Incorporation of Speciate 3.0 into EMS-2001

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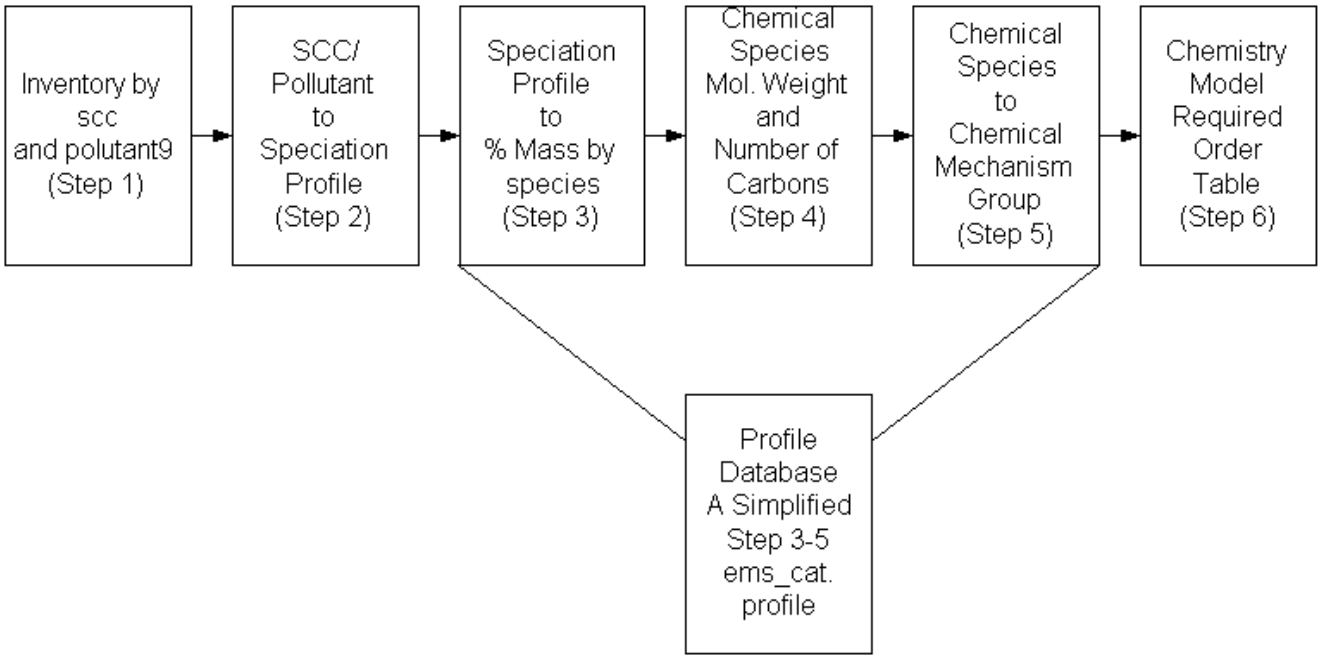
National Emissions Inventory Workshop
May 1-3, 2001
Denver Colorado

The purpose of this paper is to describe the implementation of the data in speciate 3.0 model with EMS-2001. Most of this paper will discuss data incorporation associated with Speciate 3.0 there will be some discussion of the results of modeling runs based on this work. Speciate 3.0 is the newest version of EPA's PC software for the searching and visualization of chemical speciation data for hydrocarbon(HC) and Particulate Matter (PM). Most users of the speciate model will use it to identify individual chemical species occurring from individual industrial point sources. Some users will need to use the data in Speciate to develop inputs for regional chemical transport models such as UAM-V, CAM-X or CMAQ. These models are used to simulate the transport, deposition, and transformation of chemicals in the air. To accurately reflect these processes the models requires an accurate inventory that is spatially resolved to a modeling grid cell, temporally resolved to the day of the modeling episode, and has chemical species which match the needs of the chemical mechanism of the chemical transport model.

