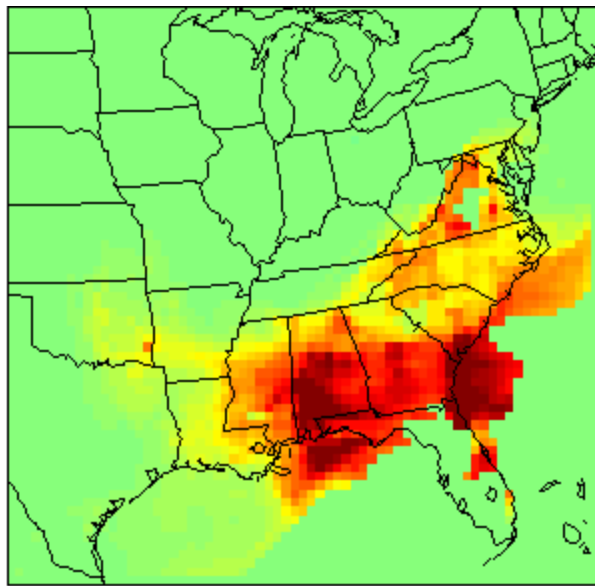
Sensitivity Analysis

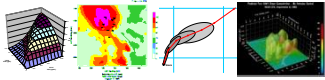
- DDM is not available for PiG
- CPU time and memory space can be significant with multiple grids
 - Increased cost may not always be worthwhile
 - Can use 1-way nesting to improve efficiency
 - Sensitivities determined for single grid
 - Can cause discrepancies in the model results
 - “Flexi-DDM”
 - Allows user to turn off sensitivity calculations for selected grids
 - Reduces CPU times but will not reduce memory requirements
 - Can’t calculate certain types of sensitivity calculations: e.g., BCs



Sensitivity Analysis

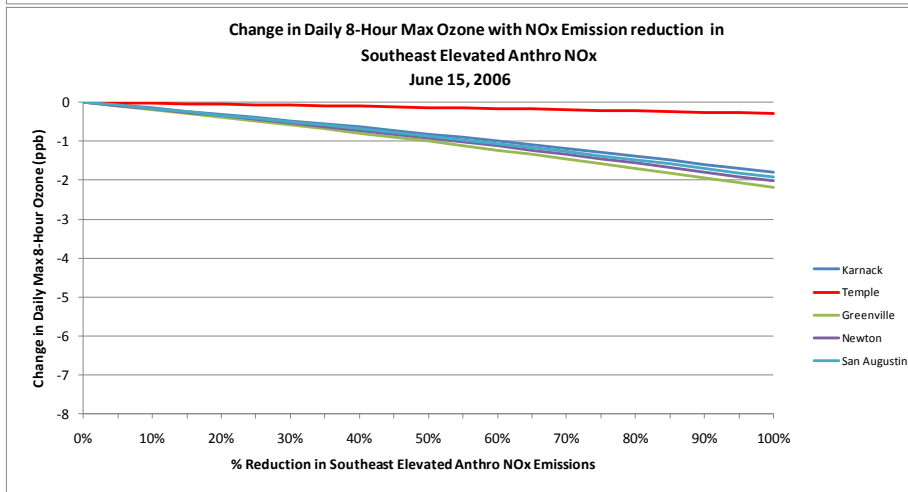
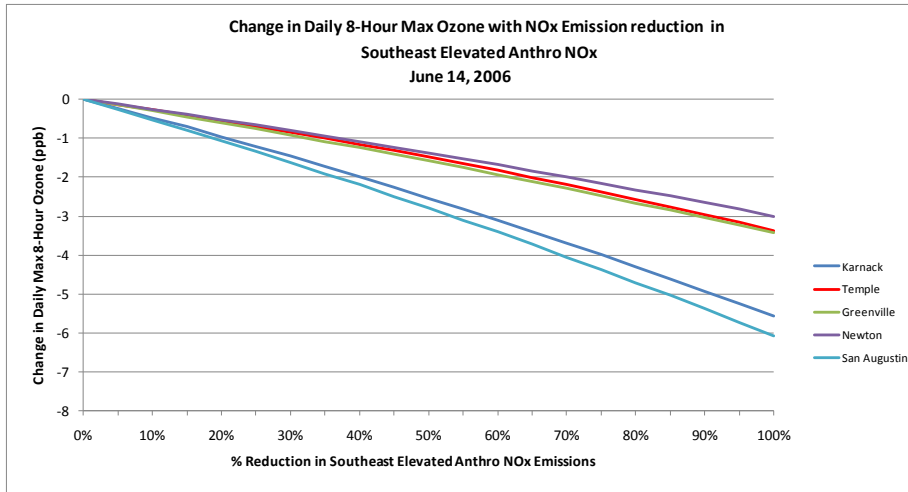
June 13-15: Average S^1_{SE} and S^2_{SE}



