# *Incorporation of Speciate3.0 into EMS-2001*

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# *Background*

- EMS-2001 : A processor/model to create emissions estimates for Chemical Transport Models(UAM-V/CAM-X/CMAQ)

- Models have one or more Chemical Mechanisms.

- Inventory VOC,NMOC,HC estimates must be converted into the Correct Chemical Mechanism

# *Chemical Mechanisms*

- CB-IV and SAPRC are common

- Different "Flavors" of each mechanism

- Approximations of atmosphere
  - too much to model each species

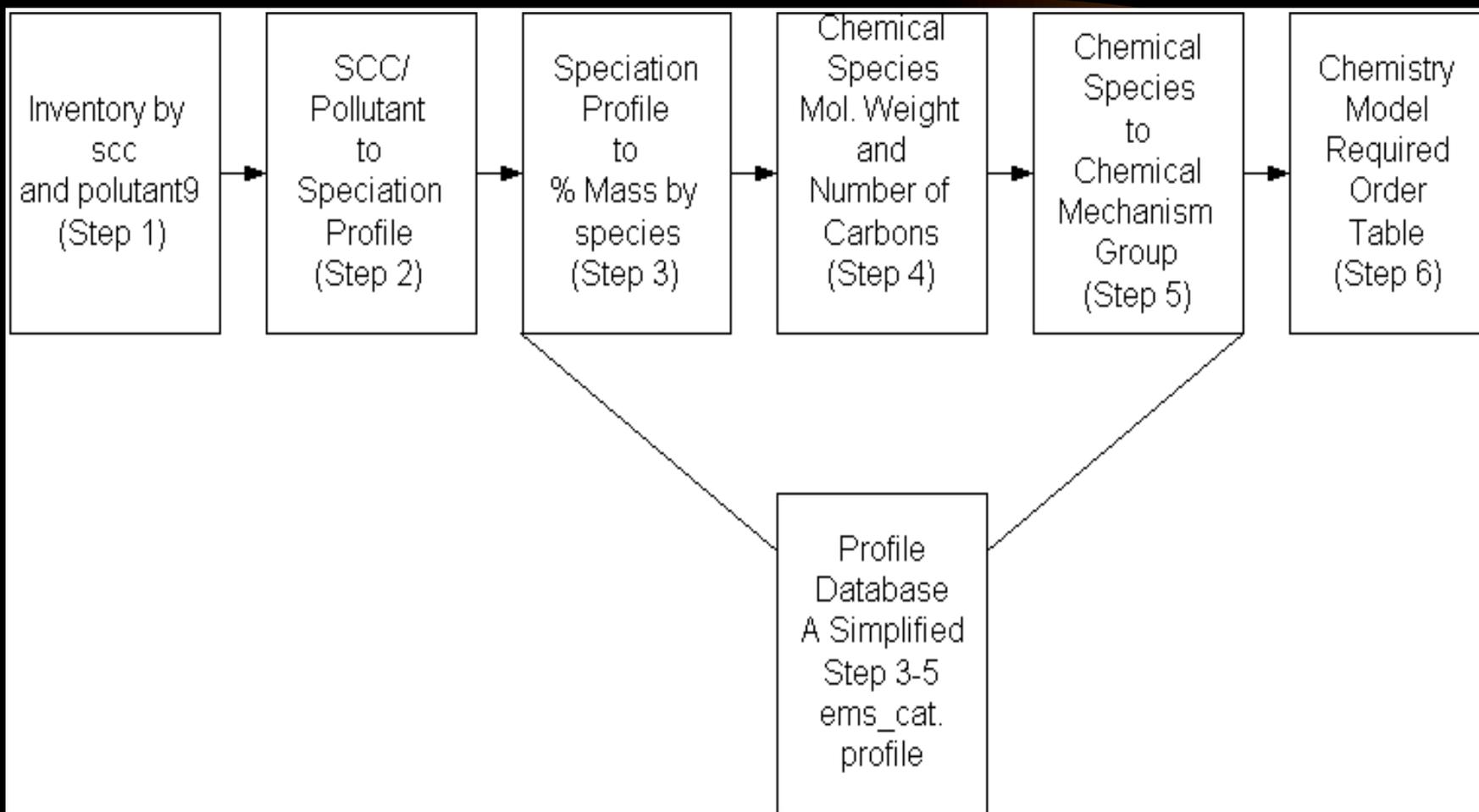- Solve chemistry by lumping species into reactivity groups

