# Summary of Updates to SCICHEM-2012 Model:

## Comparison of Results with Observations and Previous Version Results

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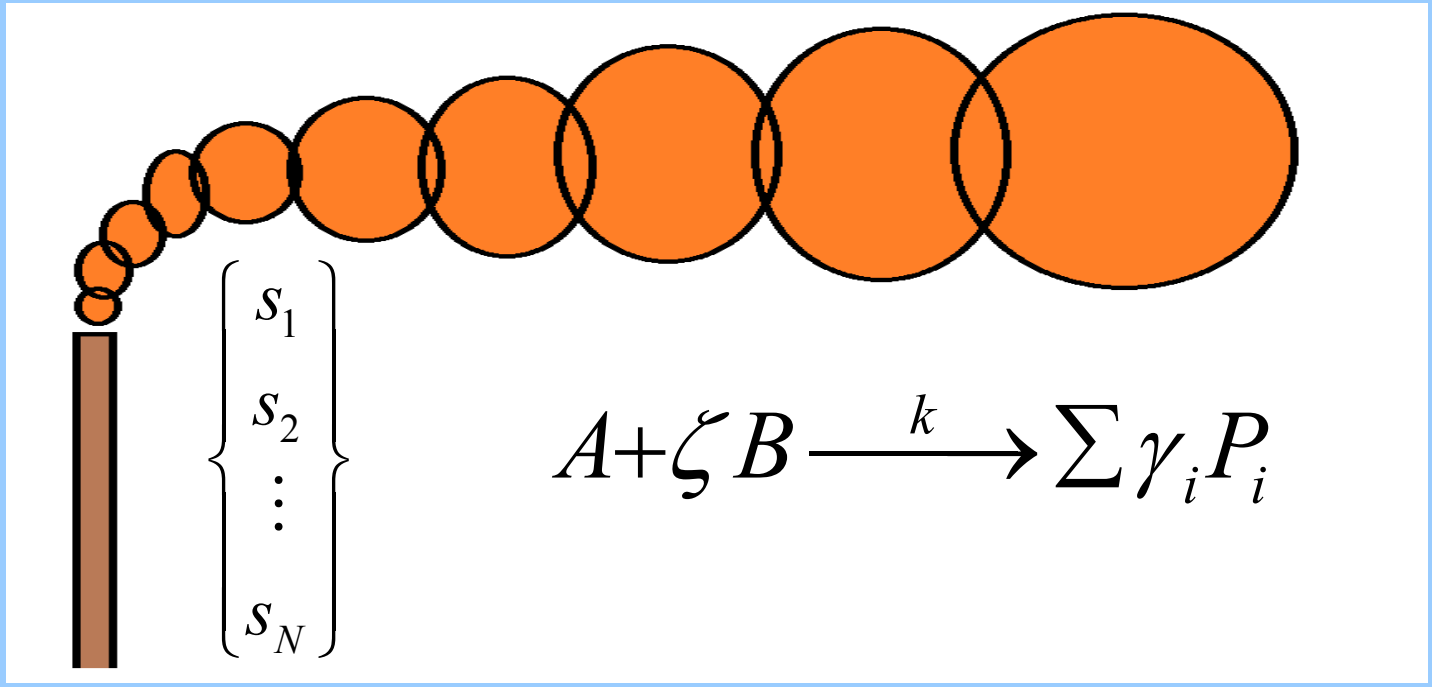
# SCICHEM

- SCIPUFF with chemistry
- Second Order Closure Integrated Puff Model



# Lagrangian Puff Model

- Concentration field
  - Collection of overlapping 3D puffs
- Puff moments
  - Solve ODE's
- Wide range of scales
  - No fixed grid
  - No diffusion errors
- Inhomogeneous conditions
  - Spatial
  - Temporal

# Improving Model Efficiency

- Puff splitting
  - Accurate treatment of wind shear
- Puff merging
  - Resolution adapted for each stage
- Adaptive time-step
  - Appropriate for resolving evolution rate

# Improving Model Efficiency

- "Static" puffs
  - Continuous releases: Steady state
- Adaptive grids & Linked lists
  - Puff overlap calculations

# Reactive Chemistry

- Species overlap concentration
  - Contribution from overlapping puffs

$$\hat{\mathrm{A}}_{\alpha} = \sum_{\beta} \mathrm{I}_{\alpha\beta} \langle A \rangle_{\beta}$$

$$\mathrm{I}_{\alpha\beta} = \int_{v} G_{\alpha}(\boldsymbol{x}) G_{\beta}(\boldsymbol{x}) dV$$

- Advance perturbation concentration
  - Exclude background reaction rate

$$\frac{d\hat{A}_{\alpha}}{dt} = -k(\hat{A}_{\alpha}\hat{B}_{\alpha} + \hat{A}_{\alpha}B_0 + A_0\hat{B}_{\alpha})$$

