# Development of GEOS-CHEM/CMAQ Interface and Comparison Studies over China during July 2001

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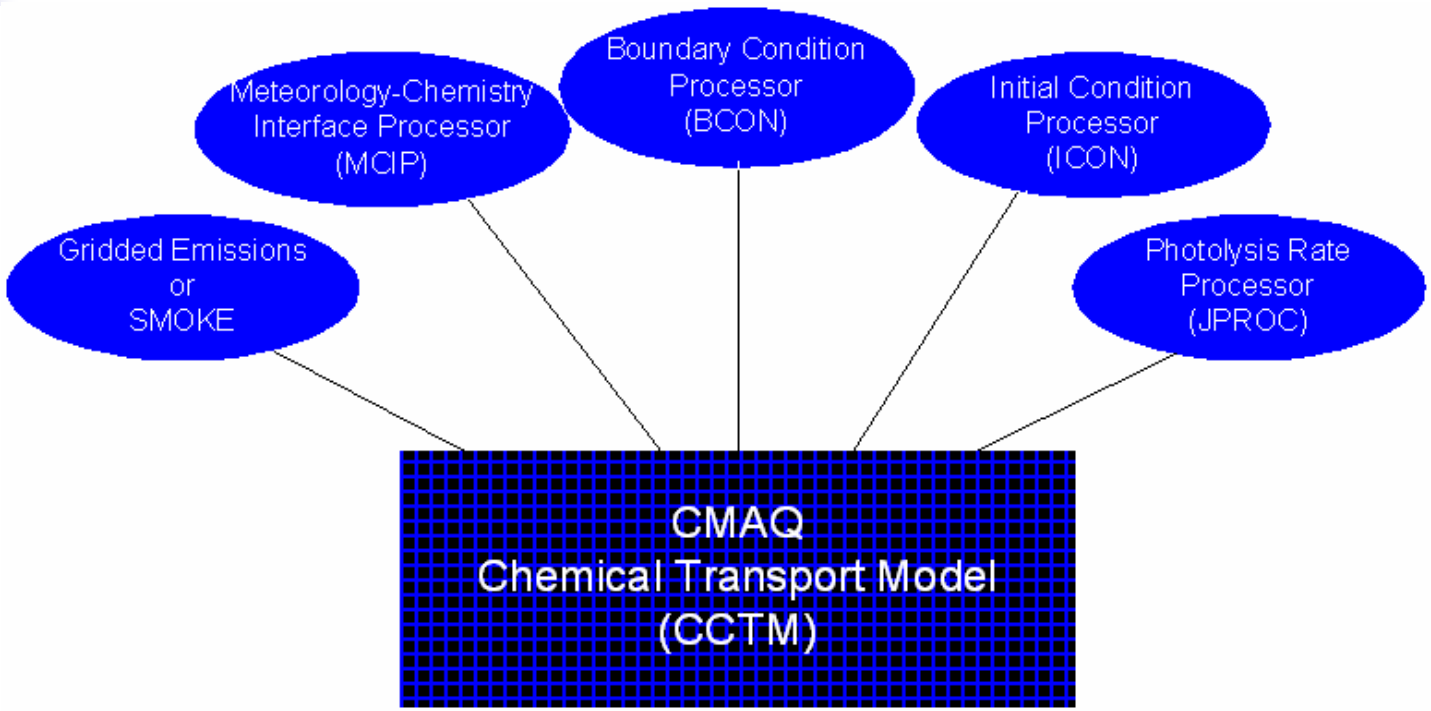
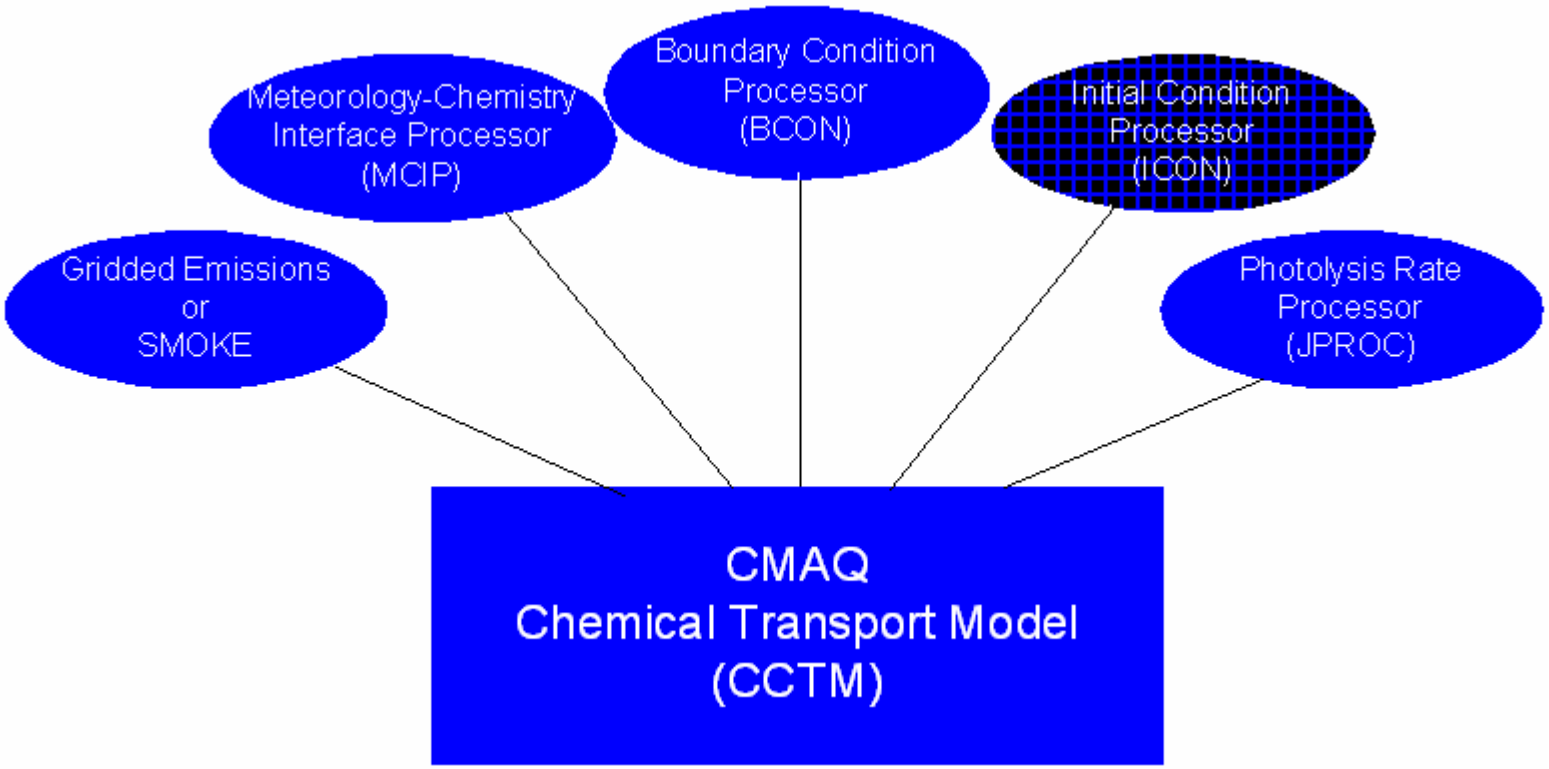
# The CMAQ Chemical Transport Model **( CCTM )**