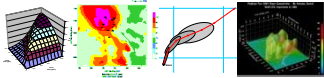


Sensitivity Analysis

Change in DM8 with SE NO_x Emission Reductions

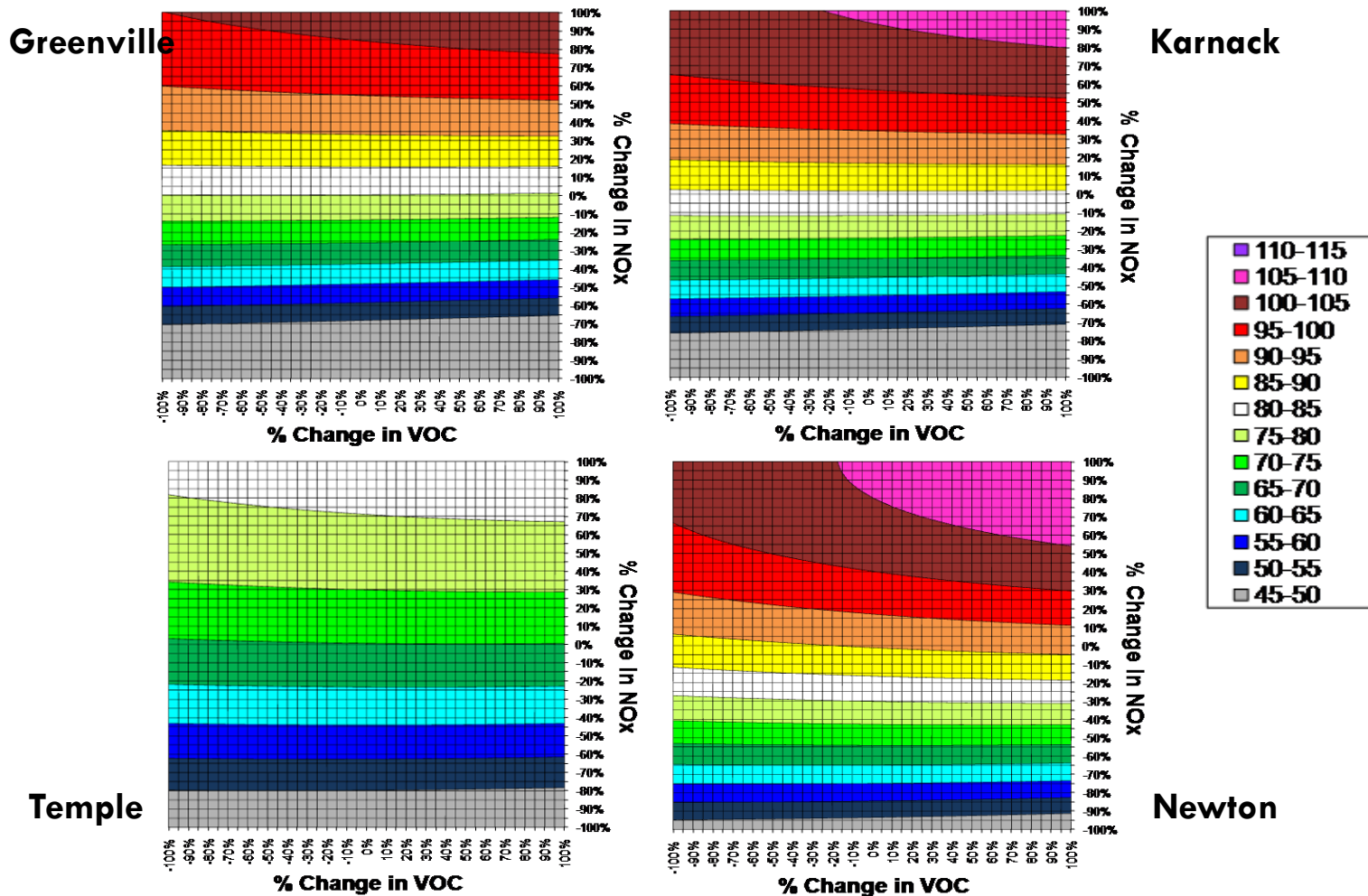


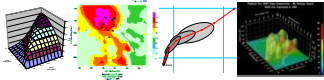
- Southeast Texas border monitors show largest sensitivity to reductions on June 14
- On June 15, smaller change



Sensitivity Analysis

June 15, 2006: 8-Hour Ozone Response Surfaces





Sensitivity Analysis

DDM sensitivity names

Emission Sources

NNNNEMGGRRMMMM

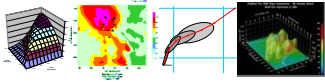
- NNNN Affected species name
- EM Indicates sensitivity is for emissions
- GG Emissions group number
- RR Emissions region number
- MMMM Influencing species name

Initial/Boundary

NNNNXXRRR_MMMM

- NNNN Affected species name
- XX IC for initial conditions; BC for boundary conditions
- RRR_ Boundary name
 - BC: WST_, EST_, STH_, NTH_, TOP_, ALL_
 - IC: _____ (four underscores)
- MMMM Influencing species name

