



# ***Accuracy and Cost Considerations in Choosing a Chemical Mechanism for Operational Use in AQ Models***

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# Background

- Accuracy
  - Air quality management decisions
    - Absolute concentration magnitudes
    - Concentration response to emissions changes
    - Gear ODE solver considered as reference solution for chemical kinetic equations
- Efficiency
  - Practical implementation in 3-D air quality models for operational use
    - Needs to work in short-term (days to weeks) and long-term (year or longer) simulations



- Need for multiple modeling iterations to examine the efficacy of various potential emissions control strategies
- Daily modeling for air quality forecasting demands high efficiency
- In single processor models from 10-20 years ago (UAM, ROM), solution of gas-phase chemistry could consume up to **80%** of total CPU time
- Today's models consume relatively less of their time in solving gas-phase chemistry
  - Additional processes
    - Aqueous chemistry, aerosols
  - More efficient solvers
  - Parallel processing



# Process contributions to runtime for CMAQ

Linux P3/1.4 GHz using 2 CPUs

Process	Relative time (% of total runtime)
Gas-phase chemistry (CB05)	33
Aerosol	25
Advection	16
Diffusion	14
Cloud	5



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# *CMAQ Mechanisms and Solvers*

- CB4
  - 41 chemical species; 93 reactions
- CB05
  - 51 chemical species; 156 reactions
- SAPRC-99
  - 72 chemical species; 214 reactions



- Solvers
  - SMV-Gear (sparse-matrix vectorized)
    - General ODE solver
    - “Gold standard” for numerical accuracy; user specifies relative tolerances
    - Relatively time-consuming
  - Rosenbrock solvers
    - Generalized solvers
    - Variable accuracy; user specifies relative tolerances
    - Less time-consuming than Gear solver



- Euler-backward iterative (EBI)
  - Customized to a particular mechanism
  - Accurate within tested bounds
  - Faster than Gear or Rosenbrock
  - May break down in extremely stiff conditions
    - e.g., within power plant plumes
    - Grid resolution issues may need consideration
  
- Others; not currently in CMAQ model
  - Quasi-steady state approximation
  - Hybrid implicit/explicit methods
  - Kinetic pre-processor (KPP)
    - Complete kinetics package
    - Has multiple generalized solvers available



## *Comparison of EBI and SMVGEAR solvers for CB05*

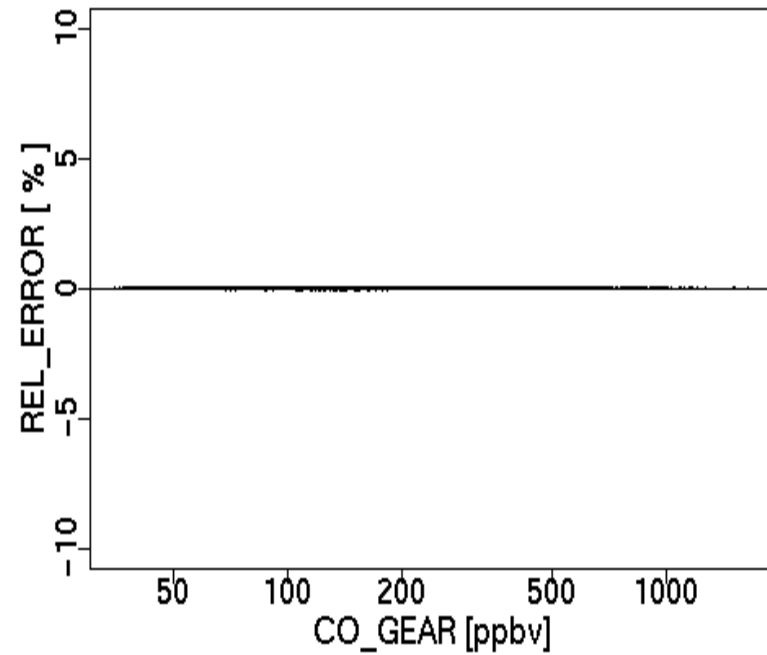
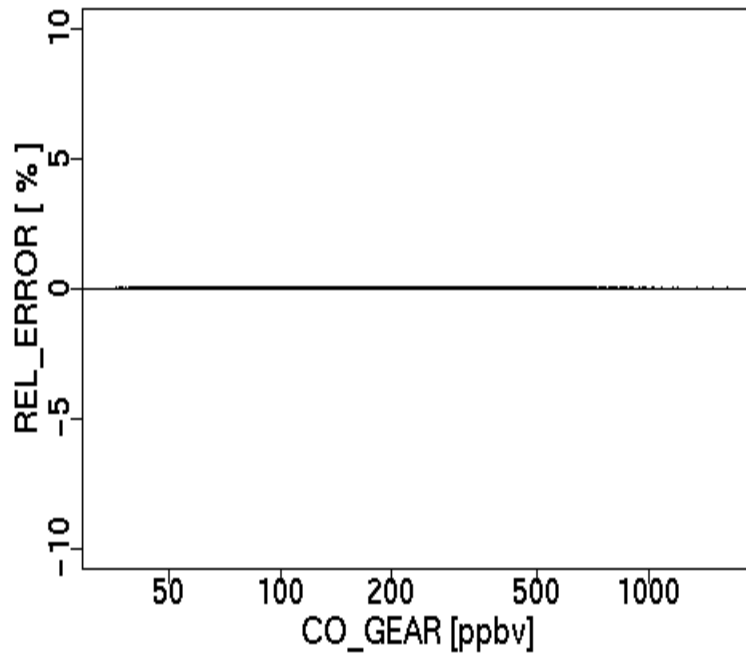
- CMAQ model - continental US domain
- 36-km horizontal grids
- July 1-5, 2001
- IC - model results for June 30, 2001
- Performed two sets of simulations with CB4, CB05
  - One with EBI solver
  - The other with smvgear solver
- First layer of model results are compared



