INTEGRATED SOURCE APPORTIONMENT METHOD (ISAM)

DECOUPLED DIRECT METHOD IN 3D (DDM-3D)

CMAQ V5.4 EDITION

SERGEY L. NAPELENOK
US EPA

CMAQV5.4 DIAGNOSTICS, TOOLS, AND INSTRUMENTED MODELS WEBINAR

22 FEBRUARY 2023

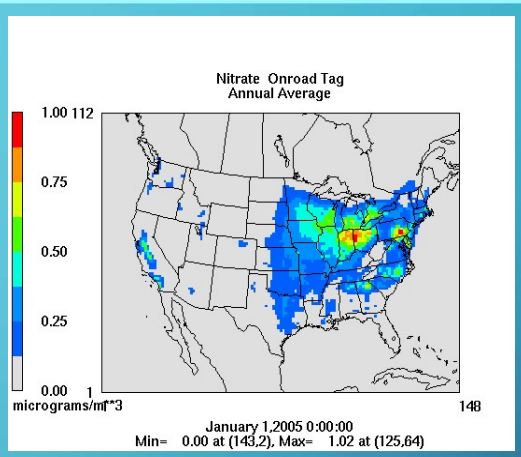
The views expressed in this presentation are those of the author and do not necessarily reflect the views or policies of the U.S. EPA.

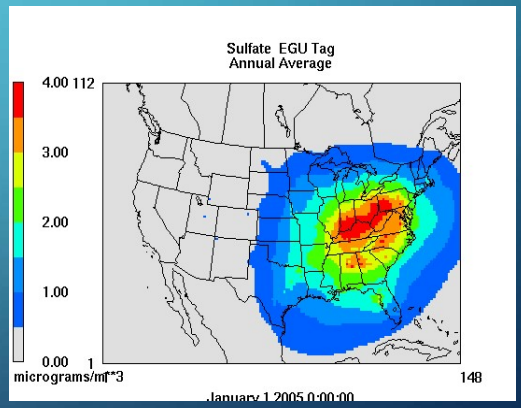
DDM-3D AND ISAM IN CMAQ 5.4

- Both models are fully integrated into the base CMAQ code.
- Both have been released as part of the CMAQ package through github.
  - See https://github.com/USEPA/CMAQ for code and documentation.
- As in the past, both models can be enabled through build script options (pre-compiler flags), but from the same source code as the base CMAQ model.
- Configuring and running both models is still done through run script options and their own specific control files.

CMAQ-ISAM

- Provides source tracking information simultaneously with the concentrations/depositions output.
- Has been released in CMAQ since version 5.0.2
- Tracks pollutants from user-selected tag classes (e.g. SULFATE, OZONE, EC, etc.)
  - In the CMAQv5.4 release, all species are now available for tracking for every supported chemical mechanism.
- Track from Emissions Streams (online and offline) either domain-wide or for user-defined geographical regions.
  - Additionally, always tracks initial conditions, boundary conditions, and "other" mass for complete mass accountability.





CMAQ-ISAM – MAIN SCIENCE UPDATES

- Added substantial flexibility for user specification on tracking assignments performed in the chemistry module.
  - Best explained through an example in the following slides

PREVIOUS ISAM IMPLEMENTATION

- The previous implementation (5.3) apportioned products of chemical reactions strictly proportionally by stoichiometry.
- For example:

ISO2 + NO -->

0.1*INTR + 0.9*NO2 + 0.673*FORM + 0.9*ISPD + 0.818*HO2 + 0.082*XO2H + 0.082*RO2

- Every source of ISO2 will get ½ of each product (proportionally by emissions amounts)
- Every source of NO will get ½ of each product (proportionally by emissions amounts).

PREVIOUS ISAM IMPLEMENTATION (2)

- The “fair” apportionment is necessary for a flexible tool design that can be used for any species in the chemical mechanism.
- However, for some features of ozone chemistry, the “fair” type of methodology may produce non-intuitive source attribution results (although strictly correct apportionment).

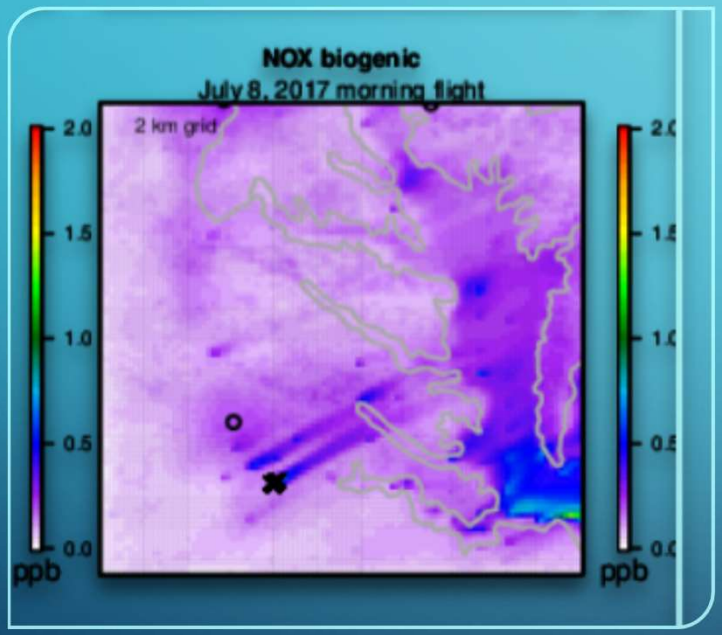
PREVIOUS ISAM IMPLEMENTATION (3)

- Looking at the same example reaction:

ISO2 + NO --> 0.1*INTR + 0.9*NO2 + 0.673*FORM + 0.9*ISPD + 0.818*HO2 + 0.082*XO2H + 0.082*RO2

- ISO2 is typically biogenic and NO is mostly from anthropogenic emissions (such as EGUs or mobile sources).
- The product NO2, therefore, becomes approximately ½ biogenic.
- Further in time and/or space, the newly tagged biogenic NO2 can cycle back to NO and retain its biogenic source identity.

PREVIOUS ISAM IMPLEMENTATION (4)

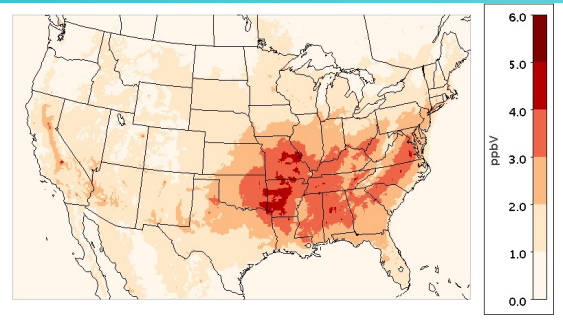


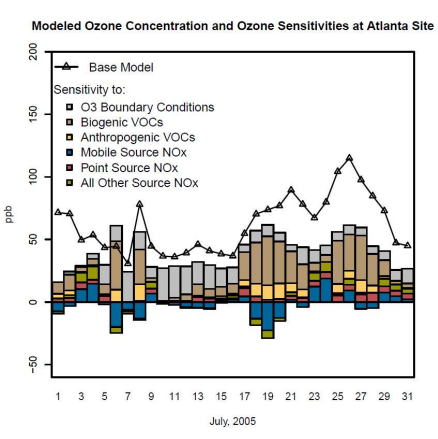
- This rapid "relabeling" of NO from anthropogenic to biogenic can lead to some results where biogenic NOx (and O3) shows up in plumes intuitively viewed as anthropogenic (such as from power plants in the illustration here).