Chemical mechanisms are simplifications of the complex chemical reactions in the atmosphere. This simplification is accomplished by grouping chemicals with similar photochemical properties into groups. The most common chemical mechanism used is Carbon Bond IV(CB-IV) It contains 11 hydrocarbon groups. In addition to the hydrocarbons, CB-IV classifies Nitric Oxide(NO), Nitrogen Dioxide(NO2) and Carbon Dioxide(CO) as discrete groups. The difficulty in using a chemical mechanism with any inventory is to group emissions inventory information into the groups required by the Chemical Mechanism. Diagram 1. Shows graphically how this is done within EMS-2001.

Figure 1.



The diagram shows that to create an inventory for the correct chemical mechanism there are 6 important pieces of information necessary. The first item is the inventory which has been classified by scc code or some equivalent. This could include Area source category code, On-road Vehicle Type(exhaust or evaporative), or simply the biogenics group. These emissions estimates are then merged with a table that references a chemical speciation profile for each scc code. An example of this is off-road Motorcycle Gasoline Hydrocarbon emissions maps to Speciation profile 1201(Gasoline Exhaust). This table can contain state or even plant specific speciation profiles. The next table defines the contents of each speciation profile by assigning weight percents by chemical species. An example of this table is speciation profile #1032. This profile contains 80.42% Acetaldehyde, and 19.58% Acrolene(propenal). Next, the model must know the molecular weight of each of the component species. This is because the model must convert from Grams in the inventory into Moles for the photochemical model. Next each species must be assigned to one or more chemical mechanism groups. It is possible to assign one species to several groups if it has the characteristics of multiple groups. An example of this is Acrolene from above, for every mole of Acrolene in the inventory there will be 1 mole of Paraffin(PAR) and 1 mole of High Molecular weight Aldehydes(ALD2). Finally, Many photochemical models require a specific order and number of pollutants be provided, Even if the inventory does not contain any emissions from that group. A table must be provided showing the order and content that the atmospheric chemistry model requires. Some Emissions models are unable to use the above tables directly but must rely on their creation elsewhere. This compressed version of the chemistry files appears very similar the EMS-2001 file ems_cat.profile.

Omission of any of the above components will result in incorrect speciation. Quality assurance throughout the process is important . Since EMS-95 already contained many of the processors capable of merging and building the above tables, most of the work of incorporating new data is assuring that complete data is available for every piece of data and that appropriate defaults are included where there are gaps.

Using the Speciate 3.0 Data.

This portion of the document will explain the LADCO implementation and methods used to identify and correct problems incorporating the National Emissions Inventory (NEI) version 3.11 with the Data in the speciate. After obtaining the NET inventory which is classified by SCC code for point and area sources and successfully run through EMS-95 and all data model interface problems were corrected with non-speciation data elements. LADCO began the incorporation by incorporating the SCC to speciation profile cross reference. The data set is named v_assign in Speciate3.0. This dataset lacks cross reference records for 204 SCC codes which are in the NEI inventory. The solution to this problem was to use the most commonly used speciation profile for the major SCC group. LADCO recognizes that it would be preferable to manually assign each of these speciation profiles. Table 1. Shows the result of applying the Speciate 3.0 default speciation profiles to industrial point and area sources in the NEI inventory. Several important facts can be gathered from this table, The first is that industrial point sources do not make the top 5 most used profiles, The second is that of the Top 10 most used profiles only 2(Architectural Coatings and Consumer Solvents) were created after 1990. Many of the dates on the older profiles were assigned and do not reflect the actual date of creation. These sources are using profiles as old as 20 years. It would be difficult to argue that in the past 20 years that solvent use has not changed

The next data set to be incorporated was the mass fraction data set. This dataset contains the percent of mass by profile for individual chemical species. Since chemical species can have any number of names, a coding scheme is necessary to define species, The two commonly used schema are SAROAD Codes and CAS Numbers. Speciate does contain information for both SAROAD and CAS, The problem is that it does not use one or the other consistently. Some profiles or species will contain CAS numbers, Others SAROAD, and still others will contain both sets of numbers. LADCO decided that since their were more profiles with SAROAD values and no table with CAS numbers could be found with good chemical mechanism data, that LADCO would continue to use SAROAD codes with the model, while making it capable of using CAS in the future. In situations where only CAS number was available, LADCO used CAS to SAROAD tables based on records in speciate where both numbers were used, and from manual assignment where other data was not available. This was not always possible since Speciate 3.0 classifies a significant mass of emissions to the SAROAD code 77777 and 99999 which are unidentified. Table 2. Show the most significant speciation profiles which classify some portion of their emissions as unidentified weighted by total VOC Mass in the NEI inventory. As we can see, There is a significant component of the inventory which can not be identified. It should also be recognized that many of the problem speciation profiles are greater than 10 years old.