# Model Evaluation Studies

- PGT curves
- Instantaneous dispersion data
- Lab dispersion and fluctuation data
- Continental-scale ANATEX field experiment
- EPRI PMV&D tall-stack emissions
- CONFLUX (short range, fluctuations)
- Dugway field tests
- Model Data Archive
- ETEX

# Major Enhancements

- Allocatable arrays
- Nested meteorology grid
- Skew turbulence
- CB-05 chemical mechanism
- CMAQ 4.7 AE5 aerosol aqueous module
- Dense gas effects
- AERMOD type input file
- Area and volume sources
- AERMET input file
- Single code for parallel runs
- Multiple PRIME sources
- New sampler capabilities

# Enhancements

- Allocatable Arrays
  - Size limits – Initialization file
  - No recompilation
- Multi/Single processor
  - Logical – Initialization file
- Nested Grid
  - High resolution terrain
  - High resolution meteorology

# Skew Turbulence in CBL

- Non-Gaussian vertical diffusion
- Vertical velocity fluctuations PDF

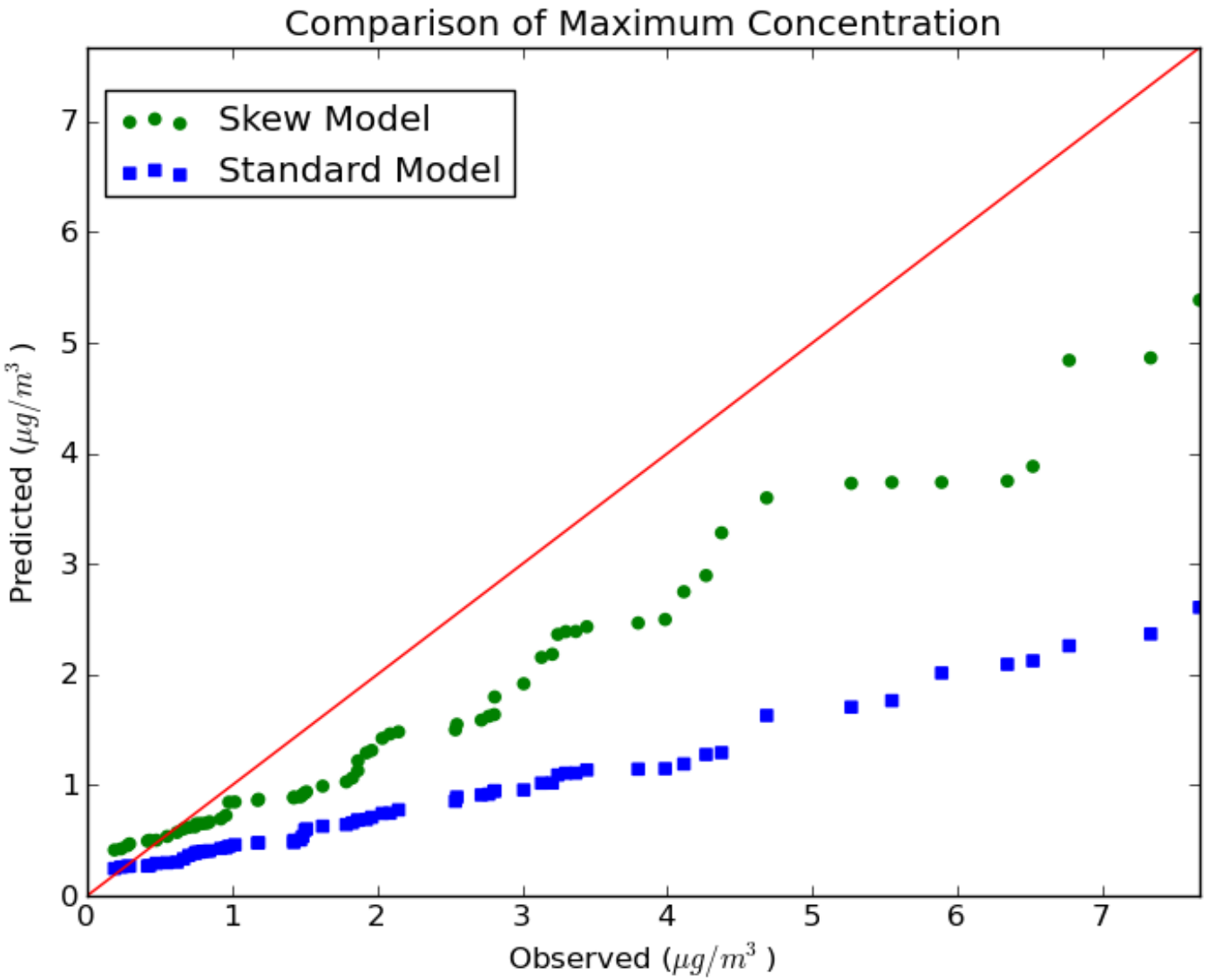
$$S = \left\langle w^3 \right\rangle \Big/ \left\langle w^2 \right\rangle^{3/2}$$