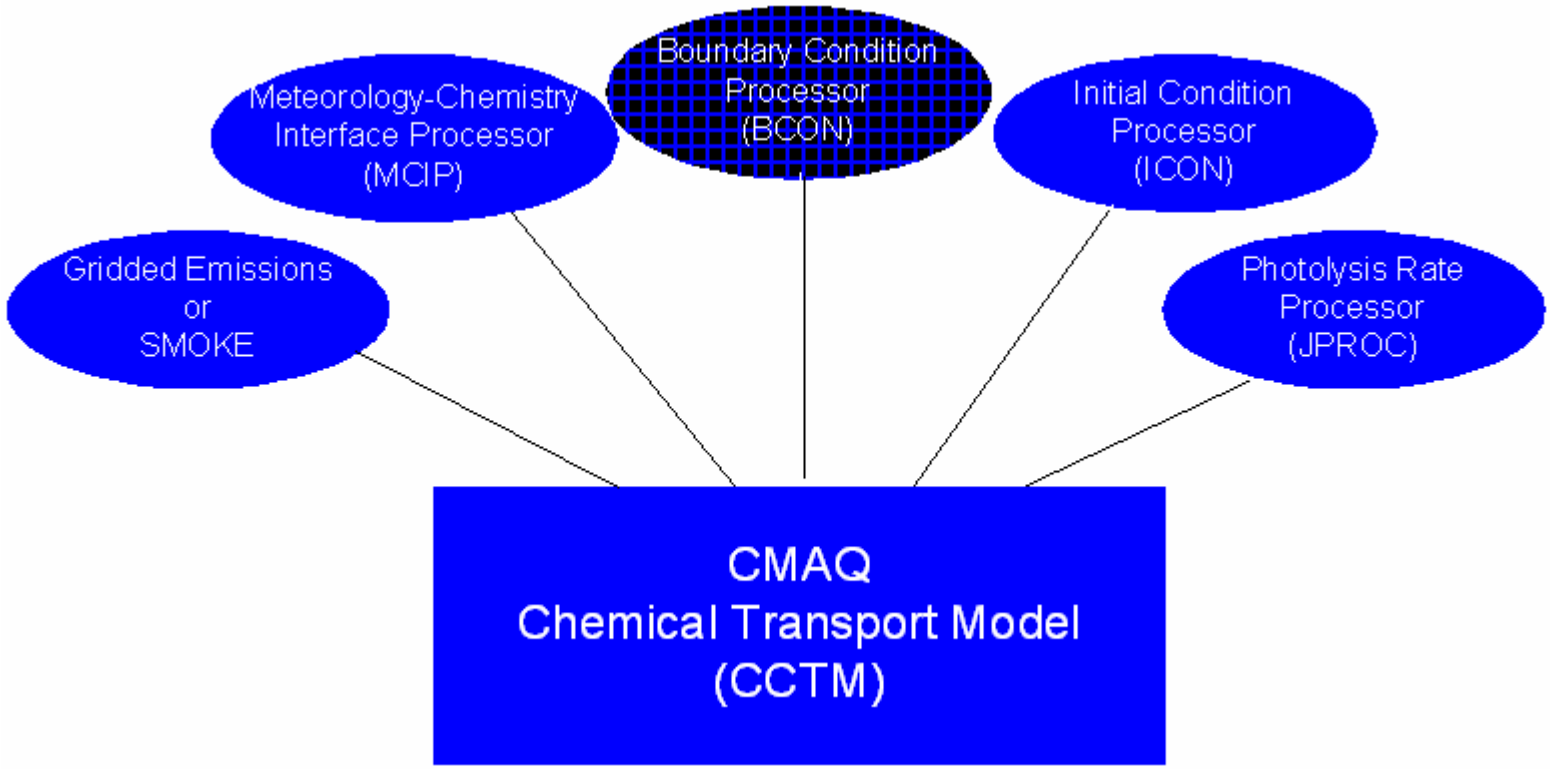

- Simulates major atmospheric chemistry, transport and deposition processes
- Requires input data from gridded emissions (or SMOKE), MCIP,BCON,ICON and JPROC processors.

# The Initial Condition Processor (ICON)



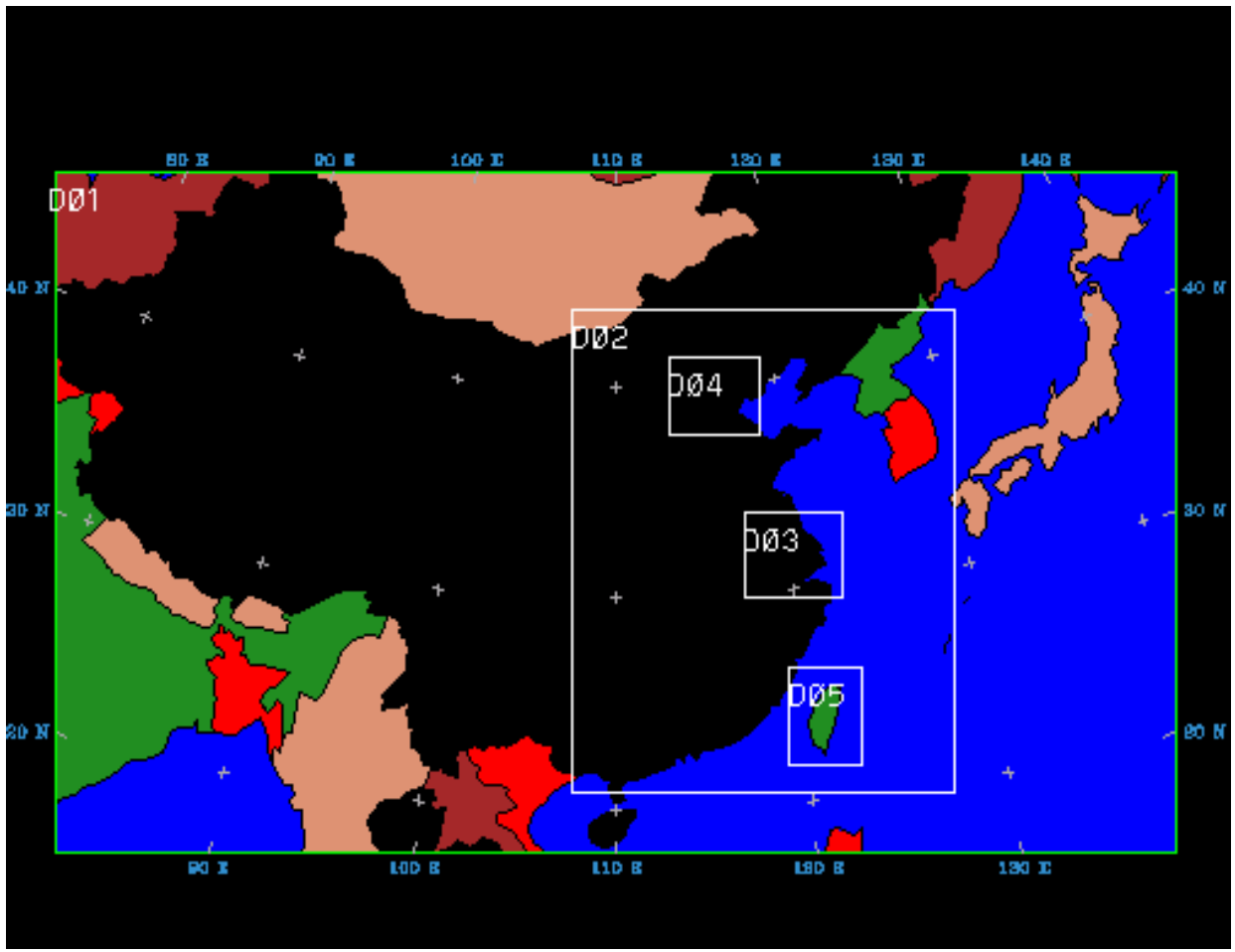

ICON provides initial species concentrations for every grid in the modeling domain

