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Canada

Impact of a Major Update to the VOC Speciation Profile Library on Regional Air Quality Model Predictions

Junhua Zhang, Michael D. Moran, Paul A. Makar, and Qiong Zheng

Air Quality Research Division, Environment and Climate Change Canada
Toronto, Ontario, Canada

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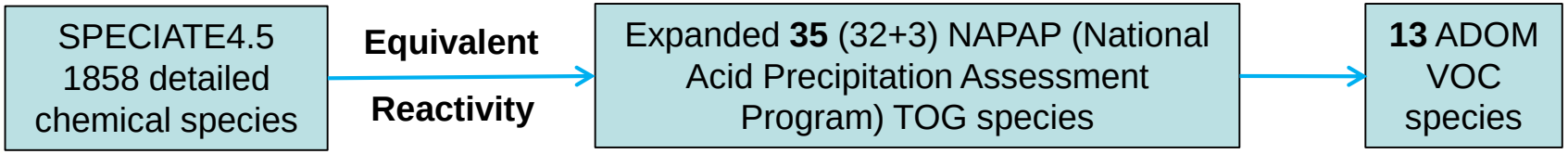
Presentation Outline

- Motivation for this study
- Overview of the methodology used to generate VOC speciation profiles for ADOM-II chemical mechanism
- Changes to emissions processing for generating AQ-model-ready VOC emissions using the new profile library
- Impacts of new processed VOC emissions on a North American modeling grid at 10-km resolution
- Sensitivity study of the impacts of the new VOC emissions on AQ predictions for a one-month summer simulation
- Conclusions

Motivation

- ADOM-II gas-phase chemical mechanism is being used by both ECCCôs operational AQ modeling system and policy platform
- Chemical speciation profiles built for ADOM-II mechanism are mainly based on VOC (TOG) speciation profiles contained in EPAôs SPECIATE V3.2 database (Makar et al., 2003)
- SPECIATE database has gone through 5 updates since V3.2; the most recent update is V4.5, which was released in September 2016
- SPECIATE V3.2 contains 567 speciation profiles and 789 individual chemical species. 1052 new VOC (TOG) profiles and 1069 new chemical species were added to newer versions of the SPECIATE database (v4.0-4.5)
- Many of the new profiles are location- and process-specific for emerging activities, such as basin-specific profiles for the oil and gas industry in the U.S.
- VOC (TOG) speciation profile library for ECCCôs operational AQ modeling system and policy platform needs to be updated

Generation of VOC Speciation Profiles (1)



ADOM Name	Description
CH4	Methane
C2H6	Ethane
C3H8	Propane and other slowly reacting organics, reacts as propane
ALKA	C4 and greater alkanes
ETHE	Ethene
ALKE	Propene and higher alkenes
TOLU	Monoalkylbenzenes, dominated by toluene
AROM	More reactive aromatics including xylenes, other polyalkyl benzenes and polycyclic aromatics
HCHO	Formaldehyde
ALD2	C2 and greater aldehydes, reacts as acetaldehyde
MEK	Lumped ketones, largely methyl ethyl ketone
CRES	Lumped cresols
ISOP	Isoprene
OTHE	Other unknown or unreactive species

Generation of VOC Speciation Profiles (2)

NAPAP NAME	ADOM NAME	NAPAP_Mass_Fraction	Reactivity Weights
Methane	CH4	1	1
Ethane	C2H6	1	1
Propane	C3H8	1	1
Alkanes (0.25-0.50)	ALKA	1	0.5447
Alkanes (0.50-1.00)	ALKA	1	0.8496
Alkanes (1.0-2.0)	ALKA	1	1.2482
Alkanes (>2.0)	ALKA	1	1.5079
Alkane/Aromatic Mixture	ALKA	0.5	1.3242
Alkane/Aromatic Mixture	AROM	0.5	0.09
Ethene	ETHE	1	1
Propene	ALKE	1	1
Alkenes (Primary)	ALKE	1	1
Alkenes (Internal)	ALKE	1	1
Alkenes (Primary/Internal Mixture)	ALKE	1	1
Benzene and Halobenzenes	C3H8	1	1.03
Aromatics (<2)	TOLU	1	1
Aromatics (>2)	AROM	1	1
Phenols and Cresols	CRES	1	1
Styrenes	TOLU	0.74032	1
Styrenes	ALKE	0.25968	1
Formaldehyde	HCHO	1	1
Higher Aldehydes	ALD2	1	1
Acetone	OTHE	1	1
Higher Ketones	MEK	1	1
Organic Acids	OTHE	1	1
Acetylene	C3H8	1	0.66
Haloalkenes	OTHE	1	1
Unreactive	OTHE	1	1
Others (<0.25)	C3H8	1	0.78
Others (0.25-0.50)	ALKA	1	0.6865
Others (0.50-1.00)	ALKA	1	0.9561
Others (>1.00)	ALKA	1	1.3364
Unidentified	OTHE	1	1
Unassigned	OTHE	1	1
Isoprene (anthropogenic)	ISOP	1	1
Alpha-Pinene (anthropogenic)	ALKE	1	1
Other monoterpenes (anthropogenic)	ALKE	1	1

Changes Made for Processing AQ-Model-Ready Emissions (1)

- Inventories: 2013 Canadian, projected 2017 U.S., and 2008 Mexican
- New VOC speciation cross-reference file based on EPA 2011 V6.3 Platform

2017 U.S.	OLD PROFILES			NEW PROFILES		
	v3.2	Legacy (CEPS)	Total	V3.2	v4.0-v4.5	Total
CMV	3	0	3	1	1	2
nonpoint	37	13	50	42	29	71
nonroad	2	0	2	0	3	3
np_oilgas	1	1	2	9	18	27
offshore	12	1	13	9	2	11
pt_oilgas	72	20	92	70	25	95
ptegu	9	0	9	10	0	10
ptnonipm	237	43	280	236	52	288
rail	1	0	1	0	1	1
rwc	2	0	2	1	1	2
seca	1	0	1	1	0	1
on-road	4	0	4	1	3	4
TOTAL	381	78	459	380	135	515

seca profile:

Old			New		
0001	External Combustion Boiler - Residual Oil	V3.2	2480	Industrial Cluster, Ship Channel, Downwind Sample - 1993	V3.2

Changes Made for Processing AQ-Model-Ready Emissions (2)

2013 CAN	OLD PROFILES			NEW PROFILES		
	v3.2	Legacy (CEPS)	Total	V3.2	v4.0-v4.5	Total
point	23	7	30	27	10	37
oarea	24	5	29	19	15	34
aircraft	3	0	3	0	1	1
marine/rail	3	0	3	1	2	3
nonroad	3	0	3	2	6	8
onroad	4	0	4	0	4	4
uog	7	2	9	6	1	7
TOTAL	67	14	81	55	39	94

2008 MEX	OLD PROFILES			NEW PROFILES		
	v3.2	Legacy (CEPS)	Total	V3.2	v4.0-v4.5	Total
point	112	19	131	111	14	125
area	16	2	18	12	12	24
nonroad	3	0	3	1	2	3
onroad	1	0	1	0	3	3
TOTAL	132	21	153	124	31	155

Changes Made for Processing AQ Model-Ready Emissions (3)

- **Last-resort default cross reference (0 0000 VOC) removed from the cross- reference file**

US np_oilgas:

Old: 2 profiles

0000 (Overall Average, v3.2) and 9015 (Legacy)

New: 45 profiles including 16 V4.5 basin-specific profiles

DJFLA	Oil and Gas -Denver-Julesburg Basin Flashing Gas Composition for Condensate Tanks	4.5
DJVNT	Oil and Gas -Denver-Julesburg Basin Produced Gas Composition from Non-CBM Gas Wells	4.5
PNC01	Oil and Gas -Piceance Basin Produced Gas Composition from Non-CBM Gas Wells	4.5
PNC02	Oil and Gas -Piceance Basin Produced Gas Composition from Oil Wells	4.5
PNC03	Oil and Gas -Piceance Basin Flash Gas Composition for Condensate Tank	4.5
PRBCB	Oil and Gas -Powder River Basin Produced Gas Composition from CBM Wells	4.5
PRBCO	Oil and Gas -Powder River Basin Produced Gas Composition from Non-CBM Wells	4.5
PRM01	Oil and Gas -Permian Basin Produced Gas Composition for Non-CBM Wells	4.5
SSJCB	Oil and Gas -South San Juan Basin Produced Gas Composition from CBM Wells	4.5
SSJCO	Oil and Gas -South San Juan Basin Produced Gas Composition from Non-CBM Gas Wells	4.5
SWFLA	Oil and Gas -SW Wyoming Basin Flash Gas Composition for Condensate Tanks	4.5
SWVNT	Oil and Gas -SW Wyoming Basin Produced Gas Composition from Non-CBM Wells	4.5
UNT02	Oil and Gas -Uinta Basin Produced Gas Composition from Non-CBM Wells	4.5
UNT03	Oil and Gas -Uinta Basin Flash Gas Composition from Oil Tanks	4.5
UNT04	Oil and Gas -Uinta Basin Flash Gas Composition from Condensate Tanks	4.5
WRBCO	Oil and Gas -Wind River Basin Produced Gas Composition from Non-CBM Gas Wells	4.5

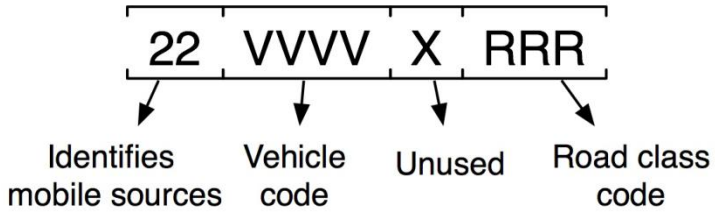
Changes Made for Processing AQ Model-Ready Emissions (4)

- **Last-resort default cross reference (0 0000 VOC) removed from the cross- reference file**

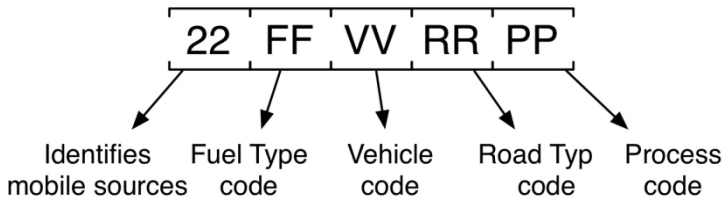
Mexican mobile:

- New set of mobile SCCs was used for 2008 Mexican mobile emissions

Structure of Old SCC



Structure of New SCC



- Due to the last-resort default VOC speciation cross reference, default profile 0000 (Overall Average, v3.2) was previously used for Mexican mobile VOC emissions

- Issue fixed with the new cross-reference file

Changed VOC-to-TOG Conversion Factors for Processing Emissions

- Inventory VOC needs to be converted to TOG because speciation profiles were built for TOG
- Updated VOC-to-TOG conversion file based on EPA 2011 Version 6.3 Platform to include new profiles and also to update conversion factors for a few v3.2 profiles: for example,

PROFILE	Old	New
0001	1.12	1.63934426
0066	1	1.63132137
0127	1	1.63132137
0333	1.91	5.71755289
1021	1	3.33333333
1025	1.21	12.87001287
1029	1	2.62950302
1030	1.04	3.09693404
1045	1	1.51515152
1195	1	1.64690382
1196	1	6.70690812

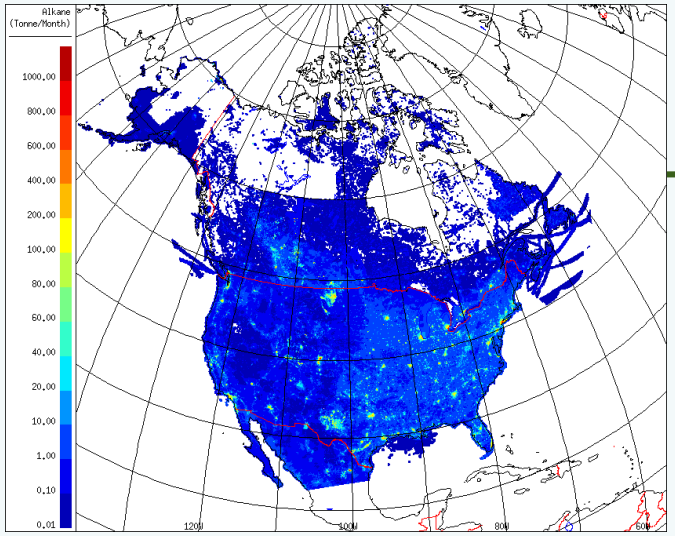
- Issue with new conversion factors for a few profiles, such as ñ0195ò (Residential Fuel - Natural Gas):
  Methane is the only species for this profile, so VOCtoTOG=0. However, it is used for processing 1.8, 26.0, and 7.7 ktons of VOC emissions for Canada, the U.S., and Mexico, respectively. All of those VOC emissions are missing due to the use of this profile