Examples: O3__EM0102NO___, HNO3_BCALL_NO2_, O3__IC____O3__



Sensitivity Analysis

DDM sensitivity names

Reaction Rates

NNNNRATE__MMMM

NNNN Affected species name

RATE__ Indicates sensitivity is for rate constants

MMMM Reaction rate sensitivity group name

HDDM

NNNNHDDMLLLMMM

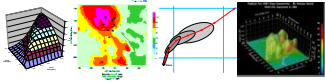
NNNN Affected species name

HDDM Indicates sensitivity is second order

LLL Index of first 1st order parameter in the internal list

MMM Index of the second 1st order parameter in the internal list

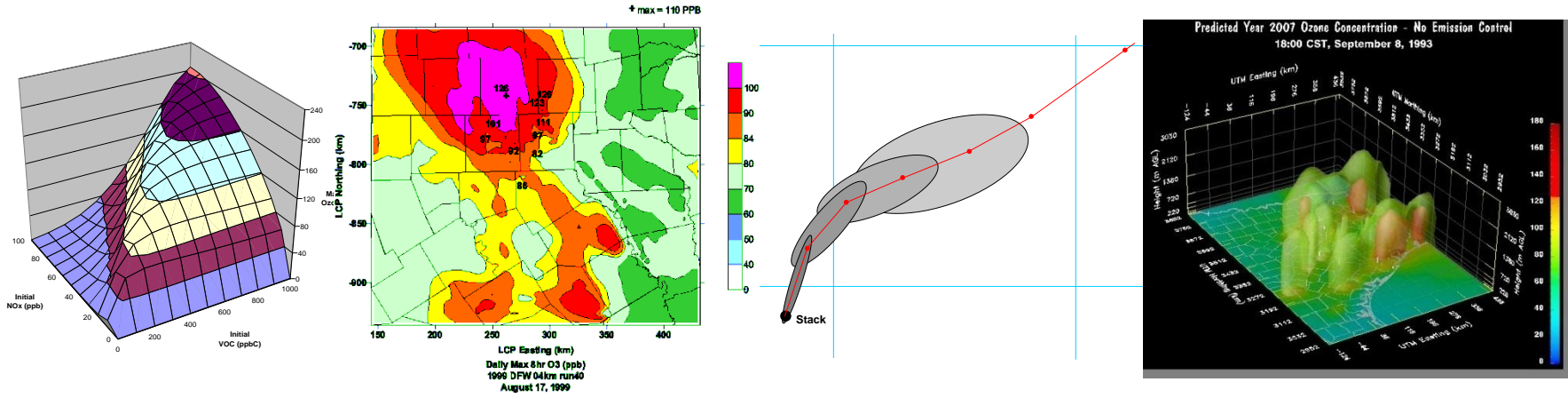
Examples: NO__RATE__RXN1, O3__HDDM001002

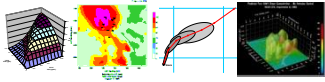


Sensitivity Analysis

- **DDM input**
 - Namelist control parameters (CAMx.in)
 - Source area map (text)
 - Receptor definition file (text)
 - Restart files (CAMx binary)
 - Point/gridded source category files (CAMx binary)
 - IC/BC files (CAMx binary)
- **DDM output**
 - Master/fine grid instantaneous sens files (CAMx binary)
 - Grid-specific average sens files (CAMx binary)
 - Receptor output file (text)

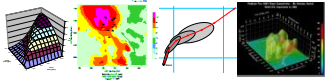
Process Analysis





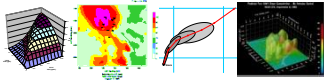
Process Analysis

- Process Analysis (PA)
 - Gather and report additional information on model processes
 - i.e., chemistry, deposition, emissions, etc.
 - Explain “how the model got the answer it got”
 - Operate for entire modeling grids or user-defined analysis domains
 - Often requires post-processing to be useful



Process Analysis

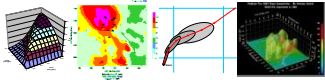
- Three components of PA
 - Integrated Process Rate (IPR)
 - Species change due to each model process (emissions, diffusion, chemistry, etc.)
 - Must post-process, straightforward to interpret
 - Integrated Reaction Rate (IRR)
 - Integrate rate of all chemical reactions
 - Difficult to interpret, seldom used
 - Chemical Process Analysis (CPA)
 - Convert IRR information to more user-friendly and accessible form, no post-processing needed