# The Boundary Condition Processor (BCON)




BCON provides species concentrations for the grids immediately surrounding the modeling domain

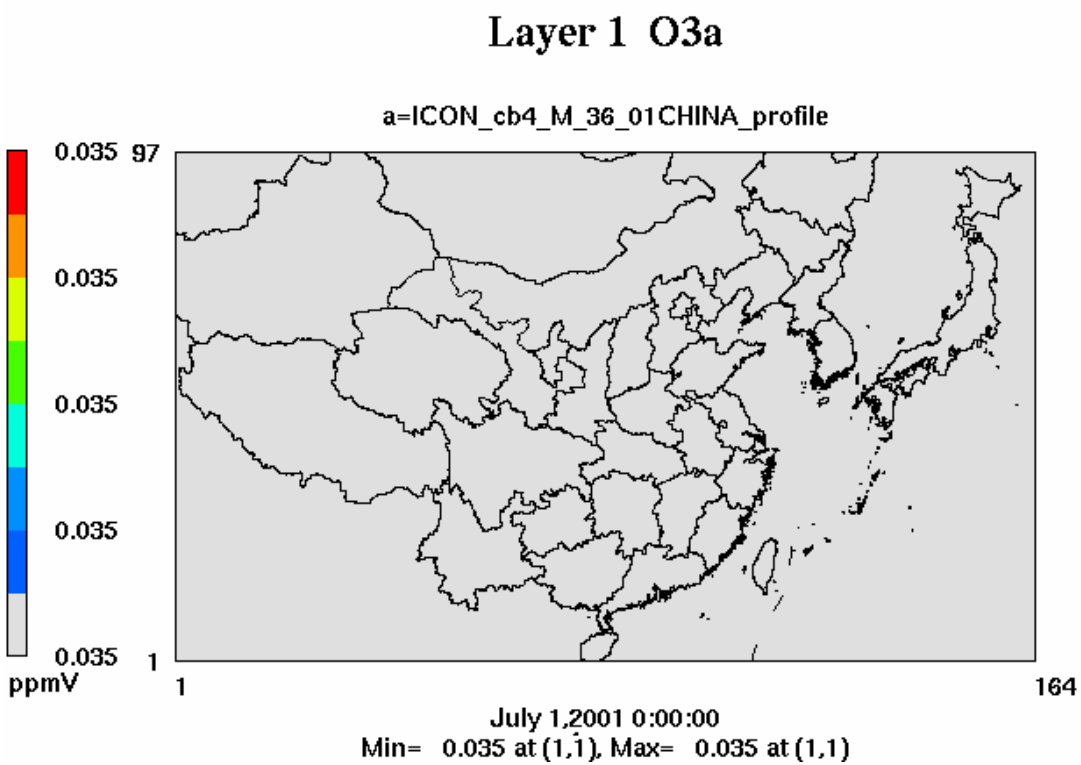
# CMAQ Domains in Great China Regions for (36km, 12km, and 4km)



# CMAQ Simulation Procedures with 36km, 12km, and 4km domains

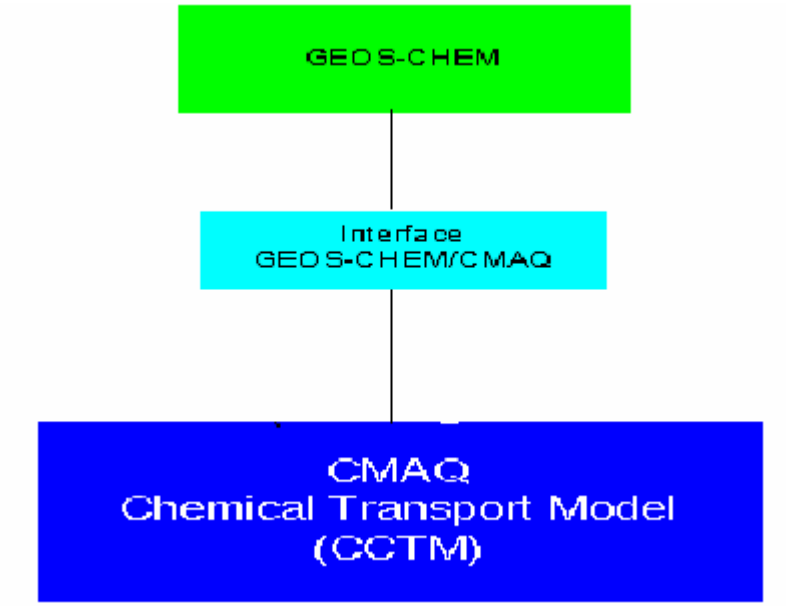
- Typical CMAQ Runs:
  - 36km -> 12km -> 4km
  - Finer domains obtain BC/IC from coarser domain results
    - 4km domains obtain IC/BC from 12km domain results
    - 12km domains obtain IC/BC from 36km domain results
  - 36 km domains use profile IC/BC
    - Time independent
    - Usually kept the same even with different scenarios and episodes
    - Add spin-out period (washout period) to initialize
      - 3, 5, 7 or even higher number of simulation days
      - Waste of time, resources, and energy.
      - Unrealistic nature