# CO

## CB05

## CB4



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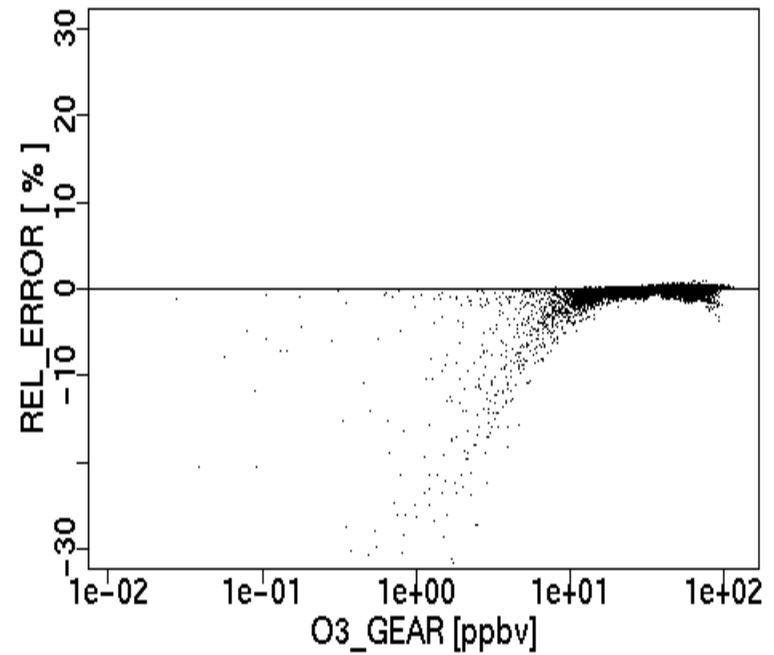
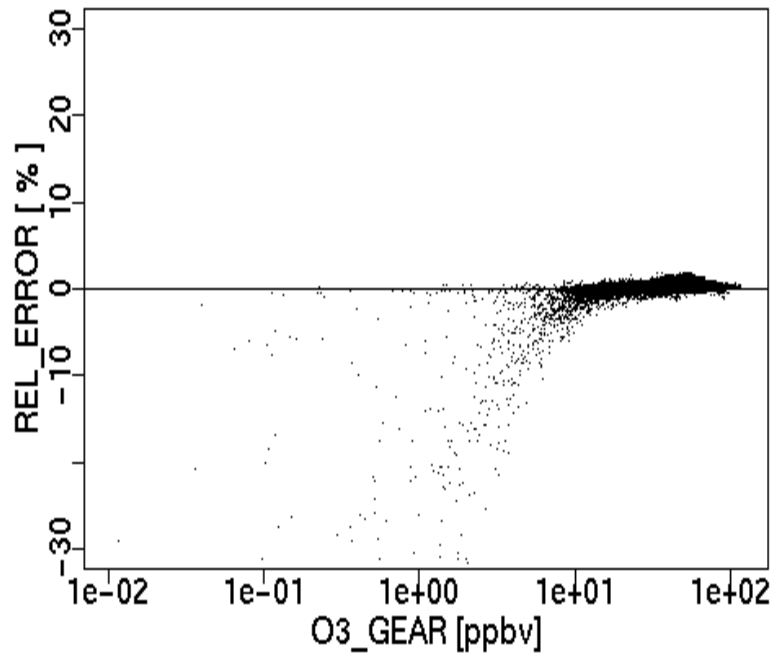
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# O3

## CB05

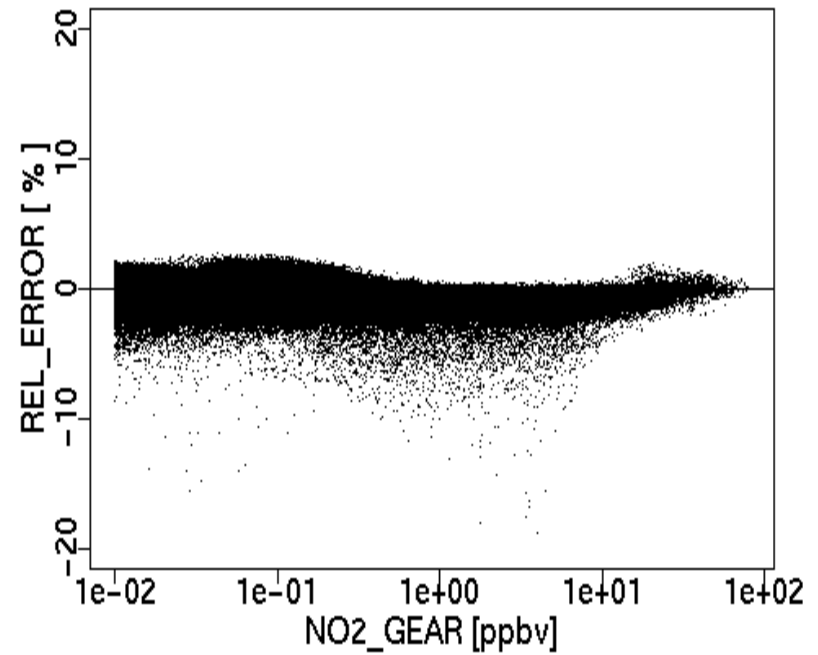
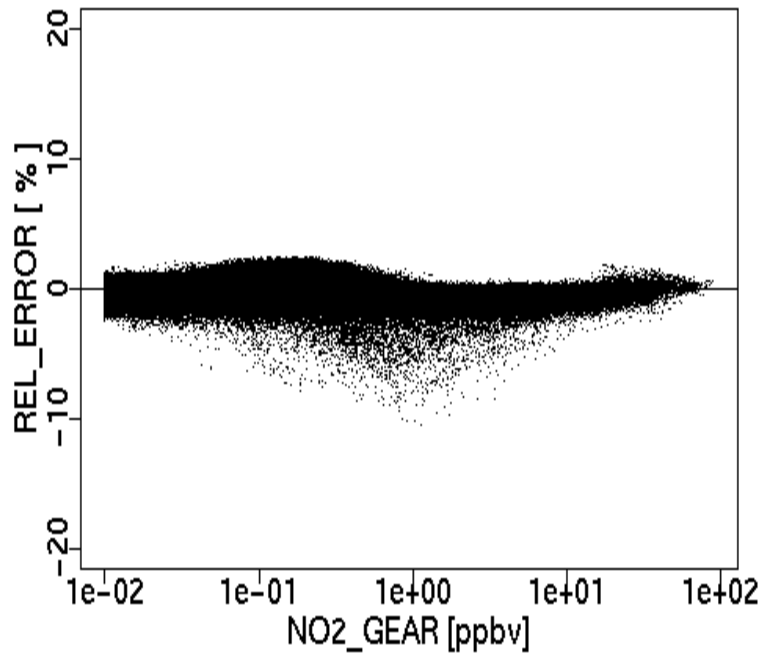
## CB4



