INVESTIGATION OF VOC REACTIVITY EFFECTS USING EXISTING REGIONAL AIR QUALITY MODELS

SUMMARY OF PROGRESS
MAY 15-16, 2002

BY

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OBJECTIVES

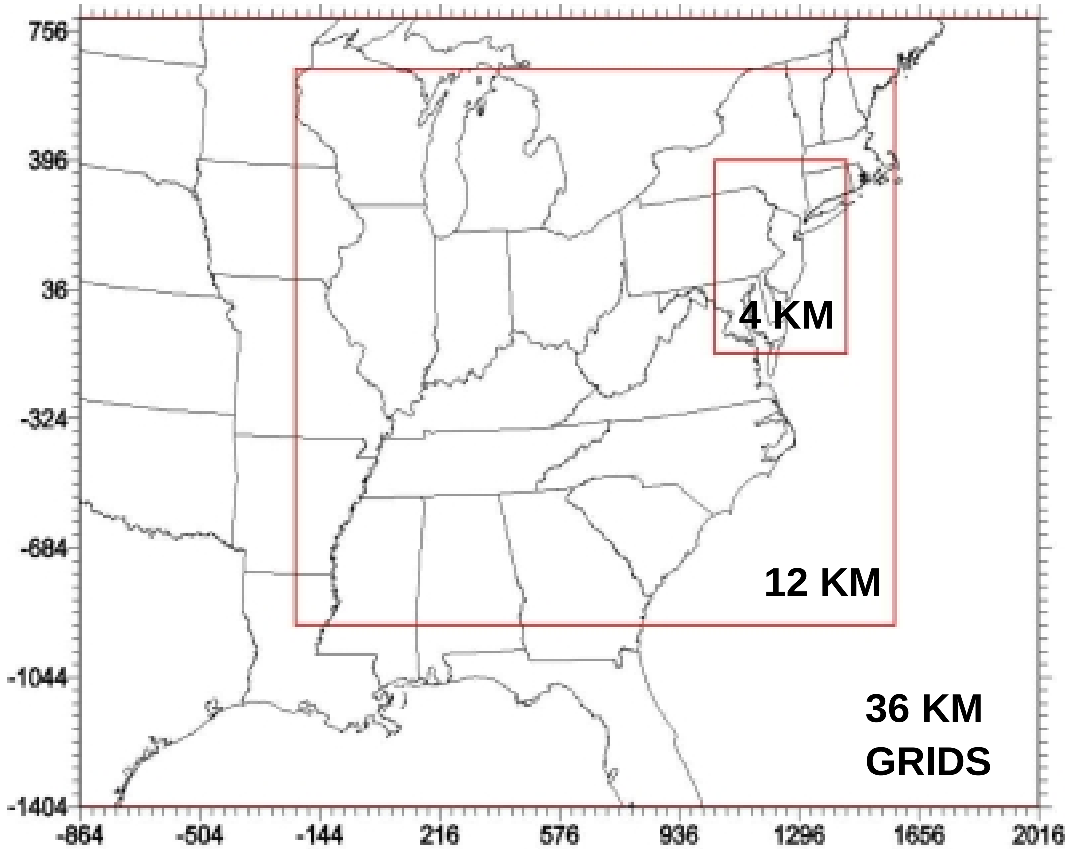
ASSESS VOC REACTIVITY EFFECTS USING AN EXISTING REGIONAL MODELING DATABASE REPRESENTING THE EASTERN U.S.

ASSESS RELATIVE INCREMENTAL OZONE IMPACTS OF VOC MODEL SPECIES WITH RESPECT TO:

- VARIATION WITHIN THE MODELING DOMAIN
- DERIVATION OF VARIOUS REACTIVITY METRICS
- COMPARISON WITH REACTIVITIES CALCULATED USING EKMA MODELS
- PREDICTIONS OF EFFECTS OF SELECTED LARGE SCALE SUBSTITUTIONS

ASSESS APPROACHES FOR DERIVING A GENERAL REACTIVITY SCALE REPRESENTING REGIONAL O_3 IMPACTS

CRC-NARSTO MODELING DATABASE



MODEL:	CAMx VERSION 3.01 WITH DDM
EPISODE DATES:	JULY 7-15, 1995 (DATA FOR 11th-14th USED IN ASSESSMENT)
EMISSIONS:	EPA NET96
MET DATA:	MM5
MECHANISM:	UPDATED CB4 (ETHANE ADDED)

(Analysis of fine grid data still underway. Current analysis uses 4 and 12 km data averaged into the 36 KM grids.)

CARBON BOND 4 MECHANISM

ADVANTAGES

- LEAST EXPENSIVE TO USE FOR INITIAL STUDY
- WIDELY USED
- REPRESENTS MOST OF THE IMPORTANT CLASSES OF REACTIVE VOCs

DISADVANTAGES

- OUT-OF-DATE (DEVELOPED IN1989)
- HIGHLY CONDENSED. CANNOT BE USED TO ASSESS MOST INDIVIDUAL VOCs
- INAPPROPRIATE OR NO REPRESENTATION OF SOME IMPORTANT TYPES OF VOCs:
  - INTERNAL ALKENES (only products represented; effects of initial OH and O_3 reaction ignored)
  - TOLUENE (reactivity characteristics significantly different than predicted using current mechanisms)
  - RADICAL INHIBITING VOCs (not represented)
- MAY BE MORE SENSITIVE TO RADICAL EFFECTS THAN CURRENT MECHANISM

NEVERTHELESS, CB4 PROBABLY SUITABLE FOR INITIAL QUALITATIVE ASSESSMENT OF VARIABILITY OF REACTIVITY WITH MODELING DOMAIN

PHASE1: DDM CALCULATIONS

DECOUPLED DIRECT METHOD (DDM) USED TO CALCULATE SENSITIVITIES OF SURFACE O_3 CONCENTRATIONS TO CHANGES IN EMISSIONS

SENSITIVITIES CALCULATED AS FUNCTION OF TIME AND SPACE AND OUTPUT AS HOURLY AVERAGES FOR ALL GROUND LEVEL CELLS.

FIRST DDM CALCULATION:

- SENSITIVITY TO TOTAL VOC AND NO_x EMISSIONS
- RESULTS GIVE PPM O_3 CHANGE RESULTING FROM 100% CHANGE IN EMISSIONS (IF LINEAR)

SECOND DDM CALCULATION:

- SENSITIVITY TO SURFACE EMISSIONS OF CO AND 9 VOC MODEL SPECIES VARIED.
- SAME TIME AND SPACE DISTRIBUTION AS TOTAL ANTHROPOGENIC VOC
- RESULTS GIVE PPM O_3 CHANGE FROM 100% CHANGE IN ANTHROPOGENIC VOC CARBON EMISSIONS AS THE SPECIES (IF LINEAR)

THE SENSITIVITIES OF O_3 TO MODEL SPECIES EMISSIONS ARE THE SAME AS THE **INCREMENTAL REACTIVITIES** OF THESE MODEL SPECIES

CARBON BOND 4 MODEL SPECIES WHOSE OZONE SENSITIVITIES WERE DETERMINED

SPECIES	APPROXIMATELY REPRESENTATIVE OF
PAR	C_4 - C_6 ALKANES
ETH	ETHENE (EXPLICIT)
OLE	PROPENE (PRIMARILY)
TOL	NO SPECIFIC COMPOUND. MAY BE INDICATIVE OF COMPOUNDS WITH VERY NO_x SENSITIVE REACTIVITIES (E.G., PHENOLS, STYRENES)
XYL	XYLENES
FORM	FORMALDEHYDE (EXPLICIT)
ALD2	ACETALDEHYDE (EXPLICIT)
ETOH	ETHANOL (EXPLICIT)
ETHA	ETHANE (ADDED FOR THIS STUDY)
CO	CARBON MONOXIDE (EXPLICIT)

OZONE IMPACT METRICS USED IN INITIAL ANALYSIS

IMPACTS BASED ON EFFECTS OF SPECIES ON DAILY MAXIMUM 1-HOUR AND 8-HOUR AVERAGE O_3

FOLLOWING CELLS NOT INCLUDED IN ANALYSIS:

- CELLS WHERE MAXIMUM O_3 LESS THAN CUTOFF
  - 80 PPB CUTOFF FOR 1-HOUR AVERAGE
  - 60 PPB CUTOFF FOR 8-HOUR AVERAGE
- CELLS WITH ZERO ANTHROPOGENIC EMISSIONS (I.E., CELLS OVER WATER)

REACTIVITIES DERIVED RELATIVE TO REACTIVITIES OF TOTAL ANTHROPOGENIC VOC EMISSIONS MIXTURE (BASE ROG)

- GIVES BENEFITS OF REDUCING A SINGLE VOC COMPARED TO REDUCING ALL VOCs EQUALLY
- BASE ROG SENSITIVITIES DERIVED FROM SENSITIVITIES OF COMPONENT SPECIES
- BASE ROG COMPOSITION DERIVED FROM EPA REGIONAL EMISSIONS DATABASE
- TOTAL VOC SENSITIVITIES COULD NOT BE USED BECAUSE THEY INCLUDED BIOGENIC VOCs

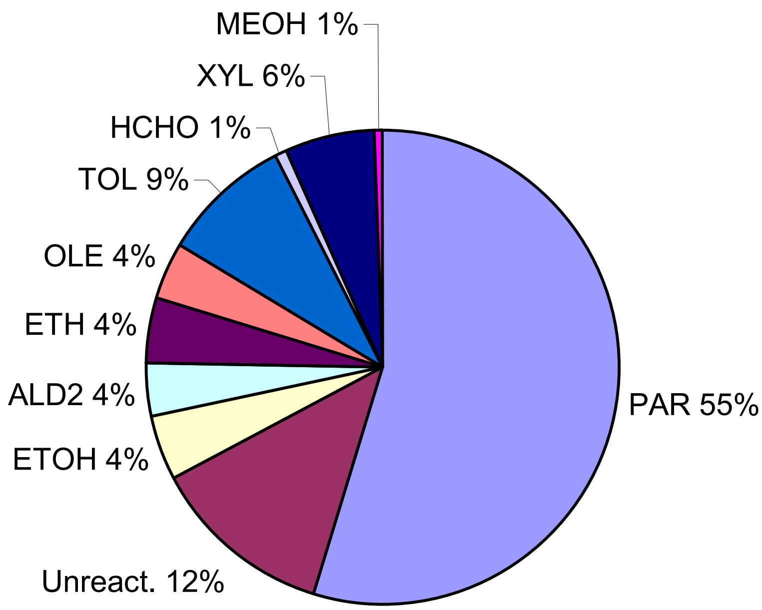
4 GLOBAL RELATIVE REACTIVITY METRICS DERIVED

- MINIMUM SUBSTITUTION ERROR (2 METHODS)
- REGIONAL MIR
- REGIONAL MAXIMUM O_3

COMPOSITION OF BASE ROG MIXTURE USED TO DERIVE RELATIVE REACTIVITIES

CB4 MODEL SPECIES:

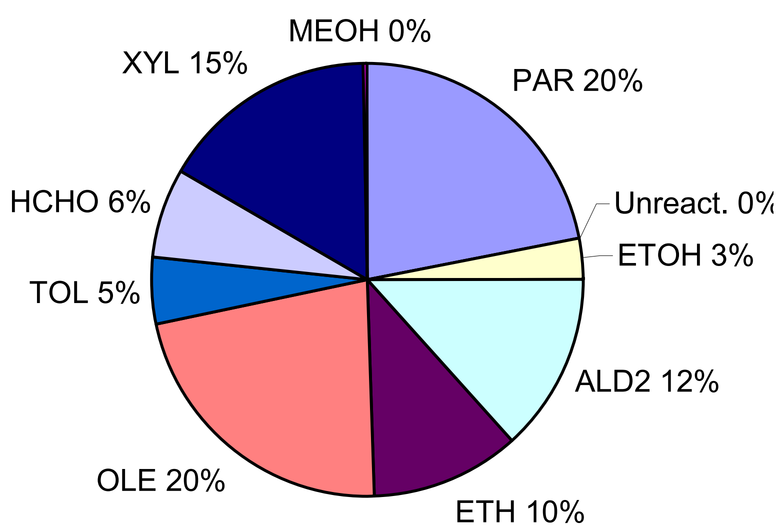
CARBON BASIS



CB4 MODEL SPECIES:

REACTIVITY BASIS

(EKMA MIR SCALE)



(BASED ON NEW EMISSIONS ASSIGNMENTS 5/02)

GLOBAL RELATIVE REACTIVITY METRIC #1

MINIMUM SUBSTITUTION ERROR: BASE ROG FOR SPECIES

DEFINITION

RELATIVE REACTIVITY TO MINIMIZE SUBSTITUTION ERROR FROM REACTIVITY-BASED SUBSTITUTION OF THE BASE ROG FOR THE MODEL SPECIES

SUBSTITUTION ERROR =

$$\Sigma_{cells} [RR(Species) \cdot IR_{cell}(Base\ ROG) - IR_{cell}(Species)]^2$$

ADVANTAGES

- WEIGHS CELLS THAT ARE SENSITIVE TO VOCs MORE HIGHLY WHILE TAKING THE MANY CELLS WITH LOWER SENSITIVITIES INTO ACCOUNT
- REPRESENTATIVE OF STRATEGIES INVOLVING REPLACING HIGHLY REACTIVE VOCs WITH VOCs OF AVERAGE REACTIVITY
- REACTIVITIES OF MIXTURES ARE LINEAR SUMS OF REACTIVITIES OF COMPONENTS

DISADVANTAGES

- MAY NOT OPTIMALLY WEIGH CONTRIBUTIONS OF DIFFERENT TYPES OF REGIONS
- NOT A PARTICULARLY REALISTIC SUBSTITUTION FOR EXEMPTION ISSUES

GLOBAL RELATIVE REACTIVITY METRIC #2

MINIMUM SUBSTITUTION ERROR: SPECIES FOR BASE ROG

DEFINITION

RELATIVE REACTIVITY TO MINIMIZE SUBSTITUTION ERROR FROM REACTIVITY-BASED SUBSTITUTION OF THE MODEL SPECIES FOR THE BASE ROG

SUBSTITUTION ERROR =

$$\Sigma_{cells}\ [IR_{cell}(\text{Base ROG}) - IR_{cell}(\text{Species})/RR(\text{Species})]^2$$

ADVANTAGES

- WEIGHS CELLS THAT ARE SENSITIVE TO VOCs MORE HIGHLY WHILE TAKING THE MANY CELLS WITH LOWER SENSITIVITIES INTO ACCOUNT
- REPRESENTATIVE OF STRATEGIES INVOLVING SUBSTITUTIONS OF CURRENT EMISSIONS WITH LOW REACTIVITY VOCs

DISADVANTAGES

- MAY NOT OPTIMALLY WEIGH CONTRIBUTIONS OF DIFFERENT TYPES OF REGIONS
- REACTIVITIES OF MIXTURES ARE NOT LINEAR SUMS OF THOSE OF COMPONENTS
- DIVERGENT RESULTS OBTAINED FOR VOCs WHOSE REACTIVITIES ARE SCATTERED AROUND ZERO

GLOBAL RELATIVE REACTIVITY METRIC #3

REGIONAL MAXIMUM INCREMENTAL REACTIVITY

DEFINITION

USE REACTIVITIES AT THE LOCATION WHERE THE INCREMENTAL REACTIVITY OF THE BASE ROG AT THE TIME OF THE O_3 MAXIMUM IS THE HIGHEST

ADVANTAGES

- COMPARABLE TO THE WIDELY-USED CARTER (1994) MIR SCALE
- REPRESENTATIVE OF IMPACTS IN REGIONS MOST SENSITIVE TO ANTHROPOGENIC VOC CONTROLS

DISADVANTAGES

- NOT A TRUE GLOBAL METRIC. DERIVED FROM IMPACTS IN ONLY ONE TYPE OF REGION
- REPRESENTS ONLY A SMALL FRACTION CELLS IN MODELING DOMAIN
- DOES NOT REPRESENT IMPACTS IN CELLS WITH THE HIGHEST O_3
- DOES NOT REPRESENT IMPACTS IN THE MANY NO_x-LIMITED CELLS

GLOBAL RELATIVE REACTIVITY METRIC #4

REGIONAL MAXIMUM OZONE REACTIVITY

DEFINITION

USE REACTIVITIES AT THE TIME AND LOCATION OF THE DOMAIN-WIDE O_3 MAXIMUM

ADVANTAGES

- ADDRESSES NEEDS TO REDUCE PEAK O_3, WHICH IS OF REGULATORY INTEREST
- SIMPLEST METRIC TO IMPLEMENT

PROBLEMS

- NOT A TRUE GLOBAL METRIC. DERIVED FROM IMPACTS IN ONLY ONE LOCATION
- NOT NECESSARILY REPRESENTATIVE OF “MOIR” CONDITIONS AS DEFINED BY CARTER (1994)
- REACTIVITY CHARACTERISTICS OF THE HIGHEST O_3 CELL CAN VARY SIGNIFICANTLY DEPENDING ON THE EPISODE
- THE DOMAIN-WIDE MAXIMUM O_3 MAY BE INSENSITIVE TO ANTHROPOGENIC VOCs

EKMA REACTIVITY SCALES FOR COMPARISON WITH REGIONAL MODEL REACTIVITIES

SAME EKMA SCENARIOS AND CALCULATION METHODS AS USED TO DERIVE “CARTER” REACTIVITY SCALES (CARTER, 1994; CARTER, 2000)

SAME VERSION OF CB4 AS USED IN THE CAMx REGIONAL MODEL CALCULATIONS

RELATIVE REACTIVITIES USE SAME BASE ROG MIXTURE AS USED FOR REGIONAL METRICS

MIR SCALE

- AVERAGES OF INCREMENTAL REACTIVITIES IN THE SCENARIOS WITH NO_x ADJUSTED TO YIELD MAXIMUM BASE ROG REACTIVITY
- ANALOGOUS TO REGIONAL MIR METRIC

MOIR SCALE

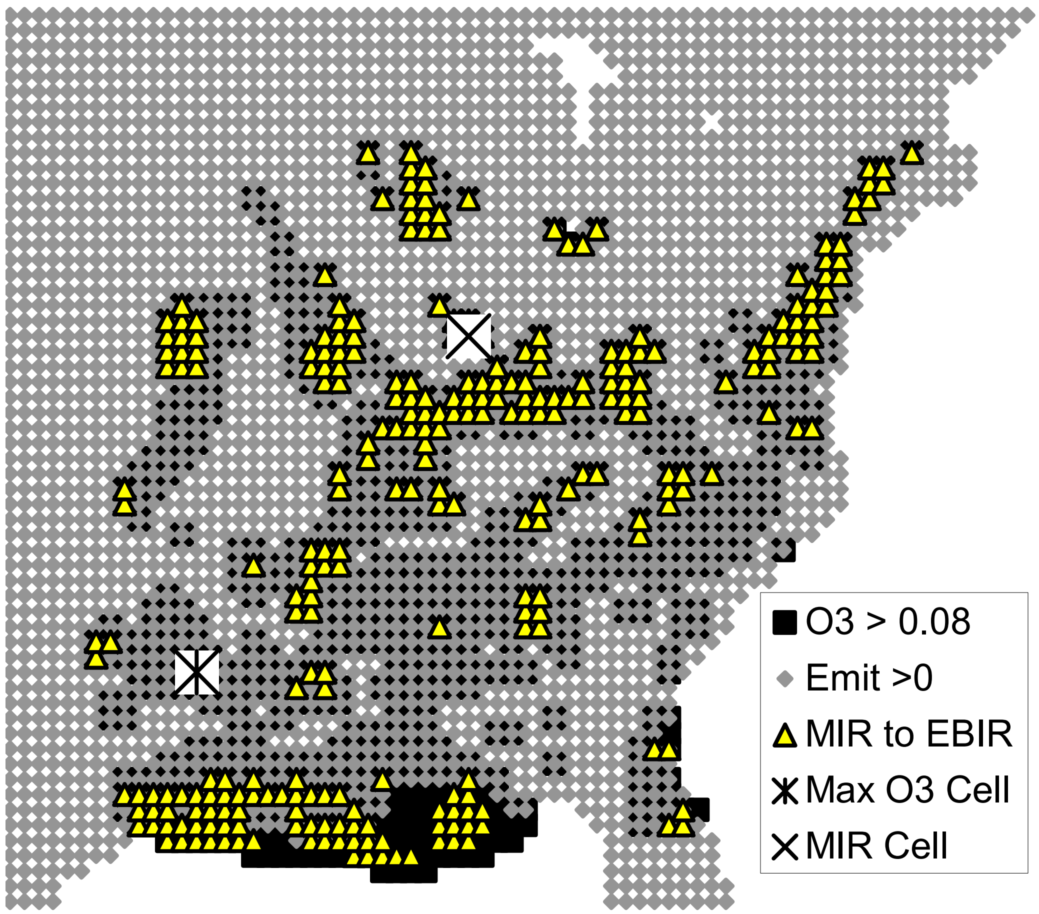
- AVERAGES OF INCREMENTAL REACTIVITIES IN THE SCENARIOS WITH NO_x ADJUSTED TO YIELD MAXIMUM PEAK O_3 CONCENTRATIONS
- **NOT** NECESSARILY ANALOGOUS TO REGIONAL MAXIMUM O_3 METRIC

BASE CASE SCALES

- RELATIVE REACTIVITIES DERIVED TO MINIMIZE SUBSTITUTION ERRORS IN THE BASE CASE (UNADJUSTED NO_x) SCENARIOS
- ANALOGOUS TO MINIMUM SUBSTITUTION ERROR METRICS #1 AND #2 FOR 1-HOUR AVG.