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# CB-IV Lumped Groups

| OBS | MDLSPAB | MDLSPNAM | MDLSPORD |
|-----|---------|----------|----------|
| 1 | OLE | Olefinic carbon bond (C=C) | 3 |
| 2 | PAR | Paraffin carbon bond (C-C) | 4 |
| 3 | TOL | Toluene (C6H5-CH3) | 5 |
| 4 | XYL | Xylene (C6H4-(CH3)2) | 6 |
| 5 | FORM | Formaldehyde (CH2=O) | 7 |
| 6 | ALD2 | High MW aldehydes (RCHO, R>H) | 8 |
| 7 | ETH | Ethene (CH2=CH2) | 9 |
| 8 | MEOH | Methanol (CH3OH) | 10 |
| 9 | ETOH | Ethanol (C2H5OH) | 11 |
| 10 | ISOP | Isoprene | 12 |
| 11 | NR | Non Reactives as methane | 13 |
| 12 | NO | Nitric Oxide | 1 |
| 13 | NO2 | Nitrogen Dioxide | 2 |
| 14 | CO | Carbon Monoxide | 14 |

# *The Problem:*

- Inventory is in mass(Tons,KG,Grams) and SCC code

- The models require moles by lumped group

- 6 steps to convert

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┌─────────────┐   ┌─────────────┐   ┌─────────────┐   ┌─────────────┐   ┌─────────────┐   ┌─────────────┐
│ Inventory by│   │    SCC/     │   │  Speciation │   │  Chemical   │   │  Chemical   │   │  Chemistry  │
│    scc      │   │  Pollutant  │   │   Profile   │   │   Species   │   │   Species   │   │    Model    │
│and polutant9│ → │     to      │ → │     to      │ → │ Mol. Weight │ → │     to      │ → │  Required   │
│  (Step 1)   │   │  Speciation │   │  % Mass by  │   │     and     │   │  Chemical   │   │    Order    │
│             │   │   Profile   │   │   species   │   │  Number of  │   │  Mechanism  │   │    Table    │
│             │   │  (Step 2)   │   │  (Step 3)   │   │   Carbons   │   │    Group    │   │  (Step 6)   │
│             │   │             │   │             │   │  (Step 4)   │   │  (Step 5)   │   │             │
└─────────────┘   └─────────────┘   └──────┬──────┘   └─────────────┘   └──────┬──────┘   └─────────────┘
                                           \                                  /
                                            \                                /
                                             \      ┌─────────────┐        /
                                              \     │   Profile   │       /
                                               \    │  Database   │      /
                                                \   │ A Simplified│     /
                                                 \  │   Step 3-5  │    /
                                                  \ │  ems_cat.   │   /
                                                    │   profile   │
                                                    └─────────────┘
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- Make Sure your inventory is using valid SCC/area-SCC

- If no SCC(Biogenics, Mobile) alter the model so that it knows how to see these categories

- Map an SCC code to a speciation profile

- Example: Off-Road motorcycle uses speciation profile 1201(Gasoline Exhaust)

- Might contain State, County or Plant specific information.

- Map a speciation profile to the chemical species that make it up.

- Example: Speciation profile 1032
  - 80.42 % Of mass goes to Acetaldehyde
  - 19.58 % Of mass goes to Acrolein(Propenal)

- Non-reactives are included in profiles.
  - (We'll solve this later)

- Apply the attributes of individual species
- Molecular weight most important
- Example Acrolein MW=56.06

- Put Each species into appropriate chemical mechanism lumping group

- Can belong to more than one group if chemical species reacts like multiple species

- Example: For each mole of Acrolein
  – 1 Mole of Paraffin and 1 mole of High Molecular Weight Aldehydes(ALD2)

# *Step 6*

- Chemistry Model Ordering
- All chemistry models require exact order and number of species
- Missing species will crash the model.
- Models expect specific order

# *Shorten The Process*

- Steps 3-6 are shortened into one file which contains lumping factors by speciation profile.

- EMS_CAT.PROFILE

- Speeds up processing

- How most models deal with speciation

- This alone limits your ability to fix speciation problems

# *Incorporating The data Step 2*

- Not all SCC's are listed in Speciates tables

- Had to update the SCC to profile crosswalk to include all currently recognized SCC's

- Each area should review this cross walk for important local sources. These are national averages.