Impact on VOC Emissions Prepared for a North American Continental Grid

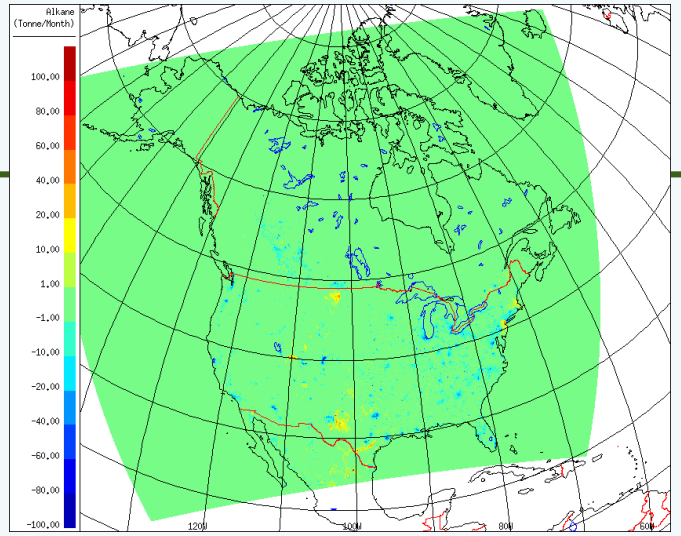
Change of domain-total VOC emissions for the ADOM-II mechanism

SPECIES	OLD (t/month)	NEW (t/month)	Change (%)	MW	Old (Mmole)	New (Mmole)	Change (%)
ALKA	658,312	614,937	-7%	93.43	7,046	6,582	-6.6%
TOLU	99,597	67,334	-32%	92.13	1,081	731	-32.4%
AROM	91,303	75,325	-17%	117.97	774	639	-17.5%
C3H8	78,760	147,902	88%	44.09	1,786	3,355	87.8%
ALKE	71,786	67,262	-6%	57.03	1,259	1,179	-6.3%
ETHE	24,347	25,316	4%	28.05	868	903	4.0%
HCHO	23,473	12,543	-47%	30.03	782	418	-46.6%
ALD2	14,363	11,662	-19%	44.05	326	265	-18.8%
MEK	11,992	9,151	-24%	72.1	166	127	-23.7%
CRES	10,619	3,118	-71%	108.13	98	29	-70.6%
ISOP	1,347	336	-75%	68.11	20	5	-75.1%
TOTAL	**1,085,899**	**1,034,887**	**-5%**		**14,206**	**14,231**	**0.2%**

Comparisons of Spatial Distribution of VOC Emissions over the Continental Grid



ALKA_Old_July_tonne



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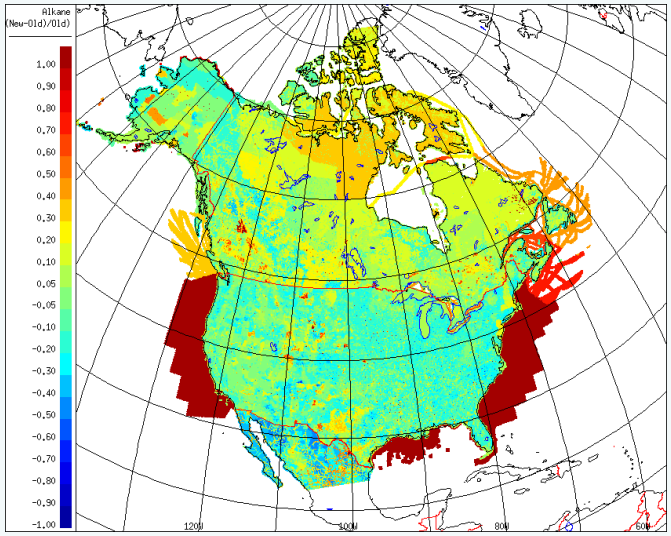

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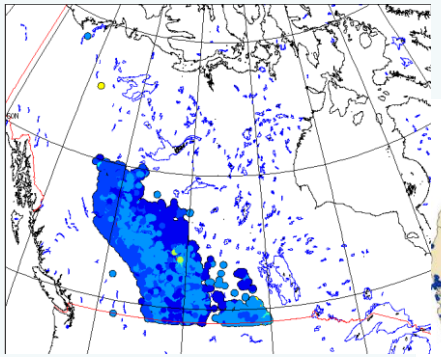


Canadian oil and gas well locations

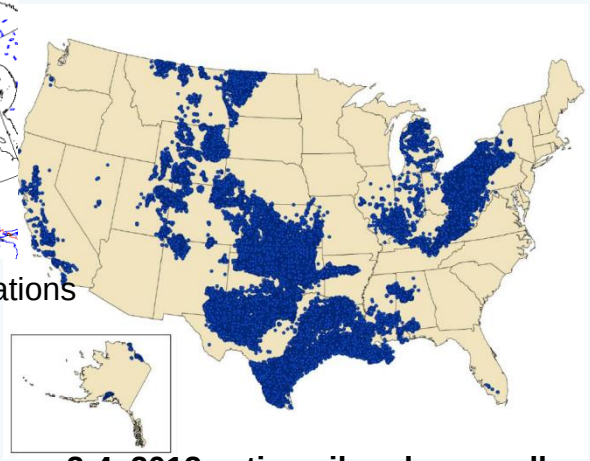
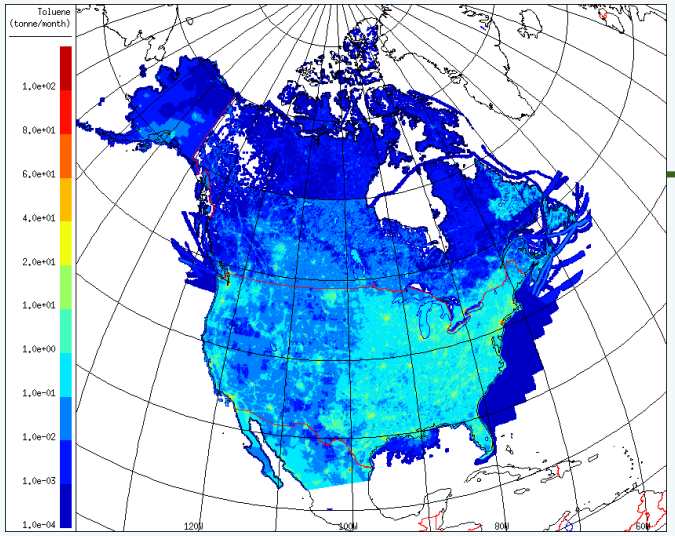


Figure 2-4. 2012 active oil and gas well locations developed by ERG, Inc.

Adelman, Z., *Emissions Modeling Platform Spatial Surrogate Documentation, prepared for EPA, 2015*



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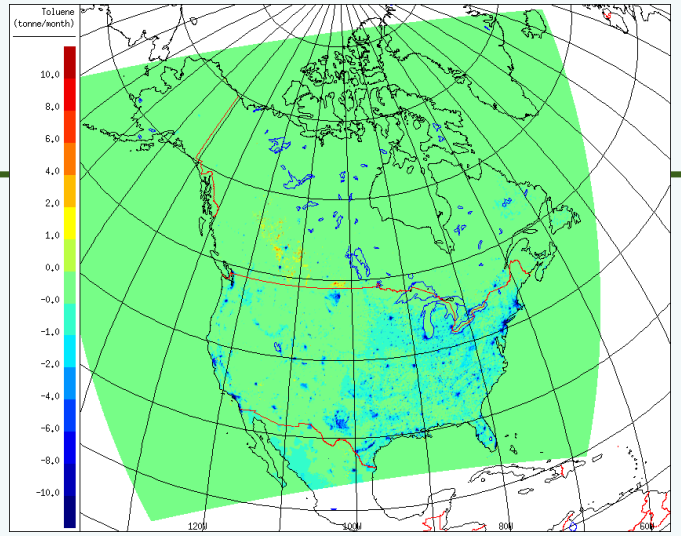

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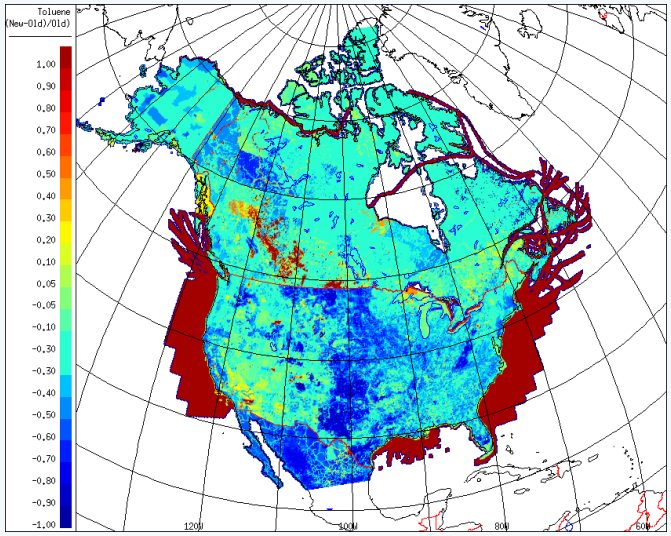

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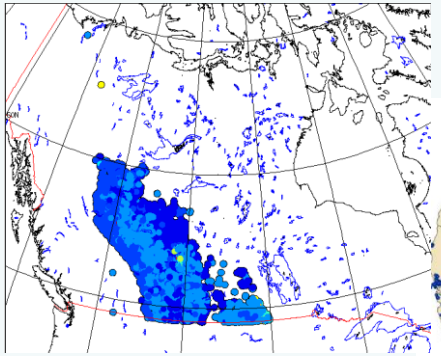

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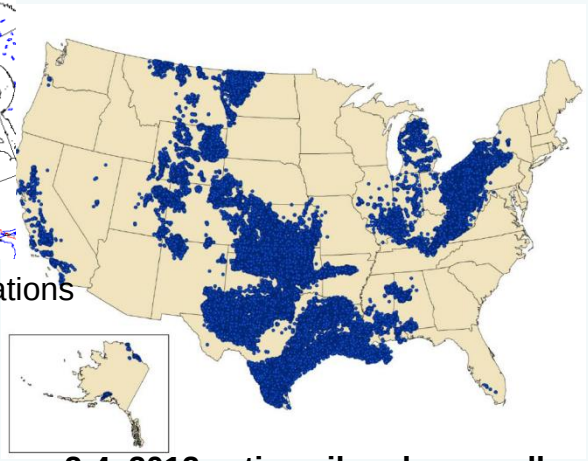

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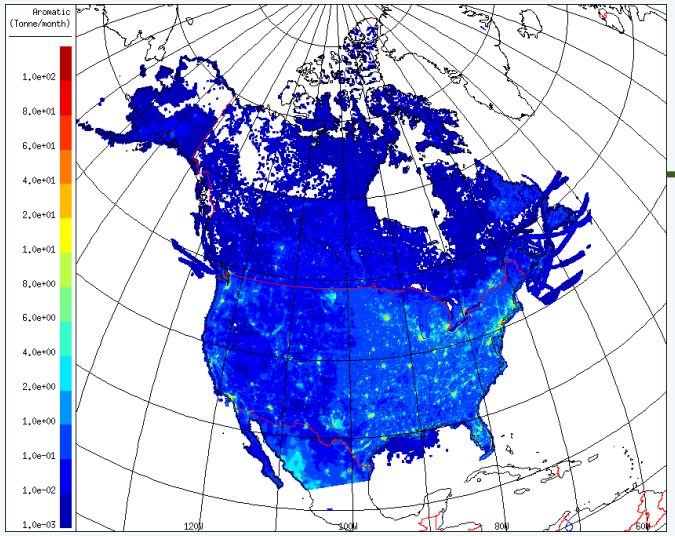

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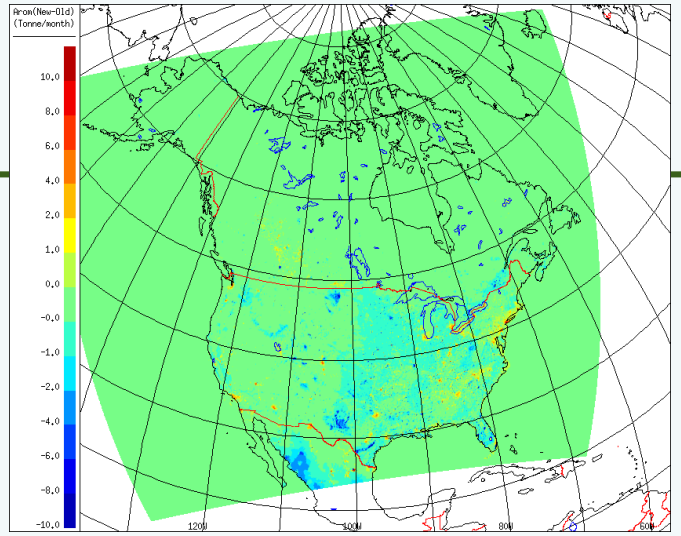