EXPANDED ISAM FUNCTIONALITY

- Option 1. Equal assignment (previous version).
- Option 2. If parent reactants include the species NO, NO2, NO3, HONO, or ANO3, assignment to these sources only. Reactions without these species proceed with equal assignment.
- Option 3. Option 2 with species list expanded to include reactive VOC species and radicals. Reactions without these species proceed with equal assignment.
- Option 4. If parent reactants include the reactive VOC species and radicals, assignment to these sources only. Reactions without these species proceed with equal assignment.
- Option 5. Assignment to VOC or Nox sources is based on the ratio of production of H2O2 to production of HNO3. Reactions without the nitrogen species listed above and reactive VOCs proceed with equal assignment.
- Additionally, the transitional value for Option 5 is also customizable (default is based on Sillman, 1995: PH2O2/PHNO3=0.35).

HCHO sensitivity to VOC emissions (Summer)





CMAQ-DDM-3D

- Provides species sensitivity information simultaneously with the concentrations/depositions output.
  - Sensitivities are in the "forward" sense, *i.e.*, sensitivity of all species concentrations/depositions to specific, user defined parameters.
- Has been released in CMAQ since version 4.7.
- Parameters can include emissions streams (online and offline), initial conditions, boundary conditions, chemical reaction rates.
- Propagates the sensitivity fields through the model processes by differentiating the governing equations associated with each process.

$$\frac{\partial C_i}{\partial t} = -\nabla(uC_i) + \nabla(K\nabla C_i) + R_i + E_i$$

Advection Diffusion Chemistry Emissions

$$\frac{\partial S_{i,j}}{\partial t} = -\nabla(uS_i)_j + \nabla(K\nabla S_i)_j + JS_{i,j} + \delta_{i,k}$$

CMAQ-DDM-3D

- The sensitivity calculations for gaseous and particulate species is done in essentially the same way as in the previous release (v5.2).
- Improvements visible to the user are from easier control file parameter definitions and full integration with the newer CMAQ emissions processing module.
- The more important improvement is the ability to calculate chemistry Jacobians inline.
  - Allows for more flexibility in using CMAQ-DDM-3D with different chemical mechanisms and allows the user to make (reasonable!) changes to the mechanism without breaking DDM-3D.

SUMMARY

- CMAQ-ISAM and CMAQ-DDM-3D can provide useful and complementary information for various purposes including development and evaluation of pollution control strategies, propagating uncertainties, future projections, and general understanding of model representation of the troposphere.
- Support for both should continue and be more timely, because they are now both fully integrated in the CMAQ model.
- There will be some minor updates/bug fixes (incorporating user feedback) to both models in CMAQv5.4+

CMAQv5.4 Diagnostics, Tools and Instrumented Models:

- **DESID**
- **ELMO**
- **Autochem**
- **Budget Tool**

Streamlining tasks to make more time for Your ideas

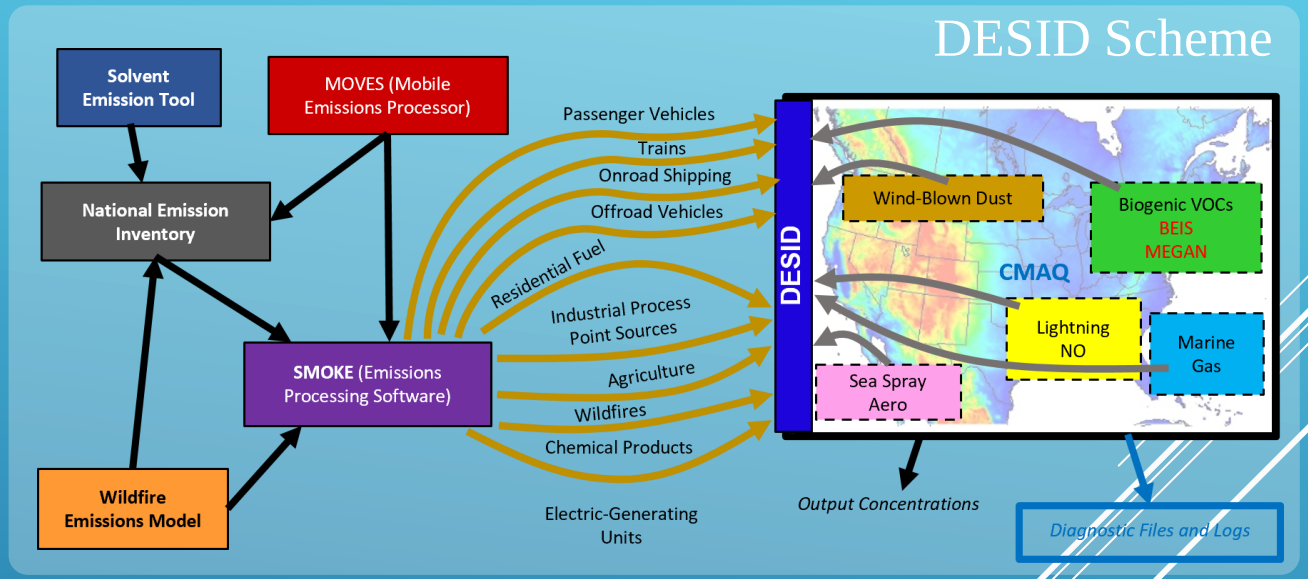
Ben Murphy

US EPA ORD

22 February 2023

DESID (The **D**etailed **E**mission **S**caling, Isolation and **D**iagnostics module)

- First released with CMAQv5.3
- Centralizes emissions processing tasks including chemical mapping, unit conversions, instrumented model source assignments, etc.
- Considers emissions from offline sources (such as those processed using SMOKE) and online sources (e.g. wind-blown dust or biogenic VOCs)
- Users can run with multiple gridded emission files, scale a species from different emissions sources independently, turn off emissions from a particular source or geographic area.
- These tasks are accomplished by modifying human readable input namelists.

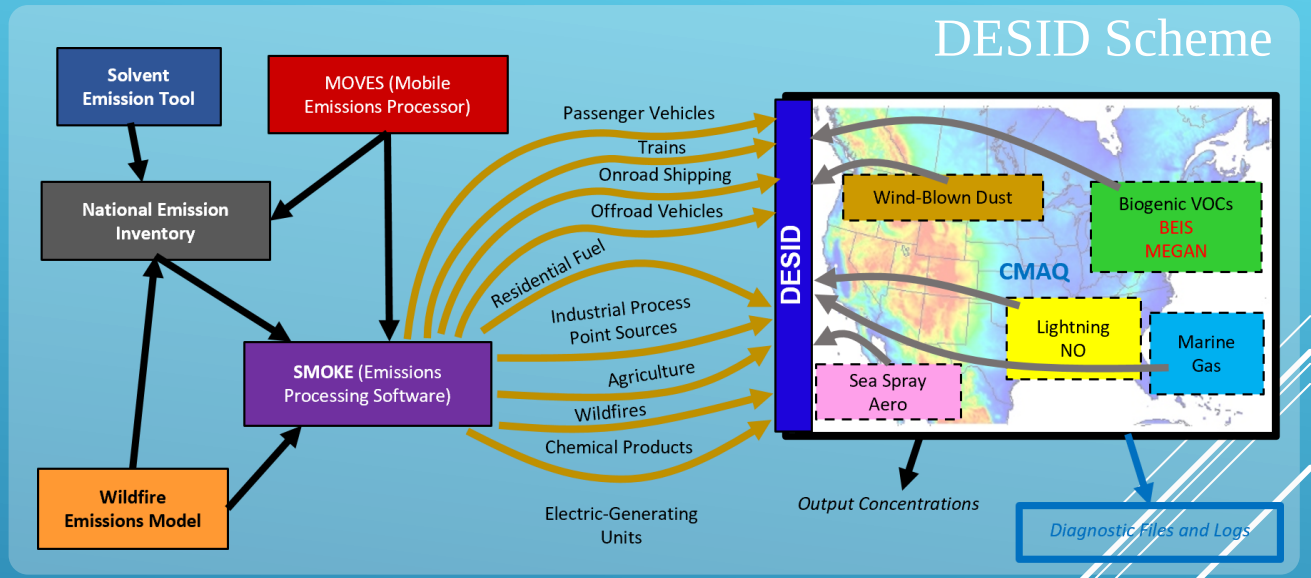


- Includes an extensive diagnostic output log to document chemical mapping and inform potential errors

Murphy et al., *Geoscientific Model Development*, 2021. https://doi.org/10.5194/gmd-14-3407-2021

DESID (The **D**etailed **E**mission **S**caling, Isolation and **D**iagnostics module)

- Biogenic emission models available: BEIS4/BELD6 or MEGANv3.2 (1 km x 1 km BELD6 files are available with the 2020 NEI package or by request).
- Diagnostic file updates:
  - Time stepping is 100% consistent with the input emission files
  - Define any number of diagnostic files
  - Sum multiple streams to one diagnostic file
  - Choose individual variables, all variables or sum variables
- Resolved region scaling problems:
  - v5.3.3 algorithm results in errors at the boundary between two specially defined regions.
  - Better algorithm was developed, issue resolved in v5.4.
- Modified the EmissCtrl file into three files to minimize maintenance of inputs that are not mechanism-dependent.