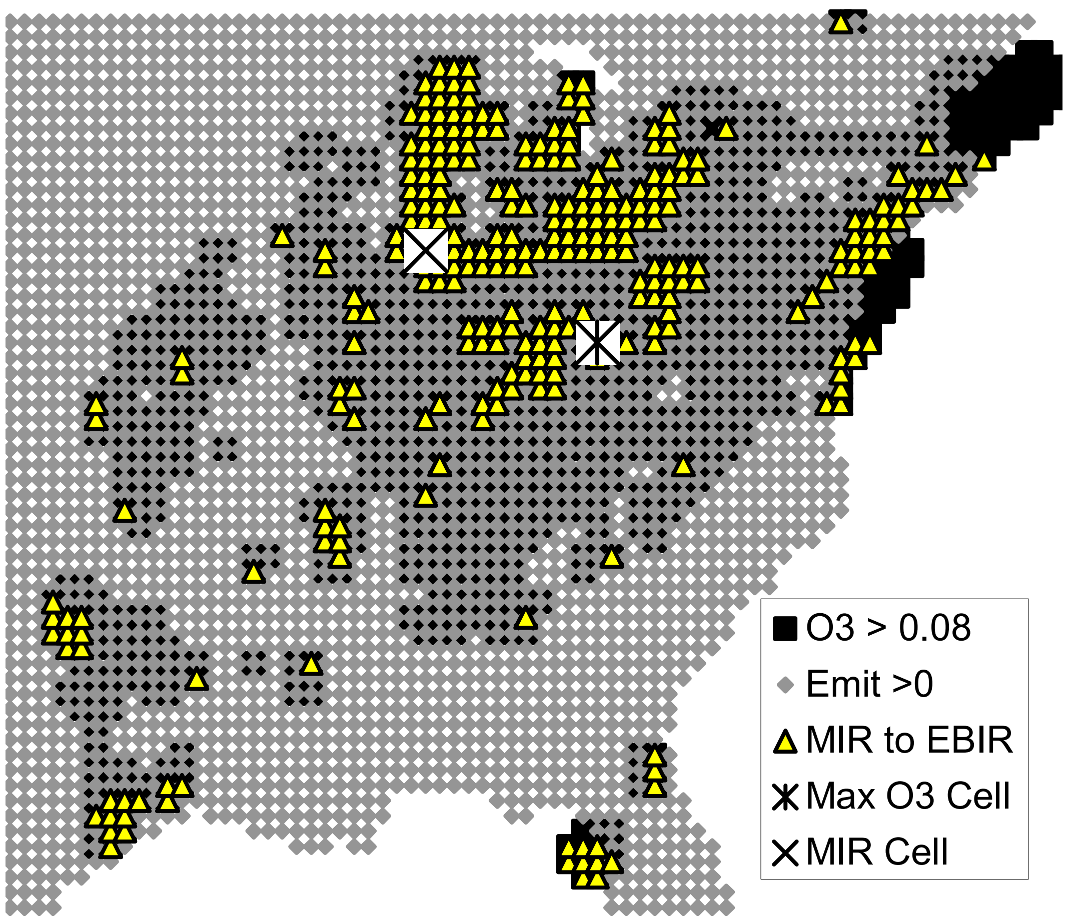
GEOGRAPHICAL DOMAIN FOR MAXIMUM 1-HOUR AVERAGE O_3 AND ANTHROPOGENIC VOC SENSITIVE REGIONS

JULY 11



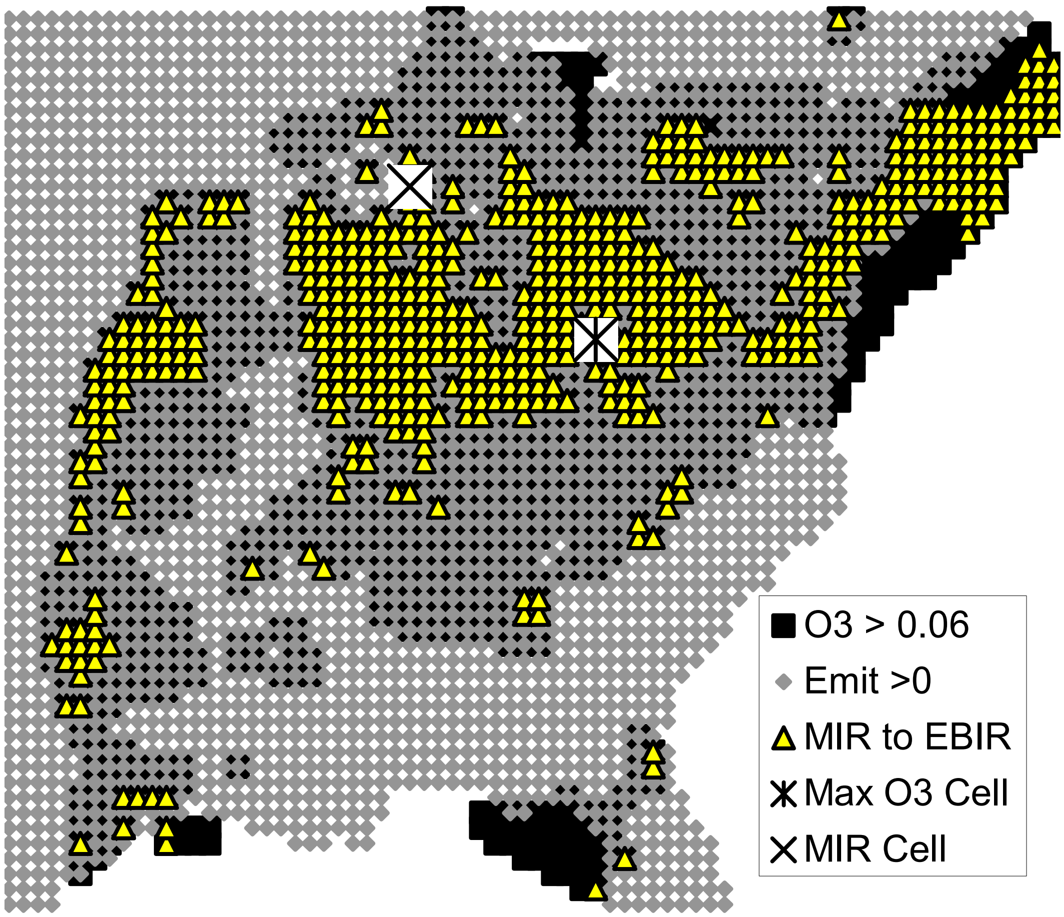
GEOGRAPHICAL DOMAIN FOR MAXIMUM 1-HOUR AVERAGE O_3 AND ANTHROPOGENIC VOC SENSITIVE REGIONS

JULY 14

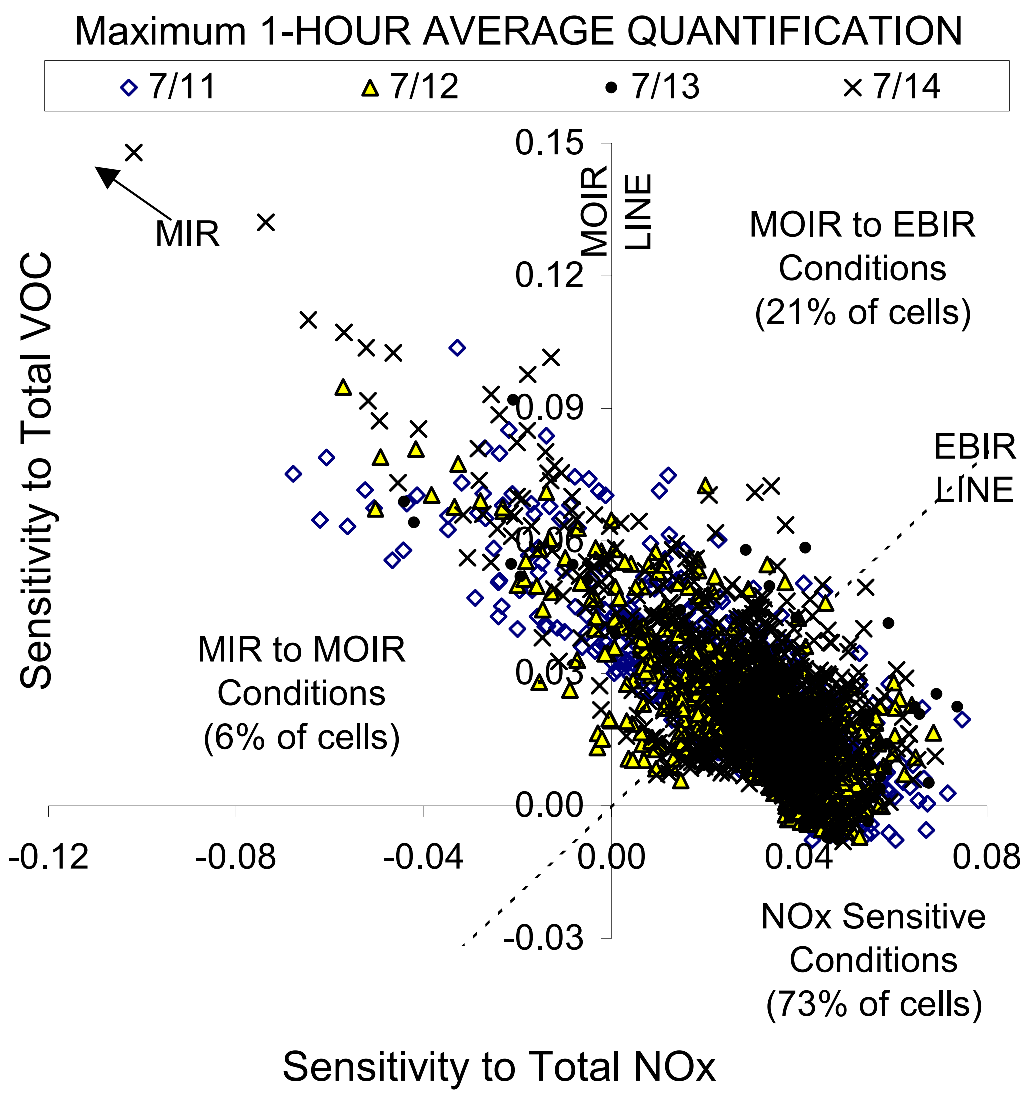


GEOGRAPHICAL DOMAIN FOR MAXIMUM 8-HOUR AVERAGE O_3 AND ANTHROPOGENIC VOC SENSITIVE REGIONS

JULY 14



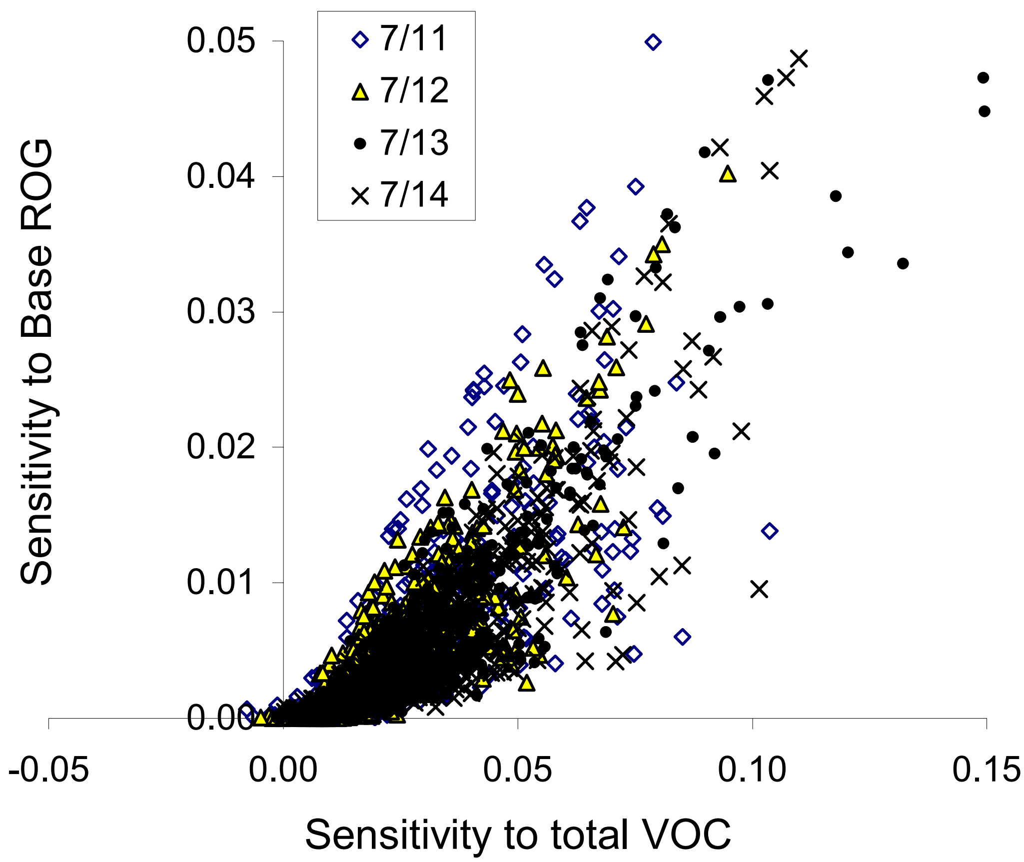
MAXIMUM 1-HOUR AVERAGE OZONE SENSITIVITIES TO VOC AND NO_x



(Cells with Maximum 1-Hour Average O_3 < 80 ppb and with Zero Emissions are Excluded)