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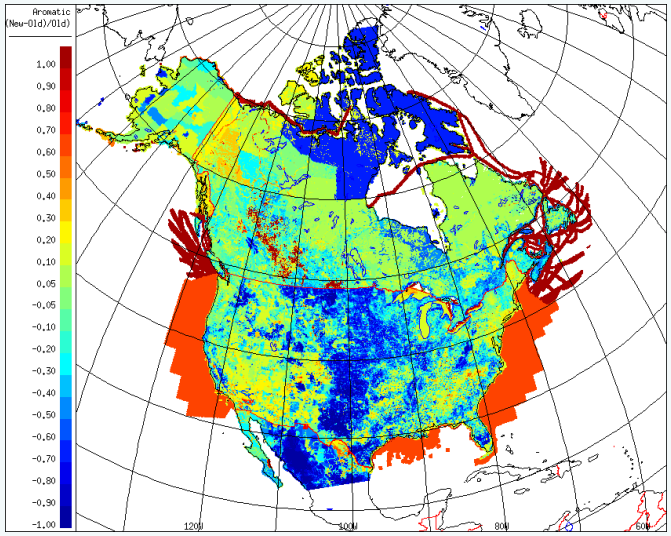

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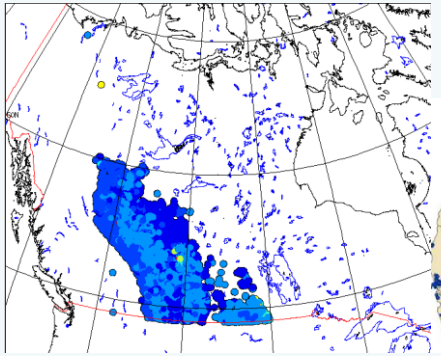

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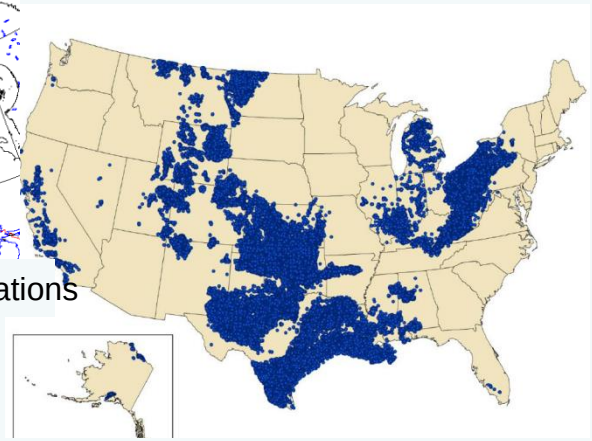

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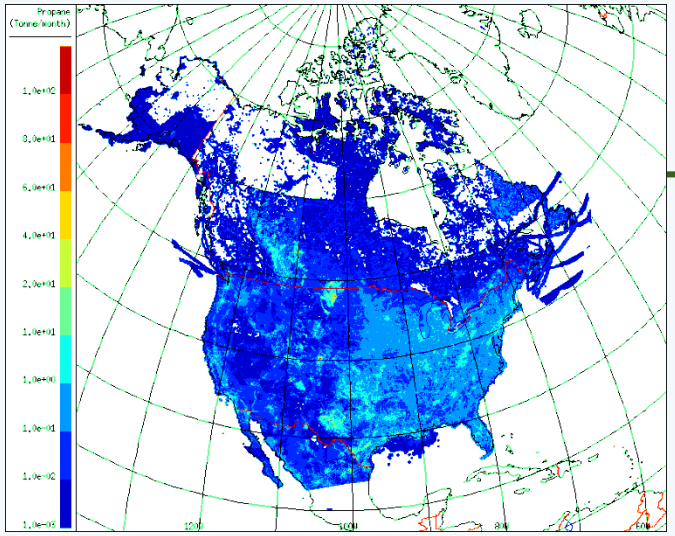
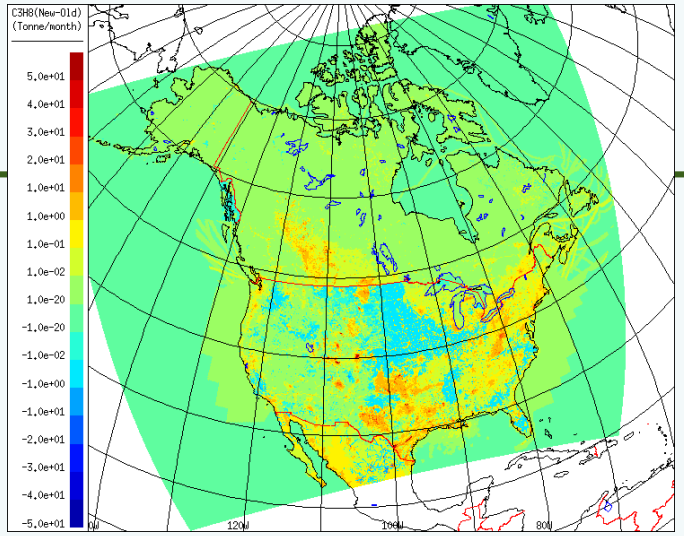


C3H8_Old_July_tonne



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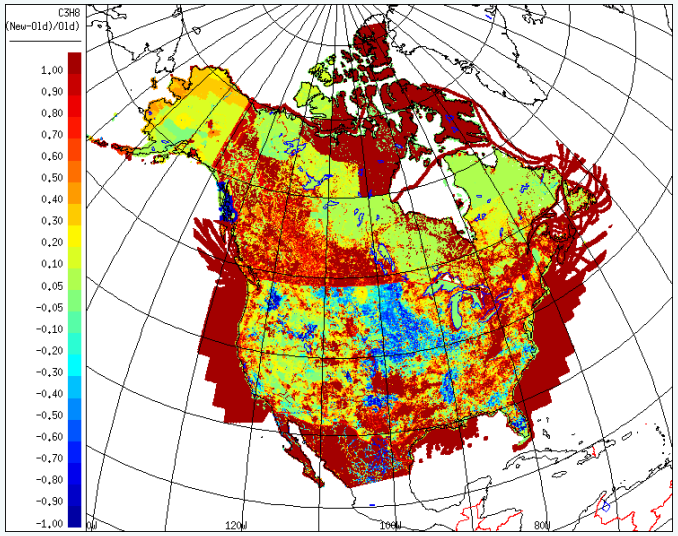

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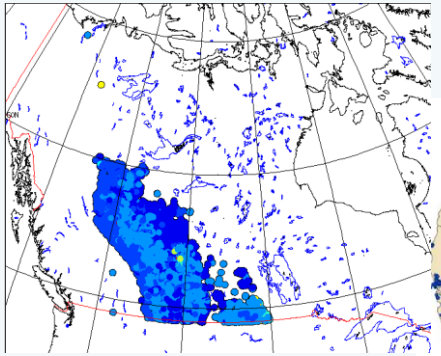

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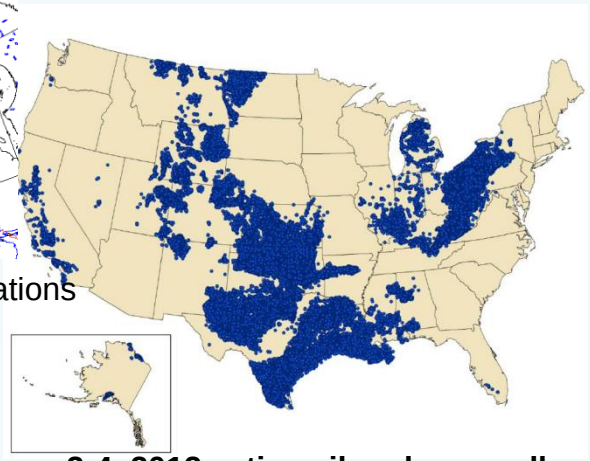

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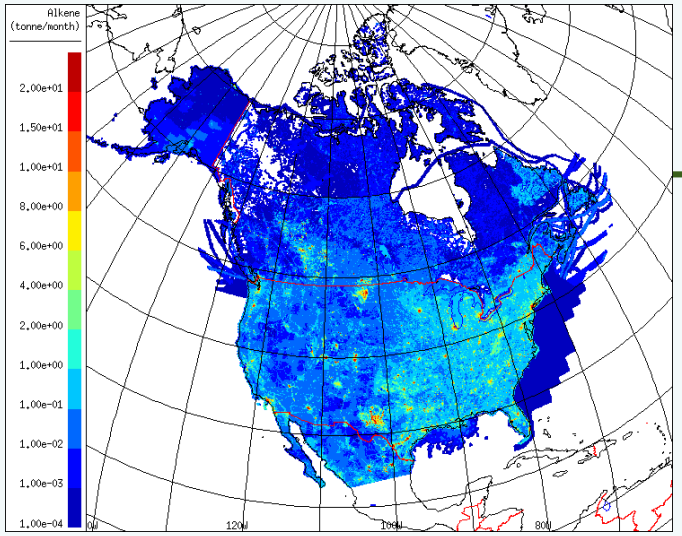
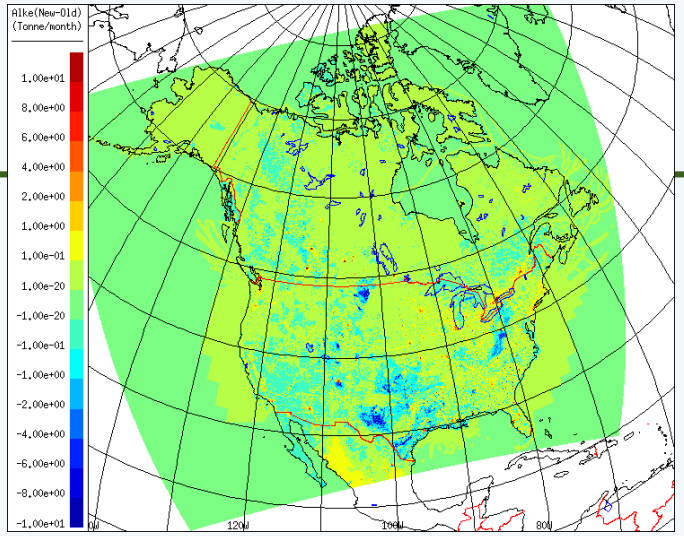


ALKE_Old_July_tonne



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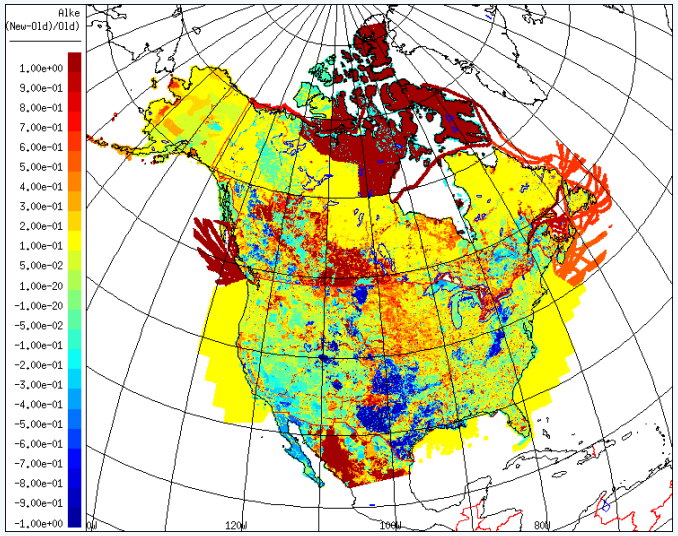

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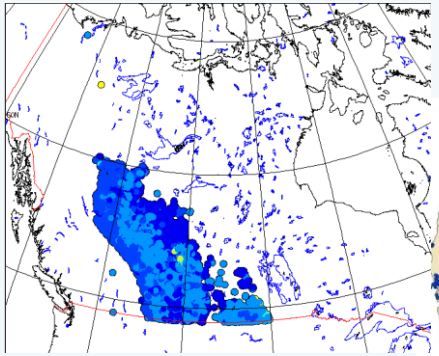
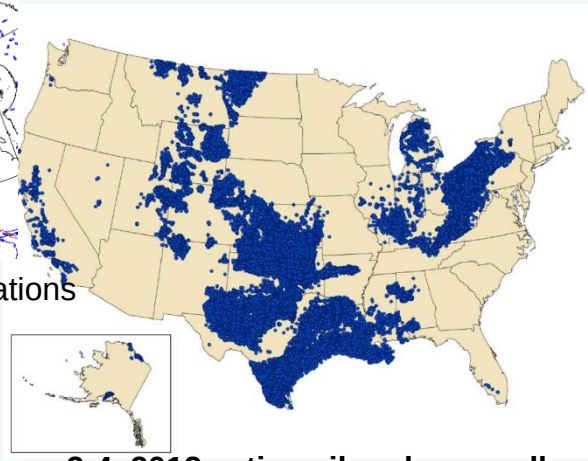