# NO2

## CB05

## CB4



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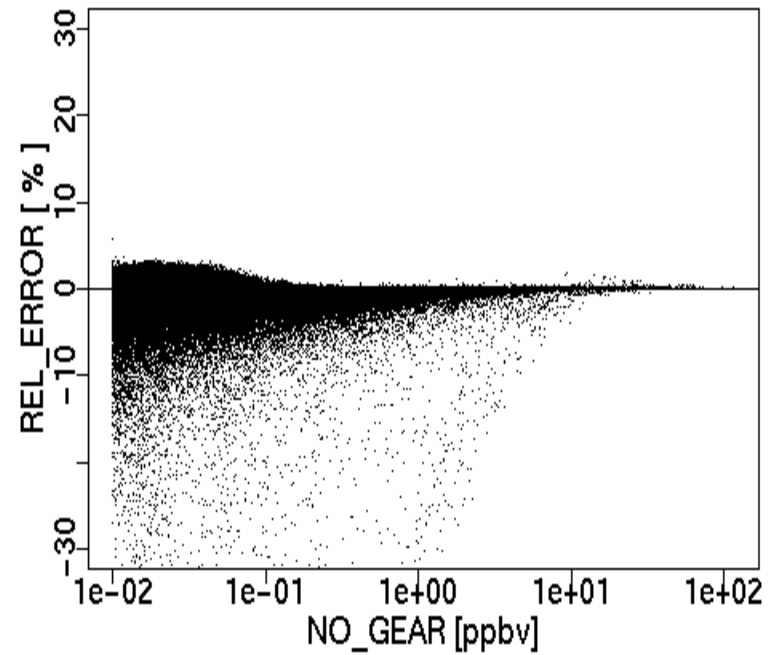
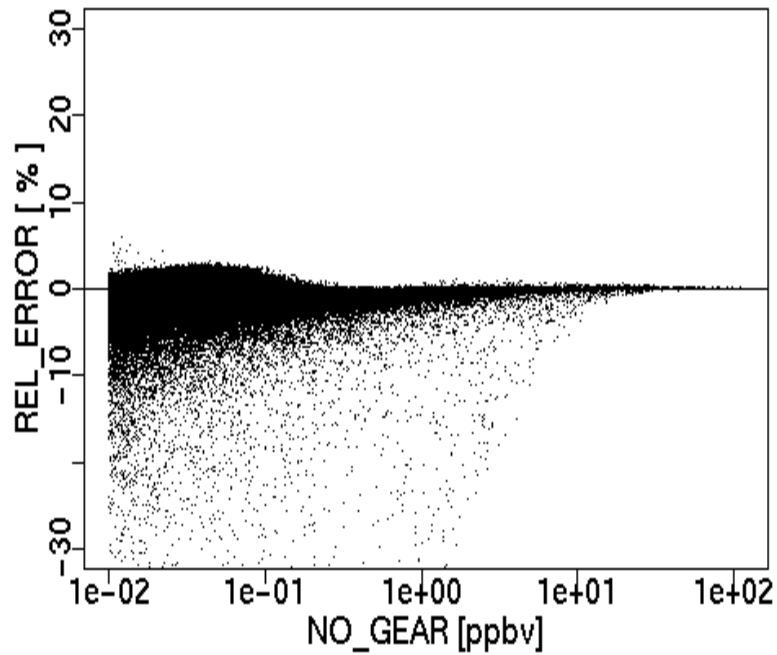
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**NO**

**CB05**

**CB4**



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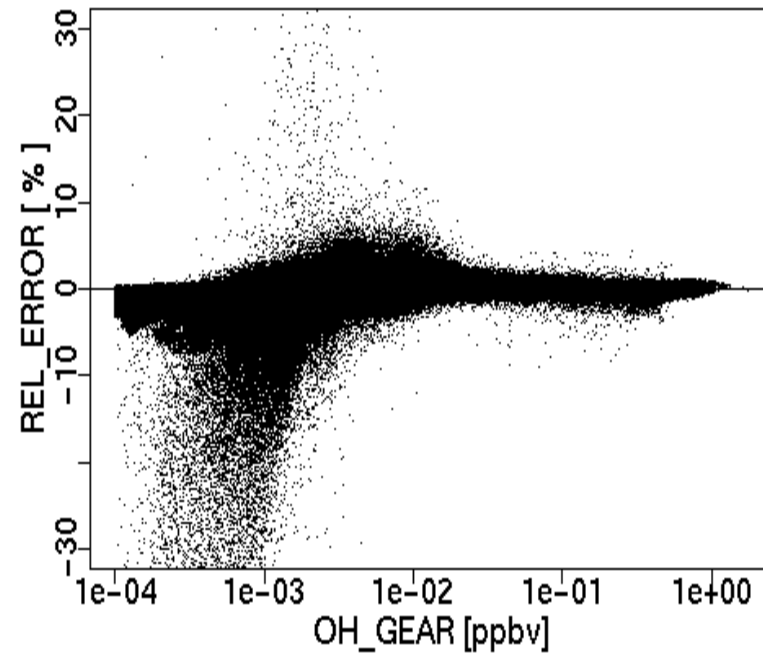
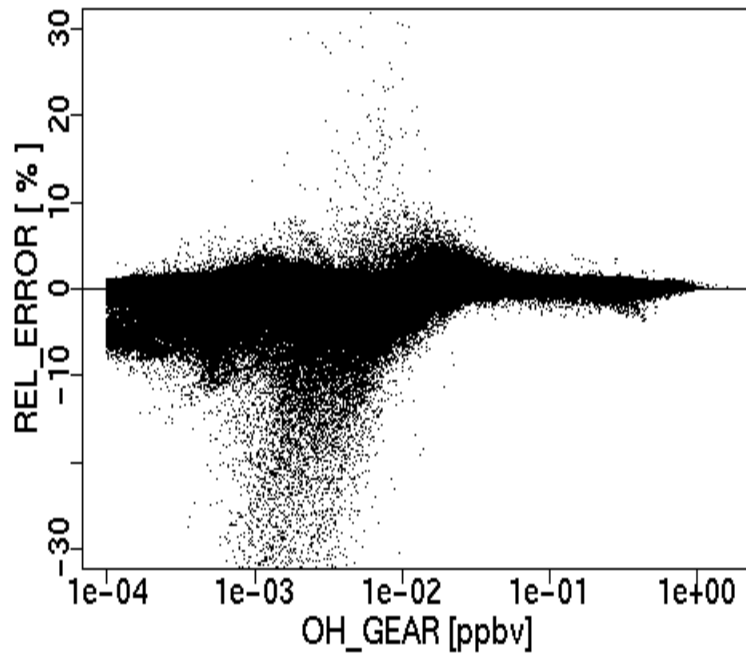
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**OH**