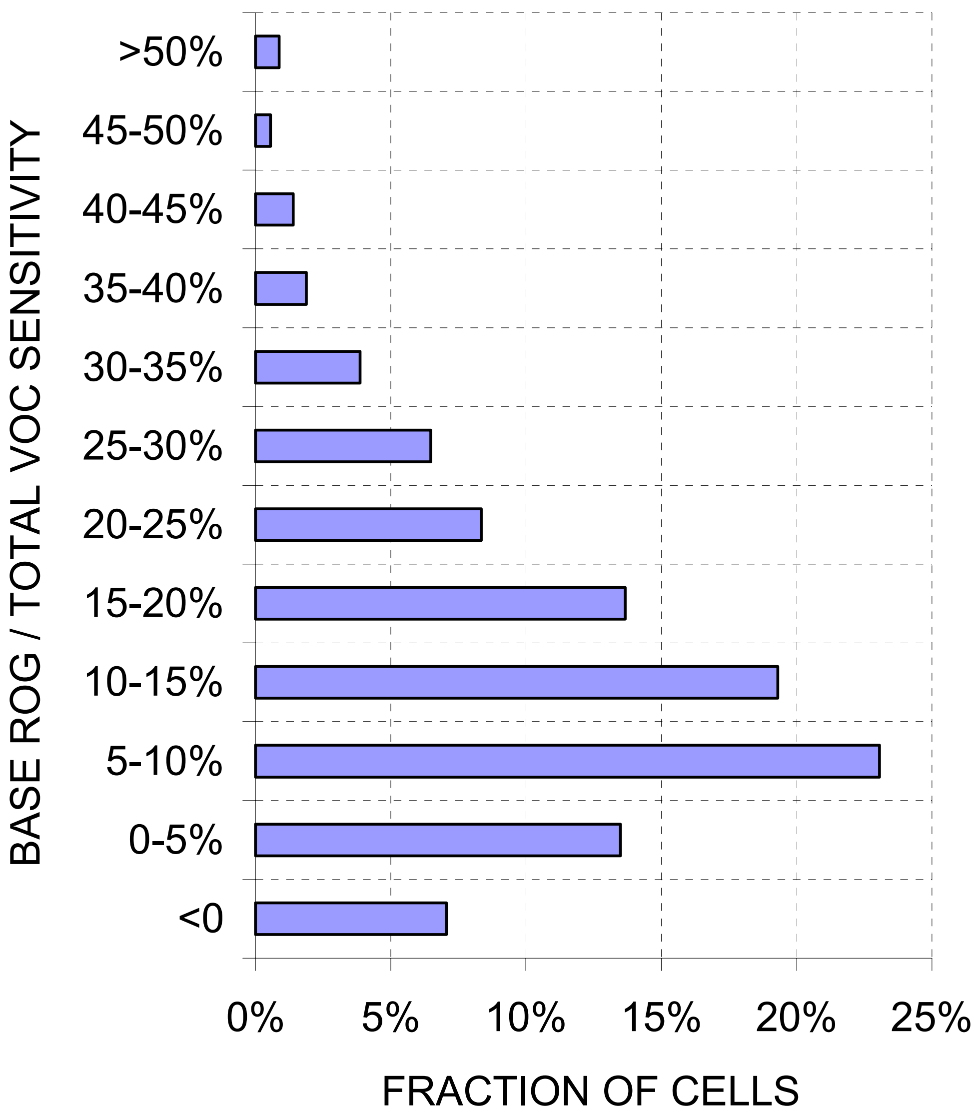
SENSITIVITIES TO BASE ROG
(REPRESENTING ANTHROPOGENIC VOCs)
<u>VS.</u> SENSITIVITIES TO TOTAL VOCs

1-HOUR AVERAGE QUANTIFICATION
ALL CELLS WHERE MAXIMUM 1-HOUR O_3 > 80 PPB



DISTRIBUTION OF BASE ROG (ANTHROPOGENIC) / TOTAL VOC SENSITIVITY RATIO

$$\frac{[O_3 \text{ SENSITIVITY TO BASE ROG}]}{[O_3 \text{ SENSITIVITY TO ALL VOCs}]}$$



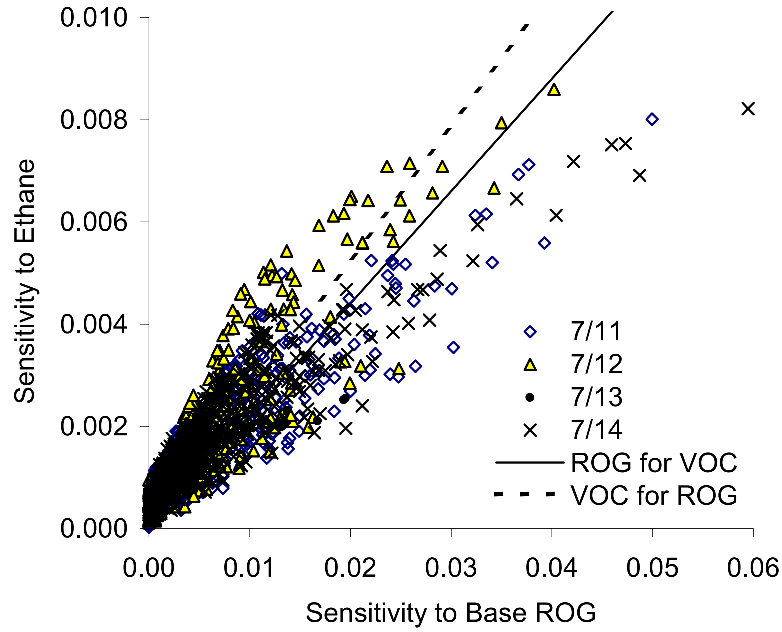
(MAXIMUM 1-HOUR AVERAGE QUANTIFICATION)
Cells with total VOC sensitivity < 0.001 excluded

REACTIVITY CHARACTERISTICS OF EPISODE DAYS

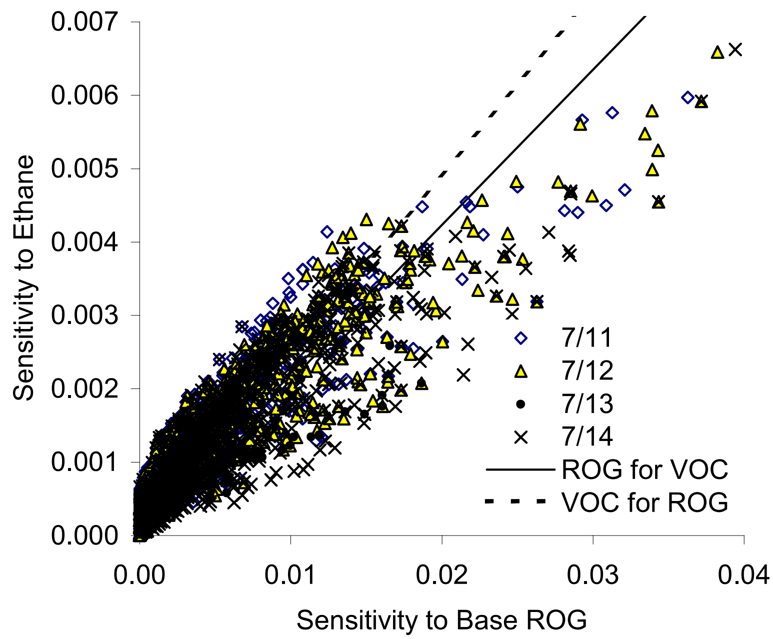
EPISODE DAY	7/11	7/12	7/13	7/14
DOMAIN-WIDE OZONE MAXIMUM (ppb)				
Peak 1-Hr Avg. O_3	165	162	187	175
Peak 8-Hr Avg. O_3	127	126	139	139
HIGH OZONE CELLS				
1-Hr Avg. > 80 ppb	18%	22%	25%	25%
1-Hr Avg. > 120 ppb	1%	1%	2%	4%
8-Hr Avg. > 60 ppb	32%	37%	38%	36%
8-Hr Avg. > 80 ppb	7%	7%	10%	12%
CELLS MORE SENSITIVE TO VOCs THAN NO_x				
1-Hour Avg. Quant.	32%	23%	27%	25%
8-Hour Avg. Quant.	25%	29%	33%	24%