Canadian oil and gas well locations



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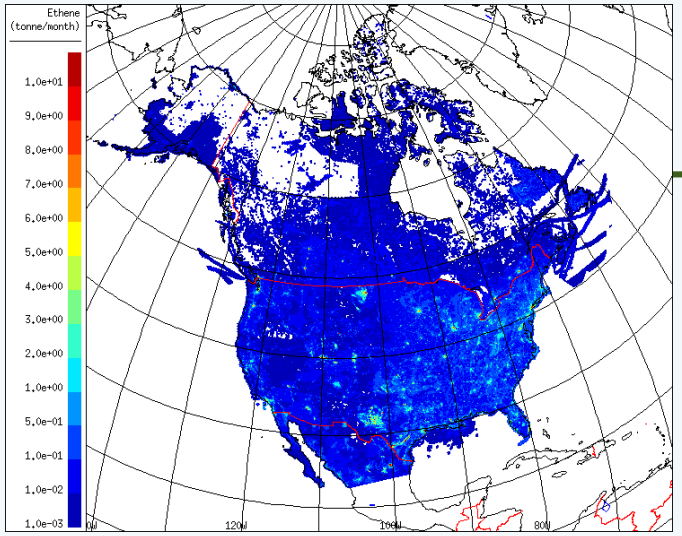
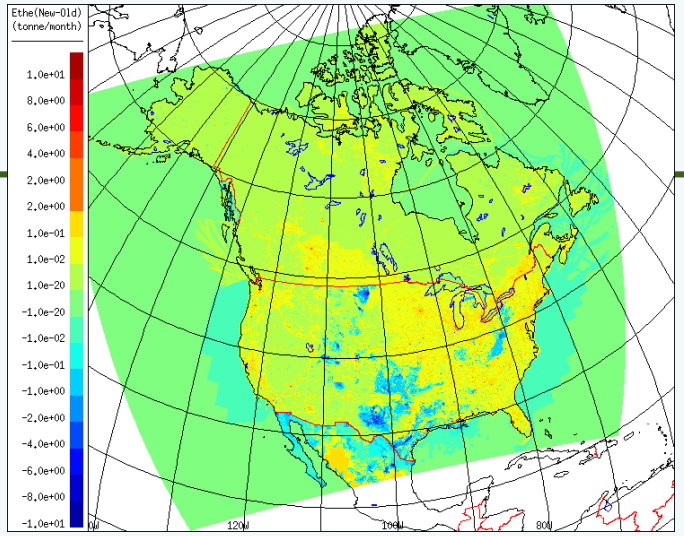
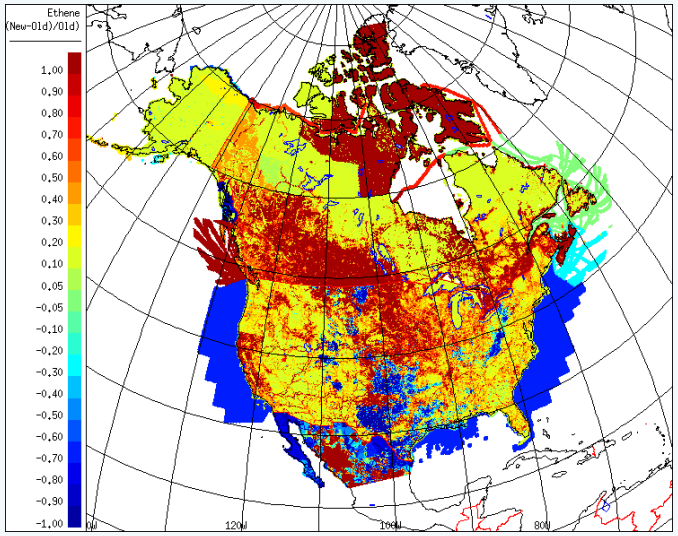


ETHE_Old_July_tonne



ETHE_New-Old_July_tonne



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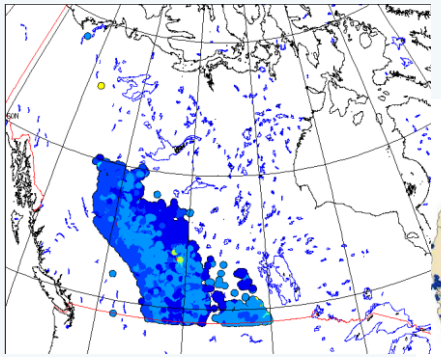
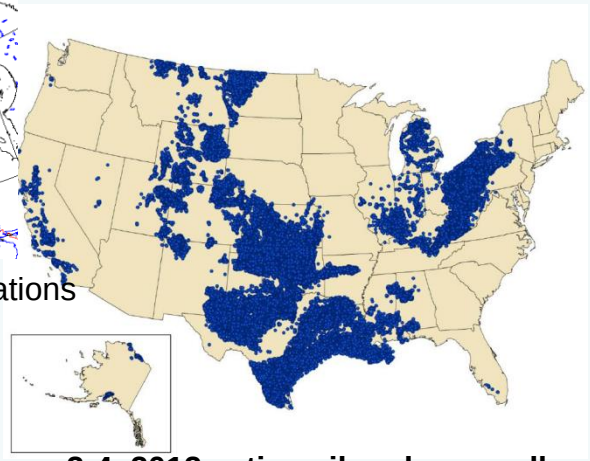


Canadian oil and gas well locations



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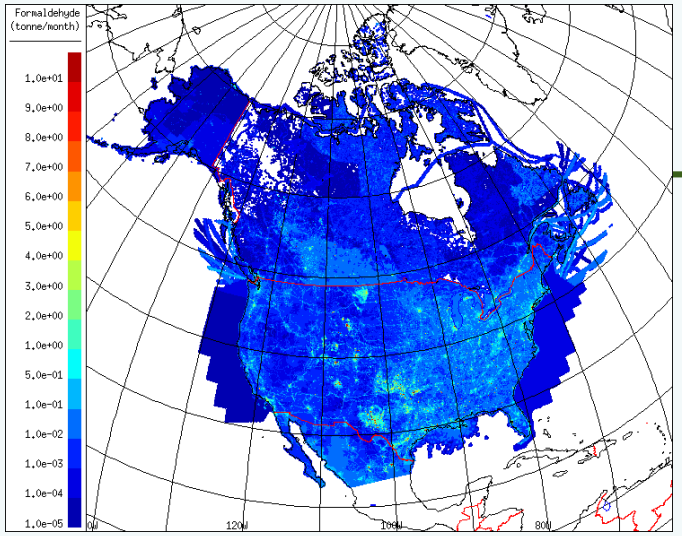
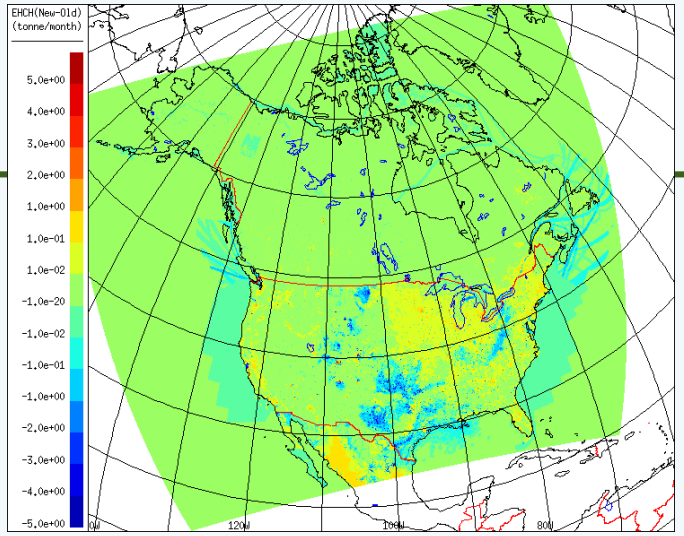
Adelman, Z., *Emissions Modeling Platform Spatial Surrogate Documentation, prepared for EPA, 2015*



HCHO_Old_July_tonne



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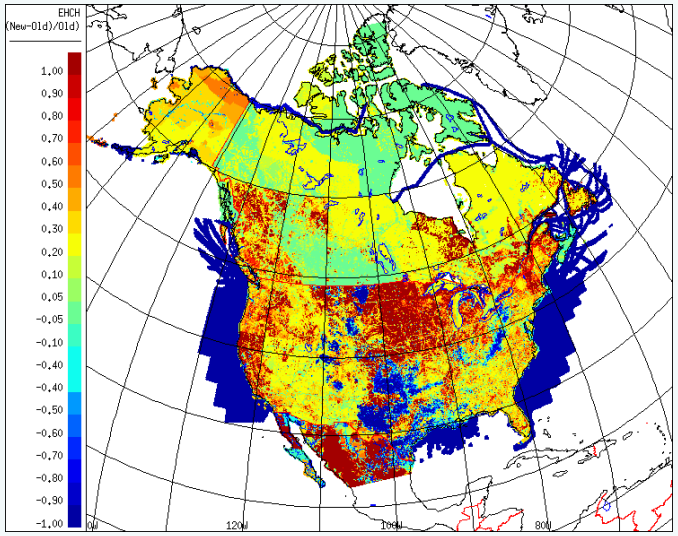

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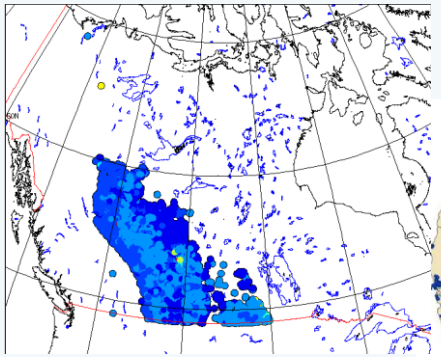

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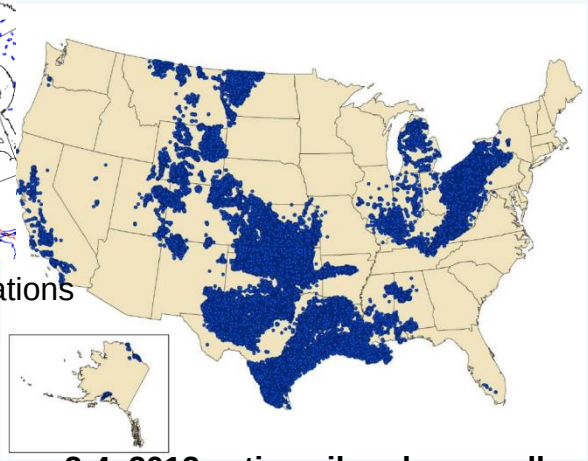

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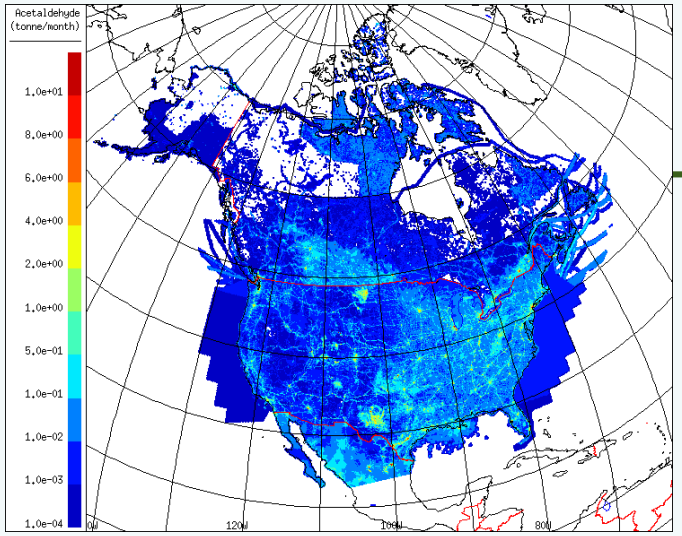
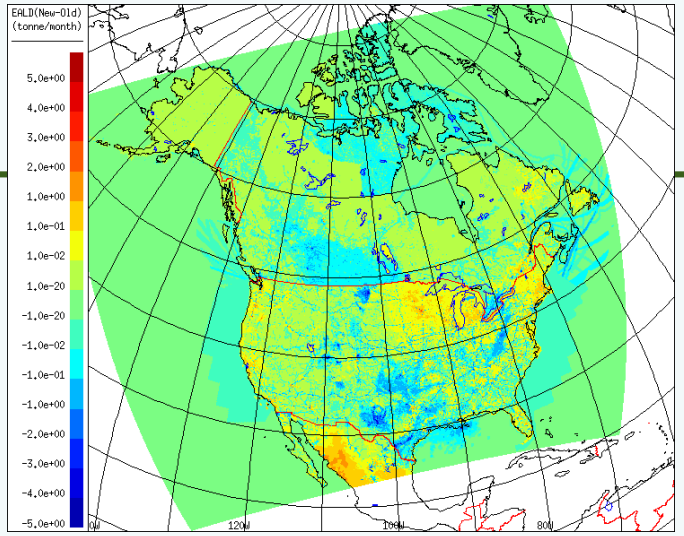