**CB05**

**CB4**



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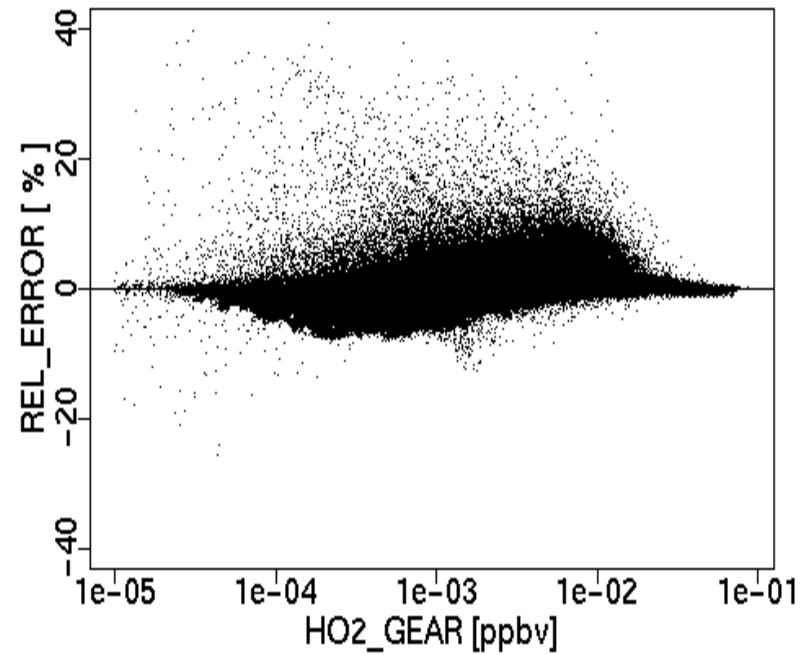
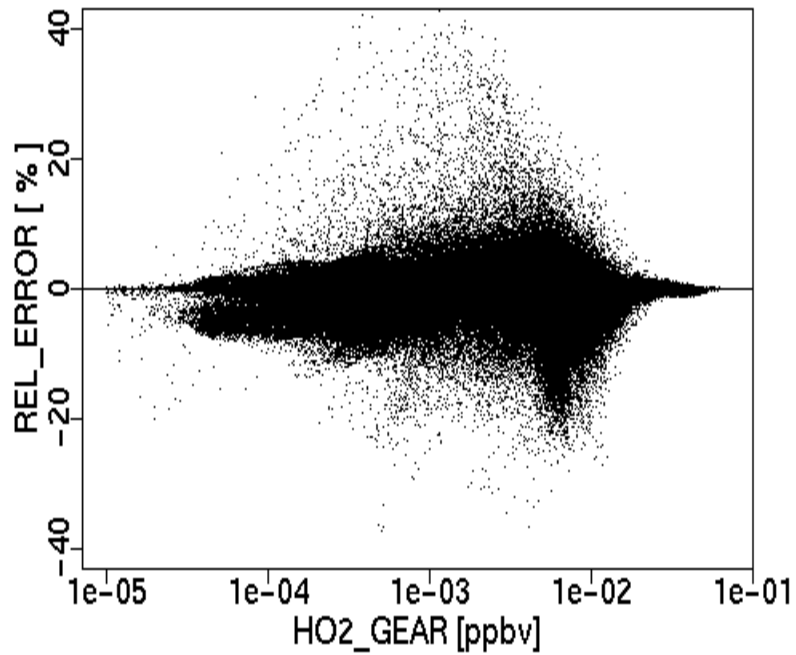
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# HO2