ETHANE VS. BASE ROG SENSITIVITIES

1-HOUR DAILY MAXIMUM O_3

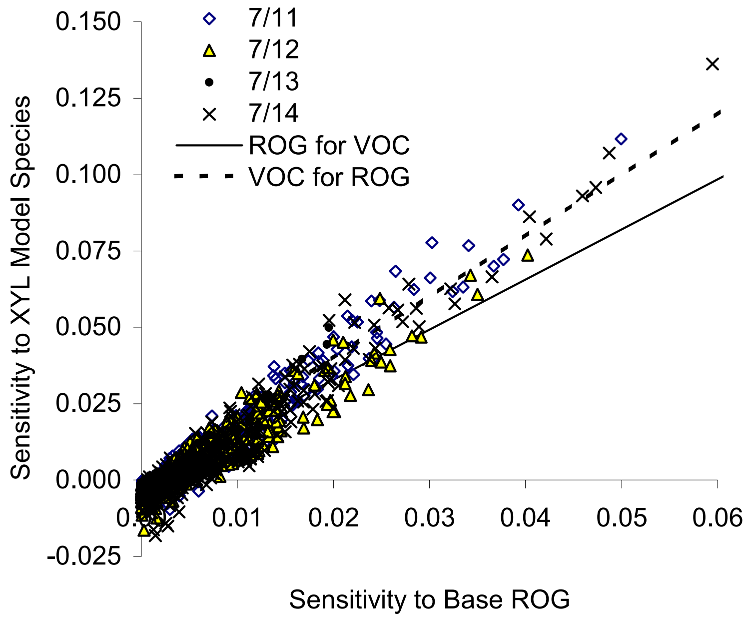


8-HOUR DAILY MAXIMUM O_3

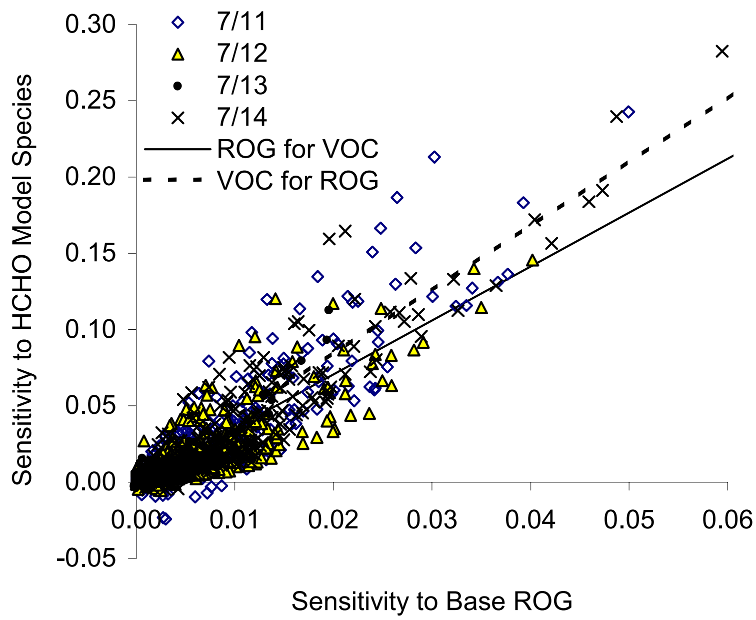


1-HOUR MAXIMUM O_3 SENSITIVITY EXAMPLES

XYLENE VS BASE ROG

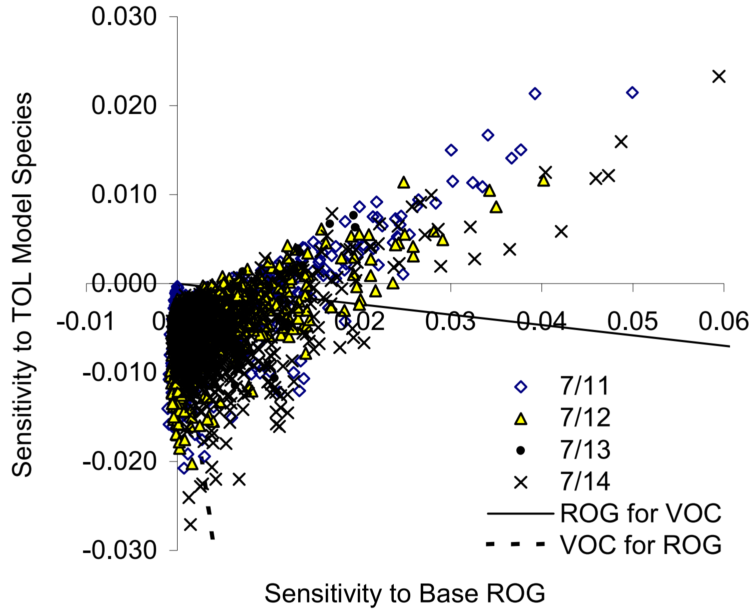


FORMALDEHYDE VS BASE ROG

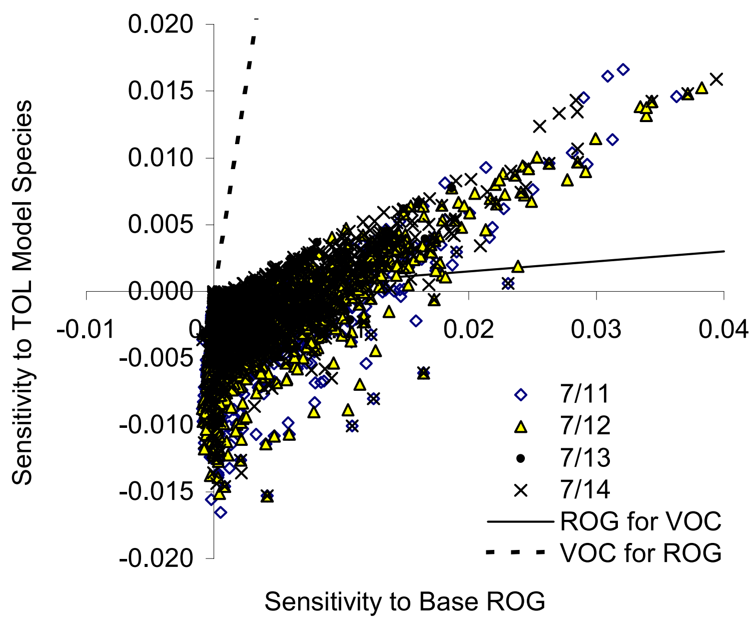


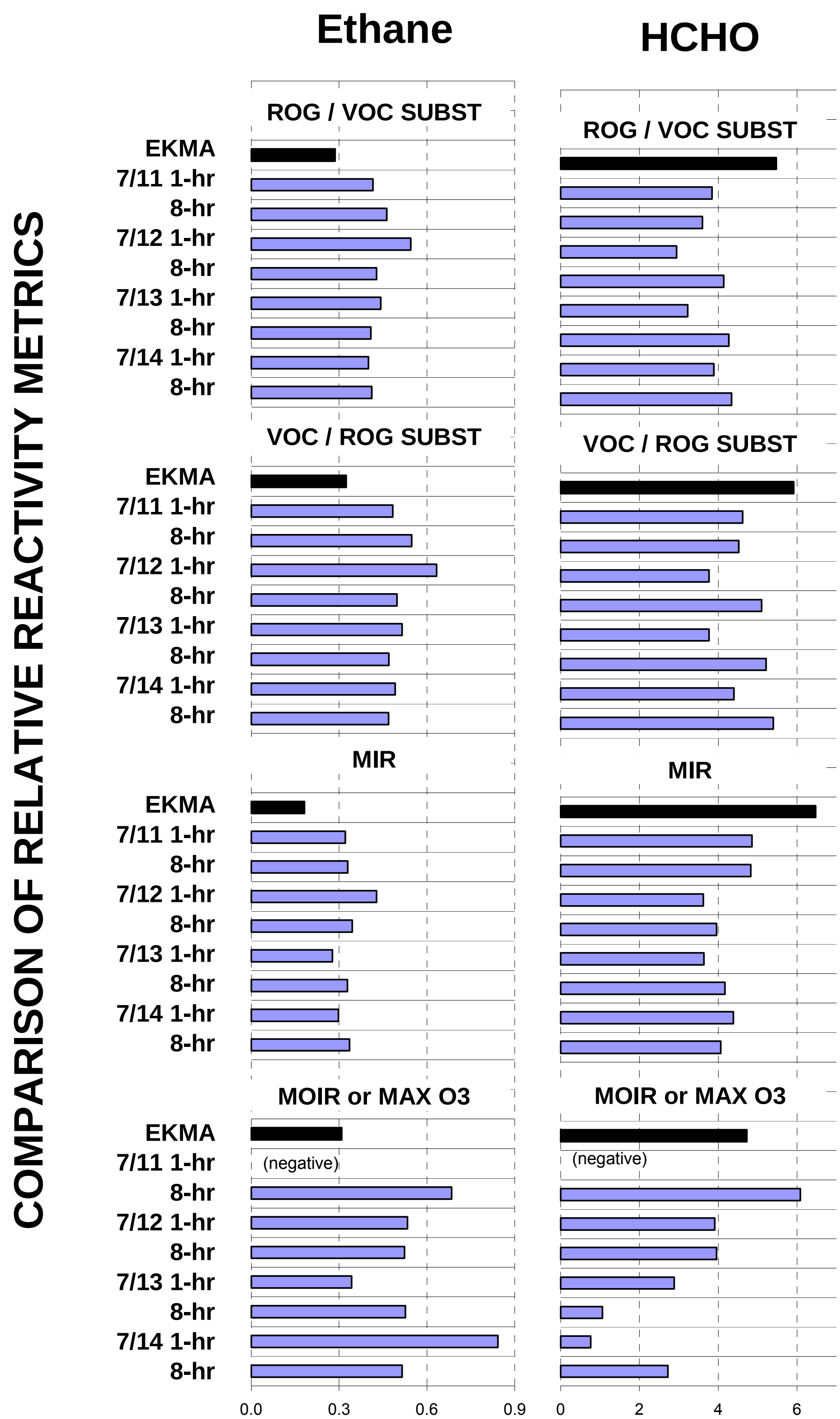
CB4 "TOL" SPECIES VS. BASE ROG SENSITIVITIES

1-HOUR DAILY MAXIMUM O_3

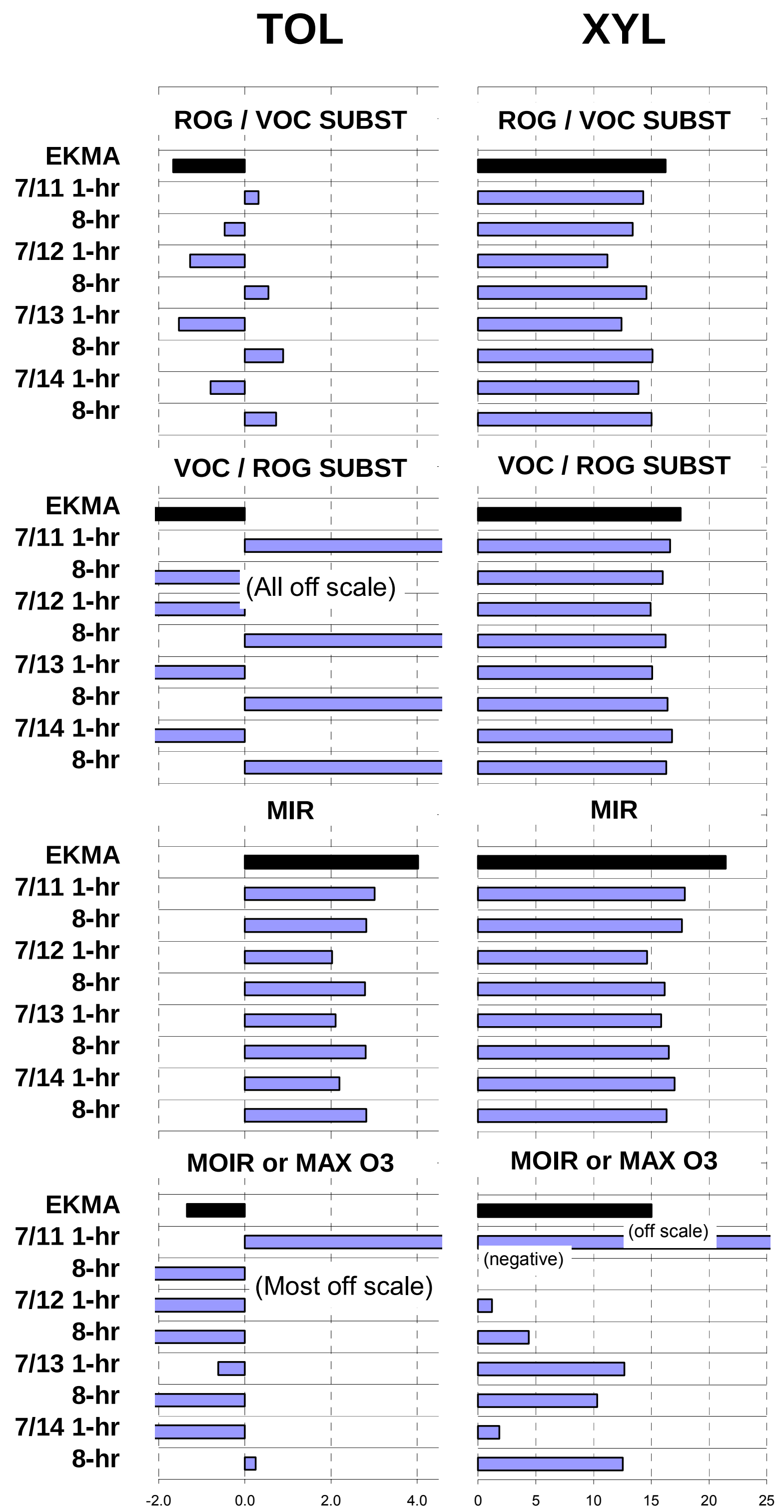


8-HOUR DAILY MAXIMUM O_3





COMPARISON OF RELATIVE REACTIVITY METRICS
Ethane
HCHO
ROG / VOC SUBST
VOC / ROG SUBST
MIR
MOIR or MAX O3
EKMA
7/11 1-hr
8-hr
7/12 1-hr
8-hr
7/13 1-hr
8-hr
7/14 1-hr
8-hr
(negative)
0.0
0.3
0.6
0.9
0
2
4
6