Since the atmospheric chemistry models need Moles by chemical mechanism and the inventory and speciation profiles are based on mass. The inventory must be converted to Moles, based on a table of molecular weights. This table is part of EMS-95 and contains a fairly comprehensive list of species although for this project 10-20 species were updated with new information. The table also contains species name and is often used in reporting.

The next step in incorporating the speciation data is to classify each chemical species into its Chemical Mechanism group. Each species must be classified to at least on group. Many species have characteristics which make it react in the atmosphere like one or more groups. The table used for this

is contained in within EMS-95 and is not part of Speciate3.0 and converts moles to moles. The species to mechanism cross reference been modified over the past 8 years to reflect new chemical species when new profiles were incorporated into the model, but does not contain an exhaustive list of all chemical species classified under either SAROAD or CAS. After incorporating this data LADCO identified a number of species which were included in Speciate 3.0 which were not identified in the species to mechanism cross reference. LADCO improved the table to fix the most problematic species where a significant portion of a profile had species which were not capable of being mapped to a mechanism group. All species which could not be matched to a CBIV group were removed from the profiles, including any species classified as "unidentified", and the speciation profile was normalized so that the mass fractions of the remaining species summed to one. In the future, LADCO will re-classify all species which were not mapped to a Mechanism group as unidentified(SAROAD=99999) and then use the traditional Species to mechanism.. traditional method assigns 6 moles of Paraffin to the model for every mole of unidentified. The rest of this document will use the older method where unidentified will be thrown out.

Finally, Each mole of a chemical mechanism group must be put into some file formatted to be read by the atmospheric chemistry model, these models tend to be inflexible and require a specific order and number of species, For example, some models need PM, NH4 and Sulphates, event if the modeler only intends to run only ozone modeling. This requires the creation table of all require species and the order which they must appear in any output files

After incorporation and modeling of this data, LADCO did show change in the modeling results, Figure 2. show the impact of Speciate 3.0 as compared to the older data used in EMS-95. This table shows increases in the 1 to 4 PPB range in some areas while there was very little ozone decrease because of the new data. Figure 3. Shows the results of changing speciation profiles for the on-road and off-road speciation profiles to one more reflective of Midwest motor-vehicles. All occurrences of speciation profile 1301 in were changed to speciation profile 2446(Evaporative) and speciation profile 1203 was replaced with 2533(Exhaust). These profiles were chosen based on their similarity to Tunnel studies in Milwaukee Wisconsin in 1999. The results of these runs indicate that changes to profiles changed modeling results as high as 8 PPB ozone in selected areas.

Conclusions:

The conclusion of this work indicates that speciate 3.0 is an important move forward, but that new data is necessary to characterize emissions correctly for modeling. The results of this analysis show 3 important future products.

1. Many of important profiles are old enough to consider them problematic. News profiles are necessary.
2. The current species to chemical mechanism databases are incomplete and to be updated.
3. Use of the default speciation profiles is not recommended for important categories.