## CB05

## CB4



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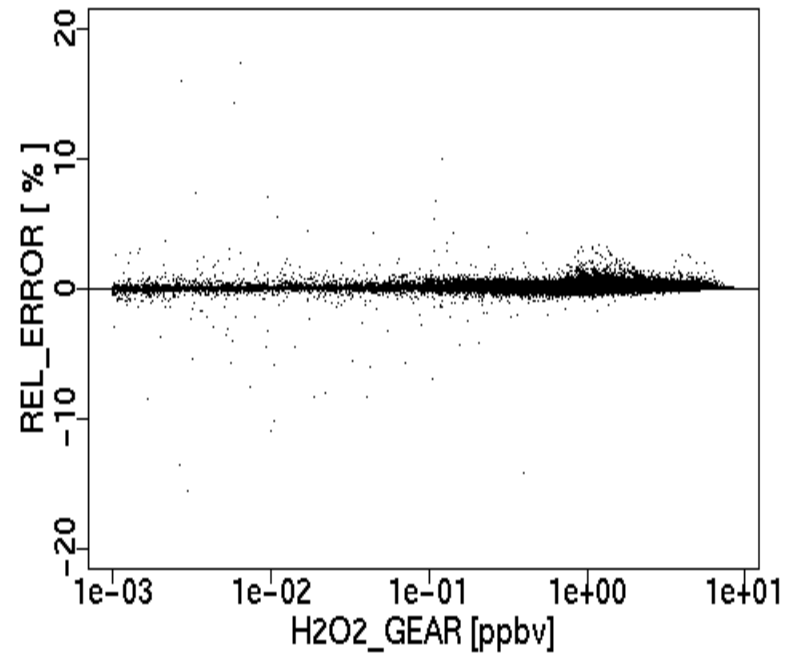
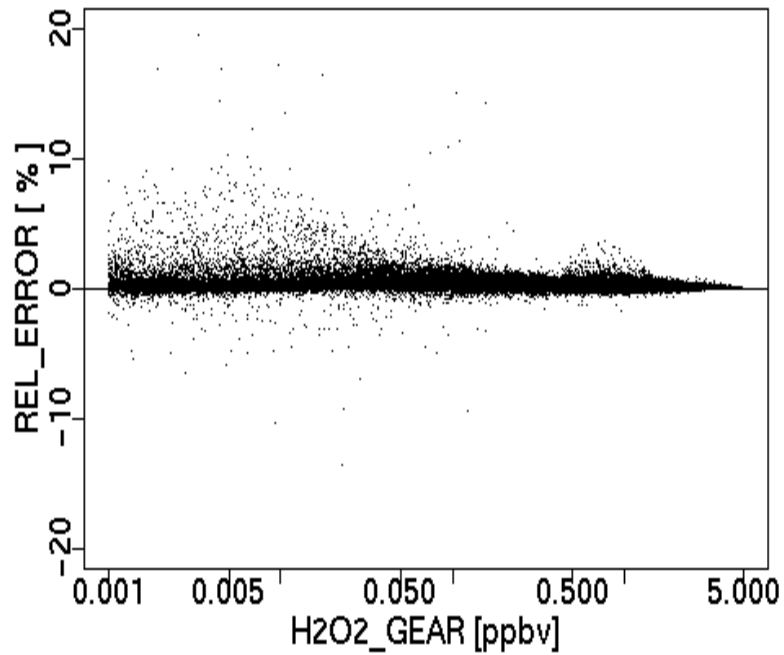
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# H2O2

## CB05

## CB4



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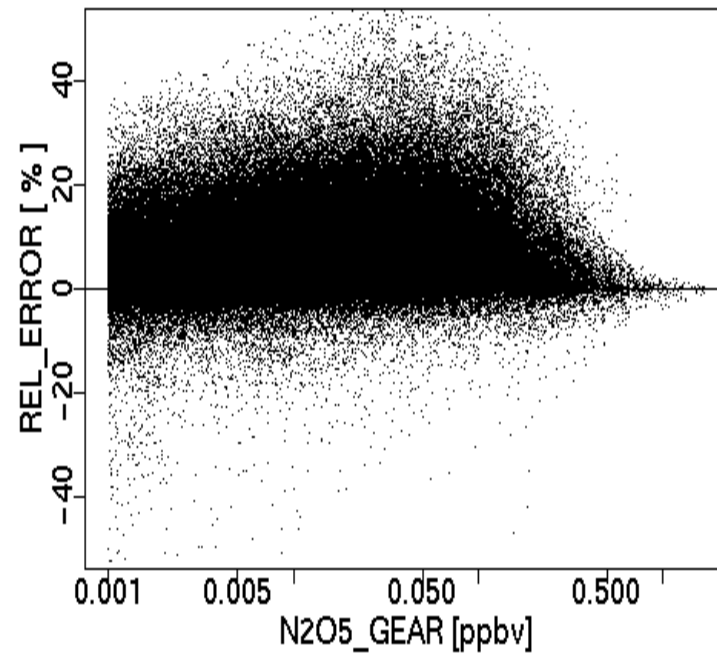
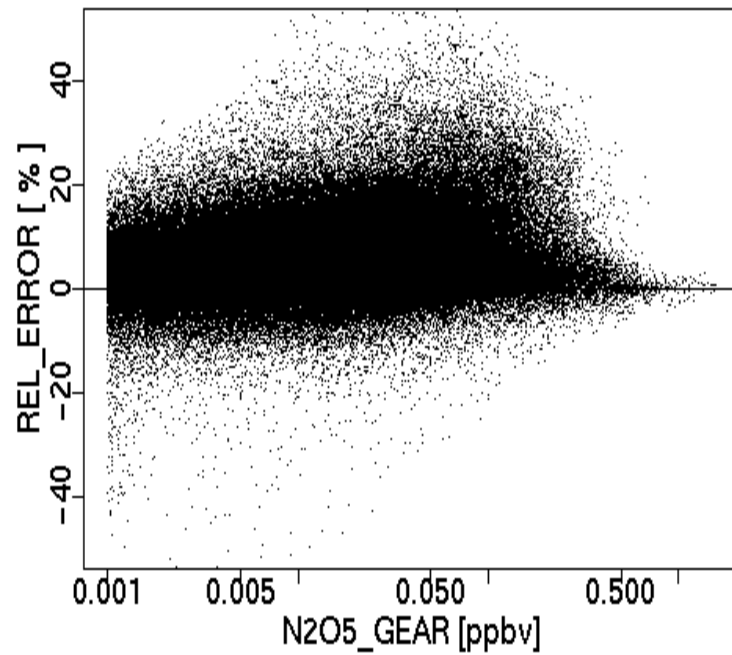
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# N2O5