Process Analysis

List of IPR variables

IPR Parameter	Process Information	Units ^a
1	Initial concentration	$\mu\text{mole}/\text{m}^3$ ($\mu\text{g}/\text{m}^3$)
2	Gas phase chemistry	$\mu\text{mole}/\text{m}^3$ ($\mu\text{g}/\text{m}^3$)
3	Gridded emissions	$\mu\text{mole}/\text{m}^3$ ($\mu\text{g}/\text{m}^3$)
4	Point source emissions	$\mu\text{mole}/\text{m}^3$ ($\mu\text{g}/\text{m}^3$)
5	Plume-in-Grid change	$\mu\text{mole}/\text{m}^3$ ($\mu\text{g}/\text{m}^3$)
6	West boundary advection	$\mu\text{mole}/\text{m}^3$ ($\mu\text{g}/\text{m}^3$)
7	East boundary advection	$\mu\text{mole}/\text{m}^3$ ($\mu\text{g}/\text{m}^3$)
8	South boundary advection	$\mu\text{mole}/\text{m}^3$ ($\mu\text{g}/\text{m}^3$)
9	North boundary advection	$\mu\text{mole}/\text{m}^3$ ($\mu\text{g}/\text{m}^3$)
10	Bottom boundary advection	$\mu\text{mole}/\text{m}^3$ ($\mu\text{g}/\text{m}^3$)
11	Top boundary advection	$\mu\text{mole}/\text{m}^3$ ($\mu\text{g}/\text{m}^3$)
12	Dilution in the vertical	$\mu\text{mole}/\text{m}^3$ ($\mu\text{g}/\text{m}^3$)
13	West boundary diffusion	$\mu\text{mole}/\text{m}^3$ ($\mu\text{g}/\text{m}^3$)
14	East boundary diffusion	$\mu\text{mole}/\text{m}^3$ ($\mu\text{g}/\text{m}^3$)
15	South boundary diffusion	$\mu\text{mole}/\text{m}^3$ ($\mu\text{g}/\text{m}^3$)
16	North boundary diffusion	$\mu\text{mole}/\text{m}^3$ ($\mu\text{g}/\text{m}^3$)
17	Bottom boundary diffusion	$\mu\text{mole}/\text{m}^3$ ($\mu\text{g}/\text{m}^3$)
18	Top boundary diffusion	$\mu\text{mole}/\text{m}^3$ ($\mu\text{g}/\text{m}^3$)
19	Dry deposition	$\mu\text{mole}/\text{m}^3$ ($\mu\text{g}/\text{m}^3$)
20	Wet deposition	$\mu\text{mole}/\text{m}^3$ ($\mu\text{g}/\text{m}^3$)
21	Inorganic aerosol chemistry	$\mu\text{mole}/\text{m}^3$ ($\mu\text{g}/\text{m}^3$)
22	Oganic aerosol chemistry	$\mu\text{mole}/\text{m}^3$ ($\mu\text{g}/\text{m}^3$)
23	Aqueous aerosol chemistry	$\mu\text{mole}/\text{m}^3$ ($\mu\text{g}/\text{m}^3$)
24	Final concentration	$\mu\text{mole}/\text{m}^3$ ($\mu\text{g}/\text{m}^3$)
25	Units conversion	$\text{ppm}/(\mu\text{mole}/\text{m}^3)$ (N/A) ^b
26	Average cell volume	m^3



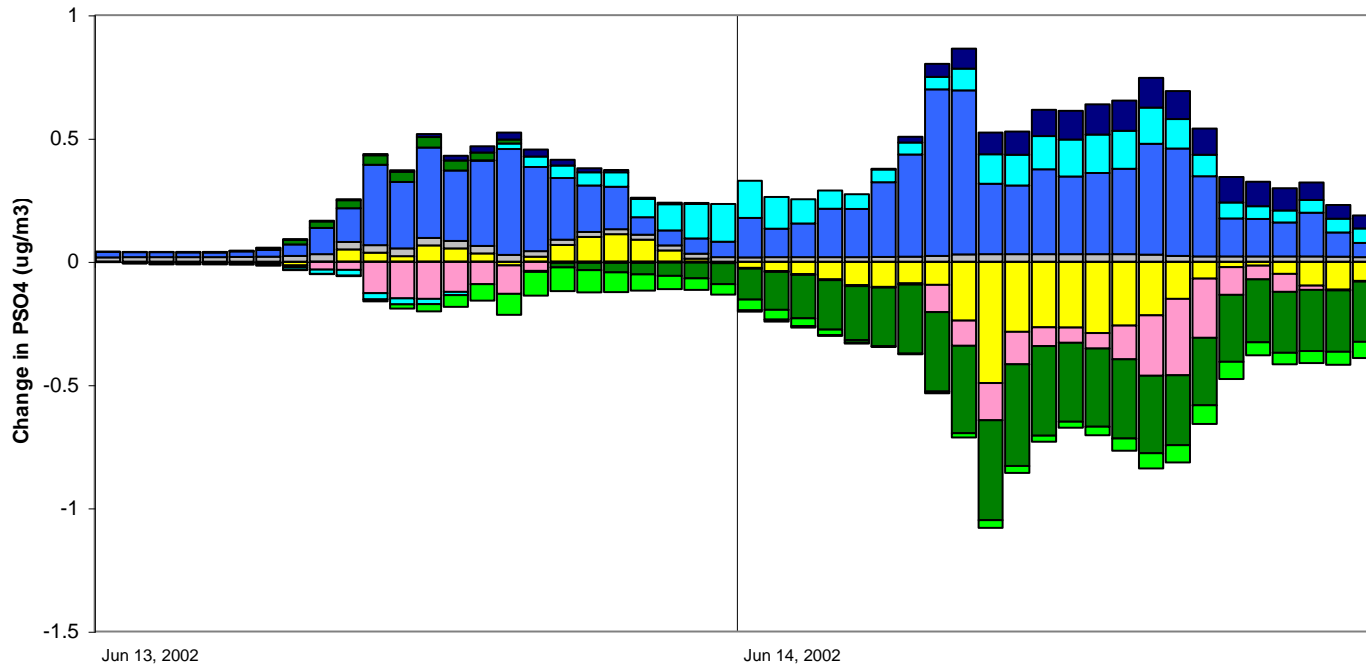
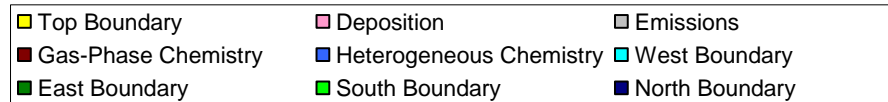
Process Analysis

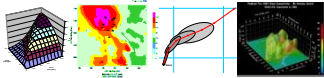
Example of PA/IPR

Hourly PSO4 Change from Different Processes in Chicago Area.