# *Missing Species in Step 3 and 4*

- What is a species is unknown:
  - C-32 Compounds, Ketones - General
  - Unidentified Petroleum Distilates, Aromatic 100, Pine Oil, Oil of Orange
- 2 Options
  - Throw out "unknown" Species
  - Define them as a category called "unknown"

# *What To Do with Unknown Species?*
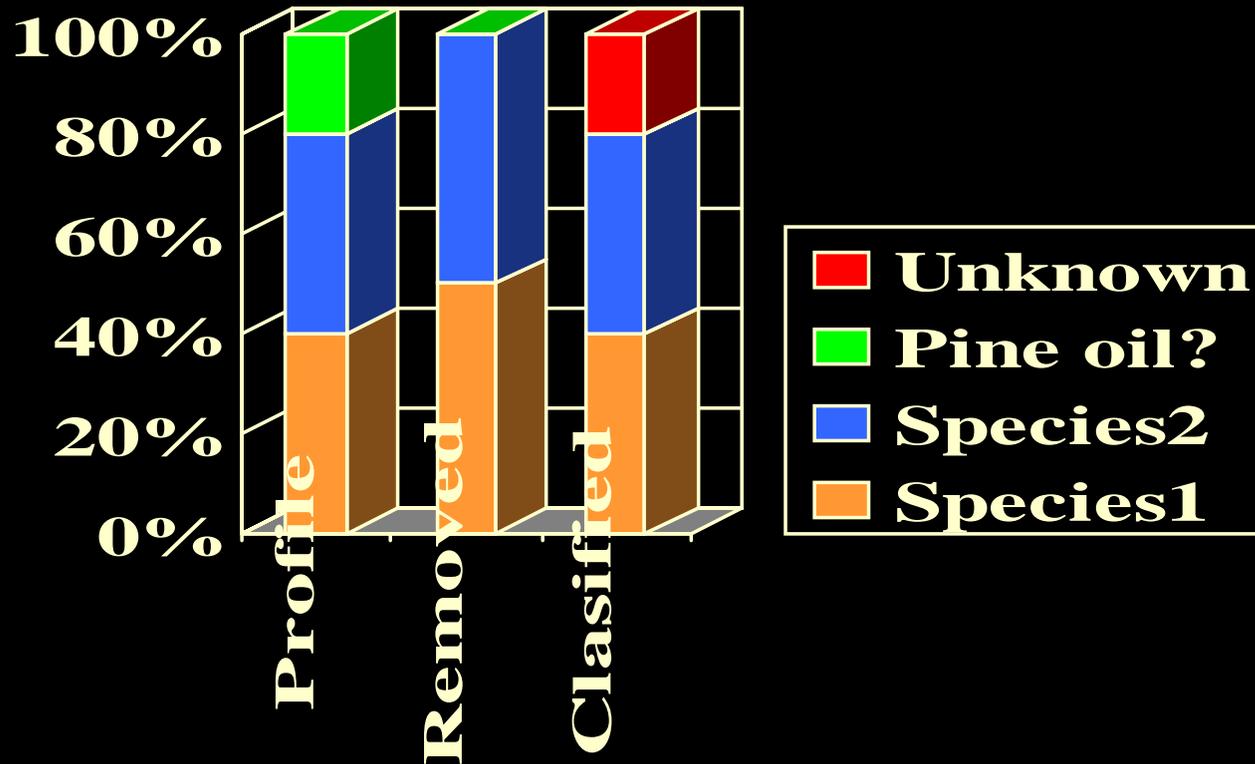
# Most Used Profiles in Point/Area/OFF-Road

| Profile NAME | Profile Number | Tons/Day (NEI) | Profile Created |
|---|---|---|---|
| Light Duty Gasoline Vehicles - | 1101 | 7406.60 | 01/05/89 |
| Architectural Coatings (Solven | 6003 | 4569.95 | 07/01/99 |
| Miscellaneous Burning - Forest | 0307 | 3023.07 | 01/05/89 |
| Gasoline Marketed - Summer Ble | 1190 | 2991.10 | 01/05/89 |
| Heavy Duty Gasoline Trucks | 1186 | 2350.71 | 01/05/89 |
| Degreasing Composite | 1195 | 2098.91 | 01/05/89 |
| Consumer and Commercial Produc | 8520 | 1968.36 | 08/01/98 |
| Light-Duty Diesel Vehicles | 1201 | 1909.39 | 01/05/89 |
| General Pesticides | 0076 | 1390.33 | 01/05/89 |
| Surface Coating Operations - A | 1088 | 1296.74 | 01/05/89 |