## CB05

## CB4



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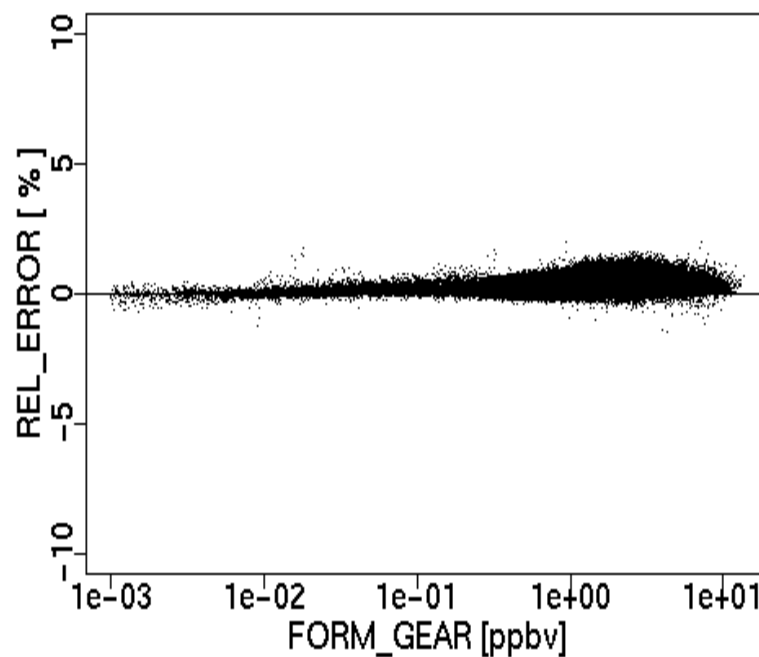
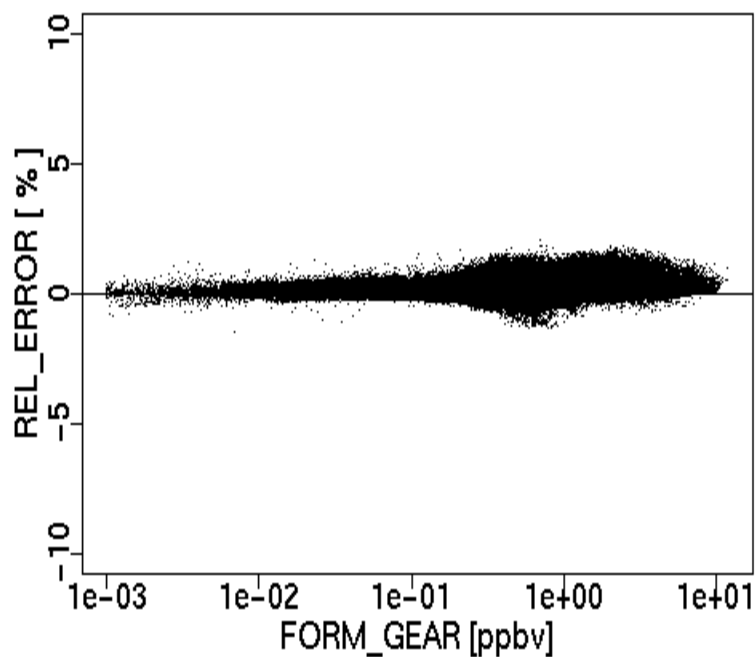
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# FORM

## CB05

## CB4



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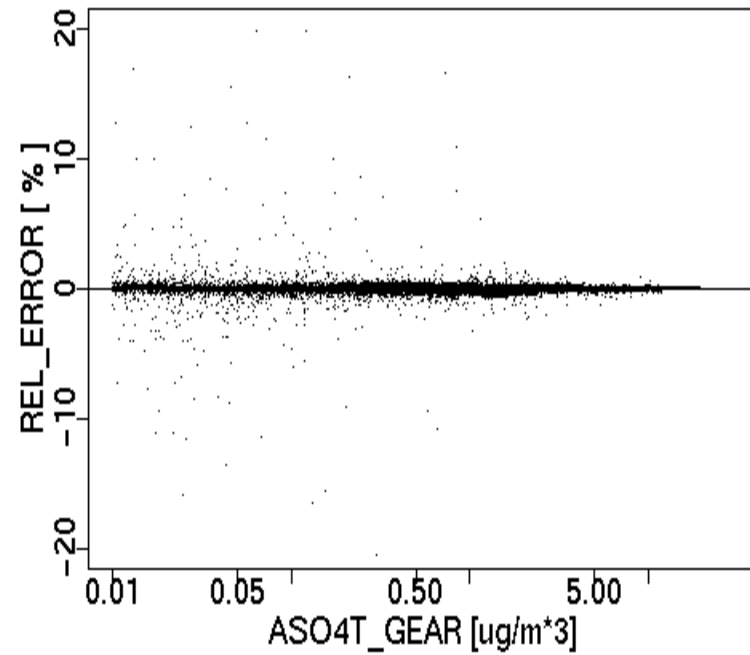
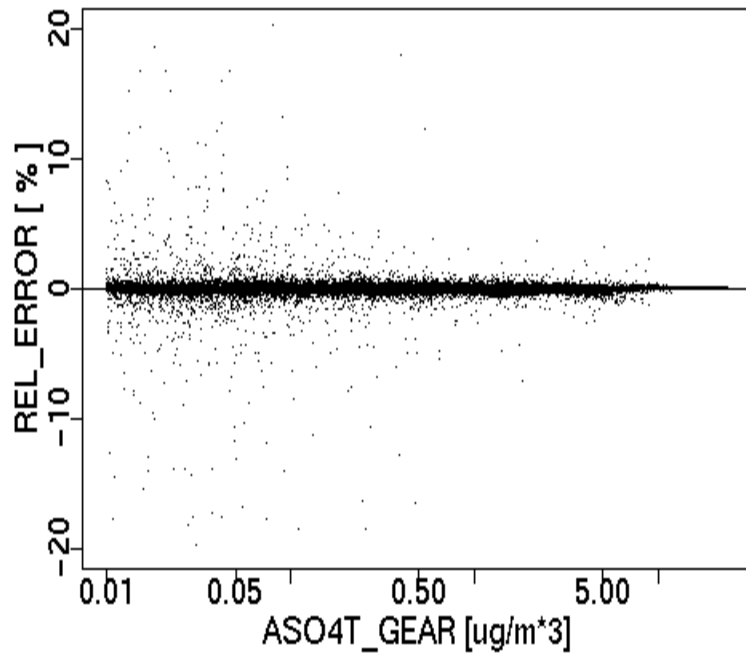
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# ASO4T