Run = postproc_test

Grid cells used from grid number 1: (43, 47) to (52, 56) using layers 1 to 5



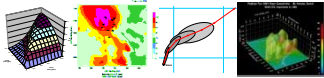


Process Analysis

List of CPA variables

CB4	CB05	SAPRC99	Description
Ozone and Oxidant Production and Loss			
OxProd	OxProd	OxProd	Production of Ox = Ozone + NOy-NO
OxLoss	OxLoss	OxLoss	Destruction of Ox
PO3_net	PO3_net	PO3_net	Net ozone produced
PO3_VOCsns	PO3_VOCsns	PO3_VOCsns	Net ozone produced under VOC sensitive conditions
PO3_NOxsns	PO3_NOxsns	PO3_NOxsns	Net ozone produced under NOx sensitive conditions
PH2O2_PHN3	PH2O2_PHN3	PH2O2_PHN3	Ratio of H ₂ O ₂ produced / HNO ₃ produced. Greater than 0.35 means NOx sensitive ozone production
O3_dest	O3_dest	O3_dest	Ozone destruction by chemical reactions
Radical Initiation			
OH_new	OH_new	OH_new	New OH produced (initiated)
HO2_new	HO2_new	HO2_new	New HO ₂ produced
HOx_new	HOx_new	HOx_new	New HOx (HOx = OH+HO ₂) produced
newOH_O1D	newOH_O1D	newOH_O1D	Production of OH from ozone photolysis
newOH_HONO	newOH_HONO	newOH_HONO	Production of OH from HONO photolysis
nOH_O3_OLE	nOH_O3_OLE	nOH_O3_OLE	Production of OH from ozone-alkene reactions
nwHO2_HCHO	nwHO2_HCHO	nwHO2_HCHO	Production of HO ₂ from formaldehyde photolysis
RO2_new	RO2_new	RO2_new	New RO ₂ produced
Radical Propagation			
OHw_CO	OHw_CO	OHw_CO	OH reacted with carbon monoxide
OHw_CH4	OHw_CH4	OHw_CH4	OH reacted with methane
OHw_PAR	OHw_ETHA	OHw_ALK1	OH reacted with alkanes
	OHw_PAR	OHw_ALK2	
		OHw_ALK3	
		OHw_ALK4	
		OHw_ALK5	
OHw_TOL	OHw_TOL	OHw_ARO1	OH reacted with toluene and mono-substituted aromatics
OHw_XYL	OHw_XYL	OHw_ARO2	OH reacted with xylenes and poly-substituted aromatics
OHw_ETH	OHw_ETH	OHw_ETHE	OH reacted with ethane
OHw_OLE	OHw_OLE	OHw_OLE1	OH reacted with terminal alkenes (R-HC=CH ₂ , e.g. propene)
	OHw_IOLE	OHw_OLE2	OH reacted with internal alkenes (R-HC=CH-R, e.g. 2-butene)
OHw_ISOP	OHw_ISOP	OHw_ISOP	OH reacted with isoprene
	OHw_TERP	OHw_TERP	OH reacted with terpenes
OHw_all_HC	OHw_all_HC	OHw_all_HC	OH reacted with all organic compounds (including CO)
ISOPwOx	ISOPwOx	ISOPwOx	Isoprene reacted with O ₃ , NO ₃ and O(³ P)
	TERPwOx	TERPwOx	Terpenes reacted with O ₃ , NO ₃ and O(³ P)
OH_rctd	OH_rctd	OH_rctd	Total OH reacted
HO2_rctd	HO2_rctd	HO2_rctd	Total HO ₂ reacted

