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# Traditional Modeling Approaches for Atmospheric Mercury Deposition

Puff Model

(source: epa.gov and www.colorado.edu)

#### Examples: ISC, AERMOD, ROME, CALPUFF, SCICHEM etc.

Examples: CMAQ, TEAM, MADRID, REMSAD, CAMx etc. 2

#### **Eulerian Gridded Model**





# Why Use Plume-in-Grid Approach?

<figure>

**Fig**. Top-down view of plumes from five point sources (hypothetical case)

Source: Godowitch, 2004

#### Limitations of Purely Grid-Based Approach

- Artificial dilution of stack emissions
- Unrealistic near-stack plume concentrations
- Incorrect representation of plume chemistry and transport

Using a plume model embedded in a grid model helps overcome these limitations. <sup>3</sup>



#### **Atmospheric Chemistry of Mercury**



4



## Mercury Chemistry in Power Plant Plumes



Schematic not to scale

- Evidence of Hg<sup>II</sup> reduction in power plant plumes from measurements and modeling (Edgerton et al., ES&T, 2006; Lohman et al., ES&T, 2006)
  - Reduction of Hg<sup>II</sup> by SO<sub>2</sub> (possibly via heterogeneous reaction on particles) is compatible with global Hg cycling budget (Seigneur et al., *J. Geophys. Res.*, 2006).
  - Rate constant for  $Hg^{II}$  reduction by  $SO_2$  was derived from nine plume events and used in modeling.



# Plume-in-grid Model Description: CMAQ-MADRID-APT

- EPA's CMAQ as host model
- MADRID: Model of Aerosol Dynamics, Reaction, Ionization and Dissolution
- APT: Advanced Plume Treatment with embedded plume model SCICHEM (state-of-the science treatment of stack plumes at the sub-grid scale)
- Mercury treatment in grid and plumes
- Consistent treatments for chemical transformations of all species in the host model and the embedded plume model
- Freely available to the public at http://www.cmascenter.org



# **Modeling Approach**

- Plume-in-grid Model CMAQ-MADRID-APT v. 4.5.1
- Time period 2001
- Modeling grid N. America domain at 36 km horizontal resolution and 14 vertical levels
- Meteorology MM5-driven from EPA
- Initial and boundary conditions –from EPA using GEOS-Chem output (10 day model spinup for each quarter)
- Mercury emissions EPA 2001 inventory based on 1999 NEI with updates by EPA to waste incinerator emissions based on MACT
- Emissions of other species EPA 2001 inventory based on 1999 NEI





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- 36 km grid resolution
- 30 large power plants with APT



### **Simulated Hg Wet Deposition in 2001**

Environmental Research, Inc.





#### **MDN Hg Wet Deposition in 2001**





# **Comparison of Hg Wet Deposition from** 2001 with MDN data



**Bias = 84%** Error = 84%

20

25

30

35

+ 2

 $R^2 = 0.7$ 







#### **Precipitation in 2001**





### **Simulated Hg Dry Deposition in 2001**

microg/m2<sup>1</sup> January 1,2001 0:00:00 Min= 2 at (24,92), Max= 114 at (98,50) \* Preliminary results



# Impact of Advanced Plume Treatment on Simulated Hg "Dry + Wet" Deposition

Change (%) in annual Hg dry + wet deposition due to plume treatment





# Conclusions

16

- A new plume-in-grid modeling system was applied to simulate mercury deposition in the United States in 2001.
- A rate constant for Hg<sup>II</sup> reduction by SO<sub>2</sub> was derived from plume measurements and used in both gridded and plume-in-grid modeling.
- Thirty large coal-fired power plants were selected for advanced plume treatment (APT).
- Model performance (r<sup>2</sup> and error) w.r.t MDN wet deposition data improved with APT.
- The model still shows a strong positive bias which is likely due to a combination of insufficient reduction of Hg<sup>II</sup> to Hg<sup>0</sup> and biased precipitation.
- The use of APT results in 3-40% decreases in annual mercury deposition compared to a purely gridded approach.



# **Questions** ?

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