# Example of Profile IC (CN36)

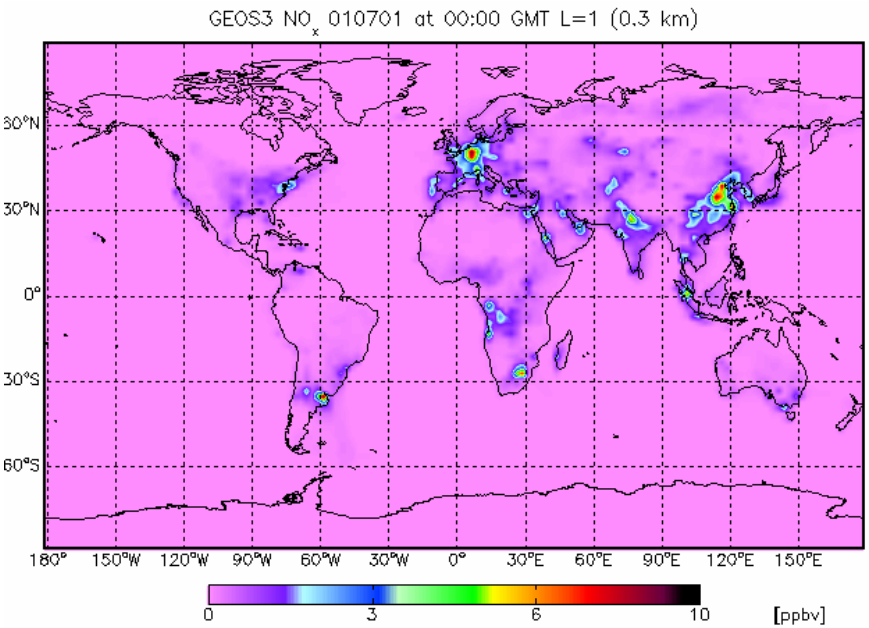


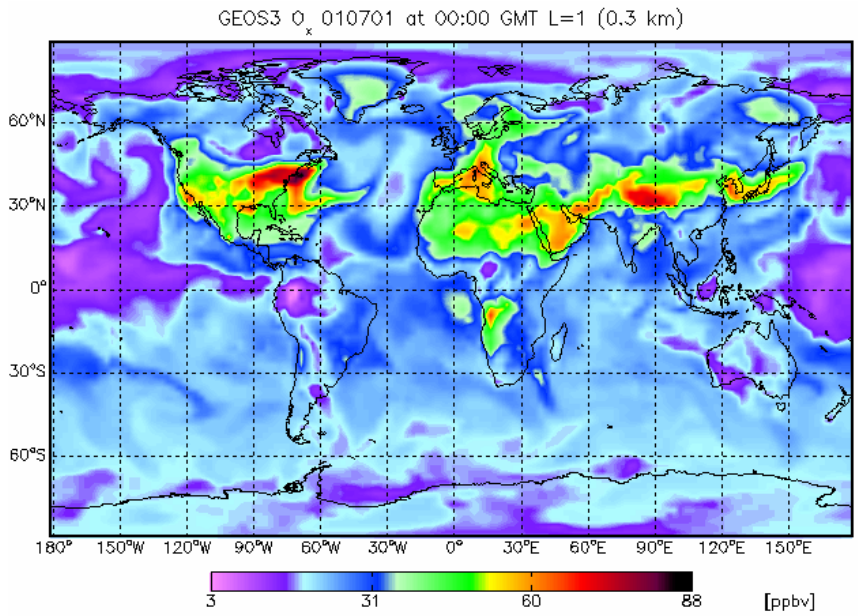
# GEOS-CHEM/CMAQ Interface

- The Goal:
  - To develop an interface to obtain more realistic IC/BC input for CMAQ from GEOS-CHEM simulation results



# To Extract IC/BC from GEOS-CHEM Simulation Results



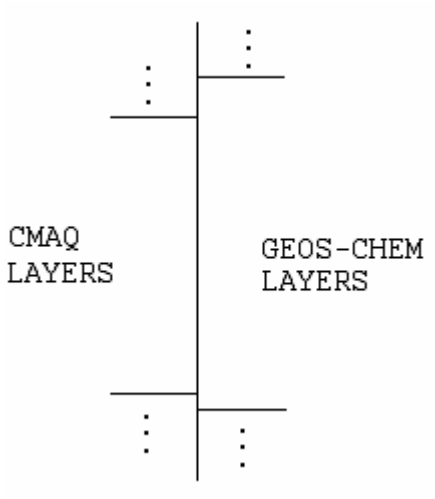
# Schematic Procedures of the Interface:

- Convert GEOS-CHEM species of interest to the corresponding CMAQ species.
- Conduct Coordinate Interpolation on GEOS-CHEM results, and transform the results to the final CMAQ coordinate system (pre-IC/BC results)
- Add profile concentrations of the species not derived from GEOS-CHEM to the pre-IC/BC results to get the final GEOS-CHEM IC/BC for CMAQ.

# Chemical Mapping Table for CB4 and SPARC-99 Mechanisms (EPA, 2003)

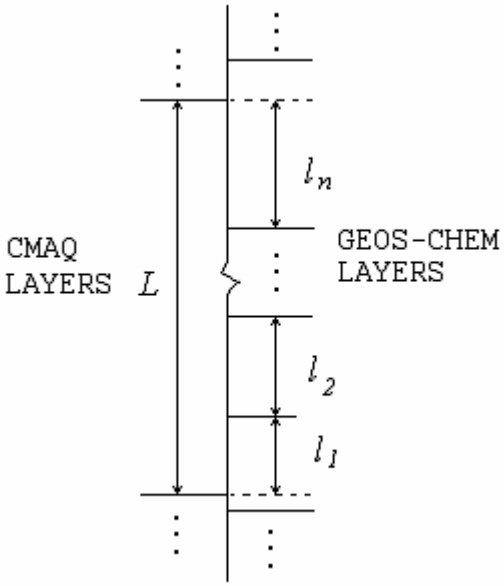
| GEOS-CHEM | | SAPRC-99 | CB4 |
|---|---|---|---|
| Ox | Ox (O3+NO2) | O3, NO2 | O3, NO2 |
| NOx | NOx (NO+NO2) | NO, NO2 | NO, NO2 |
| HNO3 | Nitric Acid | HNO3 | HNO3 |
| N2O5 | N2O5 | N2O5 | N2O5 |
| HNO4 | Peroxynitric Acid | HNO4 | PNA |
| CO | CO | CO | CO |
| H2O2 | Hydrogen Peroxide | H2O2 | H2O2 |
| CH2O | Formaldehyde | HCHO | FORM |
| SO2 | SO2 | SO2 | SO2 |
| PAN | PAN | PAN | PAN |
| PMN | MPAN | MA_PAN | PAN |
| PPN | PPN | PAN2 | PAN |
| C2H6 | Ethane | ALK1 | 0.4*PAR |
| ALK4 | Alkanes(>=C4) | ALK3+ALK4+ALK5 | 4*PAR |
| C3H8 | Propane | ALK2 | 3*PAR |
| PRPE | Propene | OLE1 | (1*OLE)+ (1*PAR) |
| ACET | Acetone | ACET | 3*PAR |
| MEK | Ketones(>C3) | MEK | 4*PAR |
| ALD2 | Acetaldehyde | CCHO | ALD2 |
| RCHO | Aldehyde(>C3) | RCHO | ALD2 |
| ISOP | Isoprene | ISOPRENE | ISOPRENE |
| MVK | Methylvinylketone | MVK | ISPD (products of isoprene rxns) |
| MACR | Methacrolein | METHACRO | ISPD (products of isoprene rxns) |
| MP | Methyl Hydroperoxide | COOH | UMHP |
| R4N2 | Alkylnitrate(>C3) | RNO3 | 2*NTR |
| | | | |
| SO4 | Sulfate | ASO4I+ASO4J | ASO4I+ASO4J |
| NH3 | Ammonia | NH3 | NH3 |
| NH4 | Ammonium | ANH4I+ANH4J | ANH4I+ANH4J |
| NO3 (p) | Particulate Nitrate | ANO3I+ANO3J | ANO3I+ANO3J |
| | | | |
| DMS | Dimethyl Sulfate | | |
| MSA | Methyl Sulfionic Acid | | |

# Vertical Interpretation (Situation I)




(a) One CMAQ layer is contained within one GEOS-CHEM layer

# Vertical Interpretation (Situation II)




$$C = \sum_{i=1}^{n} G_i \frac{l_i}{L}$$

$$L = \sum_{i=1}^{n} l_i$$

(b) One CMAQ layer covers one and more GEOS-CHEM layers

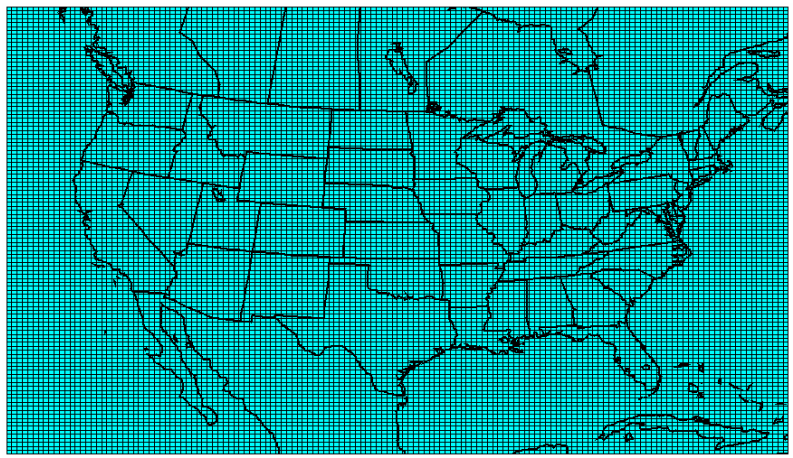
*C* is the concentration in a CMAQ unit cell to be calculated, *L* is the height of the CMAQ grid cell, *n* is the number of GEOS-CHEM layers overlapping the CMAQ cell vertically, $l_i$ is the height overlapped with $i^{th}$ of the *n* GEOS-CHEM layers, *Gi* is the estimated GEOS-CHEM concentration of the $i^{th}$ overlapping GEOSCHEM layer.