ALD2_Old_July_tonne



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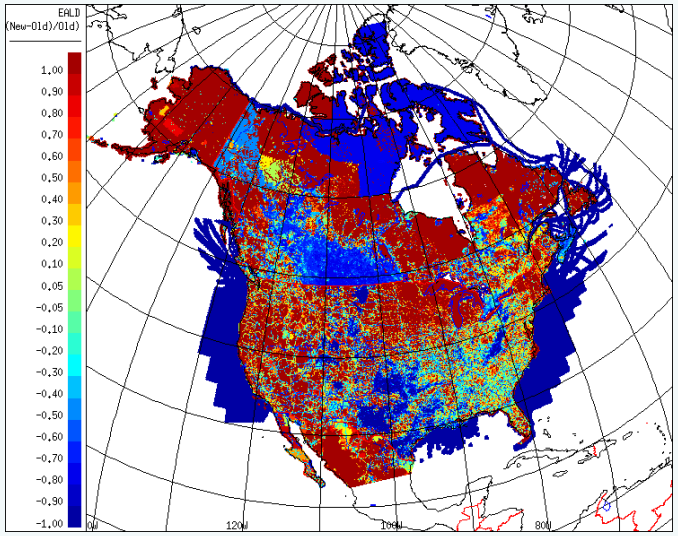

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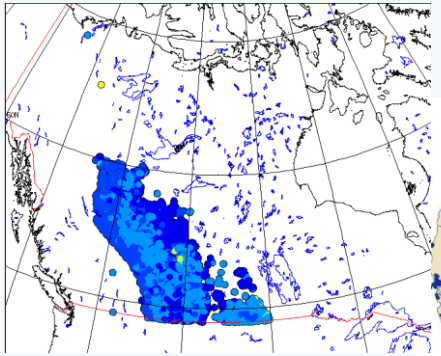

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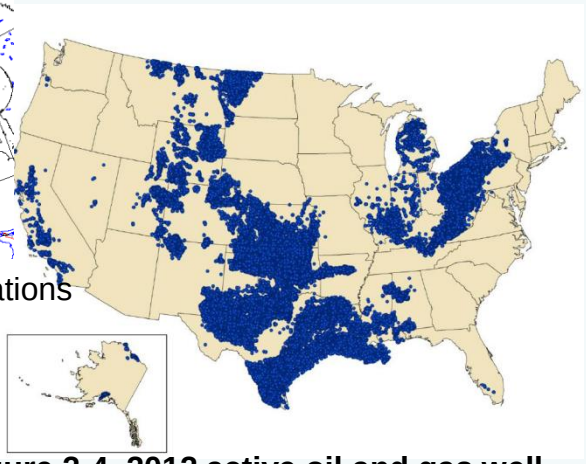

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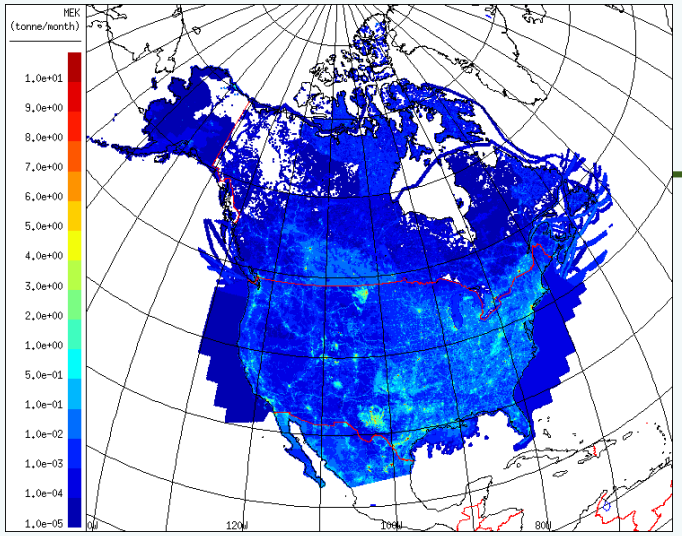

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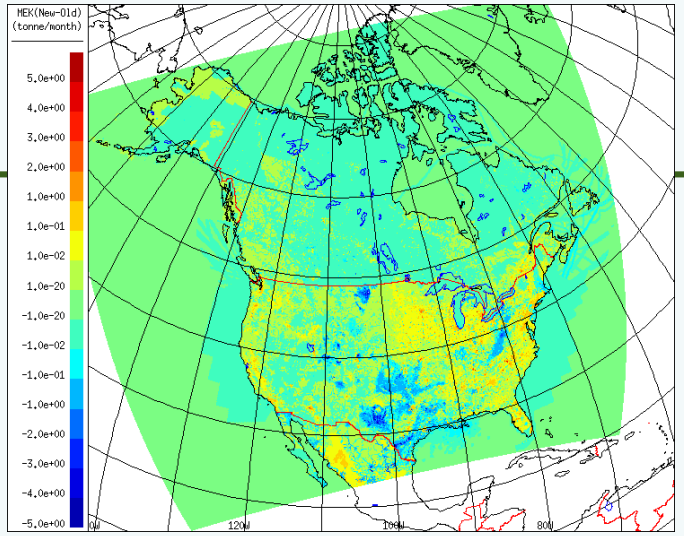

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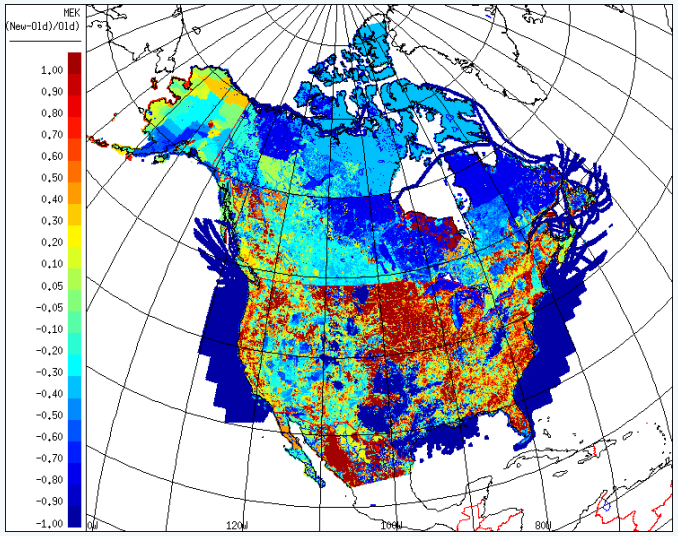

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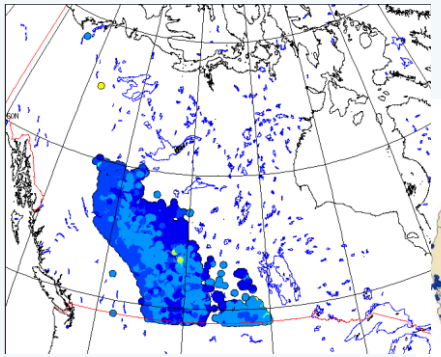

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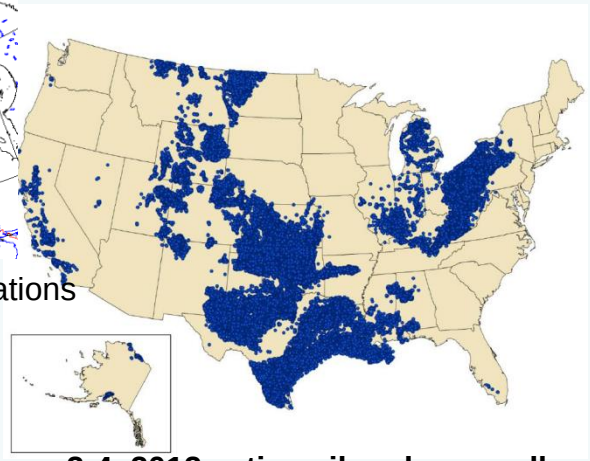

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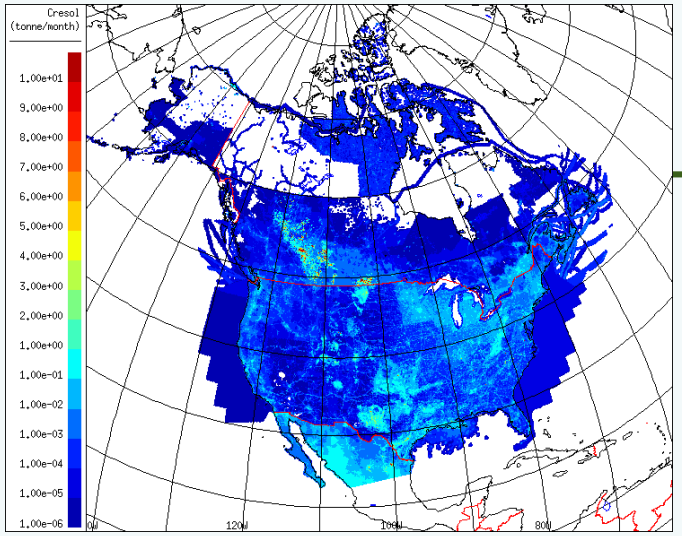
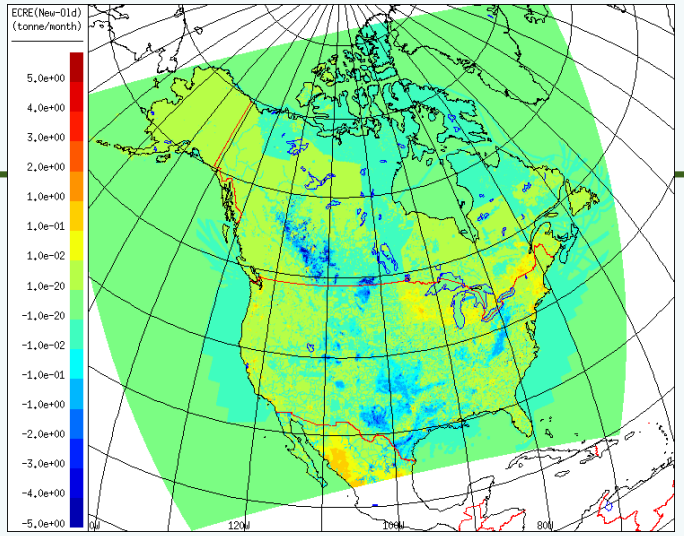


CRES_Old_July_tonne



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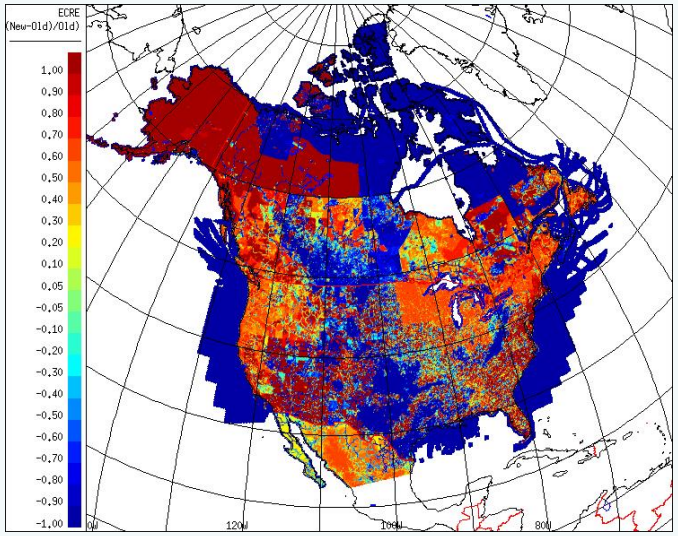

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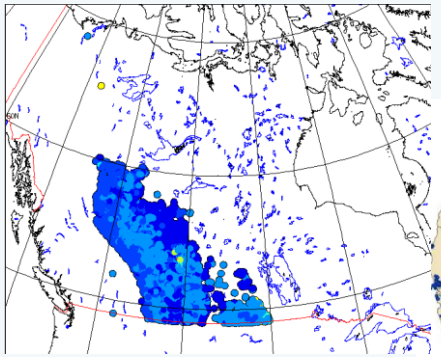
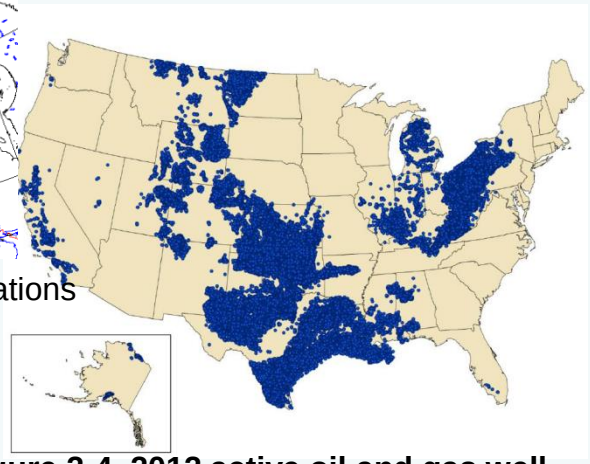