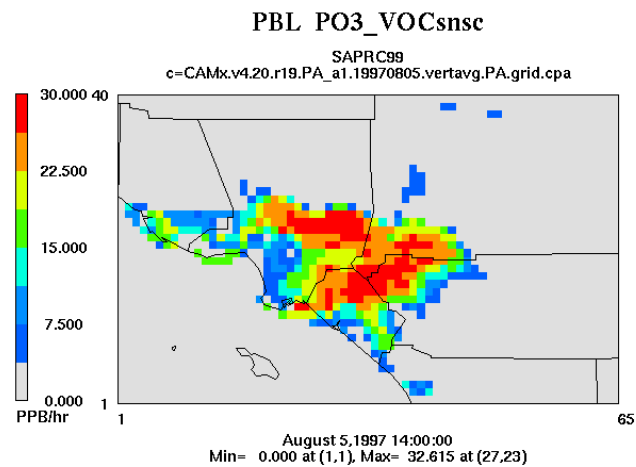
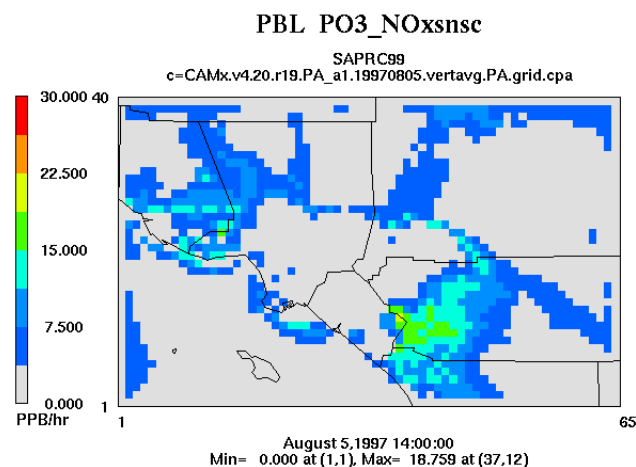
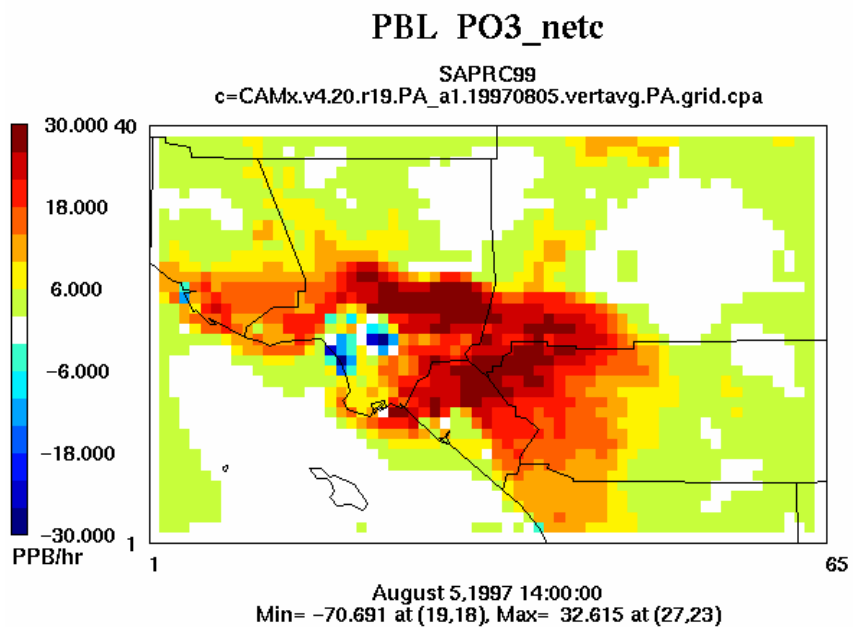
HOx_rctd	HOx_rctd	HOx_rctd	Total HOx reacted
RO2_rctd	RO2_rctd	RO2_rctd	Total RO ₂ reacted
OHfromHO2	OHfromHO2	OHfromHO2	OH produced from reactions of HO ₂
Y_OHperHO2	Y_OHperHO2	Y_OHperHO2	Yield of OH per HO ₂ reacted (= OHfromHO2 / HO ₂ _rctd)
Radical Termination and HOx Chain Length			
OH_term	OH_term	OH_term	OH terminated
HO2_term	HO2_term	HO2_term	HO ₂ terminated
HOx_term	HOx_term	HOx_term	HOx terminated
RO2_term	RO2_term	RO2_term	RO ₂ terminated
HOx_CL	HOx_CL	HOx_CL	HOx chain length (= HOx_rctd / (2 x HOx_new))
Formaldehyde Production			
HCHOp_eth	HCHOp_eth	HCHOp_ethe	Formaldehyde produced from ethene
HCHO_ole	HCHO_ole	HCHO_ole1	Formaldehyde from terminal alkenes (R-HC=CH ₂ , e.g. propene) in the first generation of products
	HCHO_iole	HCHO_ole2	Formaldehyde from internal alkenes (R-HC=CH-R, e.g. 2-butene) in the first generation of products
	HCHO_terp	HCHO_terp	Formaldehyde from terpenes in the first generation of products
HCHOp_isop	HCHOp_isop	HCHOp_isop	Formaldehyde from isoprene in the first generation of products
HCHOp_ispd	HCHOp_ispd	HCHOp_ispd	Formaldehyde from isoprene daughter products (isoprod, methacrolein and methylvinylketone)
HCHOp_Tot	HCHOp_Tot	HCHOp_Tot	Total formaldehyde produced
NOy Reactions			
HNO3_OHNO2	HNO3_OHNO2	HNO3_OHNO2	Nitric acid produced from OH reacting with NO ₂
HNO3_NO3HC	HNO3_NO3HC	HNO3_NO3HC	Nitric acid produced from NO ₃ reacting with organics
HNO3_N2O5	HNO3_N2O5	HNO3_N2O5	Nitric acid produced from N ₂ O ₅ reacting with water
PANprodNet	PANprodNet	PANSprndNet	Net PAN produced (sum of several for SAPRC99)
PANlossNet	PANlossNet	PANSlosNet	Net PAN destroyed (sum of several for SAPRC99)
RNO3_prod	RNO3_prod	RNO3prod	Organic nitrates (RNO ₃) produced
NOxrecycl	NOxrecycl	NOxrecycl	Nitrates (HNO ₃ and RNO ₃) recycled to NOx
NOw_HO2	NOw_HO2	NOw_HO2	NO reacted with HO ₂ (forming NO ₂)
NOw_RO2s	NOw_RO2s	NOw_RO2s	NO reacted with RO ₂ (forming NO ₂)
NOw_RCO3s	NOw_RCO3s	NOw_RCO3s	NO reacted with RCO ₃ (forming NO ₂)
Photolysis			
J_NO2	J_NO2	J_NO2	NO ₂ photolysis rate
J_O3O1D	J_O3O1D	J_O3O1D	O ₃ photolysis rate to O(¹ D) atoms
J_Cld_Adj	J_Cld_Adj	J_Cld_Adj	Adjustment factor
Radical Concentrations			
OH	OH	OH	OH radical concentration
HO2	HO2	HO2	HO ₂ radical concentration
NO3	NO3	NO3	NO ₃ radical concentration
N2O5	N2O5	N2O5	N ₂ O ₅ concentration