EmissCtrl_cb6r3_ae7_aq.nml

- CMAQ_Control_Misc.nml — Chemical Families, ELMO, Budget Tool
- CMAQ_Control_DESID.nml — Diagnostic file, region families, size distribution assignments
- CMAQ_Control_DESID_cb6r3_ae7_aq.nml — Mechanism-dependent emission mapping

DESID (The **D**etailed **E**mission **S**caling, Isolation and **D**iagnostics module)

Example of new diagnostics interface in CMAQ_Control_DESID.nml:

A) I'd like one file with all my emissions rates (gridded, point, online, everything) as a column sum:

```
Desid_Diag_Streams_Nml(1,:)= 'TOTAL'
Desid_Diag_Fmt_Nml(1)      = 'COLSUM'
Desid_Diag_Spec_Nml(1,:)   = 'ALL'
```

← Could also use **LAYER1** or **3D**

CMAQ_Control_DESID.nml

DESID (The **D**etailed **E**mission **S**caling, Isolation and **D**iagnostics module)

Example of new diagnostics interface in CMAQ_Control_DESID.nml:

B) I also want files for every stream, but only for SO_2 and Sulfate:

```
Desid_Diag_Streams_Nml(2,:)= 'ALL'
Desid_Diag_Fmt_Nml(2)      = 'COLSUM'
Desid_Diag_Spec_Nml(2,:)   = 'SO2','ASO4'
```

Automatically sums ASO4I, ASO4J, and ASO4K. Use 'ASO4I' if you just want Aitken mode sulfate, for example.

CMAQ_Control_DESID.nml

DESID (The **D**etailed **E**mission **S**caling, Isolation and **D**iagnostics module)

Example of new diagnostics interface in CMAQ_Control_DESID.nml:

C) I have a wildfire point file and the stack_emis_lab in the CMAQ runscript is ‘PT_WILDFIRE’. I need CO and EC from those emissions:

```
Desid_Diag_Streams_Nml(3,:)= 'PT_WILDFIRE'
Desid_Diag_Fmt_Nml(3)      = '3D'
Desid_Diag_Spec_Nml(3,:)   = 'AEC','CO'
```

CMAQ_Control_DESID.nml

DESID (The **D**etailed **E**mission **S**caling, Isolation and **D**iagnostics module)

Example of new diagnostics interface in CMAQ_Control_DESID.nml:

D) I want to output all my fire EC and CO emissions summed up in one file, and I have a stream family ‘FIRES’ defined as the sum of ‘PT_WILDFIRE’, ‘GRIDDED_RWC’, and ‘PT_RXFIRES’:

```
Desid_Diag_Streams_Nml(4,:)= 'FIRES'
Desid_Diag_Fmt_Nml(4)      = '3D'
Desid_Diag_Spec_Nml(4,:)   = 'AEC','CO'
```

```
!-------------------------------------------------------------------------------!
! Emissions Scaling Family Definitions                                          !
!    This component includes definitions for families of emission streams and   !
!    region combinations.                                                       !
!-------------------------------------------------------------------------------!
&Desid_StreamFamVars
 Desid_N_Stream_Fams = 1           ! Exact number of stream family definitions
 Desid_Max_Stream_Fam_Members = 20 ! Larger than the number of streams on all
                                   ! family definitions
/

&Desid_StreamFam
  StreamFamilyName(1)     = 'FIRES'
  StreamFamilyMembers(1,1:3)= 'PT_WILDFIRE','GRIDDED_RWC','PT_RXFIRES'
/
```

CMAQ_Control_DESID.nml

DESID (The **D**etailed **E**mission **S**caling, Isolation and **D**iagnostics module)

Example of new diagnostics interface in CMAQ_Control_DESID.nml:

E) I changed my mind. I want those fire emissions separated on their own files, not summed together:

```
Desid_Diag_Streams_Nml(4,:)= 'FIRES*'
Desid_Diag_Fmt_Nml(4)      = '3D'
Desid_Diag_Spec_Nml(4,:)   = 'AEC','CO'
```

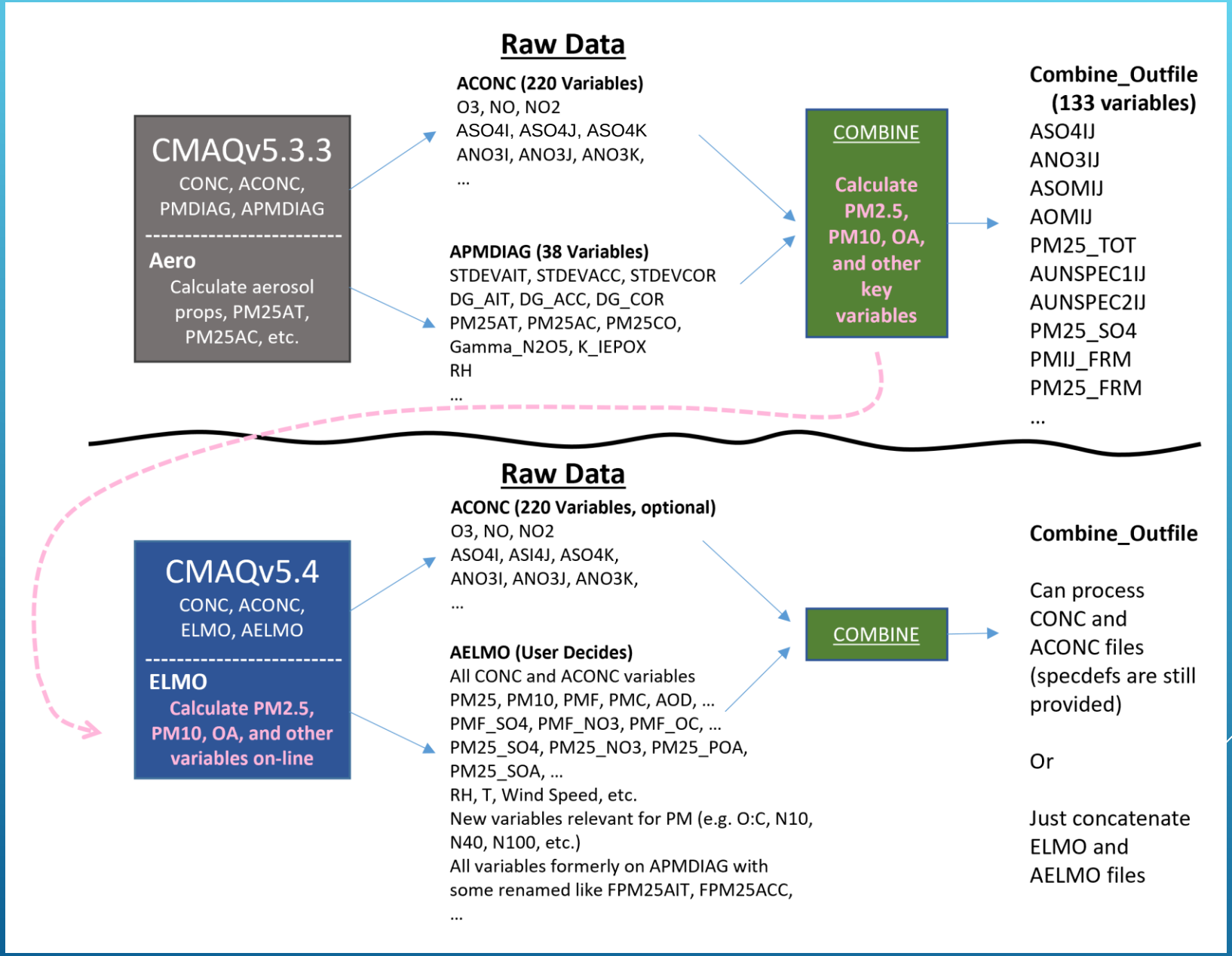
-or-

```
Desid_Diag_Streams_Nml(4,:)= 'PT_WILDFIRES'
Desid_Diag_Fmt_Nml(4)      = '3D'
Desid_Diag_Spec_Nml(4,:)   = 'AEC','CO'

Desid_Diag_Streams_Nml(5,:)= 'GRIDDED_RWC'
Desid_Diag_Fmt_Nml(5)      = '3D'
Desid_Diag_Spec_Nml(5,:)   = 'AEC','CO'

Desid_Diag_Streams_Nml(6,:)= 'PT_RXFIRES'
Desid_Diag_Fmt_Nml(6)      = '3D'
Desid_Diag_Spec_Nml(6,:)   = 'AEC','CO'
```