COMPARISON OF RELATIVE REACTIVITY METRICS

SUMMARY OF EKMA AND SELECTED REGIONAL RELATIVE REACTIVITIES FOR CB4 SPECIES

Model Species	Relative Reactivities (Carbon Basis) Effect on Maximum 1-Hour O_3			
	MIR Scales		Minimum Subst. Error: ROG for VOC	
	EKMA	Regional	EKMA	Regional
PAR	0.40	0.65 ± 0.08	0.59	0.76 ± 0.07
ETH	2.7	2.8 ± 0.2	3.0	2.9 ± 0.1
OLE	5.6	5.1 ± 0.4	5.8	5.0 ± 0.3
TOL	0.6	0.33 ± 0.07	-3.0	-0.12 ± 0.12
XYL	2.7	2.0 ± 0.2	2.2	1.6 ± 0.2
HCHO	6.6	4.1 ± 0.6	5.9	3.5 ± 0.5
ALD2	3.5	2.6 ± 0.3	3.7	2.6 ± 0.2
Ethane	0.09	0.17 ± 0.03	0.16	0.23 ± 0.03
Ethanol	0.76	0.7 ± 0.2	1.10	0.89 ± 0.08
CO	0.03	0.06 ± 0.01	0.06	0.09 ± 0.01

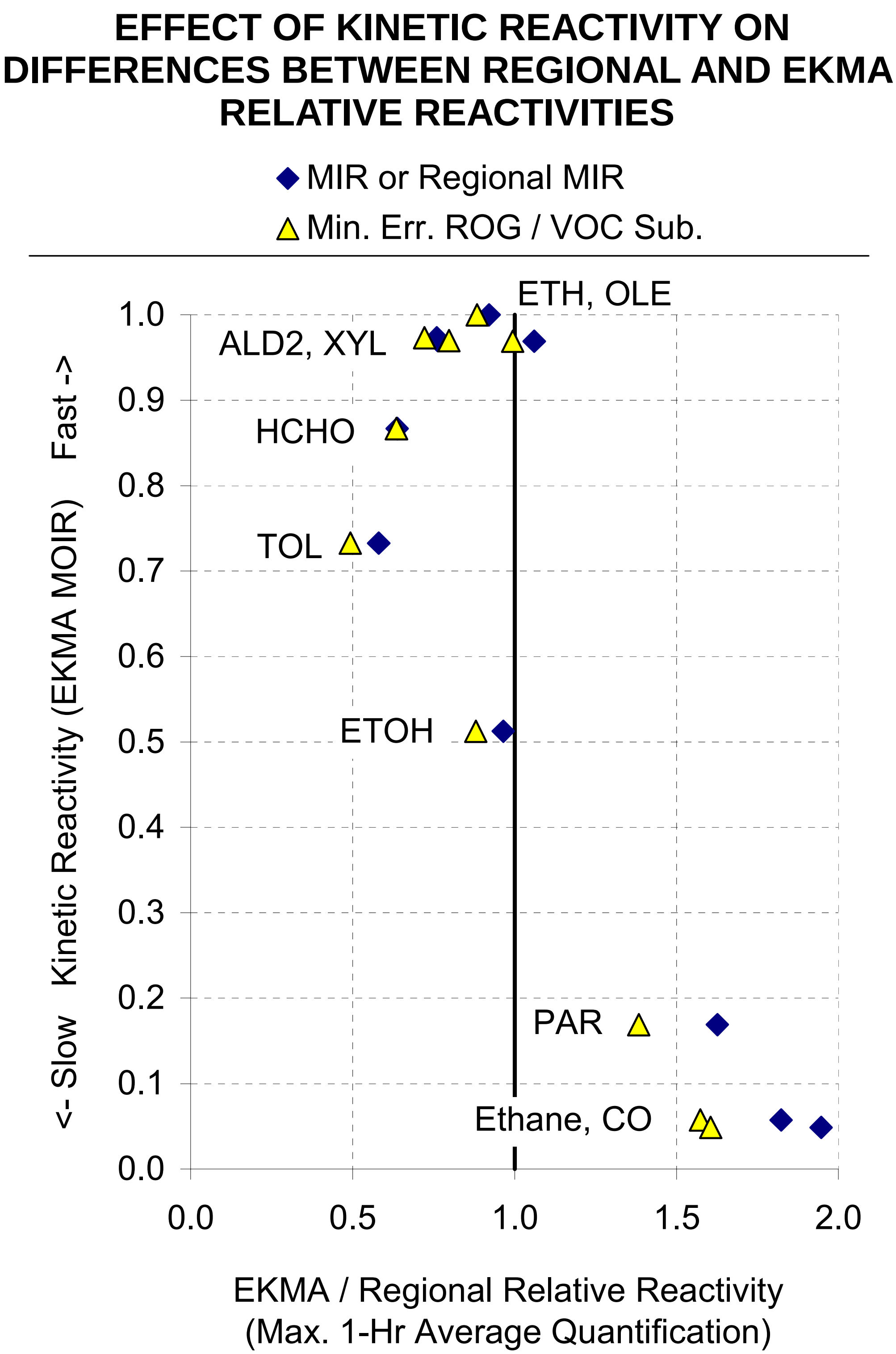
Regional data are averages of the results for the four episode-days

SUMMARY OF EKMA AND SELECTED REGIONAL RELATIVE REACTIVITIES SELECTED COMPOUNDS

Compound	Relative Reactivities - Mass Basis				
	MIR			Min Subst. Err. #1	
	SAPRC	CB4		CB4	
	EKMA	EKMA	Regional Average	EKMA	Regional Average
Ethane	0.11	0.10	0.19	0.16	0.26
n-Butane	0.46	0.47	0.76	0.65	0.89
Ethylene	3.2	3.2	3.5	3.6	3.6
Propene	4.0	4.6	4.3	4.9	4.4
m-Xylene	3.7	3.5	2.7	2.6	2.1
Formaldehyde	3.1	3.7	2.4	3.1	2.0
Acetaldehyde	2.4	2.7	2.1	2.8	2.0
Ethanol	0.59	0.56	0.58	0.76	0.66
CO	0.020	0.020	0.039	0.034	0.055

Note:

- Only compounds that are reasonably well represented in the CB4 calculations are listed.
- “SAPRC” is SAPRC-99
- CB4 n-butane is 4 PAR, propene is OLE + PAR
- “Min. Subst. Error #1” is ROG for VOC substitution


EFFECT OF KINETIC REACTIVITY ON DIFFERENCES BETWEEN REGIONAL AND EKMA RELATIVE REACTIVITIES
MIR or Regional MIR
Min. Err. ROG / VOC Sub.
ETH, OLE
ALD2, XYL
HCHO
TOL
ETOH
PAR
Ethane, CO
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
0.0
0.5
1.0
1.5
2.0
<- Slow Kinetic Reactivity (EKMA MOIR) Fast ->
EKMA / Regional Relative Reactivity
(Max. 1-Hr Average Quantification)

PRELIMINARY LARGE SCALE SUBSTITUTION CALCULATIONS

CALCULATION 1

- ALL ANTHROPOGENIC VOCS REMOVED
- RESULTS ARE COMPARED WITH PREDICTIONS USING LINEAR APPROXIMATION AND BASE ROG REACTIVITIES FROM DDM CALCULATION

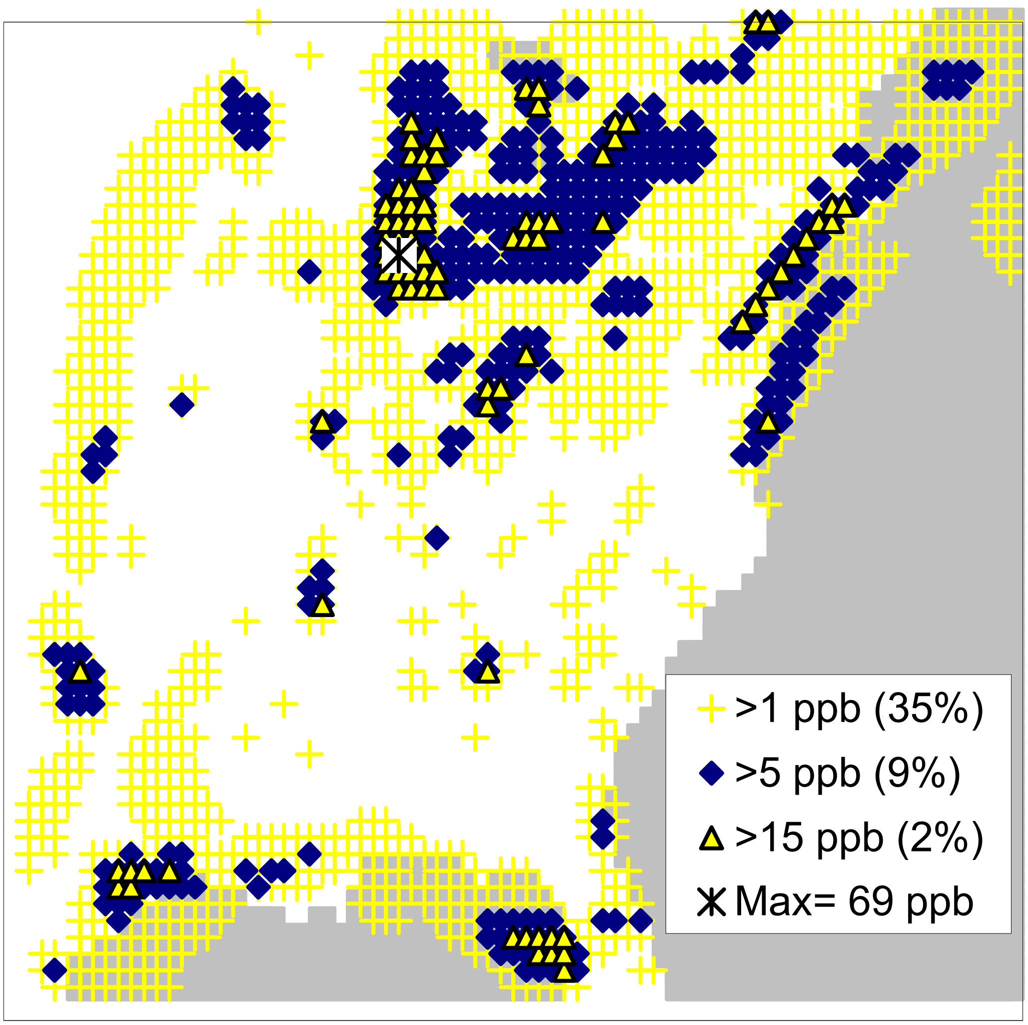
CALCULATION 2

- ALL ANTHROPOGENIC VOCs REPLACED BY ETHANE ON A CARBON FOR CARBON BASIS
- RESULTS ARE COMPARED WITH CALCULATION WITH ALL ANTHROPOGENIC VOCs REMOVED TO DETERMINE EFFECT OF ETHANE ADDITION
- RESULTS ARE COMPARED WITH EFFECTS OF ETHANE ADDITION PREDICTED BY DDM CALCULATION OF ETHANE REACTIVITY