13:37 Tuesday, December 12, 2000

OBS	Profile NAME	QUALITY	CONTROLS	Profile Number	Tons/Day (NEI)	Profile Created
1	Light Duty Gasoline Vehicles -	B	Catalyst	1101	7406.60	01/05/89
2	Architectural Coatings (Solven			6003	4569.95	07/01/99
3	Miscellaneous Burning - Forest	C	Uncontrolled	0307	3023.07	01/05/89
4	Gasoline Marketed - Summer Ble	B	Uncontrolled	1190	2991.10	01/05/89
5	Heavy Duty Gasoline Trucks	C	Uncontrolled	1186	2350.71	01/05/89
6	Degreasing Composite	B	Uncontrolled	1195	2098.91	01/05/89
7	Consumer and Commercial Produc	A	Not Applicable	8520	1968.36	08/01/98
8	Light-Duty Diesel Vehicles	C	Uncontrolled	1201	1909.39	01/05/89
9	General Pesticides	C	Uncontrolled	0076	1390.33	01/05/89
10	Surface Coating Operations - A	C	Direct flame in	1088	1296.74	01/05/89
11	Consumer and Commercial Produc	A	Not Applicable	8523	1063.23	08/01/98
12	Mineral Products - Asphaltic C	C	Uncontrolled	1007	921.42	01/05/89
13	Autobody Repair	B	Uncontrolled	1194	748.42	01/05/89
14	Consumer and Commercial Produc	A	Not Applicable	8501	727.51	08/01/98
15	Chemical Manufacturing - Avera	E	Not Applicable	9004	722.13	01/05/89
16	Wood Furniture	B		2405	695.06	07/01/99
17	Graphic Arts Coatings - 1996			2432	666.29	07/01/99
18	Consumer and Commercial Produc	A	Not Applicable	8511	551.79	08/01/98
19	Open Burning Dump - Landscape/	C	Uncontrolled	0121	550.74	01/05/89
20	Can Coating	B		2408	513.84	07/01/99
21	Oil and Gas Production - Avera	E	Not Applicable	9015	502.21	01/05/89
22	Petroleum Industry - Average	E	Not Applicable	9012	415.30	01/05/89
23	Pulp and Paper Industry - Aver	E	Not Applicable	9013	411.76	01/05/89
24	Consumer and Commercial Produc	A	Not Applicable	8535	353.97	08/01/98
25	Surface Coating Primer - Napth	E	Uncontrolled	0282	333.58	01/05/89
26	Metal Furniture	B		2406	331.08	07/01/99
27	Industrial Maintenance	B		2418	292.92	07/01/99
28	Solid Waste Landfill Site - Cl	C	Uncontrolled	0202	292.74	01/05/89
29	Electrical Insulation	B		2410	285.80	07/01/99
30	Food and Agriculture - Average	E	NOT APPLICABLE	9008	285.07	01/05/89
31	Residential Wood Combustion	C	Uncontrolled/Ca	1167	263.03	01/05/89
32	Traffic Markings	B		2403	262.95	07/01/99
33	Surface Coating Operations - A	E	Not Applicable	9021	235.01	01/05/89
34	Perchloroethylene - Dry Cleani	E	Uncontrolled	0085	232.70	01/05/89
35	Solid Waste - Animal Waste Dec	C	Uncontrolled	0203	230.71	01/05/89
36	Aircraft Landing/Takeoff (LTO)	B	Uncontrolled	1098	226.72	01/05/89
37	Bar Screen Waste Incinerator	D	Uncontrolled	0122	221.26	01/05/89
38	Internal Combustion Engine - N	C	Not reported	1001	213.49	01/05/89
39	Auto Refinishing	B		2402	201.97	07/01/99
40	Gasoline Headspace Vapors (Unb			6000	198.61	07/01/99
41	Printing Press - Gravure Gener	C	Uncontrolled	0182	198.20	01/05/89
42	Consumer and Commercial Produc	A	Not Applicable	8500	192.45	08/01/98
43	Paper, Foil, Film	B		2407	184.31	07/01/99
44	Industrial Processes - Average	E	Not Applicable	9003	182.91	01/05/89
45	External Combustion Boiler - N	B	Uncontrolled	0003	178.25	01/05/89

Table 2. Lost Emissions Due to chemical species with Bad Species codes or No CB-IV data.
13:31 Tuesday, December 12, 2000