CMAQ_Control_DESID.nml

Pause for Check-in

ELMO: Explicit and Lumped CMAQ Model Output Module



ELMO: **E**xplicit and **L**umped CMAQ **M**odel **O**utput Module

- Online processing of aggregate variables you love
- Writes out raw (i.e., CONC and ACONC) variables too
- Instantaneous and/or average daily files with hourly resolution (COMBINE tool is used to make monthly files with hourly resolution)
- Can choose 2D or 3D
- Can make your own variables (tried to make it user friendly; recommend asking for help if you get stuck)
- Future:
  - make any number of files you want and select which variables you want on which files
  - Support other CMAQ modules: deposition, ISAM, etc.

ELMO: **E**xplicit and **L**umped CMAQ **M**odel **O**utput Module

All of these variables can be output directly from CMAQ on request!
Just use the CMAQ_Control_Misc.nml file.

Aerosol Mass
PM_MASS
PMU_MASS
PMF_MASS
PMC_MASS
PMNUC_MASS
PMAIT_MASS
PMACC_MASS
PM01
PM1
PM25
PM10
PM25TO10
PMAMS

PM2.5 Speciation
PM25_SO4
PM25_NO3
PM25_NH4
PM25_CL
PM25_NA
PM25_EC
PM25_OC
PM25_OA
PM25_MG
PM25_K
PM25_CA
PM25_OTHER
PM25_FE
PM25_SI
PM25_TI
PM25_MN
PM25_AL
PM25_SOIL
PM25_UNSP1
PM25_UNSPCRS
PM25_HP

ELMO: Explicit and Lumped CMAQ Model Output Module

All of these variables can be output directly from CMAQ on request!
Just use the CMAQ_Control_Misc.nml file.

Aerosol Properties
STDEV
DRY_DG
WET_DG
WET_M2
DRY_M3
WET_M3
DRY_DENS
WET_DENS
PM_SRF
PMU_SRF
PMF_SRF
PMC_SRF
FPM01
FPM1
FPM25
FPM10
FPM25TO10
FAMS

Aerosol Mass
PM_MASS
PMU_MASS
PMF_MASS
PMC_MASS
PMNUC_MASS
PMAIT_MASS
PMACC_MASS
PM01
PM1
PM25
PM10
PM25TO10
PMAMS

PM1.0 Speciation
PM1_SO4
PM1_NO3
PM1_NH4
PM1_CL
PM1_NA
PM1_EC
PM1_OC
PM1_OA
PM1_MG
PM1_K
PM1_CA
PM1_OTHER
PM1_FE
PM1_SI
PM1_TI
PM1_MN
PM1_AL
PM1_SOIL
PM1_UNSP1
PM1_UNSPCRS
PM1_HP

PM2.5 Speciation
PM25_SO4
PM25_NO3
PM25_NH4
PM25_CL
PM25_NA
PM25_EC
PM25_OC
PM25_OA
PM25_MG
PM25_K
PM25_CA
PM25_OTHER
PM25_FE
PM25_SI
PM25_TI
PM25_MN
PM25_AL
PM25_SOIL
PM25_UNSP1
PM25_UNSPCRS
PM25_HP

AMS-Relevant Speciation
PMAMS_SO4
PMAMS_NO3
PMAMS_NH4
PMAMS_CL
PMAMS_OA
PMAMS_OTOC

Fine Speciation
PMF_SO4
PMF_NO3
PMF_NH4
PMF_CL
PMF_NA
PMF_EC
PMF_OC
PMF_OA
PMF_FE
PMF_AL
PMF_SI
PMF_TI
PMF_CA
PMF_MG
PMF_K
PMF_MN
PMF_H2O
PMF_SOILIMPV
PMF_UN_IMPV1
PMF_UN_IMPV2
PMF_HP
PMF_HPMOLAL
PMF_PH
PMF_POC
PMF_SOC
PMF_POA
PMF_SOA
PMF_NCOM
PMF_OMOC
PMF_OTOC
PMF_ASOA
PMF_BSOA
PMF_CLDGLY
PMF_ISOPSOA
PMF_IEPOXSOA
PMF_MTNSOA
PMF_MTSOA

Coarse Speciation
PMC_SO4
PMC_NO3
PMC_NH4
PMC_CL
PMC_NA
PMC_MG
PMC_K
PMC_CA

"PMF" = i-mode + j-mode
"PMC" = k-mode

These variables are repeated for each mode (e.g., when STDEV is selected, STDEVACC, STDEVAIT, and STDEVCOR will all be output)

ELMO: Explicit and Lumped CMAQ Model Output Module

All of these variables can be output directly from CMAQ on request!
Just use the CMAQ_Control_Misc.nml file.

Aerosol Properties
STDEV
DRY_DG
WET_DG
WET_M2
DRY_M3
WET_M3
DRY_DENS
WET_DENS
PM_SRF
PMU_SRF
PMF_SRF
PMC_SRF
FPM01
FPM1
FPM25
FPM10
FPM25TO10
FAMS

Aerosol Mass
PM_MASS
PMU_MASS
PMF_MASS
PMC_MASS
PMNUC_MASS
PMAIT_MASS
PMACC_MASS
PM01
PM1
PM25
PM10
PM25TO10
PMAMS

Meteorology
RH
TA
TSURF
PRES
DZ
ZH
CFRAC
PV
DENS
RHOJ

Aerosol Number
PM_NUM
PMU_NUM
PMF_NUM
PMC_NUM
N10
N20
N40
N100

Other Variables
TNO3
TNO3TOT
PM25_FRM
PMF_FRM
AOD_550
PM_EXT_550
GAMMA_N2O5
GAMMA_N2O5K
YIELD_CLNO2
YIELD_CLNO2K
GAMMA_IEPOX
K_IEPOX
GAMMA_IMAE

PM1.0 Speciation
PM1_SO4
PM1_NO3
PM1_NH4
PM1_CL
PM1_NA
PM1_EC
PM1_OC
PM1_OA
PM1_MG
PM1_K
PM1_CA
PM1_OTHER
PM1_FE
PM1_SI
PM1_TI
PM1_MN
PM1_AL
PM1_SOIL
PM1_UNSP1
PM1_UNSPCRS
PM1_HP

PM2.5 Speciation
PM25_SO4
PM25_NO3
PM25_NH4
PM25_CL
PM25_NA
PM25_EC
PM25_OC
PM25_OA
PM25_MG
PM25_K
PM25_CA
PM25_OTHER
PM25_FE
PM25_SI
PM25_TI
PM25_MN
PM25_AL
PM25_SOIL
PM25_UNSP1
PM25_UNSPCRS
PM25_HP