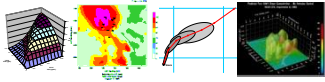


Process Analysis

Example of PA/CPA

Net ozone production (left), and NO_x-sensitive (right top) and VOC-sensitive (right bottom) ozone production

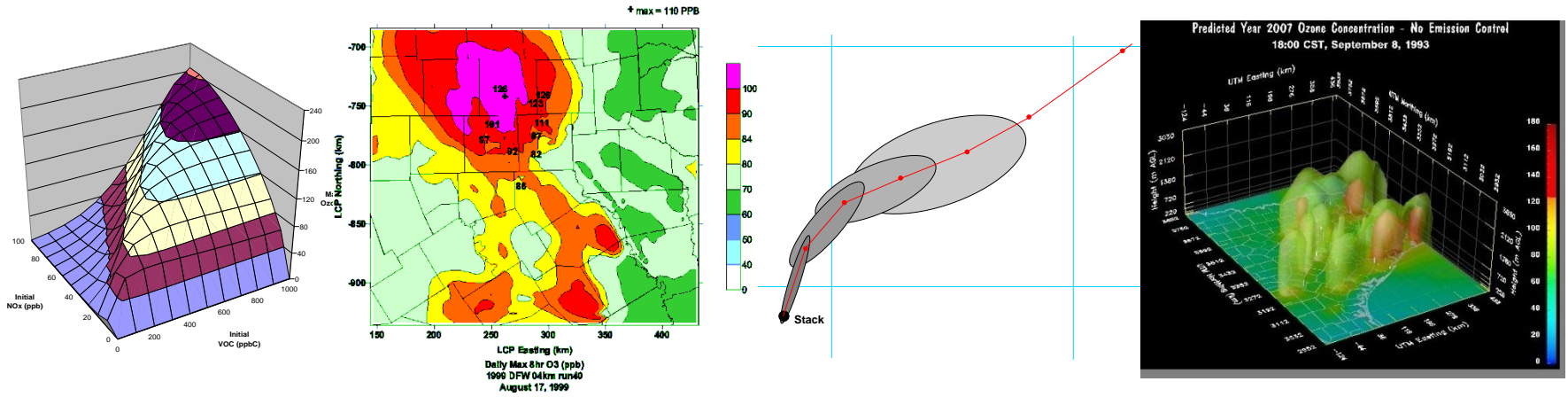


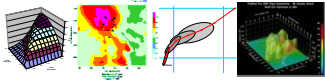


Process Analysis

- PA input
 - Namelist control parameters (CAMx.in)
- PA output
 - IPR files for user-defined PA sub-domain (CAMx binary)
 - IRR files for user-defined PA sub-domain (CAMx binary)
 - Grid-specific CPA files (CAMx binary)
- Postprocessors
 - Ext_ipr and ext_irr generate comma-delimited text files
 - Reports individual or cell-aggregated rates
 - Excel macro can generate time-series of IPR rates
 - Needs to be updated for later versions of MS Office

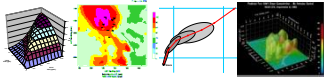
Reactive Tracers





Reactive Tracers

- Reactive Tracers (RTRAC)
 - Independent reactive gas and/or inert particle tracers
 - e.g., modeling *air toxics*
 - Assumes reactive species have minimal impact on photochemistry
 - Each tracer can be “tagged” for source apportionment
 - Tracers operate in parallel to the CAMx host model
 - Tracer decay/production driven by modeled oxidant levels and photolysis rates
 - “Recursive tracers” allows for several generations of products: *secondary toxics*
 - Can use IRON PiG and sampling grid for “fenceline” dispersion calculations