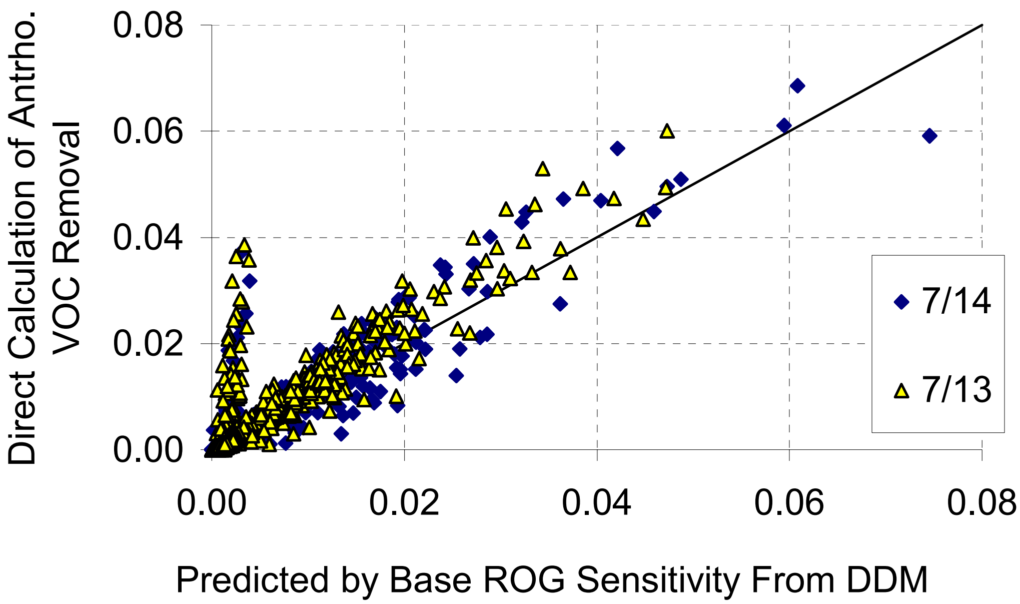
ONLY DATA FOR JULY 13 AND 14 ARE CURRENTLY ANALYZED

MAXIMUM 1-HOUR AVERAGE O_3 REDUCTION FROM REMOVING ALL ANTHROPOGENIC VOCs

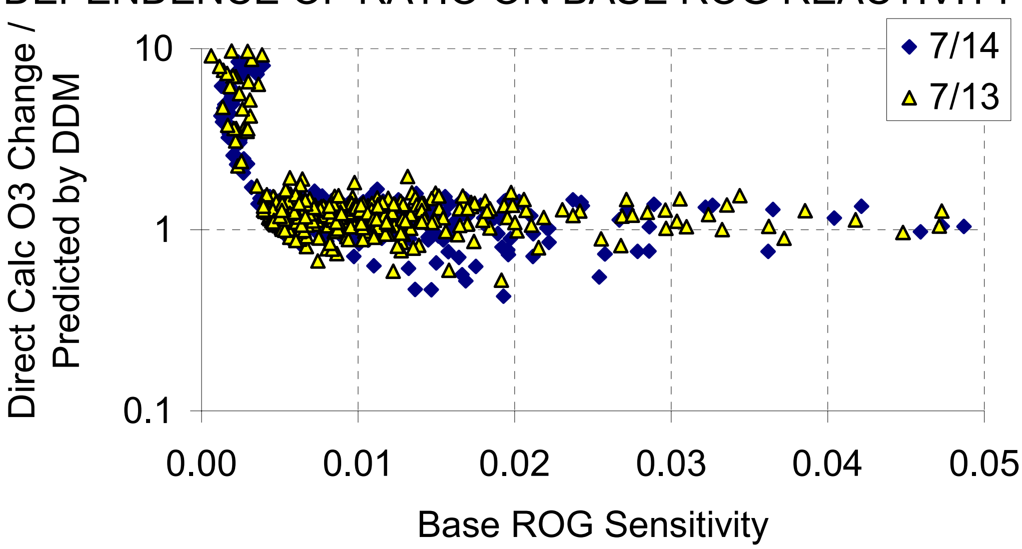
JULY 14



PLOT OF CHANGE IN MAXIMUM 1-HOUR O_3 FROM REMOVING ANTHROPOGENIC VOCs VS. ΔO_3 PREDICTED BY BASE ROG REACTIVITY



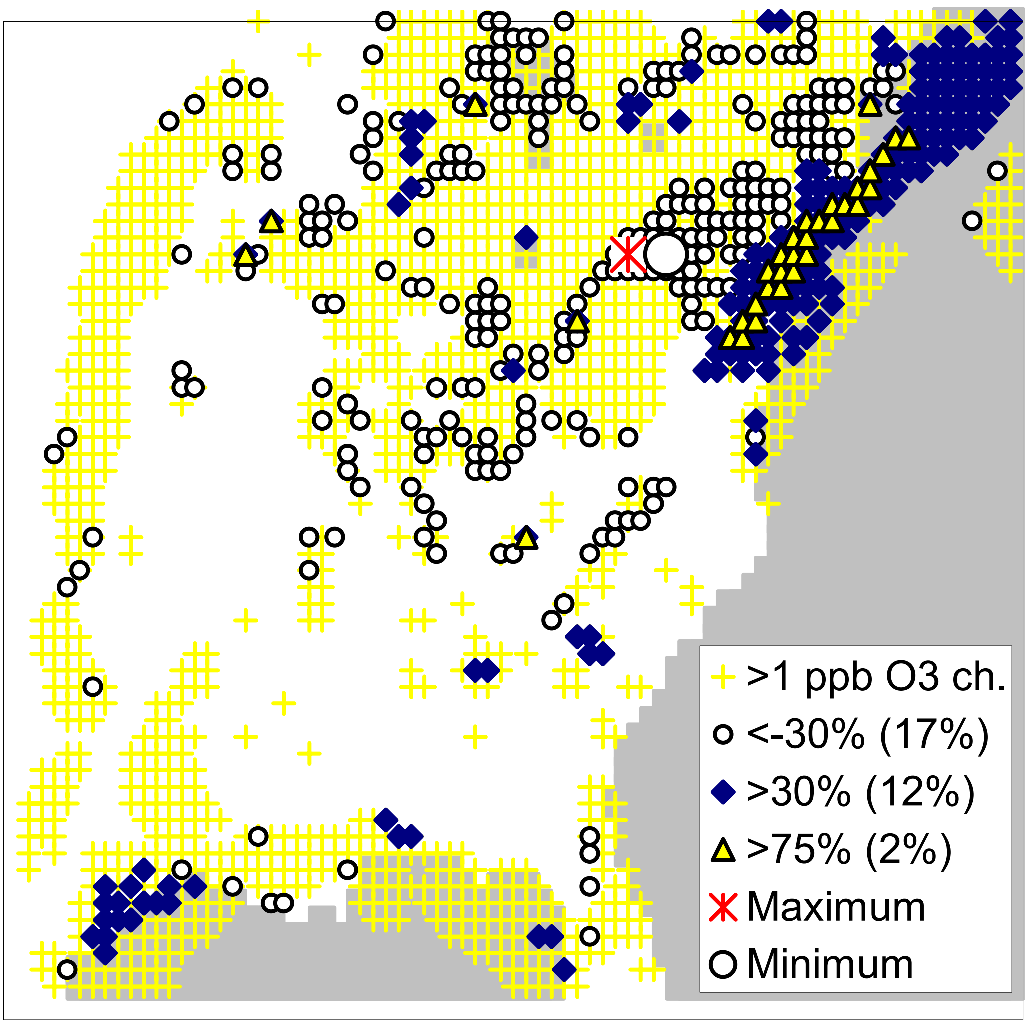
DEPENDENCE OF RATIO ON BASE ROG REACTIVITY



ERROR IN LINEAR APPROXIMATION PREDICTION OF ΔO_3 FOR ANTHROPOGENIC VOC REMOVAL

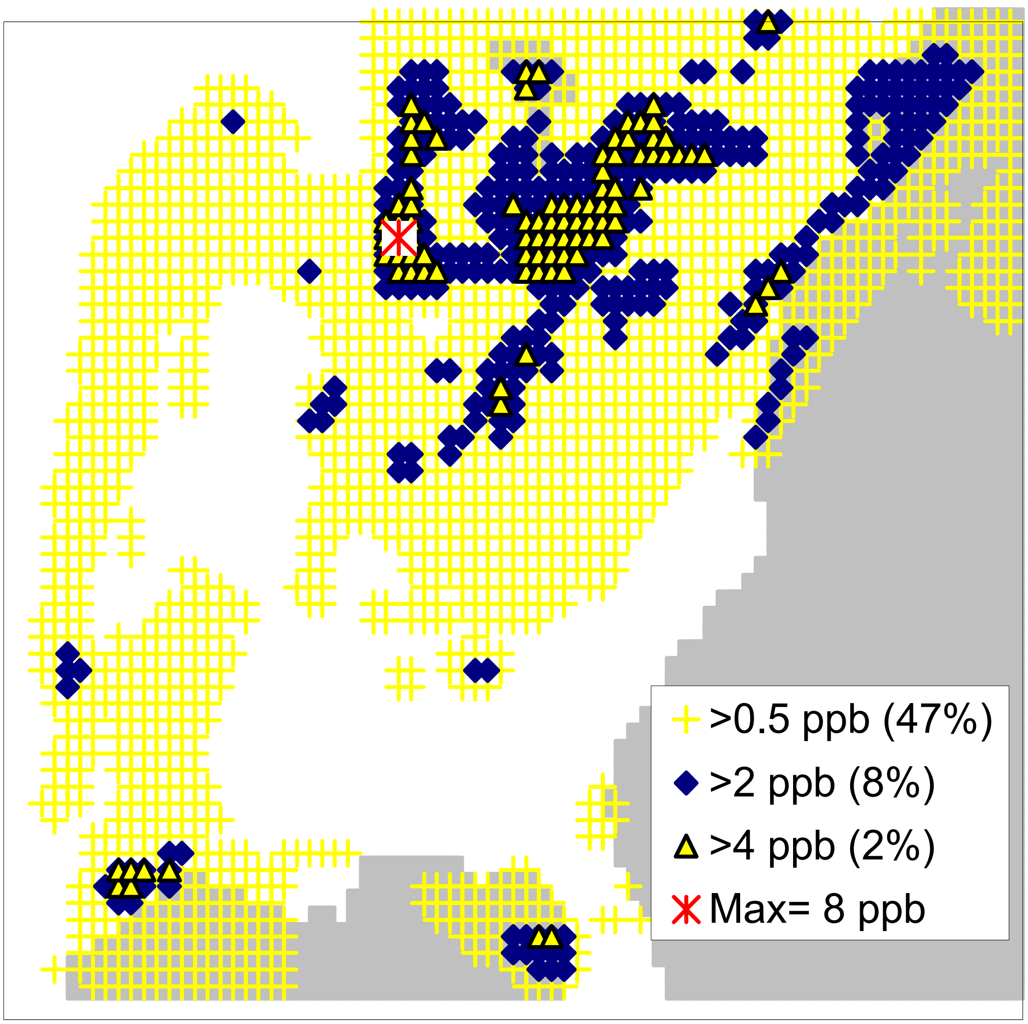
$$\frac{\text{[DIRECT CALC]} - \text{[DDM ESTIMATE (BASE ROG)]}}{\text{[DIRECT CALC]}}$$