AMS-Relevant Speciation
PMAMS_SO4
PMAMS_NO3
PMAMS_NH4
PMAMS_CL
PMAMS_OA
PMAMS_OTOC

PM2.5 - PM10.0 Speciation
PM25TO10_SO4
PM25TO10_NO3
PM25TO10_NH4
PM25TO10_CL
PM25TO10_NA

PM Toxics
PM25_HDIESEL
PM25_HBE
PM25_HCD
PM25_HCR3
PM25_HCR6
PM25_HCR
PM25_HPB
PM25_HMN
PM25_HNI
PM25_HAS
PM25_HG
PM10_HDIESEL
PM10_HBE
PM10_HCD
PM10_HCR3
PM10_HCR6
PM10_HCR
PM10_HPB
PM10_HMN
PM10_HNI
PM10_HAS
PM10_HG
PM25_BENAPY
PM10_BENAPY
PMF_BENAPY
GAS_BENAPY
BENAPY_FAERO

Fine Speciation
PMF_SO4
PMF_NO3
PMF_NH4
PMF_CL
PMF_NA
PMF_EC
PMF_OC
PMF_OA
PMF_FE
PMF_AL
PMF_SI
PMF_TI
PMF_CA
PMF_MG
PMF_K
PMF_MN
PMF_H2O
PMF_SOILIMPV
PMF_UN_IMPV1
PMF_UN_IMPV2
PMF_HP
PMF_HPMOLAL
PMF_PH
PMF_POC
PMF_SOC
PMF_POA
PMF_SOA
PMF_NCOM
PMF_OMOC
PMF_OTOC
PMF_ASOA
PMF_BSOA
PMF_CLDGLY
PMF_ISOPSOA
PMF_IEPOXSOA
PMF_MTNSOA
PMF_MTSOA

Coarse Speciation
PMC_SO4
PMC_NO3
PMC_NH4
PMC_CL
PMC_NA
PMC_MG
PMC_K
PMC_CA

"PMF" = i-mode + j-mode
"PMC" = k-mode

These variables are repeated for each mode (e.g., when STDEV is selected, STDEVACC, STDEVAIT, and STDEVCOR will all be output)

ELMO: Explicit and Lumped CMAQ Model Output Module

All of these variables can be outp
Just use the CMAQ_Control_Mis

All raw gas and particle species are available too!

Aerosol Properties
STDEV
DRY_DG
WET_DG
WET_M2
DRY_M3
WET_M3
DRY_DENS
WET_DENS
PM_SRF
PMU_SRF
PMF_SRF
PMC_SRF
FPM01
FPM1
FPM25
FPM10
FPM25TO10
FAMS

Aerosol Mass
PM_MASS
PMU_MASS
PMF_MASS
PMC_MASS
PMNUC_MASS
PMAIT_MASS
PMACC_MASS
PM01
PM1
PM25
PM10
PM25TO10
PMAMS

Meteorology
RH
TA
TSURF
PRES
DZ
ZH
CFRAC
PV
DENS
RHOJ

Aerosol Number
PM_NUM
PMU_NUM
PMF_NUM
PMC_NUM
N10
N20
N40
N100

Other Variables
TNO3
TNO3TOT
PM25_FRM
PMF_FRM
AOD_550
PM_EXT_550
GAMMA_N2O5
GAMMA_N2O5K
YIELD_CLNO2
YIELD_CLNO2K
GAMMA_IEPOX
K_IEPOX
GAMMA_IMAE

PM1.0 Speciation
PM1_SO4
PM1_NO3
PM1_NH4
PM1_CL
PM1_NA
PM1_EC
PM1_OC
PM1_OA
PM1_MG
PM1_K
PM1_CA
PM1_OTHER
PM1_FE
PM1_SI
PM1_TI
PM1_MN
PM1_AL
PM1_SOIL
PM1_UNSP1
PM1_UNSPCRS
PM1_HP

PM2.5 Speciation
PM25_SO4
PM25_NO3
PM25_NH4
PM25_CL
PM25_NA
PM25_EC
PM25_OC
PM25_OA
PM25_MG
PM25_K
PM25_CA
PM25_OTHER
PM25_FE
PM25_SI
PM25_TI
PM25_MN
PM25_AL
PM25_SOIL
PM25_UNSP1
PM25_UNSPCRS
PM25_HP

AMS-Relevant Speciation
PMAMS_SO4
PMAMS_NO3
PMAMS_NH4
PMAMS_CL
PMAMS_OA
PMAMS_OTOC

PM2.5 - PM10.0 Speciation
PM25TO10_SO4
PM25TO10_NO3
PM25TO10_NH4
PM25TO10_CL
PM25TO10_NA

PM Toxics
PM25_HDIESEL
PM25_HBE
PM25_HCD
PM25_HCR3
PM25_HCR6
PM25_HCR
PM25_HPB
PM25_HMN
PM25_HNI
PM25_HAS
PM25_HG
PM10_HDIESEL
PM10_HBE
PM10_HCD
PM10_HCR3
PM10_HCR6
PM10_HCR
PM10_HPB
PM10_HMN
PM10_HNI
PM10_HAS
PM10_HG
PM25_BENAPY
PM10_BENAPY
PMF_BENAPY
GAS_BENAPY
BENAPY_FAERO

Fine Speciation
PMF_SO4
PMF_NO3
PMF_NH4
PMF_CL
PMF_NA
PMF_EC
PMF_OC
PMF_OA
PMF_FE
PMF_AL
PMF_SI
PMF_TI
PMF_CA
PMF_MG
PMF_K
PMF_MN
PMF_H2O
PMF_SOILIMPV
PMF_UN_IMPV1
PMF_UN_IMPV2
PMF_HP
PMF_HPMOLAL
PMF_PH
PMF_POC
PMF_SOC
PMF_POA
PMF_SOA
PMF_NCOM
PMF_OMOC
PMF_OTOC
PMF_ASOA
PMF_BSOA
PMF_CLDGLY
PMF_ISOPSOA
PMF_IEPOXSOA
PMF_MTNSOA
PMF_MTSOA

Coarse Speciation
PMC_SO4
PMC_NO3
PMC_NH4
PMC_CL
PMC_NA
PMC_MG
PMC_K
PMC_CA

"PMF" = i-mode + j-mode
"PMC" = k-mode

These variables are repeated for each mode (e.g., when STDEV is selected, STDEVACC, STDEVAIT, and STDEVCOR will all be output)

ELMO: **E**xplicit and **L**umped CMAQ **M**odel **O**utput Module

A) I don't want a million variables. I just want O_3, NO_x and $PM_{2.5}$.

```
&elmo_avrg
  Avrg_Layer_Top = 1
  Avrg_Layer_Bot = 1
  Avrg_Vars_Nml  = 'NO2','NO','O3','PM25'
```

If you have not defined NO_X as a chemical family

```
&elmo_avrg
  Avrg_Layer_Top = 1
  Avrg_Layer_Bot = 1
  Avrg_Vars_Nml  = 'NOX','O3','PM25'
```

If you have defined NO_X as a chemical family

CMAQ_Control_Misc.nml

ELMO: **E**xplicit and **L**umped CMAQ **M**odel **O**utput Module

B) I want to look at all fine-mode species, but I forget which ones are available. I also want to check total $PM_{2.5}$ as well as isoprene and OH levels against some measurements or other model data.

```
&elmo_avrg
  Avrg_Layer_Top = 1
  Avrg_Layer_Bot = 1
  Avrg_Vars_Nml  = 'FINE_SPECIES','PM25','ISOP','OH'
```

CMAQ_Control_Misc.nml

ELMO: **E**xplicit and **L**umped CMAQ **M**odel **O**utput Module

C) I'm going to compare to AMET, and I don't want to forget any important variables. Oh, and I would like to compare to satellite data too.

```
&elmo_avrg
  Avrg_Layer_Top = 1
  Avrg_Layer_Bot = 1
  Avrg_Vars_Nml  = 'AMET','SAT'
```

SAT Variables	
Met Vars	***Chem Vars***
DENS	NO2
DZ	SO2
ZH	O3
CFRAC	CO
PV	FORM
PRES	NH3
TA	AOD_550

CMAQ_Control_Misc.nml

ELMO: **E**xplicit and **L**umped CMAQ **M**odel **O**utput Module

D) Please stop all this foolishness! Just give me what I had in v5.3.3.