# Data Structures in the Interface

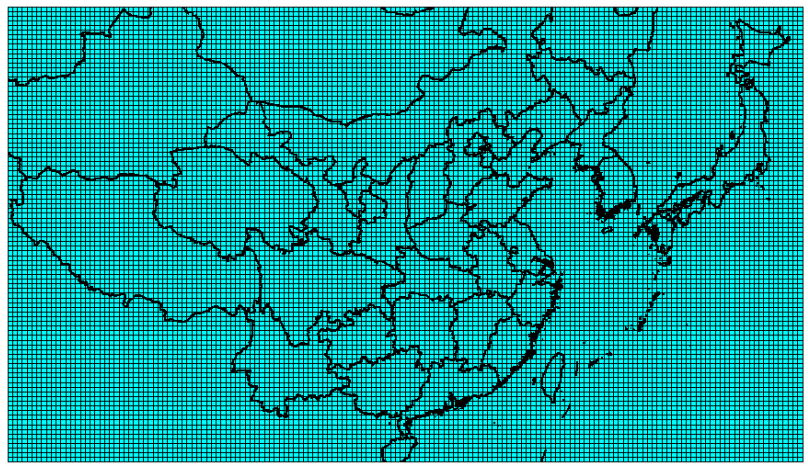
- Concentration Matrix:
  - **Data0**(NI, NJ, NL, **NP**) ->
  - **Data1**(NI, NJ, NL, **NVAR**)->
  - **Data2**(NCOL, NROW, NL, NVAR) ->
  - **Data3**(NCOL, NROW, NLAY, NVAR)
  - Note:
    - NI, NJ, NL, NP represent COLS, ROWS, LAYERS, SPECIES in GEOS-CHEM system
    - NCOL, NROW, NLAY, and NVAR are counterparts in CMAQ system

# CMAQ 36km Domain (US36 and CN36)

US 36km



CN 36km



# CMAQ Domains

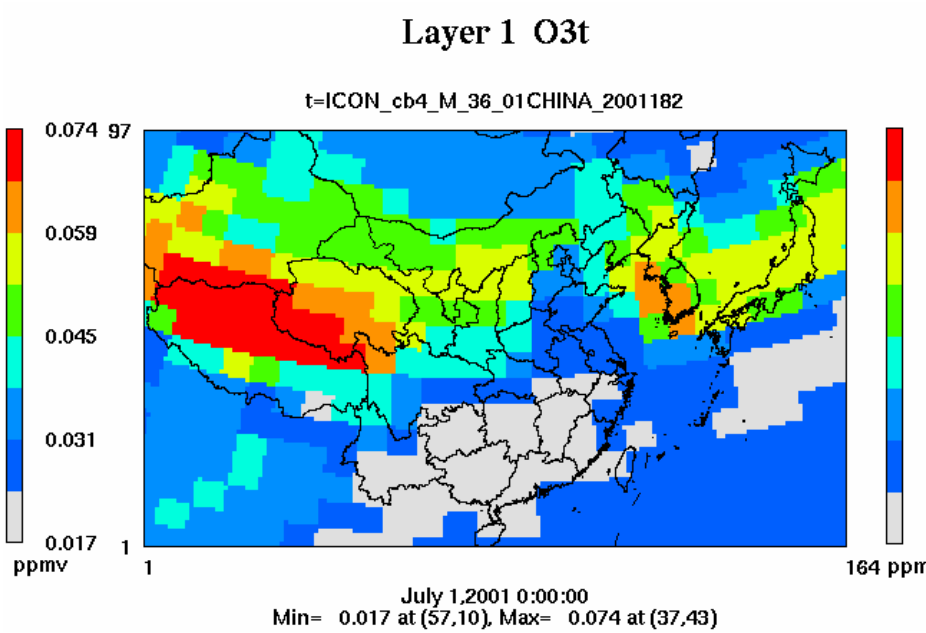
- US Domain
  - Grid cell size (36km)
  - 16 Layers
- East Asia/China Domains
  - Grid cell size (36km)
  - 14 Layers

# Input to GEOS-CHEM/CMAQ Interface

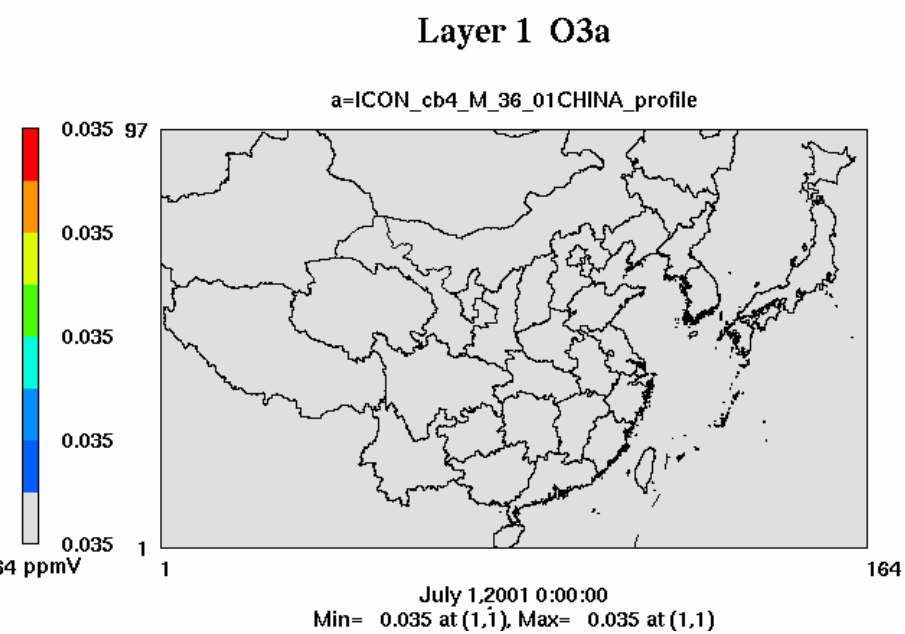
- GEOS-CHEM Results (2001) from Harvard
  - 3-hourly average concentration(NI, NJ, NL, NP)
  - Monthly Average BXHGHT Data
- Species Converting Formula from EPA
- CMAQ Domain Info
  - NCOL, NROW, NVAR
  - Vertical Layers Info (NLAY, Height of each layer)
  - Map projection info
    http://www.baronams.com/products/ioapi/LAMBERT.html
  - Air Density Data from MM5