## CB05

## CB4



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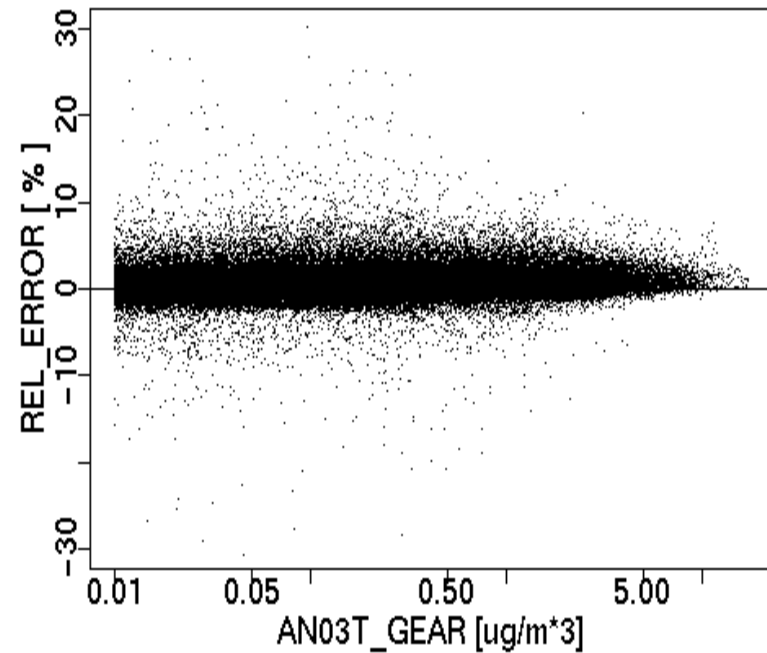
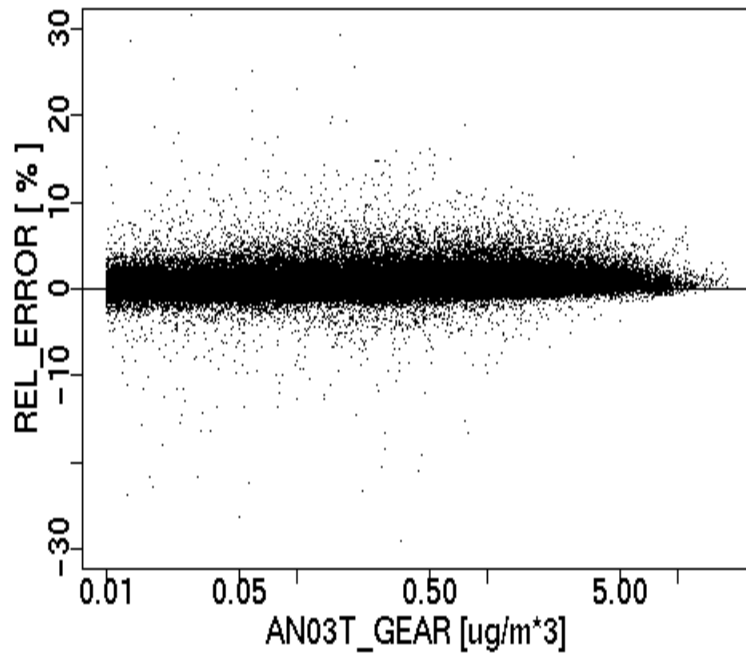
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# ANO3T

## CB05

## CB4



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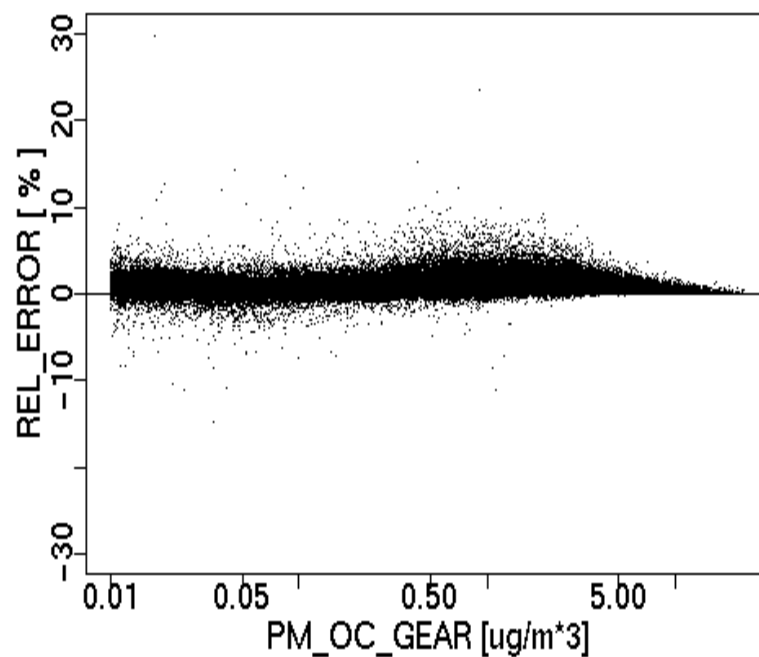
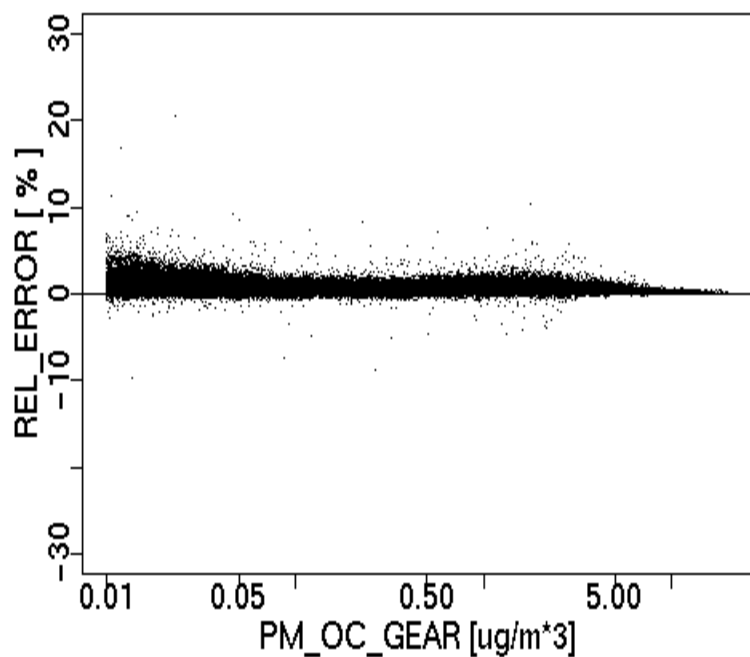
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# PM\_OC