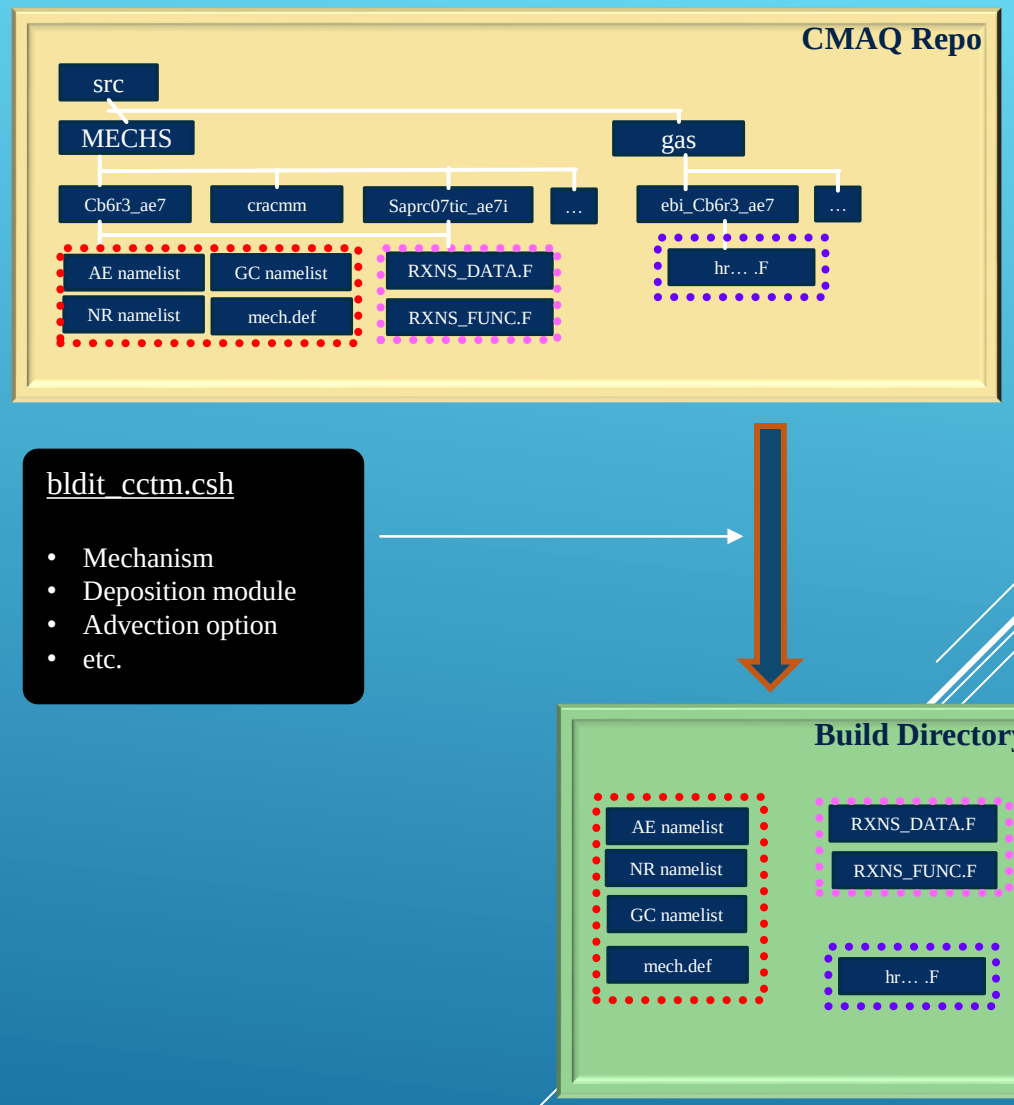
```
&elmo_avrg
  Avrg_Layer_Top = 1
  Avrg_Layer_Bot = 1
  Avrg_Vars_Nml  = 'DEFAULT'
```

Pause for Check-in

CMAQ_Control_Misc.nml

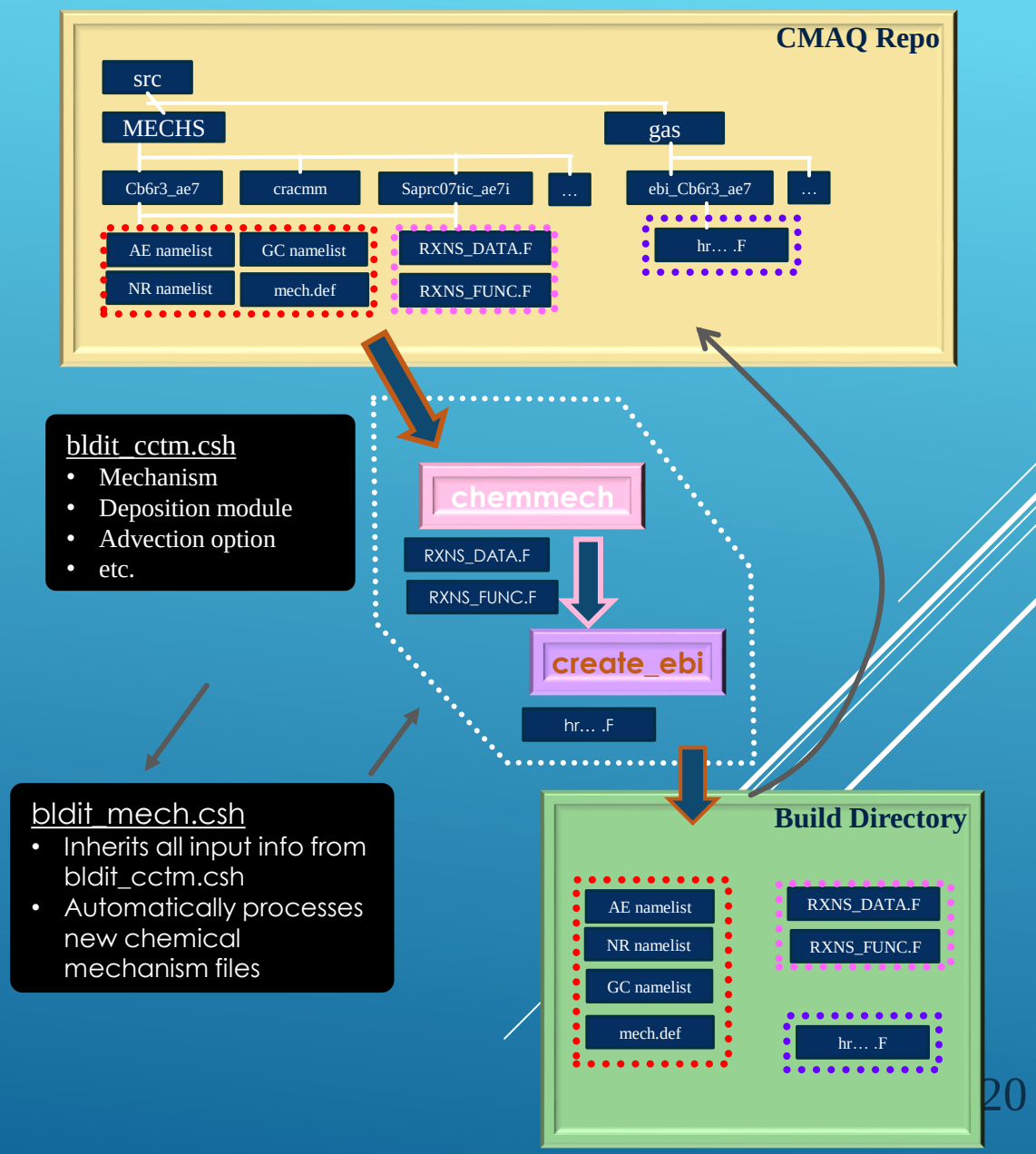
Autochem: easily generate mechanisms

Many chemical mechanism-relevant files are copied from the CMAQ repo to the build directory by the build process, kicked off by the bldit_cctm.csh script.