# IC for CN Domain from GEOS-CHEM and Profile

## GEOS-CHEM IC

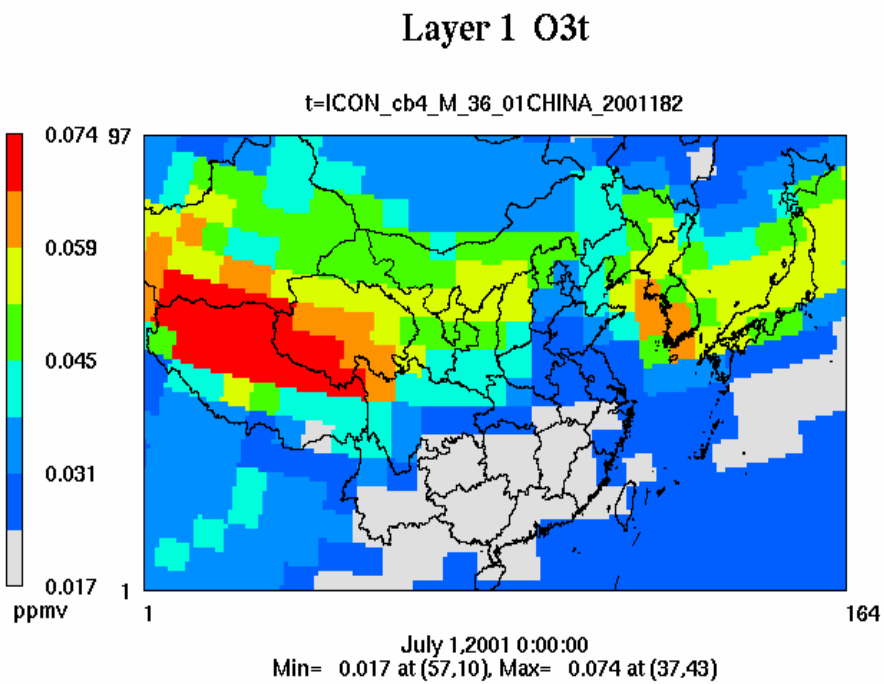



## Profile IC

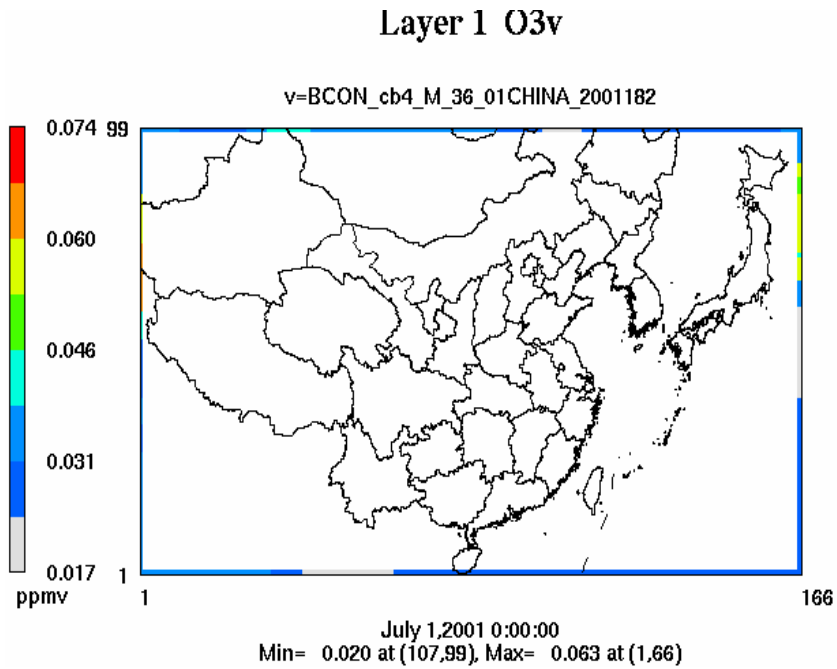


# IC/BC for CN Domain from GEOS-CHEM Results

## GEOS-CHEM IC

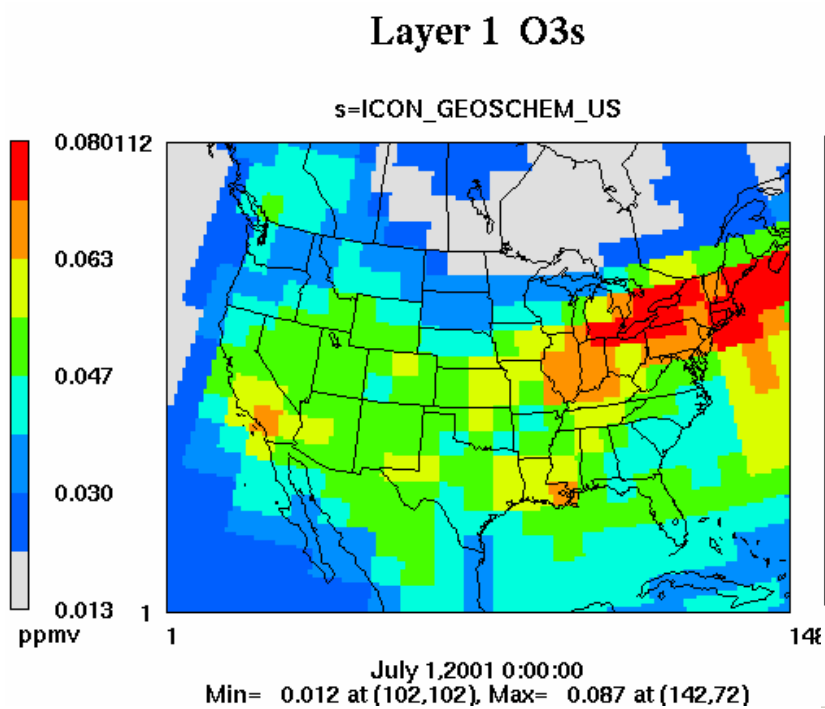



## GEOS-CHEM BC

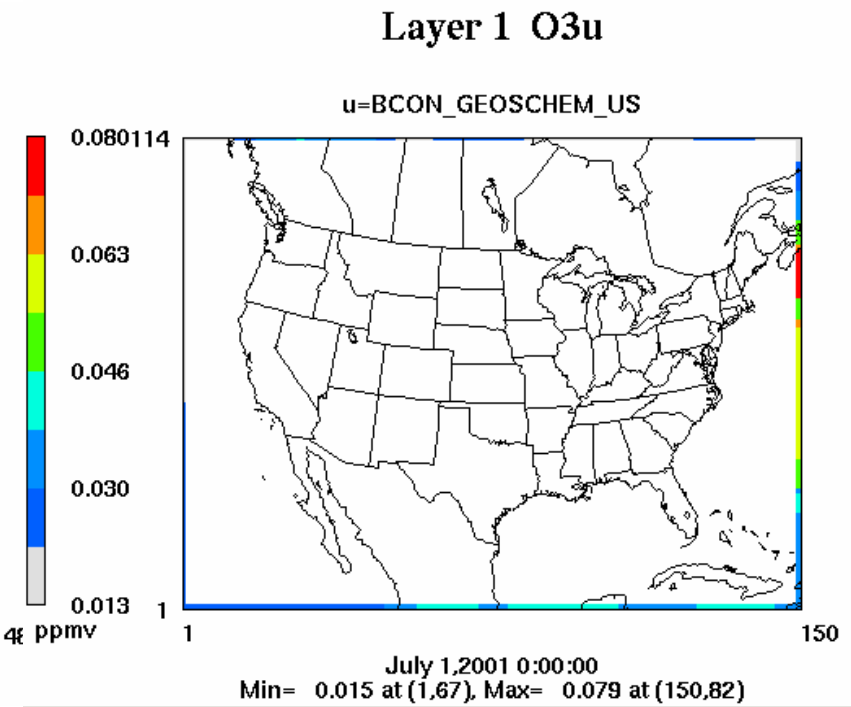


# IC/BC for US Domain from GEOS-CHEM Results

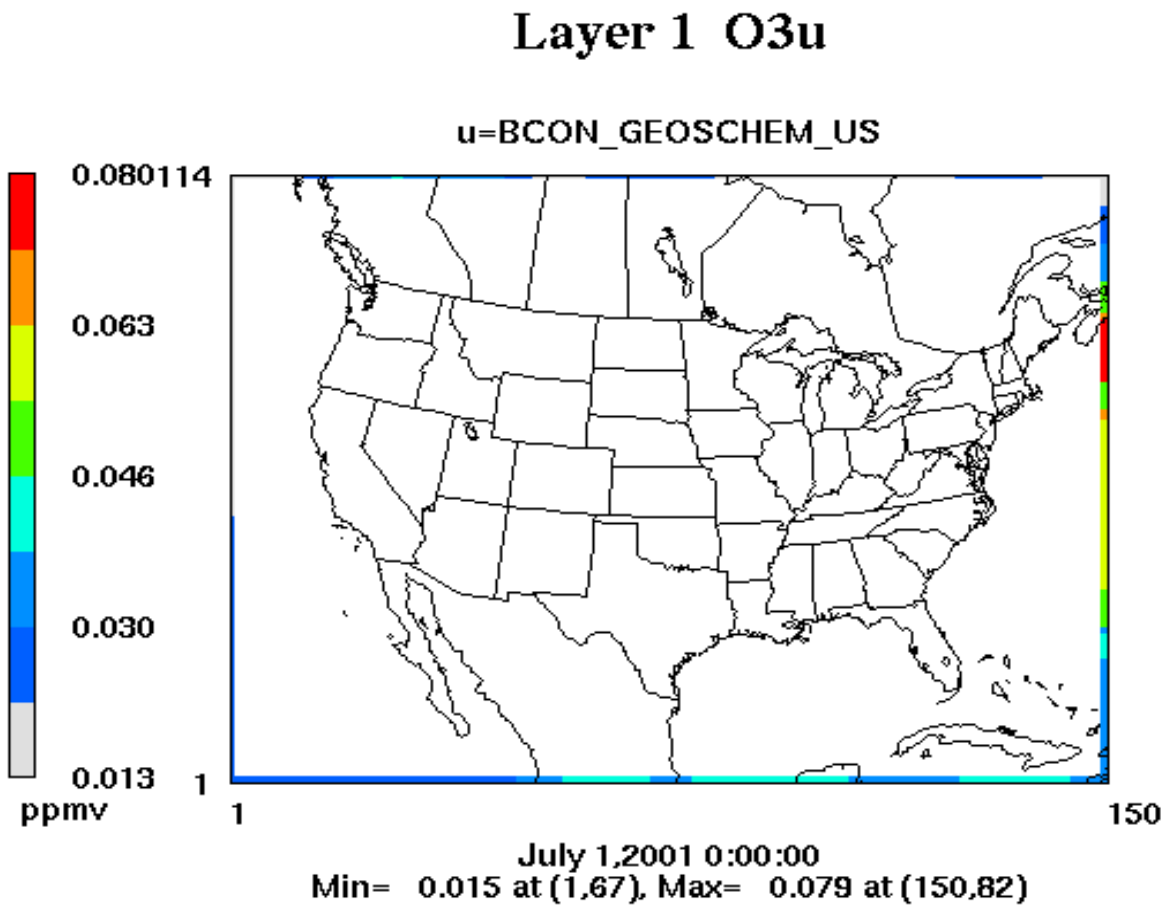
## GEOS-CHEM IC



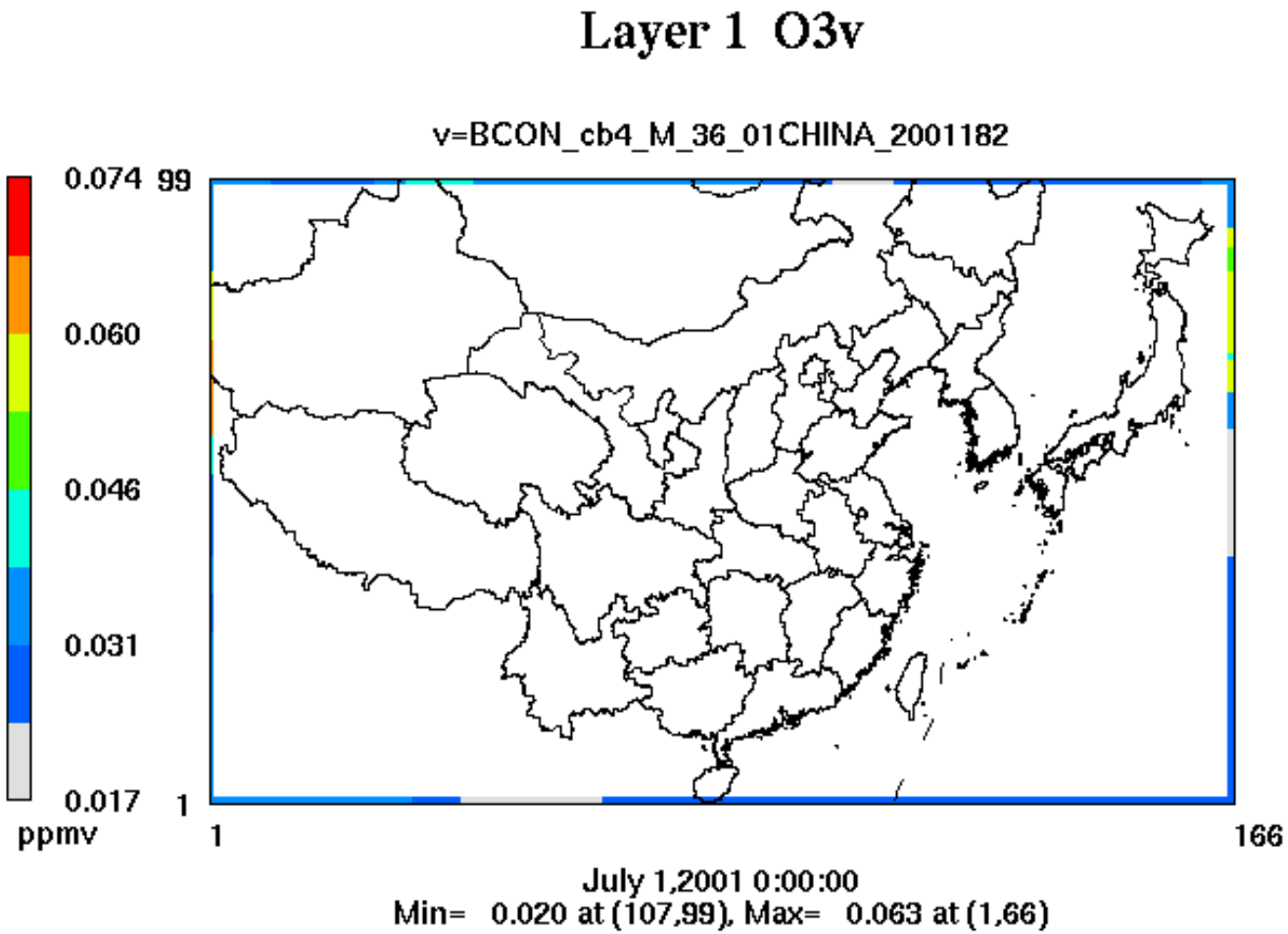

## GEOS-CHEM BC



# 3-Hourly BC(O3) Animation for US Domain from GEOS-CHEM Results



# 3-Hourly BC(O3) Animation for CN Domain from GEOS-CHEM Results

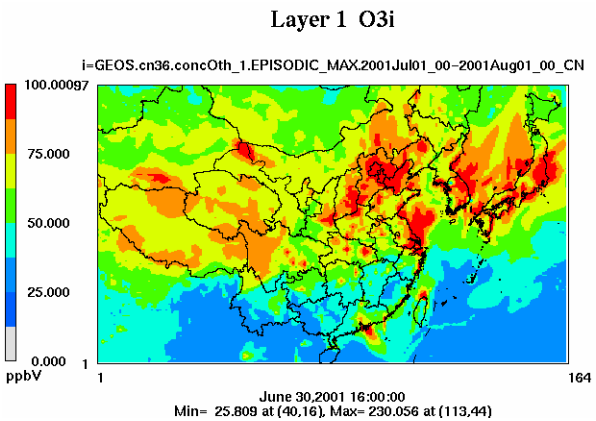


# Simulations

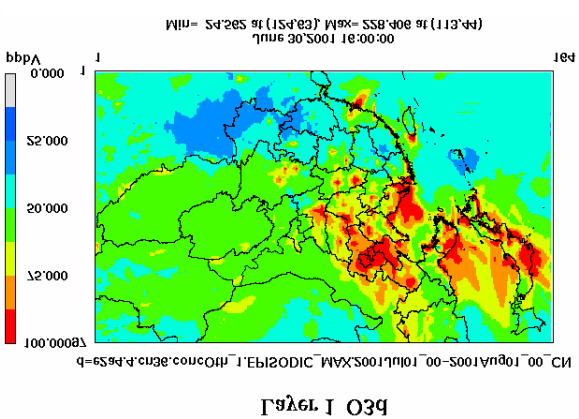