- Two "streams"
  - Updrafts
  - Downdrafts
- Switch type on reflection

# Copenhagen

- Elevated release
  - 115 m
  - 7 Convective releases
  - 3 Neutral releases
- Surface concentration
  - Arcs – 2 to 6 km

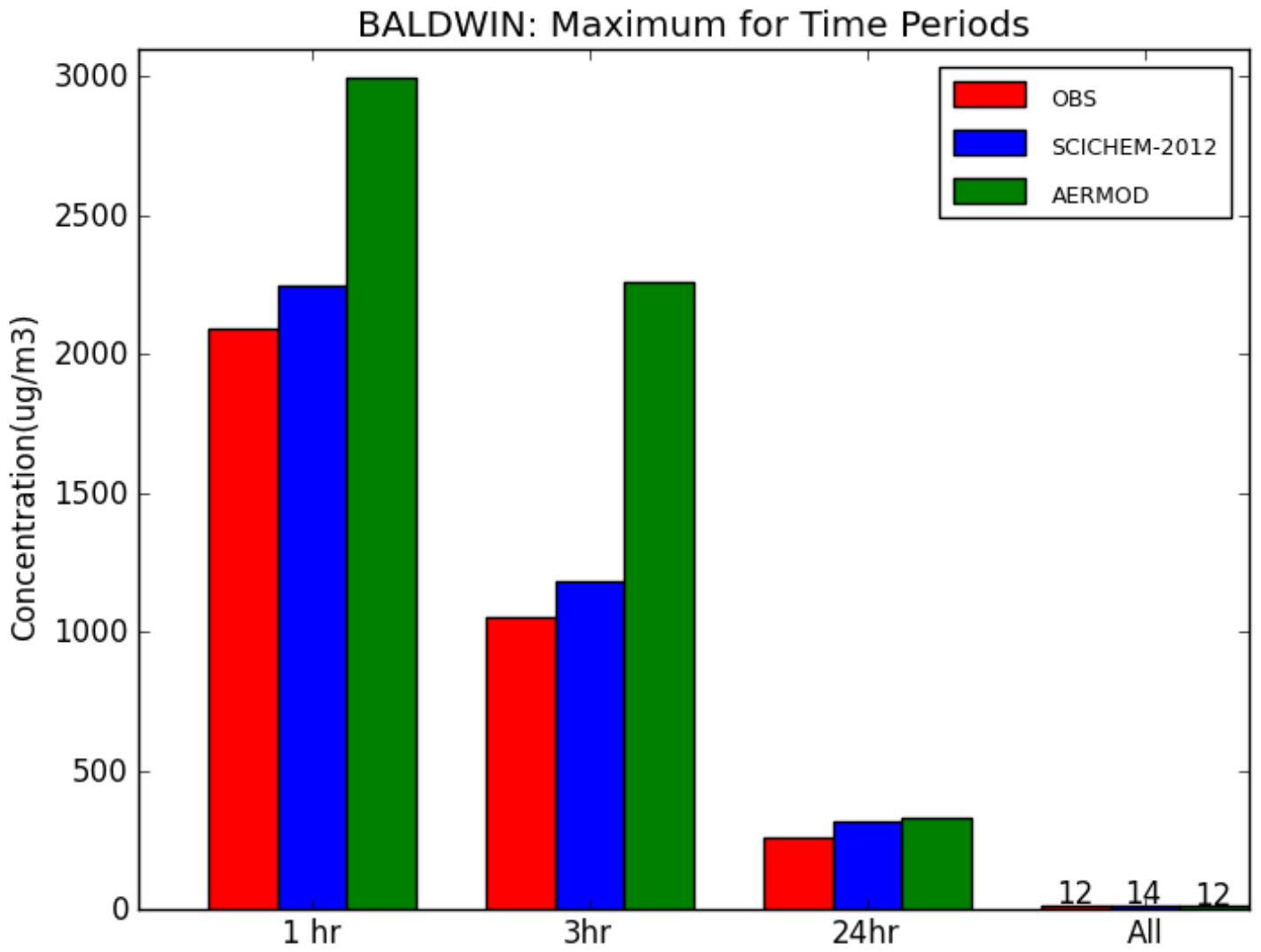
# Copenhagen


Comparison of Maximum Concentration
Skew Model
Standard Model
Predicted ($\mu g/m^3$)
Observed ($\mu g/m^3$)
0
1
2
3
4
5
6
7

# Enhancements

- Dense gas effects
  - Lateral spreading
  - Suppressed vertical diffusion
- New Sampler Format
  - Moving samplers
  - Line of sight sampler
  - Integrated concentration
  - Time averaged concentration
  - Meteorological samplers