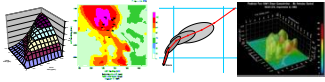
Reactive Tracers

RTRAC Chemistry Parameters File

```

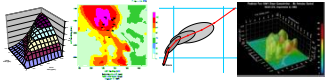
CAMx Version      |VERSION5.2
Description       |MATES Toxics for CRC project A-42
No of gas tracers |6
No of aero tracers|8
No photolysis rxns|4
No thermal rxns  |12
Gas Tracers
No.  Name      P/S  SNAM  lower bnd    H-law    T-fact    Diffrat    Reactvty    Rscale
  1  PACET     PRIM  SNAM  1.00E-12    6.30e+03 -6492.    1.56        0.0         1.0
  2  HCHO      PRIM  SNAM  1.00E-12    6.30e+03 -6492.    1.29        0.0         1.0
  3  BENZ      PRIM  SNAM  1.00E-12    1.80e-01  0.        2.08        0.0         1.0
  4  BUTA      PRIM  SNAM  1.00E-12    1.00e-02  0.        1.73        0.0         1.0
  5  SACET     SEC   ALD2  1.00E-12    6.30e+03 -6492.    1.56        0.0         1.0
  6  SFORM     SEC   FORM  1.00E-12    6.30e+03 -6492.    1.29        0.0         1.0
Aero Tracers
No.  Name      lower bnd    Density    Low cut    Upper cut
  7  DSLF      1.00E-09     1.5         0.10       2.50
  8  ECF       1.00E-09     1.5         0.10       2.50
  9  CRF       1.00E-09     1.5         0.10       2.50
 10  CR6F      1.00E-09     1.5         0.10       2.50
 11  DSLC      1.00E-09     1.5         2.50       10.00
 12  ECC       1.00E-09     1.5         2.50       10.00
 13  CRC       1.00E-09     1.5         2.50       10.00
 14  CR6C      1.00E-09     1.5         2.50       10.00
Photolysis reactions
Toxic   Rxn #    Factor
PACET   45       1.0
SACET   45       1.0
HCHO    39       1.6
SFORM   39       1.6
Thermal reactions and rates
Toxic   React A (ppm-lmin-1)    Ea (K)    B    Tref
PACET   OH    8.2015E+03 -3.1099E+02    0.0  300.0
PACET   NO3   2.0689E+03  1.8599E+03    0.0  300.0
HCHO    OH    1.6699E+03 -6.4815E+02    2.0  300.0
HCHO    NO3   4.1377E+03  2.5161E+03    0.0  300.0
BENZ    OH    3.6944E+03  1.9978E+02    0.0  300.0
BUTA    OH    2.1871E+04 -4.4787E+02    0.0  300.0
BUTA    O3    4.8766E+01  2.5000E+03    0.0  300.0
BUTA    NO3   2.1871E+04  1.4890E+03    0.0  300.0
SACET   OH    8.2015E+03 -3.1099E+02    0.0  300.0
SACET   NO3   2.0689E+03  1.8599E+03    0.0  300.0
SFORM   OH    1.6699E+03 -6.4815E+02    2.0  300.0
SFORM   NO3   4.1377E+03  2.5161E+03    0.0  300.0

```



Reactive Tracers

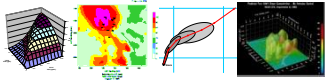
- New chemistry capability: Reactive Tracer Chemical Mechanism Compiler (RTCMC)
 - Reads external mechanism from text file
 - Builds mechanism for LSODE solver at model startup
 - Performs independent chemical integration
 - Complex non-linear interactions among tracers and CAMx “core” species
 - Adds mechanism flexibility
 - Removes need to code mechanism by hand
 - Tracer apportionment possible, depends on chemical complexity



Reactive Tracers

RTCMC Chemistry Parameters File

```
#Control
  rate_species_units = 'ppm'
  rate_time_units = 'min'
  solver = 'dlsode'
  Jacobian = 'numeric'
#Species, Type, Ambient, Tolerance, deposition vel, wet scav
O3      A      1.0      1.0E-12    0.0      0.0
OH      A      1.0      1.0E-12    0.0      0.0
ATRAC   F      1.0      1.0E-12    0.010    0.0
BTRAC   F      1.0      1.0E-12    0.001    0.0
CTRAC   F      1.0      1.0E-12    0.020    0.0
DTRAC   F      1.0      1.0E-12    0.001    0.0
ETRAC   F      1.0      1.0E-12    0.030    0.0
FTRAC   F      1.0      1.0E-12    0.001    0.0
#Table
  0          0.      15.      30.      45.      60.      75.
    80.      86.      87.      88.
  1 4.1590E-04 4.0600E-04 3.7540E-04 3.27E-04 2.6040E-04 9.4990E-05 2.9930E-
05 4.8590E-06 8.3030E-08 1.0000E-09
#Equations
  1 [ATRAC] -> (2.0) [BTRAC] ; 0 0.000E-00
  2 (1.5) [CTRAC] + [OH] -> (0.5) [DTRAC] ; 1 4.2000E+04
  3 [ETRAC] + [O3] -> [FTRAC] ; 1 1.8000E-02
```



Reactive Tracers

- **RTRAC input**
 - Namelist control parameters (CAMx.in)
 - Chemistry parameters file (text)
 - Receptor definition file (text)
 - Restart files (CAMx binary)
 - Point/gridded emission files (CAMx binary)
 - IC/BC files (CAMx binary)
- **RTRAC output**
 - Master/fine grid instantaneous files (CAMx binary)
 - Grid-specific average files (CAMx binary)
 - IRON PiG sampling file (CAMx binary)
 - Receptor output file (text)