## CB05

## CB4



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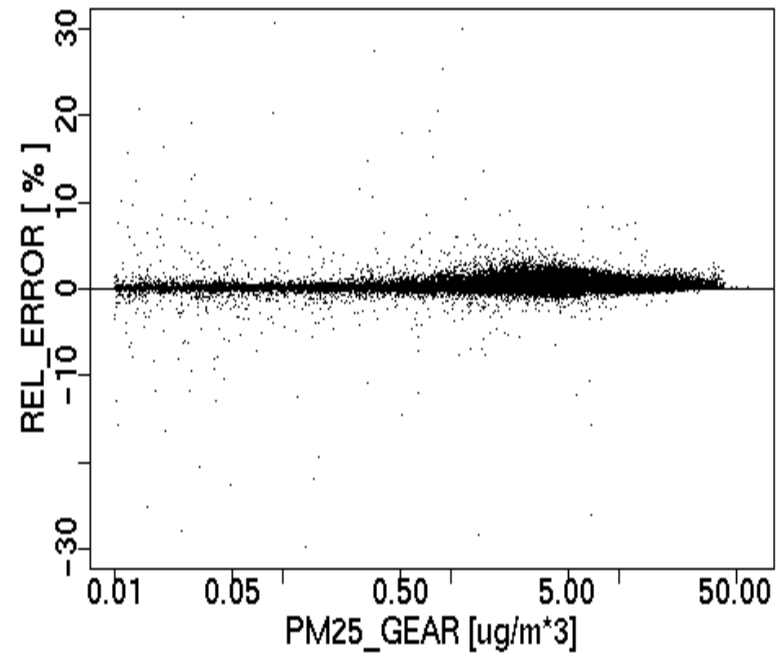
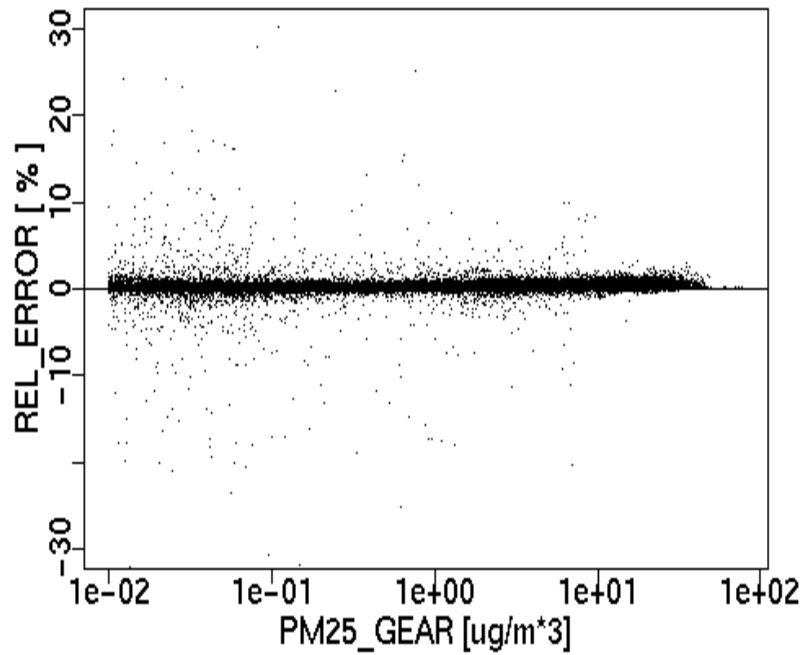
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# PM2.5

## CB05

## CB4



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# *Numerical Accuracy Considerations*

- Errors in target species
  - O<sub>3</sub>, PM components
- Errors in primary driver species
  - NO, NO<sub>2</sub>, VOCs
- Errors in radicals/intermediates
  - Should be monitored
  - Can be important if the error significantly changes the *response of the mechanism target species to emissions perturbations*



# ***Solvers: EBI, ROS3, and SMVGEAR CMAQ Model: Run Time Comparisons***

CONUS domain, 36-km grid-cells / (112 x 148 x 14 grid-cells) July 1, 2001  
Linux P3/1.4 GHz using 2 CPUs

Solver (CB05)	Time (min)	Ratio
SMVGEAR	135	-
ROS3	92	1.4
EBI	53	2.5



## *Additional Considerations*

- Future capabilities moving toward more multipollutant modeling
  - Base capabilities: photooxidants, aerosols, acid/nutrient species deposition
  - Additions: HAPS/air toxics, mercury, semi-volatile species, metals
  - Additional demands on chemistry mechanisms and solvers to consider concurrent multiple pollutant regimes



- Additional computer power does not necessarily mean an end to the need for compact mechanisms and fast/accurate solvers
  - More process description
  - Larger domains
  - Higher spatial resolution
  - Longer simulation periods
- Another major resource constraint in mechanism choice
  - Implementation of emissions processing
    - Rules for organic lumping



- Continuing tension between accuracy and speed
  - Balance is application-dependent
  - Generally, a reasonable compromise exists for any application



**Disclaimer:** The research presented here was performed under the Memorandum of Understanding between the U.S. Environmental Protection Agency (EPA) and the U.S. Department of Commerce's National Oceanic and Atmospheric Administration (NOAA) and under agreement number DW13921548. This work constitutes a contribution to the NOAA Air Quality Program. Although it has been reviewed by EPA and NOAA and approved for publication, it does not necessarily reflect their policies or views.



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