# Unidentified species in the top profiles

| | Profile Name | PROF# | NET VOC Tons/Day | Profile Created | Percent Unident. | Mass Unident. |
|---|---|---|---|---|---|---|
| 1 | Miscellaneous Burning - Forest | 0307 | 2936.28 | 01/05/89 | 0.46414 | 1362.85 |
| 2 | Consumer and Commercial Produc | 8520 | 1968.36 | 08/01/98 | 0.39489 | 777.28 |
| 3 | Degreasing Composite | 1195 | 2047.34 | 01/05/89 | 0.36633 | 750.01 |
| 4 | Light Duty Gasoline Vehicles - | 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 | 8523 | 1063.23 | 08/01/98 | 0.41237 | 438.44 |
| 7 | Consumer and Commercial Produc | 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 | 2410 | 285.80 | 07/01/99 | 0.73679 | 210.57 |
| 10 | Heavy Duty Gasoline Trucks | 1186 | 2344.25 | 01/05/89 | 0.06281 | 147.23 |

# *LADCO Sensitivity Tests*

- Test the impact of Speciate 3.0
- Run 3 runs
  - Old speciation profiles
  - New speciate with default speciation profiles
  - Extreme Speciation(not as extreme as we thought!)

# Peak 1hr Ozone

camx mplus 36 base1 vs hotmv
=xymax.980718.mplus.36.base1.O3.1.bin, j=xymax.980718.mplus.36.hotmv
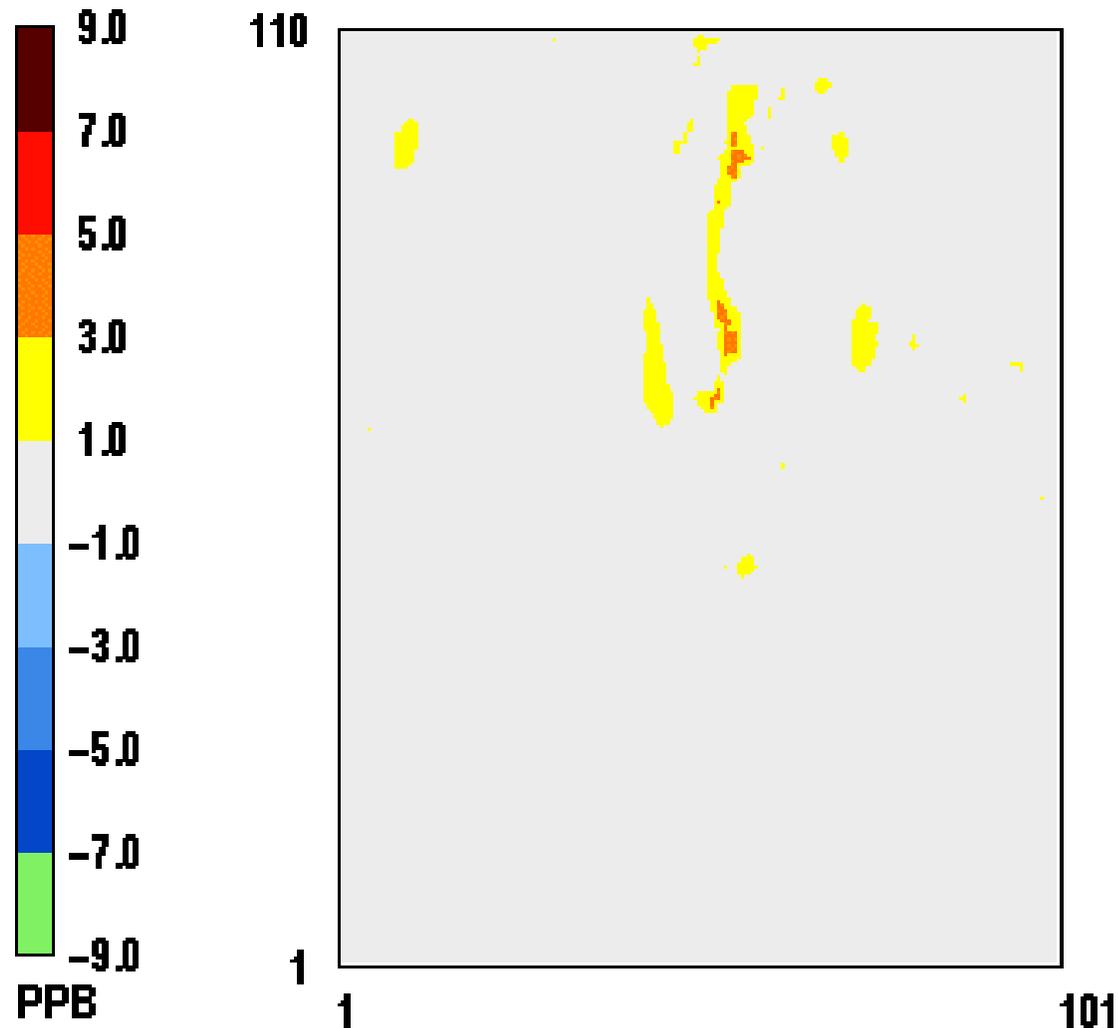
PPB
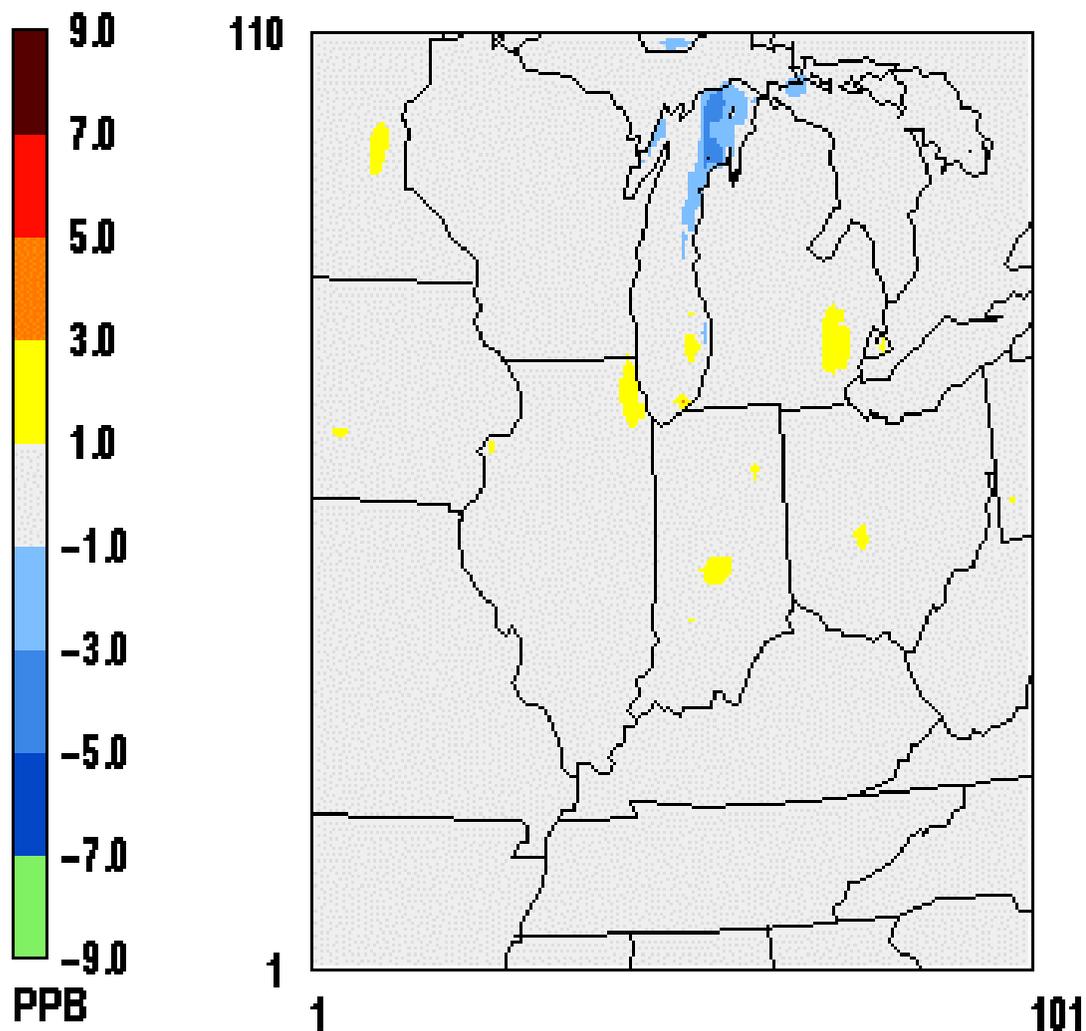
PAVE
by
MCNC

July 18,1998 23:00:00
Min=-4.2 at (56,98), Max= 4.3 at (53,67)

# Peak 1hr Ozone



camx mplus 36 base1 vs spec3b

:ymax.980718.mplus.36.base1.O3.1.bin, j=xymax.980718.mplus.36.spec3

9.0
7.0
5.0
3.0
1.0
−1.0
−3.0
−5.0
−7.0
−9.0

PPB

110

1

1                    101

PAVE
by
MCNC

July 18,1998 23:00:00
Min=−1.0 at (89,36), Max= 4.8 at (54,77)

# *Future Directions*

- EIIP Emissions Modeling Group
  - Update Species to Mechanism X-ref.
  - Update Profiles
- Incorporate SAPRC Chemistry Tables
- Further sensitivity with unidentified retained
- Load PM data