Canadian oil and gas well locations



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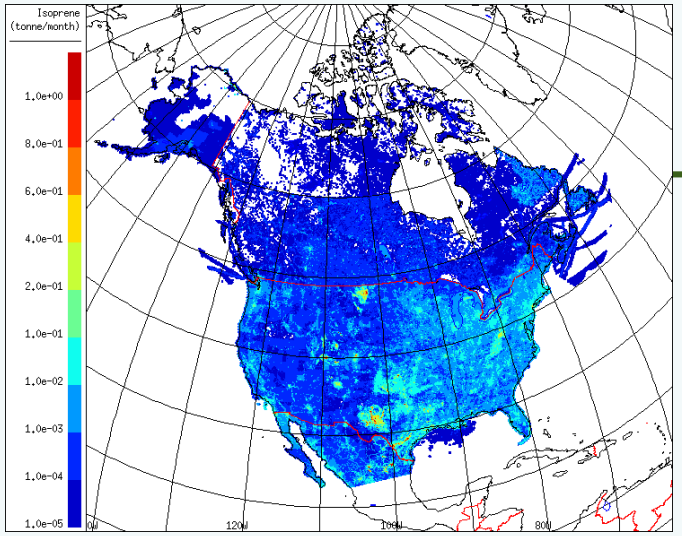
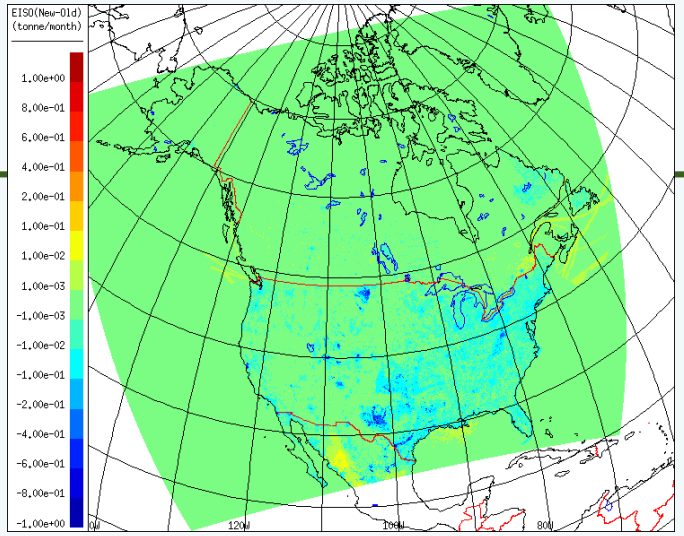


ISOP_Old_July_tonne



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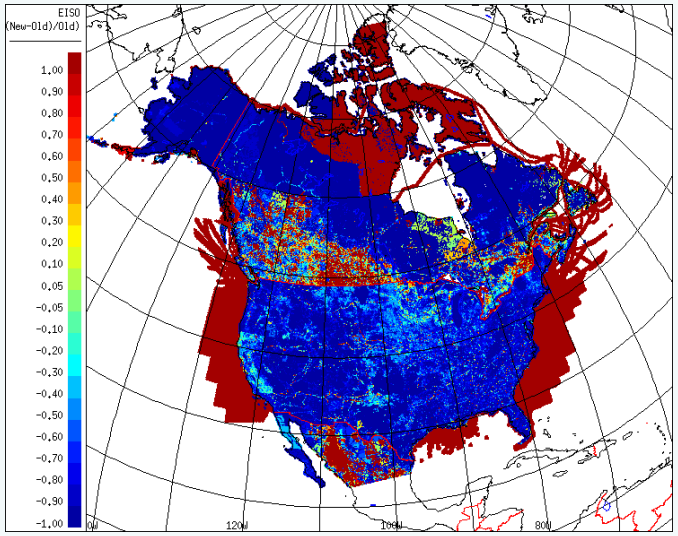

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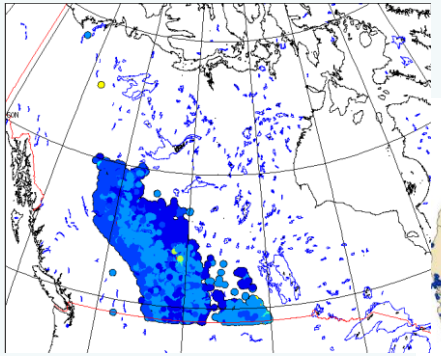

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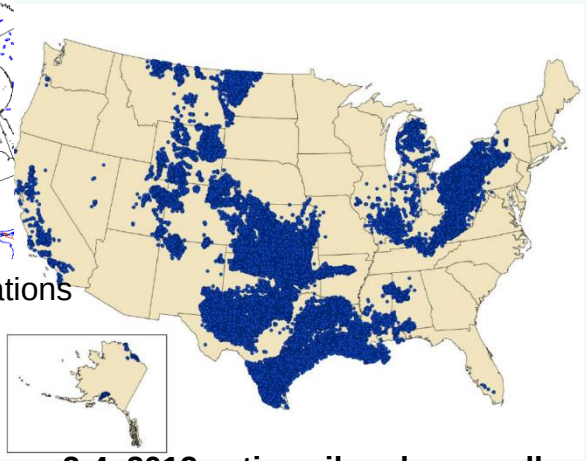

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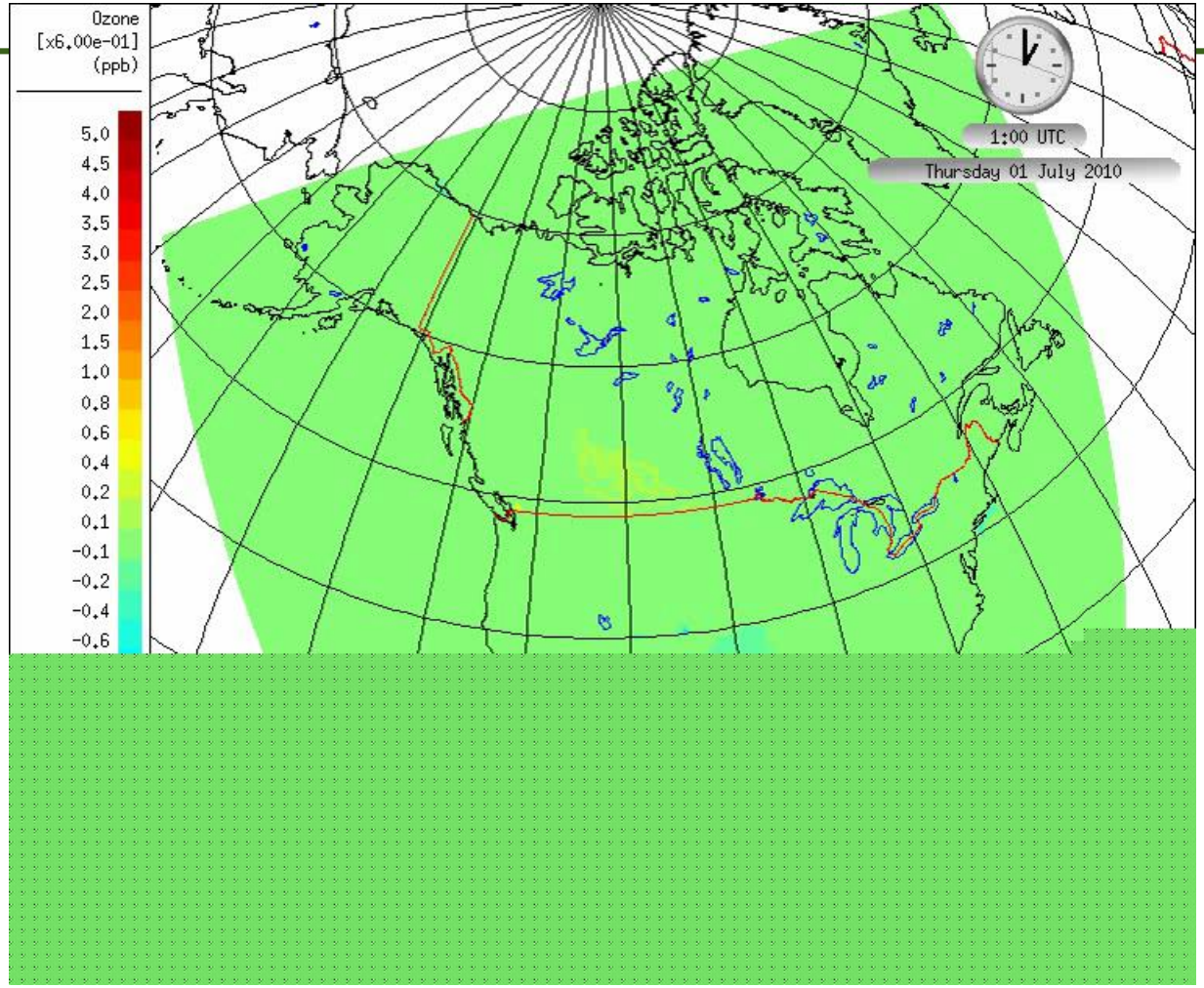
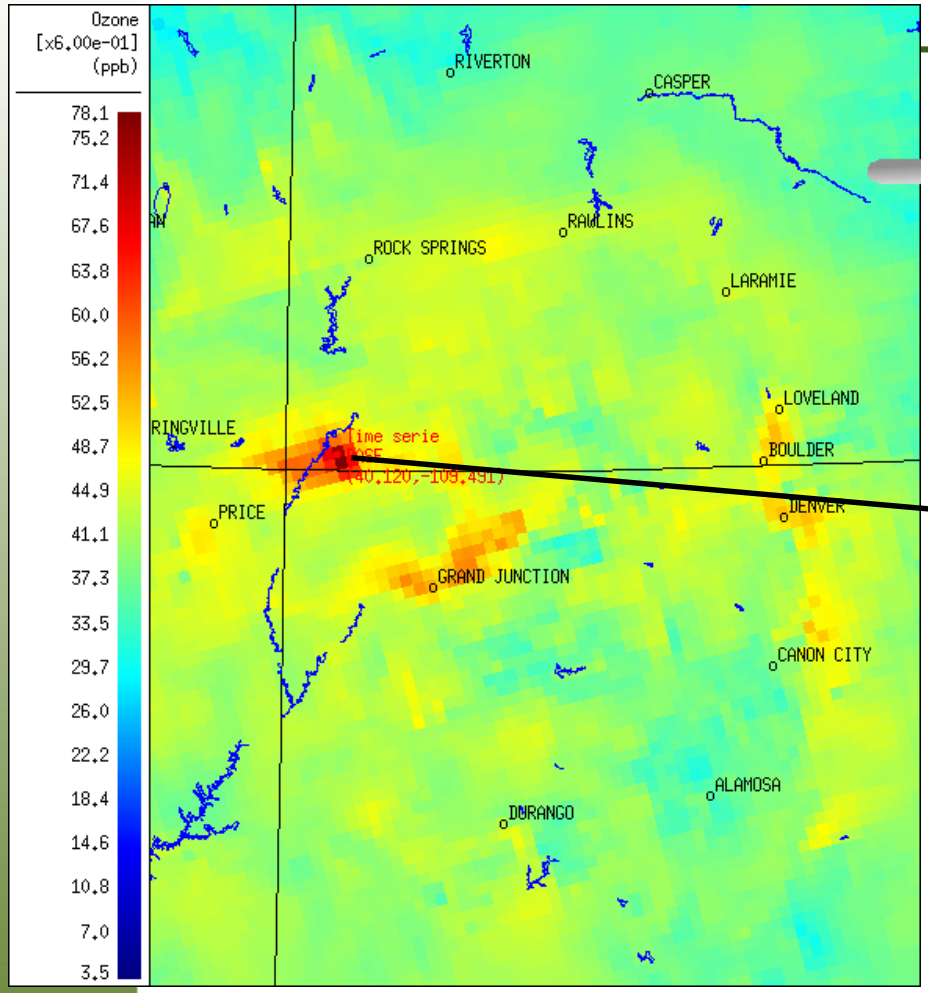
Impacts on AQ Model (GEM-MACH) Predictions of Gas and Particulate Species