OBS	NAME	QUALITY	CONTROLS	Profile Number	VOC Tons/Day	Profile Created	Mass Fraction	Mass Lost
1	Miscellaneous Burning - Forest	C	Uncontrolled	0307	2936.28	01/05/89	0.46414	1362.85
2	Consumer and Commercial Produc	A	Not Applicable	8520	1968.36	08/01/98	0.39489	777.28
3	Degreasing Composite	B	Uncontrolled	1195	2047.34	01/05/89	0.36633	750.01
4	Light Duty Gasoline Vehicles -	B	Catalyst	1101	7406.60	01/05/89	0.09763	723.11
5	Graphic Arts Coatings - 1996			2432	646.24	07/01/99	0.72253	466.93
6	Consumer and Commercial Produc	A	Not Applicable	8523	1063.23	08/01/98	0.41237	438.44
7	Consumer and Commercial Produc	A	Not Applicable	8511	551.79	08/01/98	0.50991	281.36
8	Architectural Coatings (Solven			6003	4313.23	07/01/99	0.05233	225.72
9	Electrical Insulation	B		2410	285.80	07/01/99	0.73679	210.57
10	Heavy Duty Gasoline Trucks	C	Uncontrolled	1186	2344.25	01/05/89	0.06281	147.23
11	General Pesticides	C	Uncontrolled	0076	1389.33	01/05/89	0.10384	144.27
12	Consumer and Commercial Produc	A	Not Applicable	8501	727.51	08/01/98	0.13442	97.79
13	Light-Duty Diesel Vehicles	C	Uncontrolled	1201	1899.05	01/05/89	0.04631	87.95
14	Wastewater Treatment Plants -			2542	102.49	07/01/99	0.85687	87.82
15	Consumer and Commercial Produc	A	Not Applicable	8535	353.97	08/01/98	0.22286	78.88
16	Consumer and Commercial Produc	A	Not Applicable	8500	192.45	08/01/98	0.35039	67.43
17	Traffic Markings	B		2403	262.95	07/01/99	0.20493	53.89
18				NONE	38.35	.	1.00000	38.35
19	Chemical Manufacturing - Avera	E	Not Applicable	9004	220.87	01/05/89	0.12411	27.41
20	Can Coating	B		2408	438.82	07/01/99	0.06087	26.71
21	Wastewater Treatment Plants -			2541	27.06	07/01/99	0.91930	24.88
22	Industrial Maintenance	B		2418	292.92	07/01/99	0.07603	22.27
23	Wood Furniture	B		2405	526.71	07/01/99	0.03605	18.99
24	Metal Furniture	B		2406	177.39	07/01/99	0.10136	17.98
25	Residential Wood Combustion	C	Uncontrolled/Ca	1167	263.03	01/05/89	0.03693	9.71
26	Drycleaning Composite	B	Uncontrolled	1196	53.64	01/05/89	0.17868	9.58
27	Auto Refinishing	B		2402	201.97	07/01/99	0.04443	8.97
28	Paper, Foil, Film	B		2407	83.69	07/01/99	0.06714	5.62
29	Over All Average	E	NOT APPLICABLE	0000	69.32	10/03/94	0.07834	5.43
30	Appliances	B		2411	55.05	07/01/99	0.08058	4.44
31	Pulp and Paper Industry - Aver	E	Not Applicable	9013	7.18	01/05/89	0.52710	3.79
32	Marine Paints	B		2415	54.98	07/01/99	0.04731	2.60
33	Aircraft	B		2414	29.49	07/01/99	0.07273	2.14
34	Autobody Repair	B	Uncontrolled	1194	605.97	01/05/89	0.00318	1.93
35	Organic Chemical Storage - Ave	E	Not Applicable	9028	14.76	01/05/89	0.06154	0.91
36-72	Deleted for Report length							
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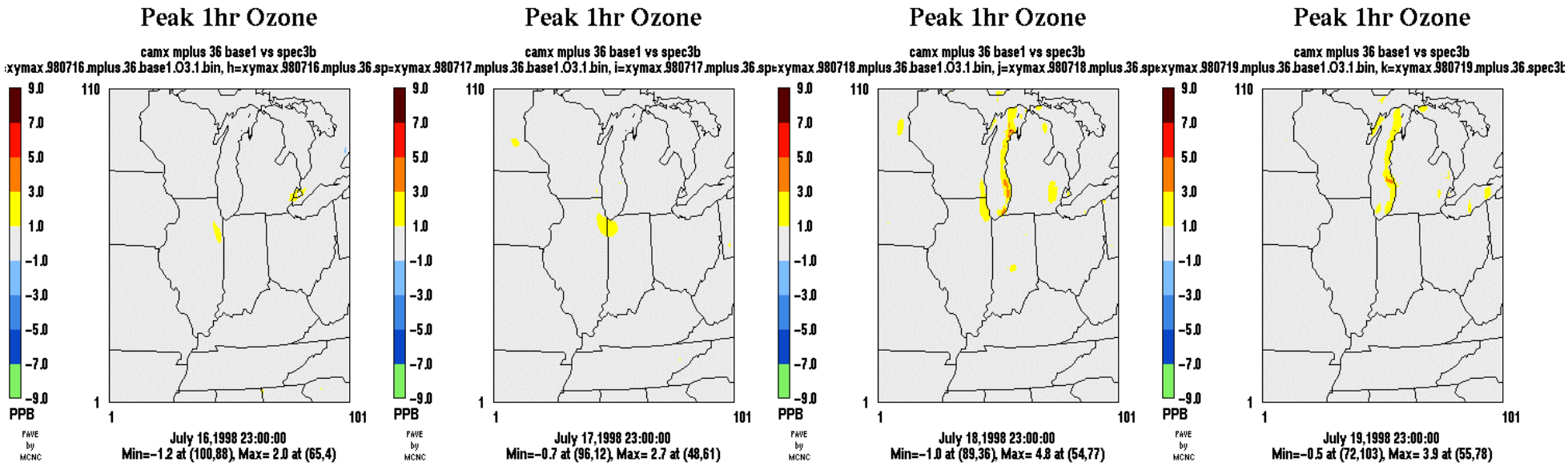
								40114.00