Autochem: easily generate mechanisms

- The chemmech and create_ebi utilities are now available to generate source code files for new mechanisms.
- The bldit_cctm.csh script passes model configuration options (e.g. mechanism choice) to the bldit_mech.csh script which executes the reaction code generation utilities and moves files into the build directory as required.



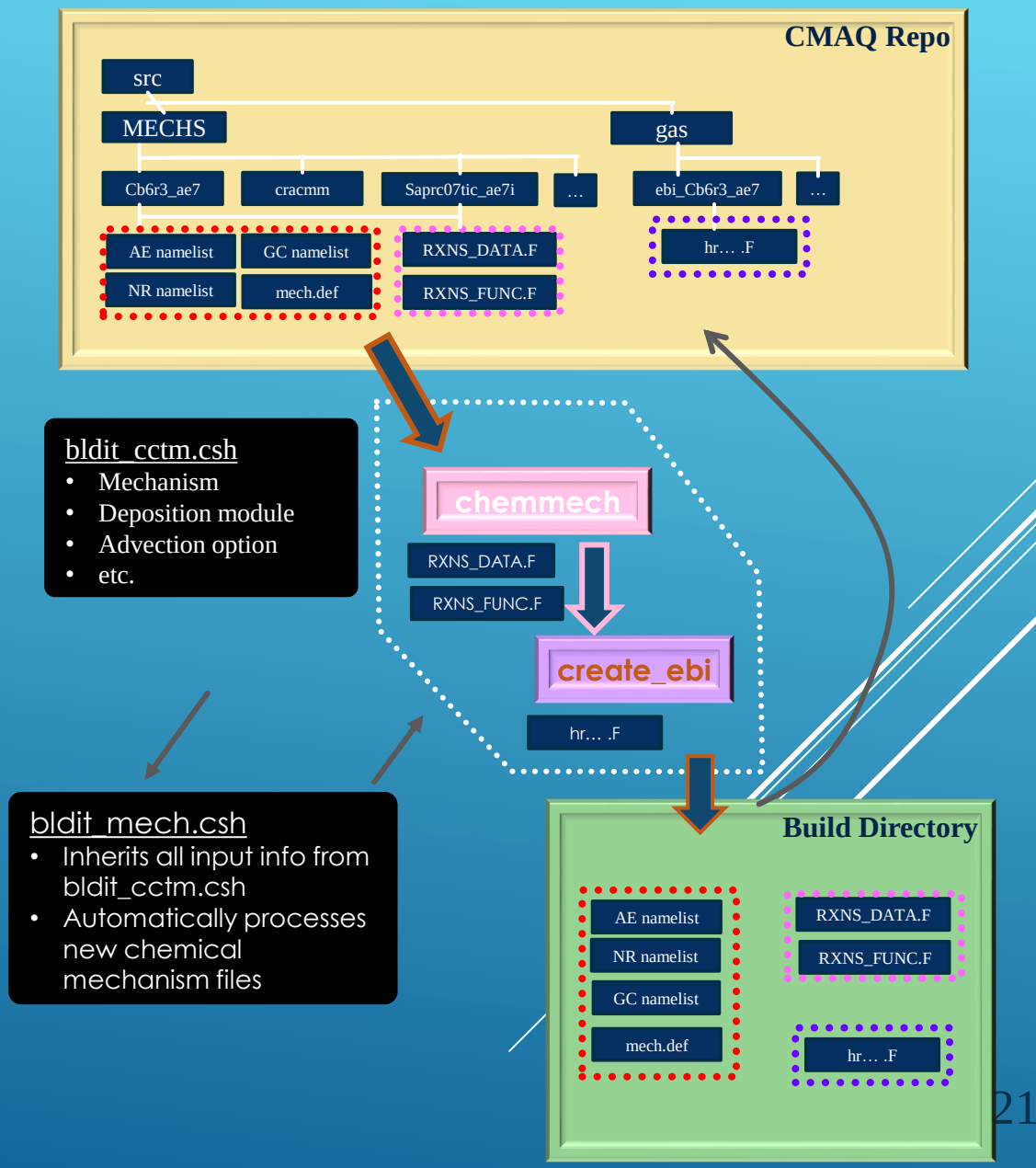
Autochem: easily generate mechanisms

- If you want to make a new mechanism by changing the reactions in mech.def or species in the GC namelist, uncomment one line of code in bldit_cctm.csh to reprocess new mechanism source code files.

```
set build_mech       #> uncomment to build mechanism source code files using the
                      #>   chemmech utility.
```

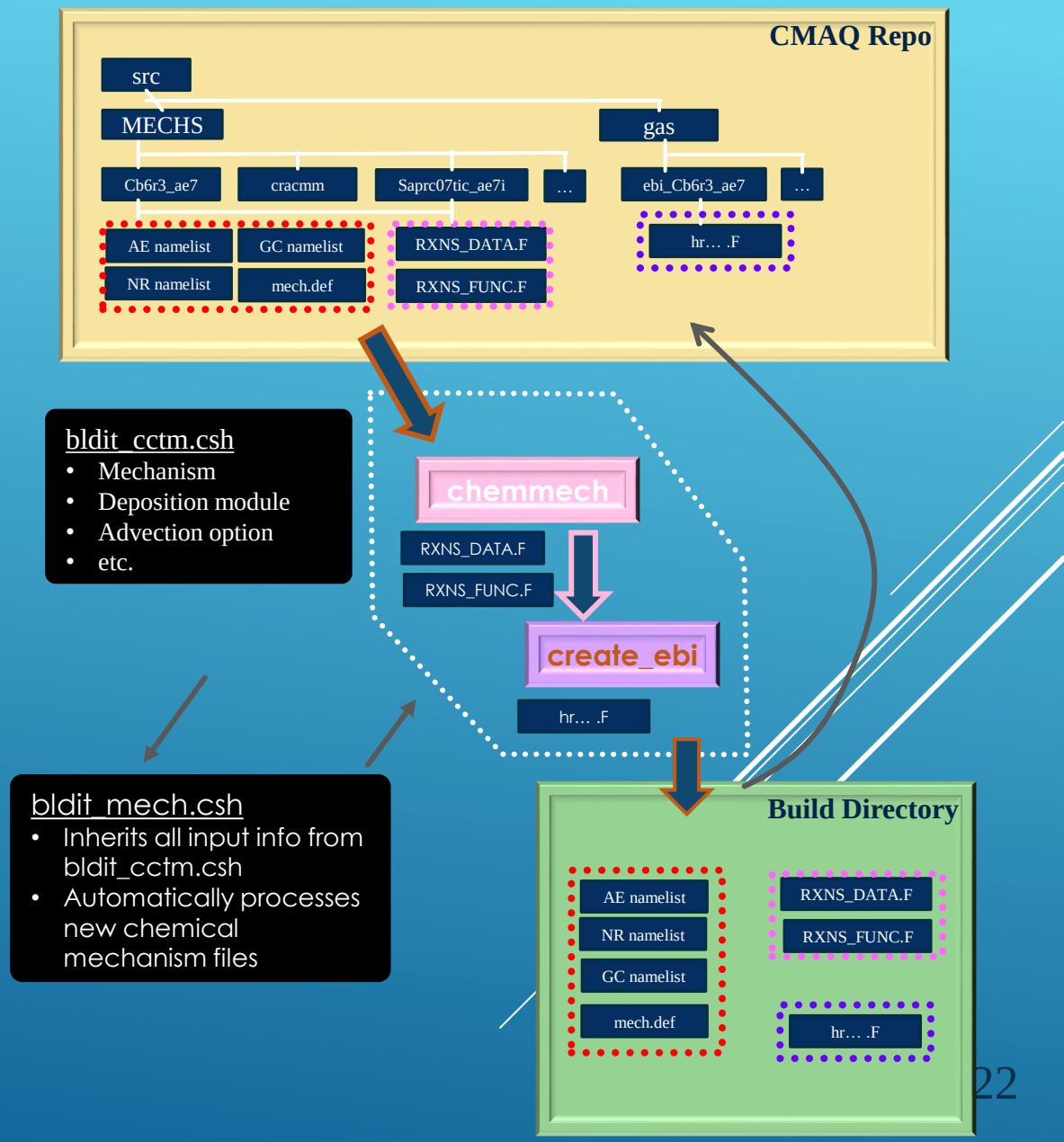
- If you want your new mechanism to overwrite an existing mechanism, uncomment the next line as well

```
set clobber_mech     #> when commented, the bldit_mech.csh script will halt if
                      #>   newly created mechanism files are attempting replace
                      #>   existing ones. When uncommented, the existing files
                      #>   will be overwritten.
```