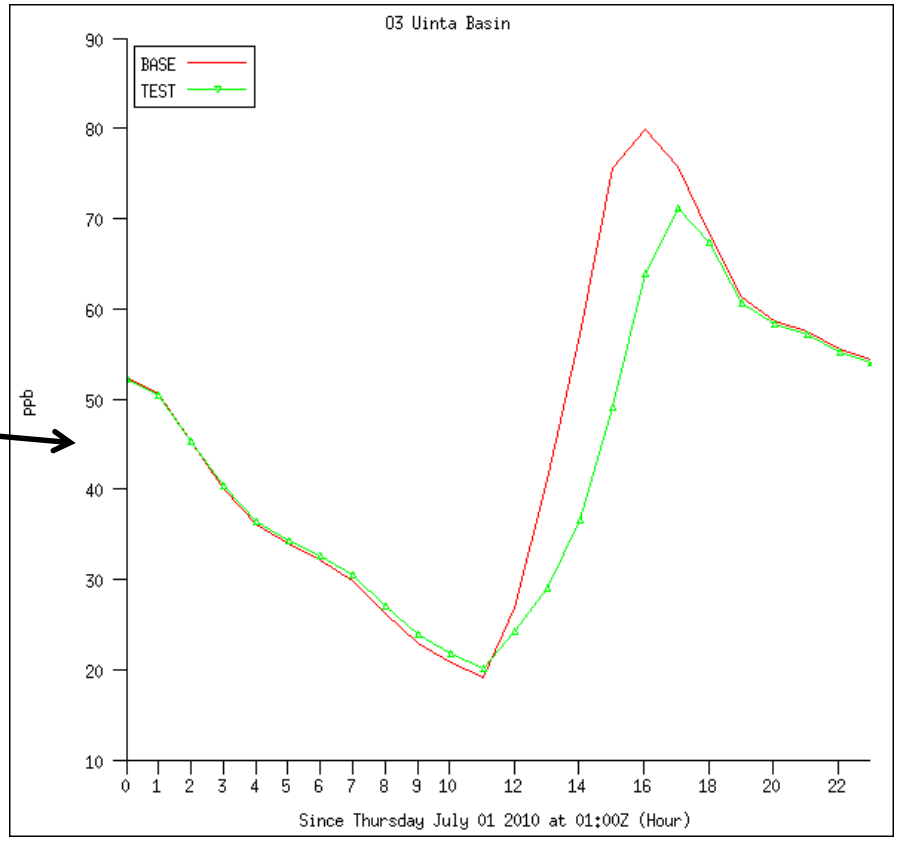
Gridded Average Hour-Specific Differences over 4-Week Summer Simulation

O3 Hourly Differences: TEST –BASE



O_3 Time Series over a Grid Cell in Uinta Basin, Utah





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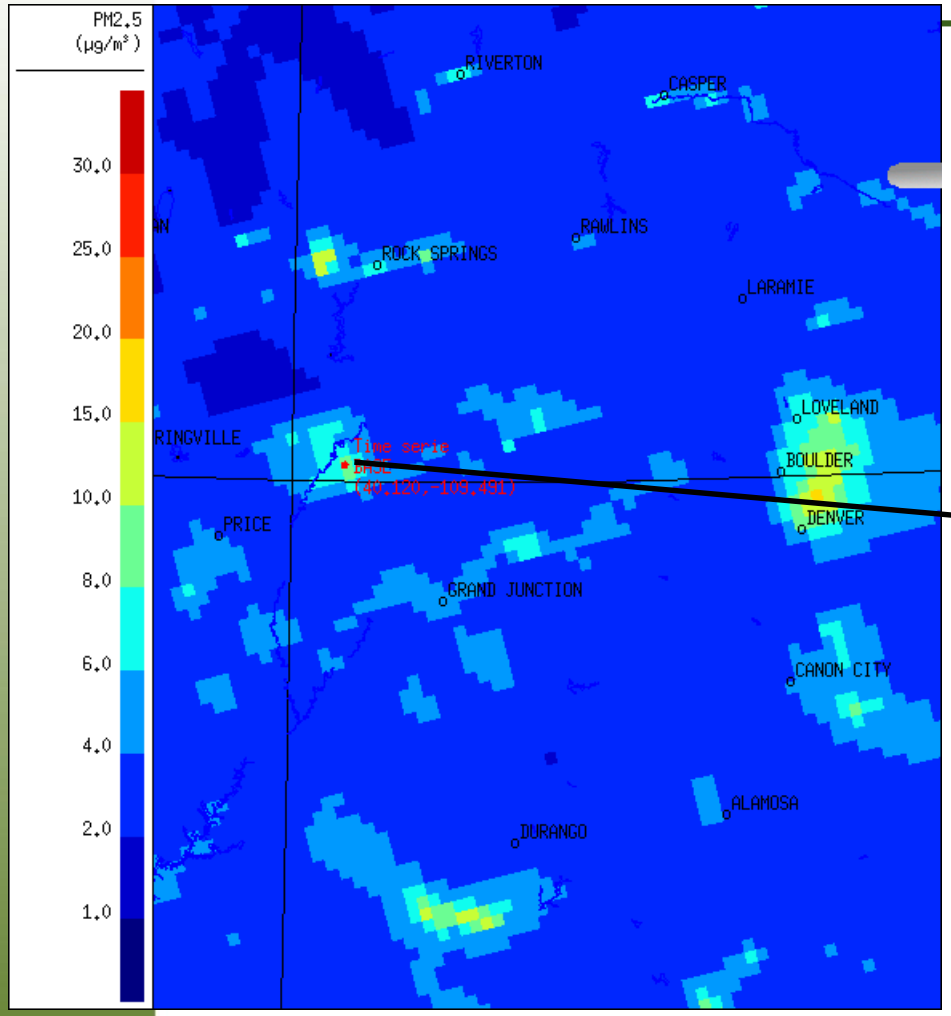
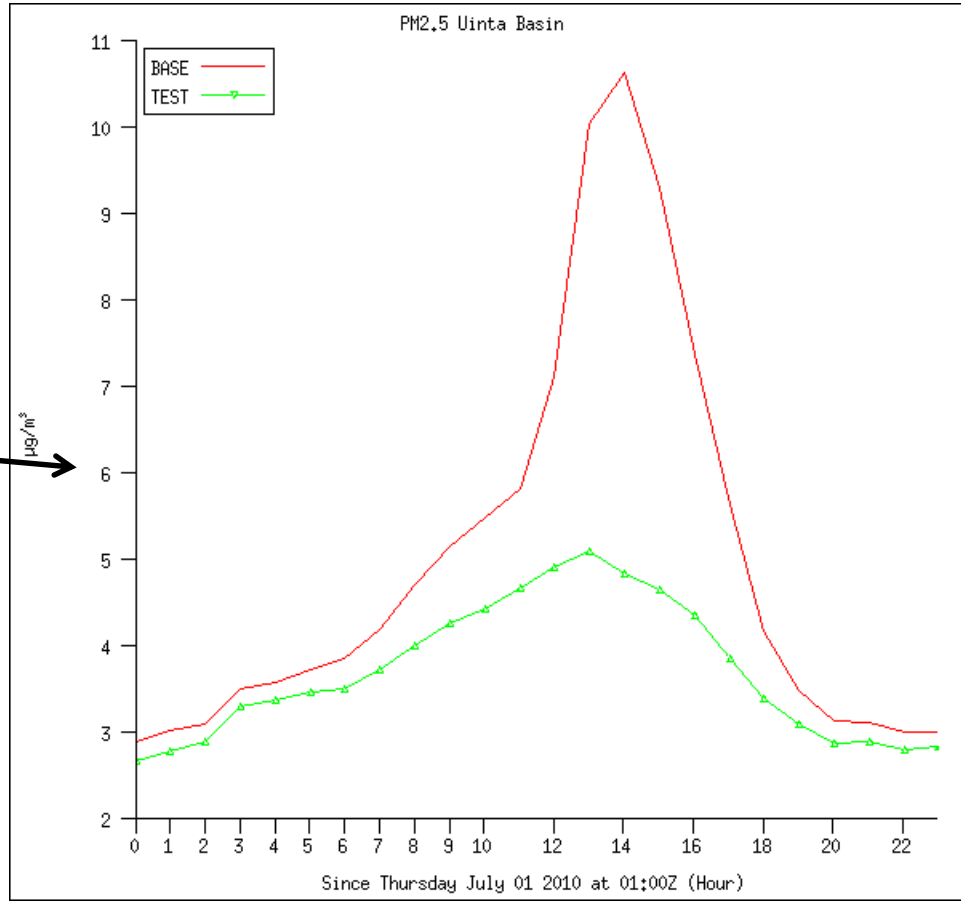
$PM_{2.5}$ Time Series over a Grid Cell in Uinta Basin, Utah





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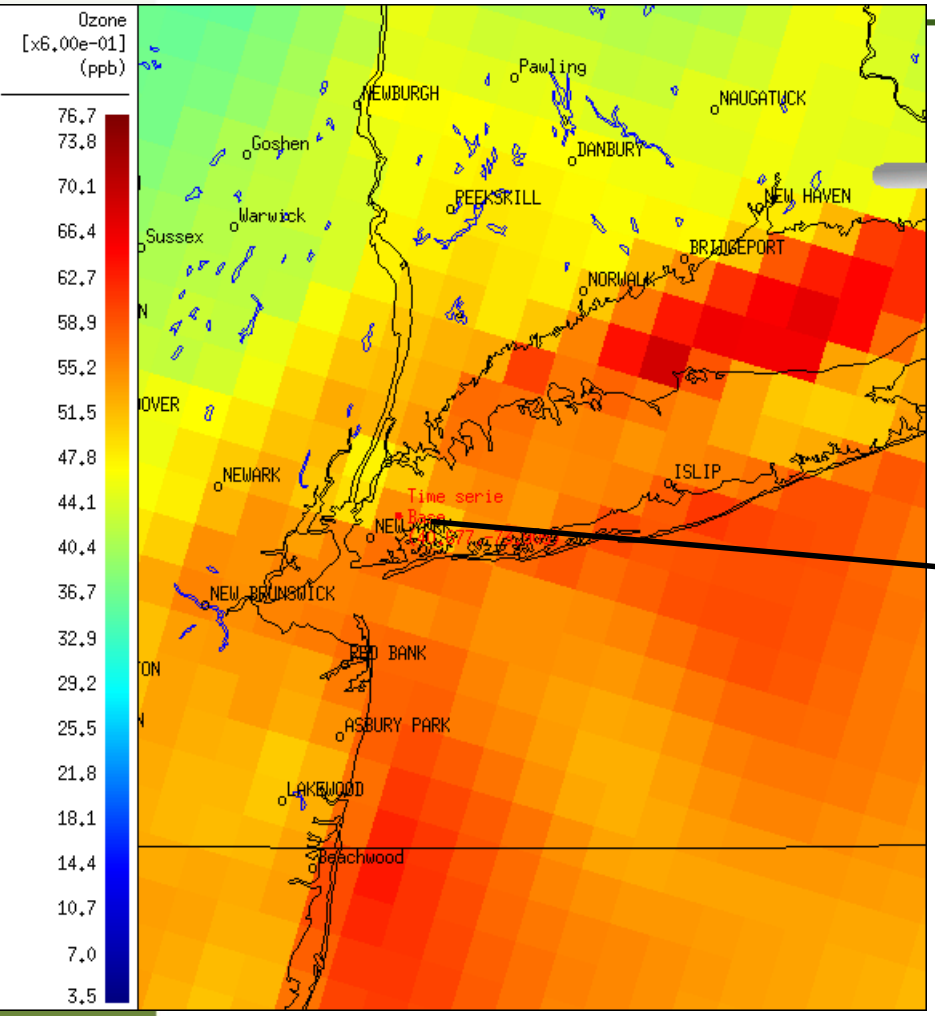
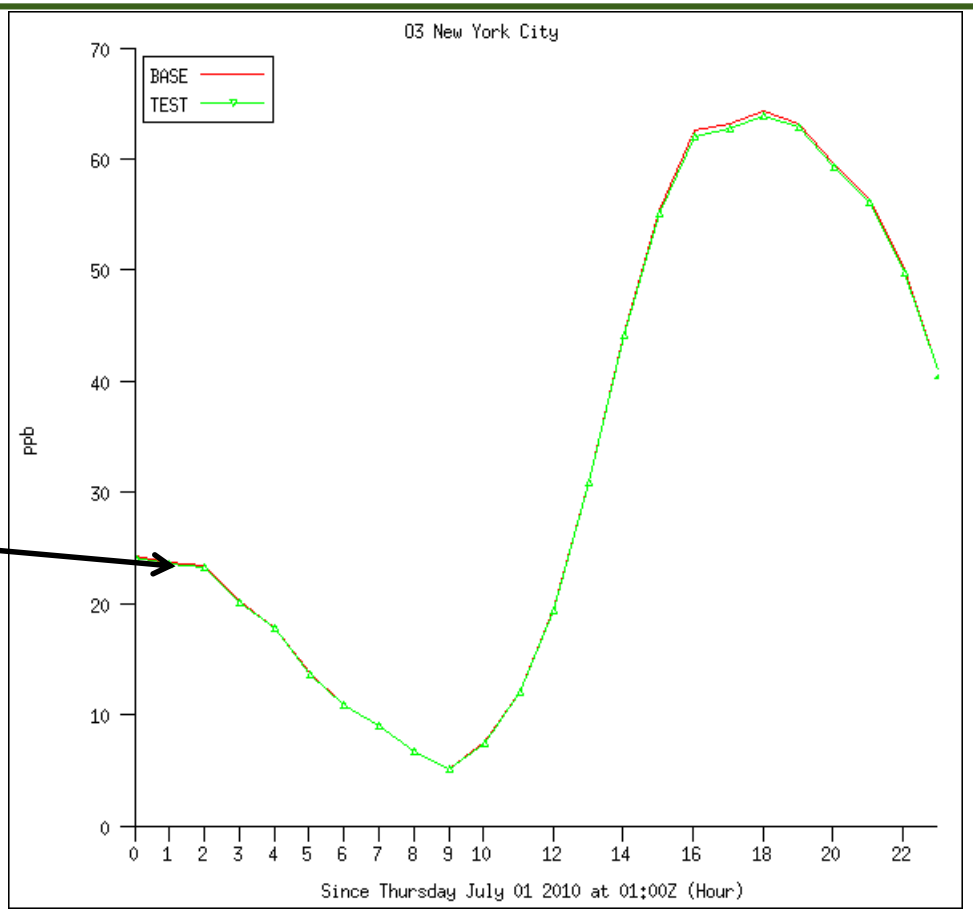
O_3 Time Series over a Grid Cell in New York City