(FOR CELLS WHERE ΔO_3 > 1 PPB ONLY)



MAXIMUM 1-HOUR AVERAGE O_3 INCREASE FROM ADDING BACK ETHANE TO REPLACE THE ANTHROPOGENIC VOCs THAT WERE REMOVED

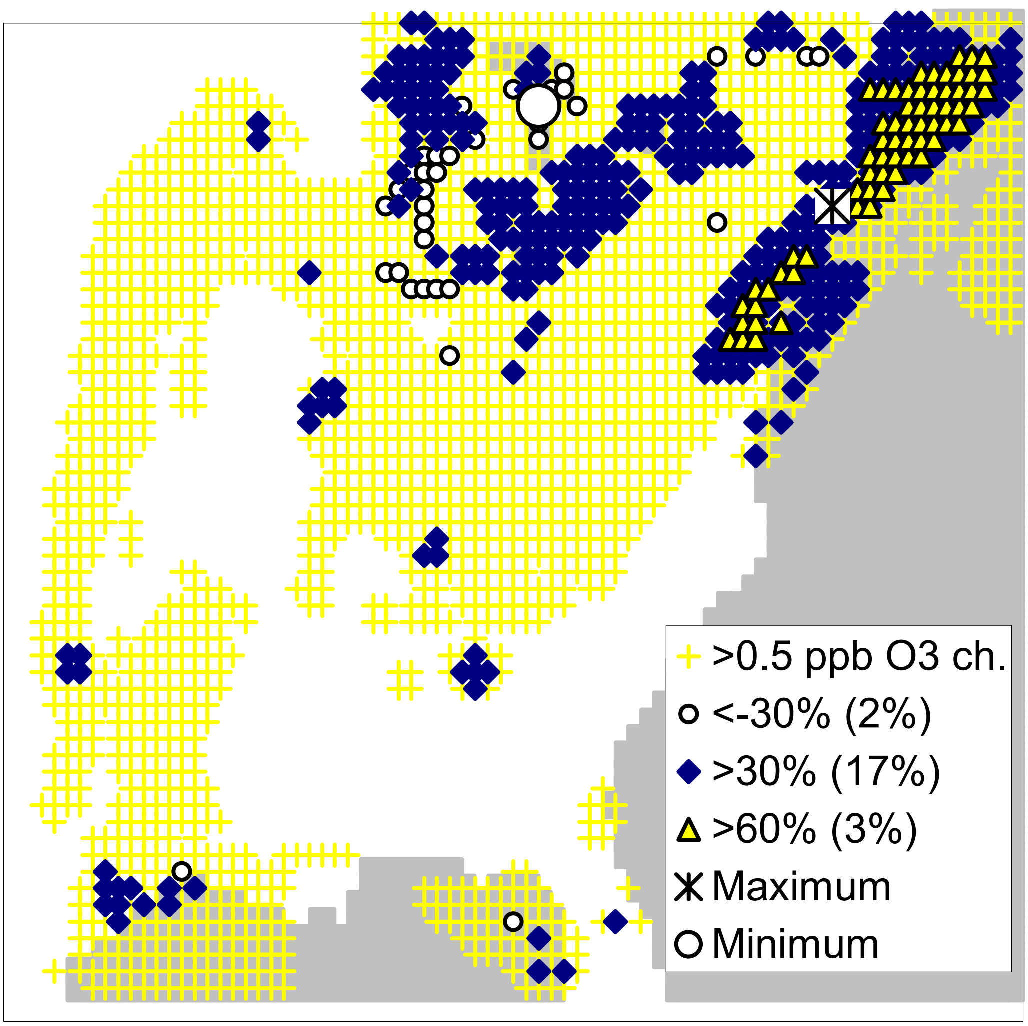
JULY 14



ERROR IN LINEAR APPROXIMATION PREDICTION OF ΔO_3 FOR ADDING BACK ETHANE AFTER ANTHROPOGENIC VOCs REMOVED

$$\frac{\text{[DIRECT CALC]} - \text{[ETHANE I.R. ESTIMATE]}}{\text{[DIRECT CALC]}}$$

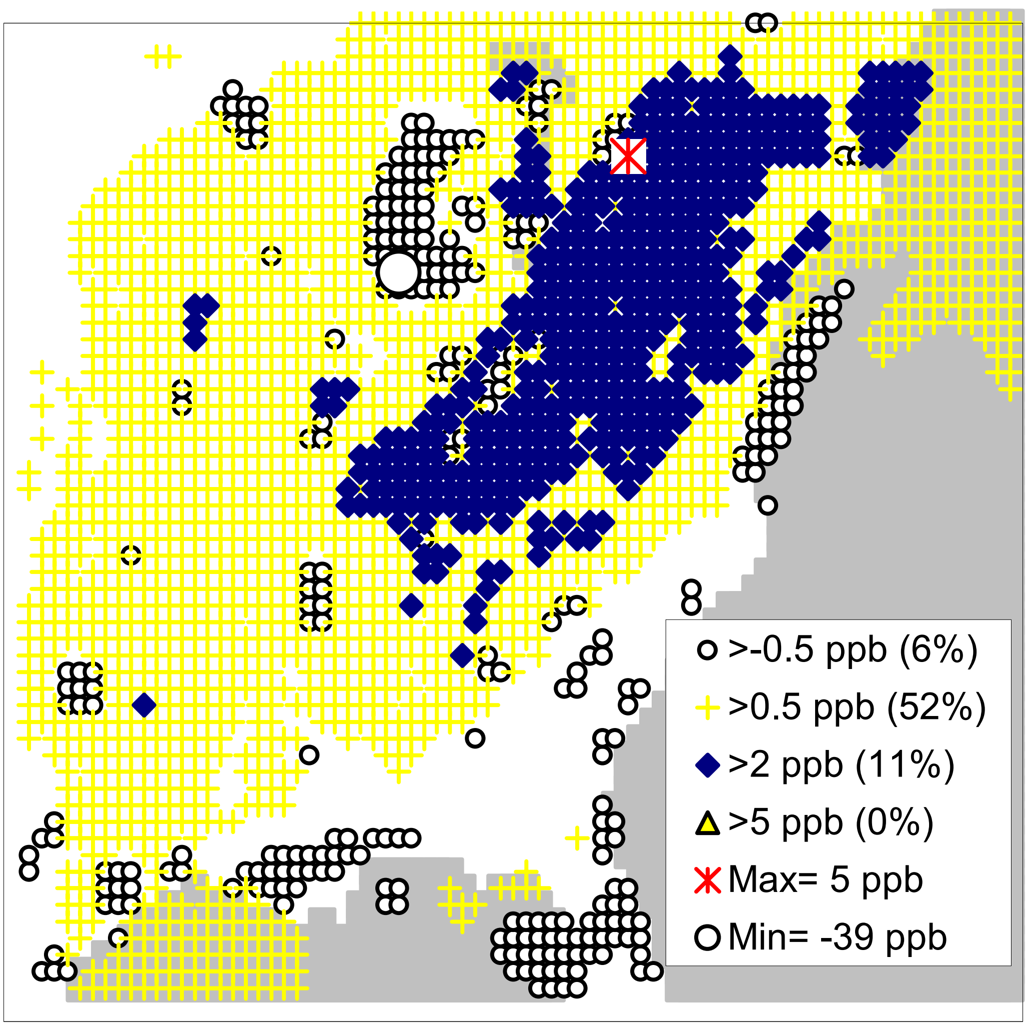
(FOR CELLS WHERE ΔO_3 > 0.5 PPB ONLY)



SPATIAL DISTRIBUTION OF O_3 CHANGES CAUSED BY REPLACING EACH CARBON IN THE BASE ROG WITH 3.9 CARBONS OF ETHANE

THE OPTIMUM FACTOR WAS DERIVED FROM THE MINIMUM ETHANE-FOR-VOC SUBSTITUTION ERROR FOR ALL CELLS (INCLUDING OVER H_2O AND LOW O_3)

O_3 CHANGE IN PPB IF 100% SUBSTITUTED (IF LINEAR)



PRELIMINARY CONCLUSIONS

NO_x CONTROL IS MORE EFFECTIVE THAN VOC CONTROL IN MOST OF THIS MODELING DOMAIN

BIOGENIC VOCs DOMINATE OVER ANTHROPOGENICS IN MOST IN MOST OF THIS MODELING DOMAIN

RELATIVE REACTIVITIES ARE HIGHLY VARIABLE, BUT VARIABILITY IS LESS IN MORE VOC-SENSITIVE CELLS

RELATIVE REACTIVITIES VARY FROM DAY TO DAY IN ANY GIVEN REGION

THE MINIMUM SUBSTITUTION ERROR (MSE) METHOD PROVIDES A MEANS TO DERIVE REACTIVITY METRICS BASED ON VARYING REGIONAL IMPACTS

THE MINIMUM SUBSTITUTION ERROR AND REGIONAL MIR METRICS GIVE CONSISTENT RESULTS FOR MOST CB4 SPECIES EXCEPT TOL

THE REGIONAL MAXIMUM O_3 METRIC DOES NOT GIVE CONSISTENT REACTIVITY RESULTS

EKMA-BASED REACTIVITY SCALES ARE REASONABLY CONSISTENT WITH REGIONAL MSE AND MIR METRICS, BUT SOME BIASES EXIST

- EKMA SCALES OVERESTIMATE AROMATIC AND FORMALDEHYDE REACTIVITIES (but this needs to be verified using current mechanisms)
- EKMA SCALES UNDERESTIMATES REACTIVITIES OF SLOWLY REACTING SPECIES (E.G., ETHANE)

PRELIMINARY CONCLUSIONS
(CONTINUED)

NEED TO VERIFY THESE CONCLUSIONS WITH ANALYSIS OF FINE GRID DATA

NEED TO TEST THE ASSUMPTION THAT THE BASE ROG SENSITIVITIES CAN BE USED TO ESTIMATE SENSITIVITIES TO TOTAL ANTHROPOGENIC VOCs

PRELIMINARY CONCLUSIONS FROM 100% ANTHROPOGENIC VOC REMOVAL CALCULATION

- MAXIMUM ΔO_3 IS ~70 PPB, BUT ONLY ~10% OF THE CELLS HAVE ΔO_3 > ~5 PPB, 2%>15 PPB.
- EFFECT PREDICTED REASONABLY WELL BY DDM EXCEPT SOME CELLS LOW BASE ROG SENSITIVITY PREDICTED TO HAVE LARGE ΔO_3.

PRELIMINARY CONCLUSIONS FROM 100% ETHANE SUBSTITUTION CALCULATION ON EFFECT OF ADDING BACK ETHANE AFTER ANTHRO. VOCs REMOVED

- MAXIMUM ΔO_3 IS ~8 PPB, BUT ONLY ~10% OF THE CELLS HAVE ΔO_3 > 2 PPB
- INCREMENTAL REACTIVITY ANALYSIS PREDICTS ΔO_3 REASONABLY WELL IN ~95% OF THE CELLS

PREDICTIONS OF EFFECTS OF “OPTIMUM” SUBSTITUTIONS BASED ON INCREMENTAL REACTIVITY ANALYSIS STILL NEED TO BE TESTED WITH LARGE SCALE SUBSTITUTION CALCULATIONS

NEED TO FINALIZE WHICH OF THE LARGE SCALE SUBSTITUTION CALCULATIONS WILL BE CONDUCTED