Figure 2. Ozone Difference Peak Plots, Speciate 3.0 Minus EMS-95 Data.



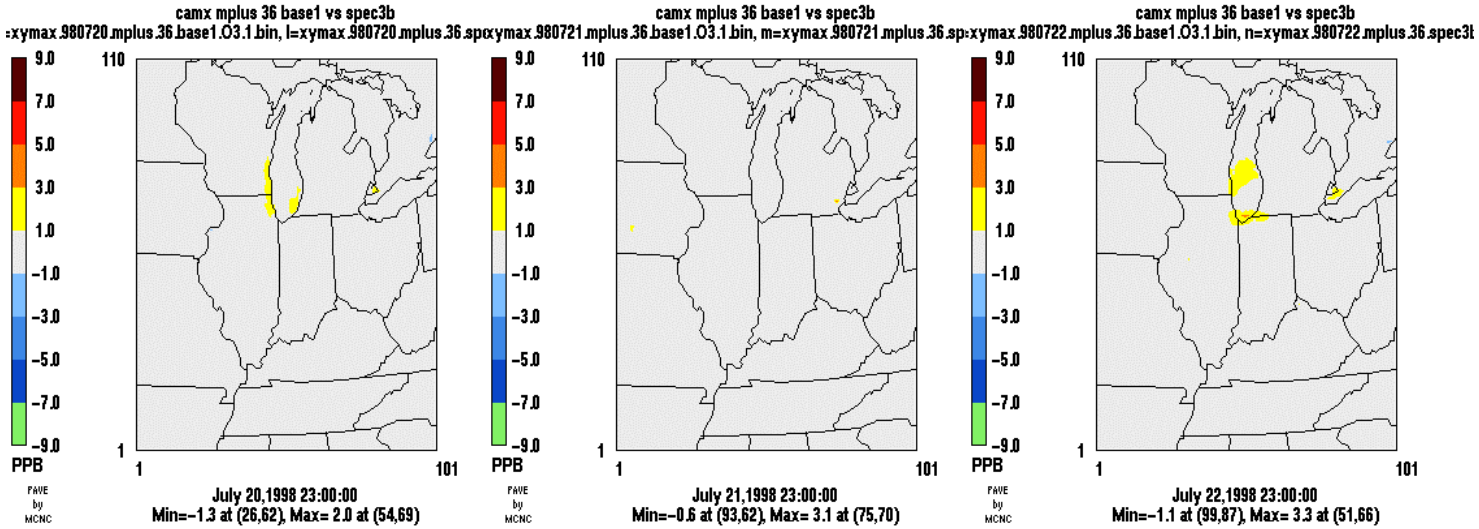


Figure 3. Ozone Difference Peak Plots, Hot MV minus Speciate 3.0