Autochem: easily generate mechanisms

- If you are adding an aerosol, there are more places in the source code to add information including:
  - AERO_DATA registry table of aerosol chemical species
  - SOA_DEFN registry table of organic aerosol properties
  - hlconst table of Henry's Law coefficient parameters
  - CMAQ_Control_STAGE.nml deposition parameters if using STAGE



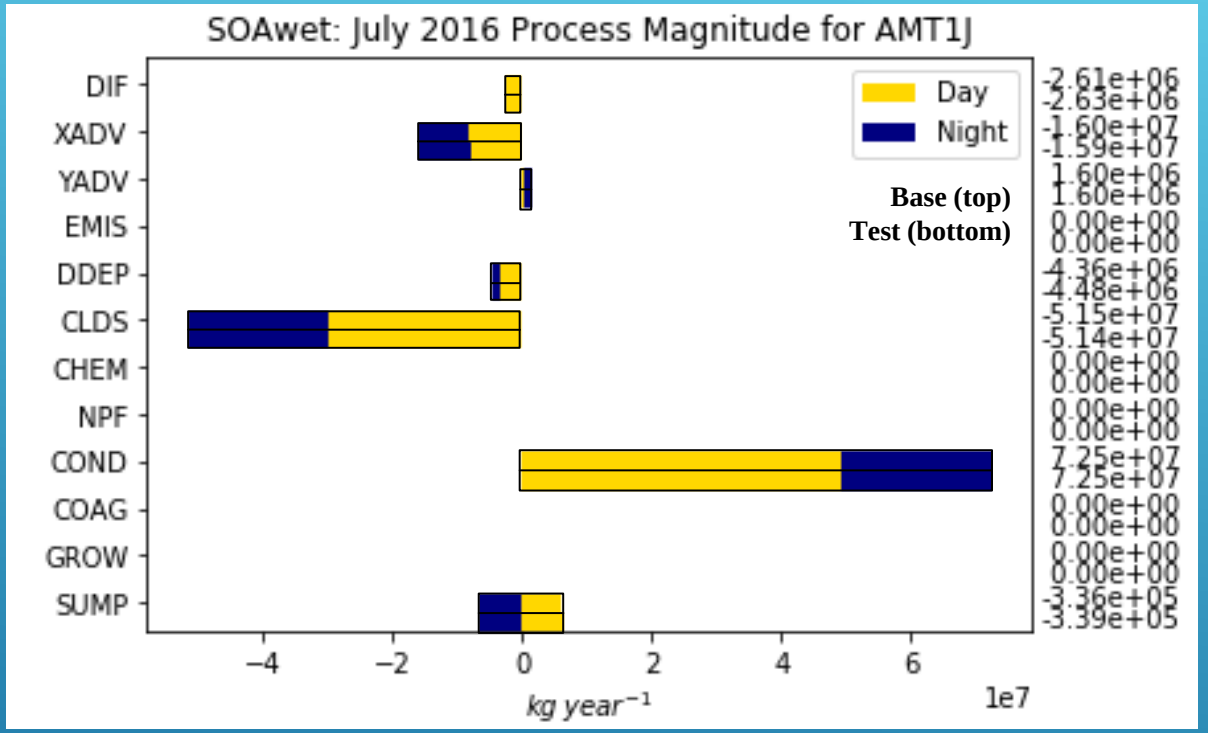
Pause for Check-in

Budget Tool: Quantify process contributions to domain-wide total

- A new Budget Reporting Tool is available to quantify the impact of individual model processes on each atmospheric species across the modeling domain.
- CCTM_BUDGET_[…].txt
- Hourly resolution, total mass (kg hr^{-1}).
- Makes a text file for every species you select. You can also ask for a sum of species.
- Helps diagnose problematic model configurations like:
  - Emissions are present for a species that shouldn't be emitted.
  - Boundary gains/losses are not as expected.
  - Cloud/Dry deposition scavenging relative doesn't match chemical properties.
- Helps inform which processes are driving domain-wide burden (e.g., deposition, advection, chemistry).
- Can detect mass conservation issues.

Available Processes	
Transport	***Non-Transport***
VDIFF	EMIS
ZADV	DRY DEP
HDIFF	PVO3
WEST_IN	CLOUDS
WEST_OUT	CHEM
EAST_IN	CONDENS
EAST_OUT	COAG
NORTH_IN	NPF
NORTH_OUT	GROWTH
SOUTH_IN	
SOUTH_OUT	RESIDUAL

Budget Tool: Quantify process contributions to domain-wide total



Example: made a model change for SOA (simulated one year). Verified that the total rates in kg yr^{-1} of each process did not change when going from base (top) to new (bottom). Stratified results by day and night as well.

Budget Tool: Quantify process contributions to domain-wide total

A) Request all CMAQ chemical species be output to budget file.

```
&Budget_Options
  Budget_Diag = .TRUE.
  BudgetVariables  = 'ALL'
/
```

CMAQ_Control_Misc.nml

Budget Tool: Quantify process contributions to domain-wide total

B) Limit budget output to just O_3, NO_2, and accumulation-mode EC.

```
&Budget_Options
  Budget_Diag = .TRUE.
  BudgetVariables  = 'O3','NO2','AECJ'
/
```

CMAQ_Control_Misc.nml

Budget Tool: Quantify process contributions to domain-wide total

C) Output budget for all EC summed together (AECI + AECJ). If the mode-suffix letter is omitted, the bulk aerosol species is assumed. Also output for O_3, NO_2, and a chemical family names VOC that should be defined in the "ChemicalFamilies" section of CMAQ_Control_Misc.nml.

```
&Budget_Options
  Budget_Diag = .TRUE.
  BudgetVariables  = 'O3','NO2','AEC','VOC'
/
```

CMAQ_Control_Misc.nml

Summary and Resources

- DESID – new diagnostic approaches to help you confirm and document emission perturbations.
- ELMO – simplified output. Just get $PM_{2.5}$ if you just want $PM_{2.5}$.
- Autochem – frictionless implementation of new chemistry or chemical species.
- Budget Tool – domain-wide output of species burden and process rates (hourly resolution; human readable).

- User Guide and Tutorials:
  - DESID: Appendix B: Emission Control | Tutorial: Prescribing Emissions Using DESID
  - ELMO: Appendix F: ELMO
  - Autochem: Tutorial: Modifying a Chemical Mechanism in CMAQ
  - Budget Tool: Chapter 9: Process Analysis and Budget (Section 9.7)
  - Online Help: CMAS Forum

Thank you to CMAS, the CMAQ Team, and **You**
for listening and using CMAQ to further Science and Environmental Quality!