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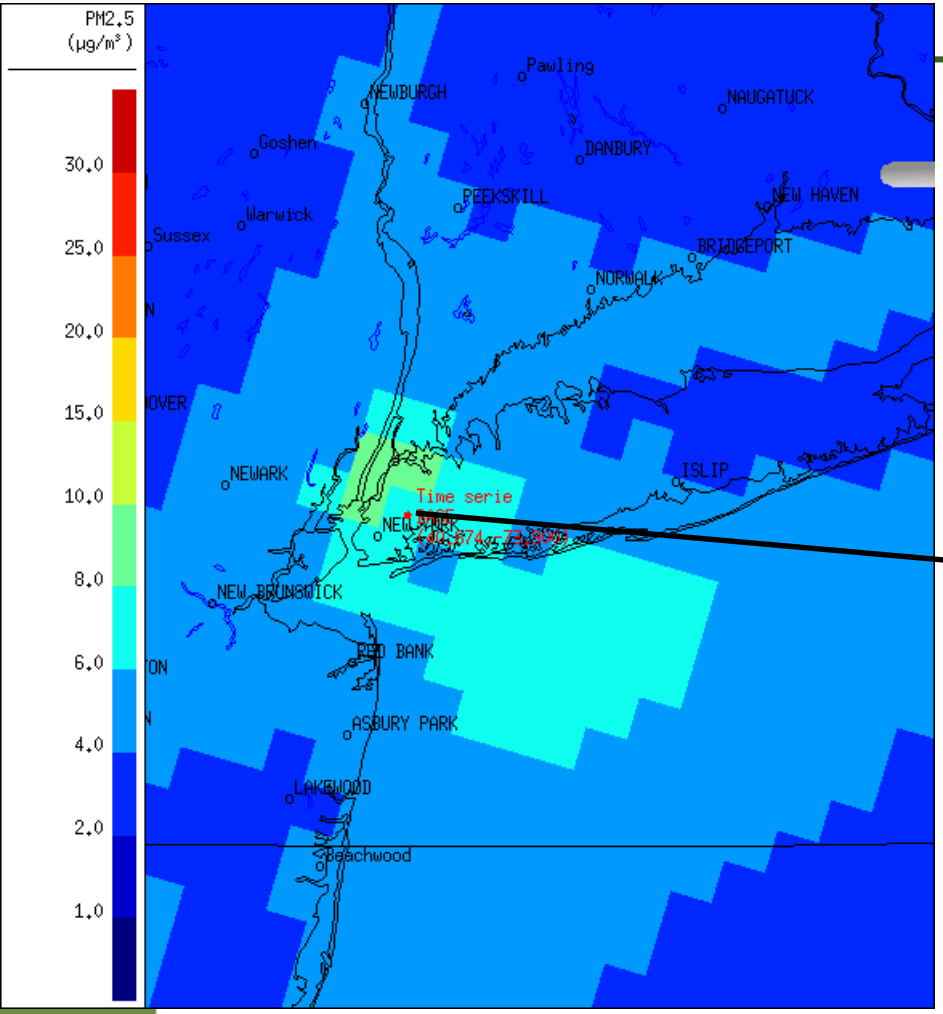
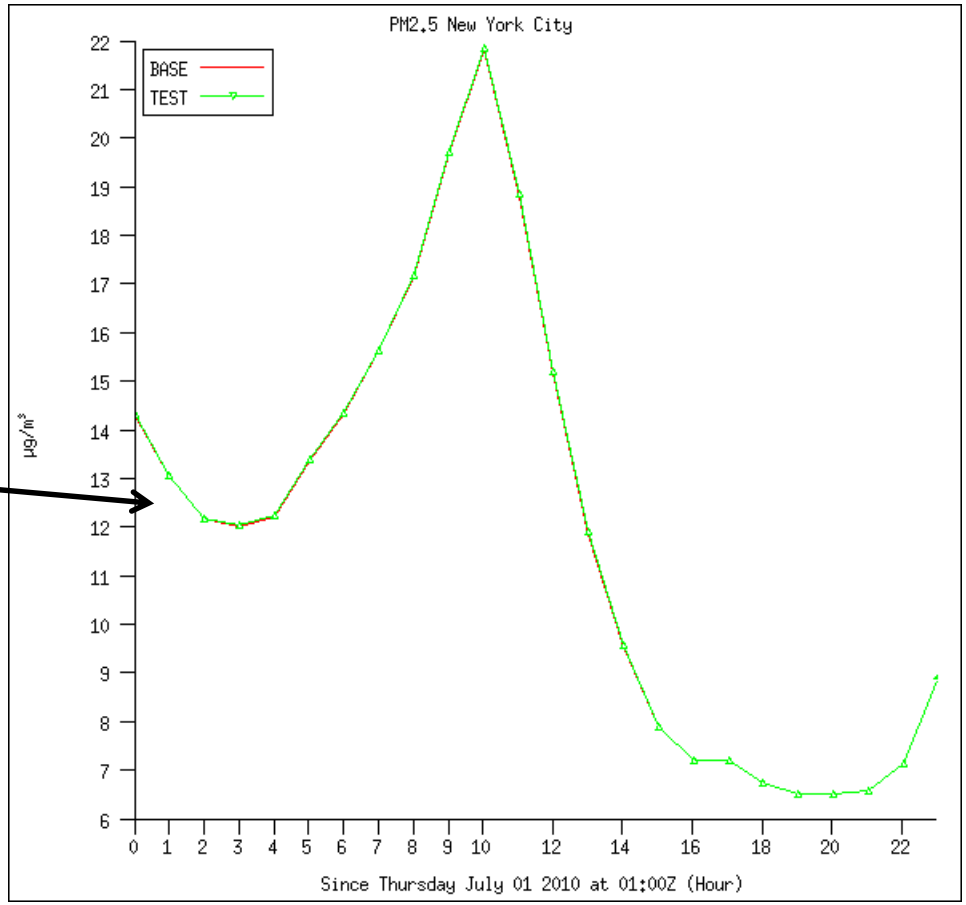
$PM_{2.5}$ Time Series over a Grid Cell in New York City





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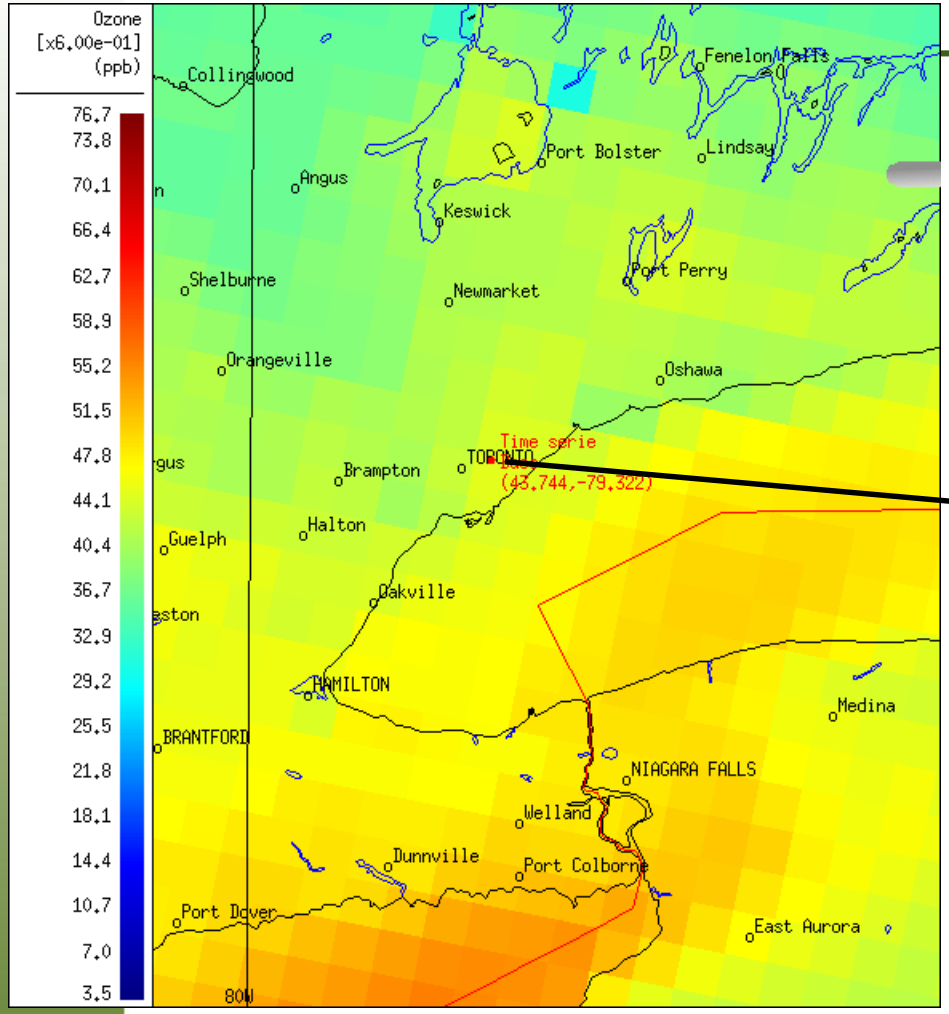
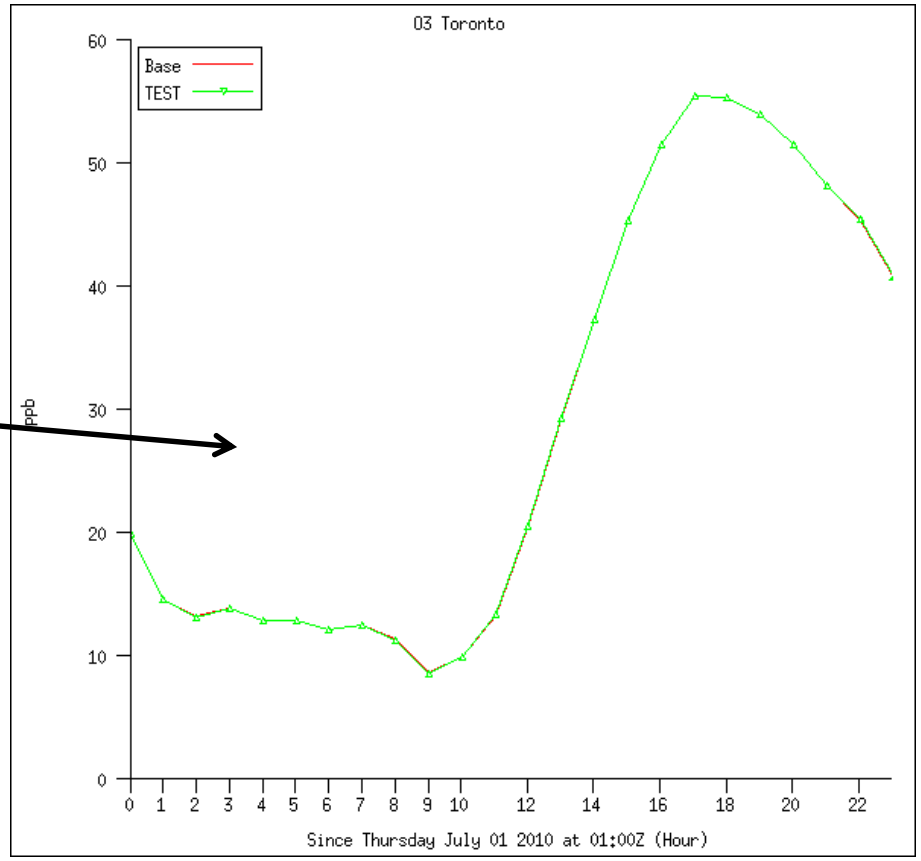
O_3 Time Series over a Grid Cell in Toronto, Ontario





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CONCLUSIONS

- Use of an updated VOC profile library significantly changes speciated VOC emissions for AQ modeling
- Oil and gas industry (38% and 27% of national total VOC emissions for Canada and U.S., respectively) is affected the most, while changes over large cities are also seen
- Changes to model VOC emissions have a significant impact on predicted O_3 and $PM_{2.5}$ concentrations locally, particularly over oil and gas fields
- Impact on AQ predictions for large cities is relatively small
- Comparison with observations remains to be done to evaluate changes to model performance for new VOC emissions (*16th CMAS Conference*, Oct. 23-25, 2017)

THANK YOU!

QUESTIONS?