- Simulations with different IC/BC
  - Simulation 1: with Profile IC/BC(Regular CMAQ run)
  - Simulation 2: with GEOS-CHEM IC/BC
- Domain: cn36
- Episode: July 01-31, 2001 (spin-out: 5 days)

# Monthly Maximum (O3)

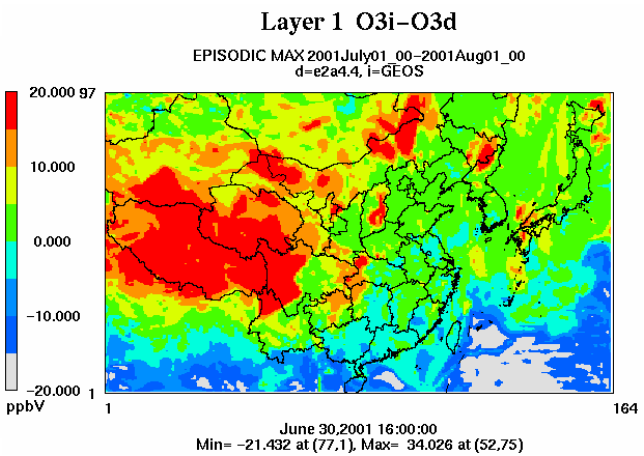
**GEOS-CHEM IC/BC**




**Profile IC/BC**



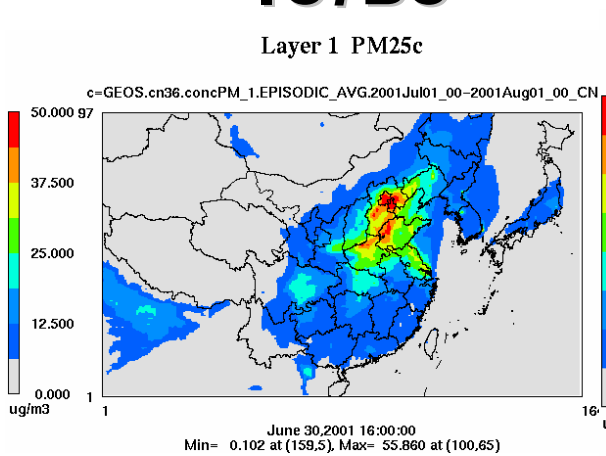
**Difference**



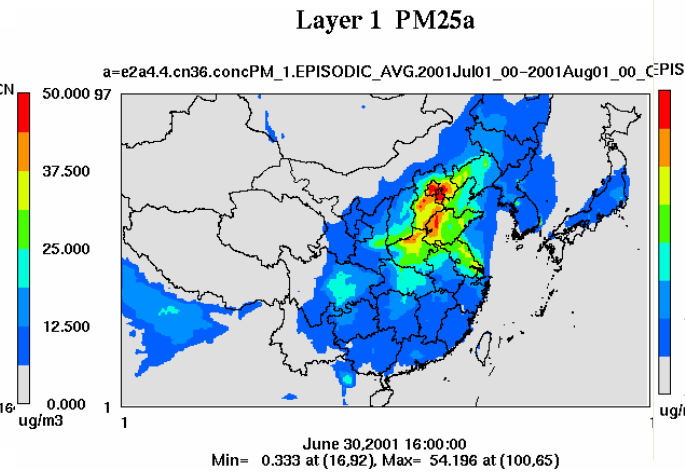

Does GEOSCHEM IC/BC generate higher O3 concentrations around Beijing Areas?

# Monthly Average (PM2.5)

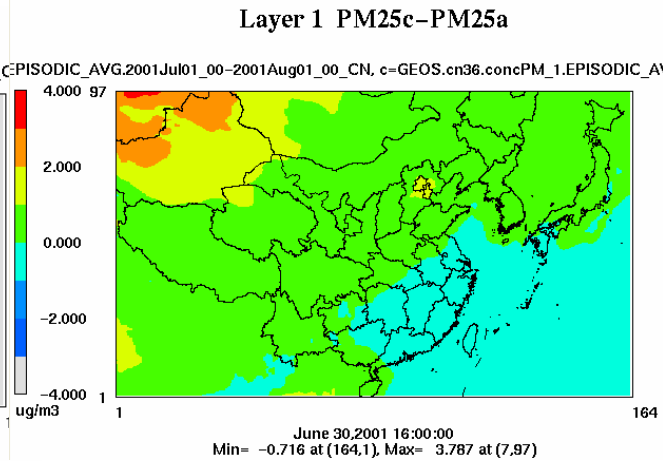
**GEOS-CHEM IC/BC**




**Profile IC/BC**




**Difference**




GEOS-CHEM IC/BC run does get a little bit higher PM2.5 values than the profile run around the Beijing area ( 1 – 2 ug/m$^3$)

# Summary

- The GEOS-CHEM/CMAQ Interface can provide CCTM IC/BC inputs from GEOS-CHEM simulation results, and CCTM runs smoothly with the GEOS-CHEM IC/BC inputs
- The output demonstrated apparently different monthly maximum O3 results between the simulation using profile IC/BC and the simulation using GEOS-CHEM IC/BC. Results also shows a slight increasing trend of PM2.5 values.

# Future Work

- CMAQ simulation studies will be conducted for CONUS 36km domain with GEOS-CHEM IC/BC generated by the GEOS-CHEM/CMAQ interface

# Acknowledgement


- NCAR's supports of computing resources through projects #35991003 and #35991004
- USEPA’s STAR and ICAP financial support