# AERMOD Test Cases



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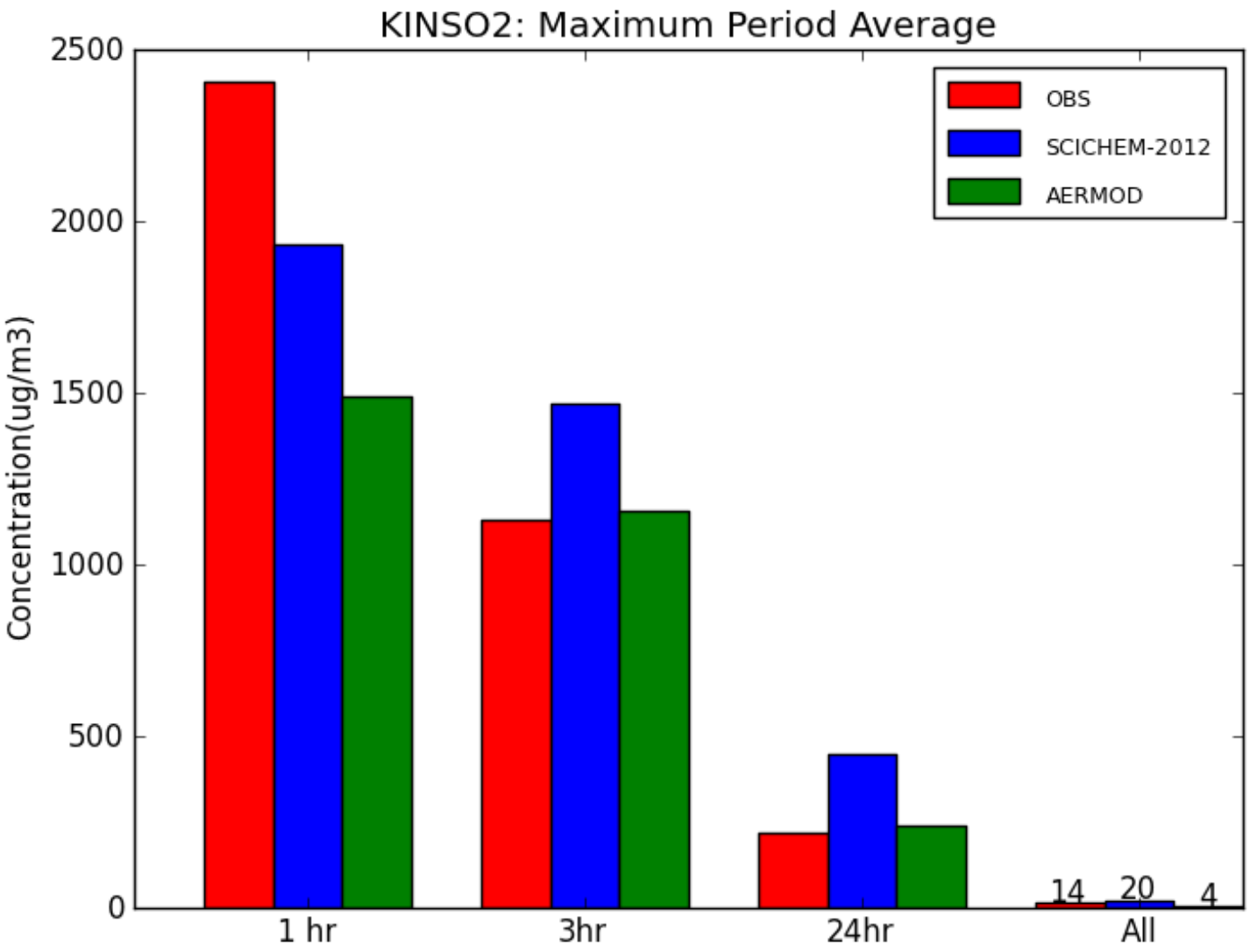


# SCICHEM-2012 Chemistry

Carbon Bond (CB05) Mechanism-
Yarwood et al. (2005)

CMAQ 4.7.1 Aerosol module (AE5) –
Edney et al (2007)

CMAQ 4.7.1 Aqueous
Foley et. al (2010)

# SCICHEM-2012 CB05-AE5

- TVA, Cumberland, TN
- 2 stacks, coal fired, both with $SO_2$ scrubbers
- Low $NO_x$ burner installed on 1 stack in 1999
- Stack Parameters (each stack)
  - Height = 194 m
  - Diameter = 11.7 m
  - Exit temperature = 48° C
  - Exit velocity = 20 m/s

# Simulations

- Performed for 2 days: 8/25/98, 7/15/99
- Used hourly emissions data for each day

Average Emissions

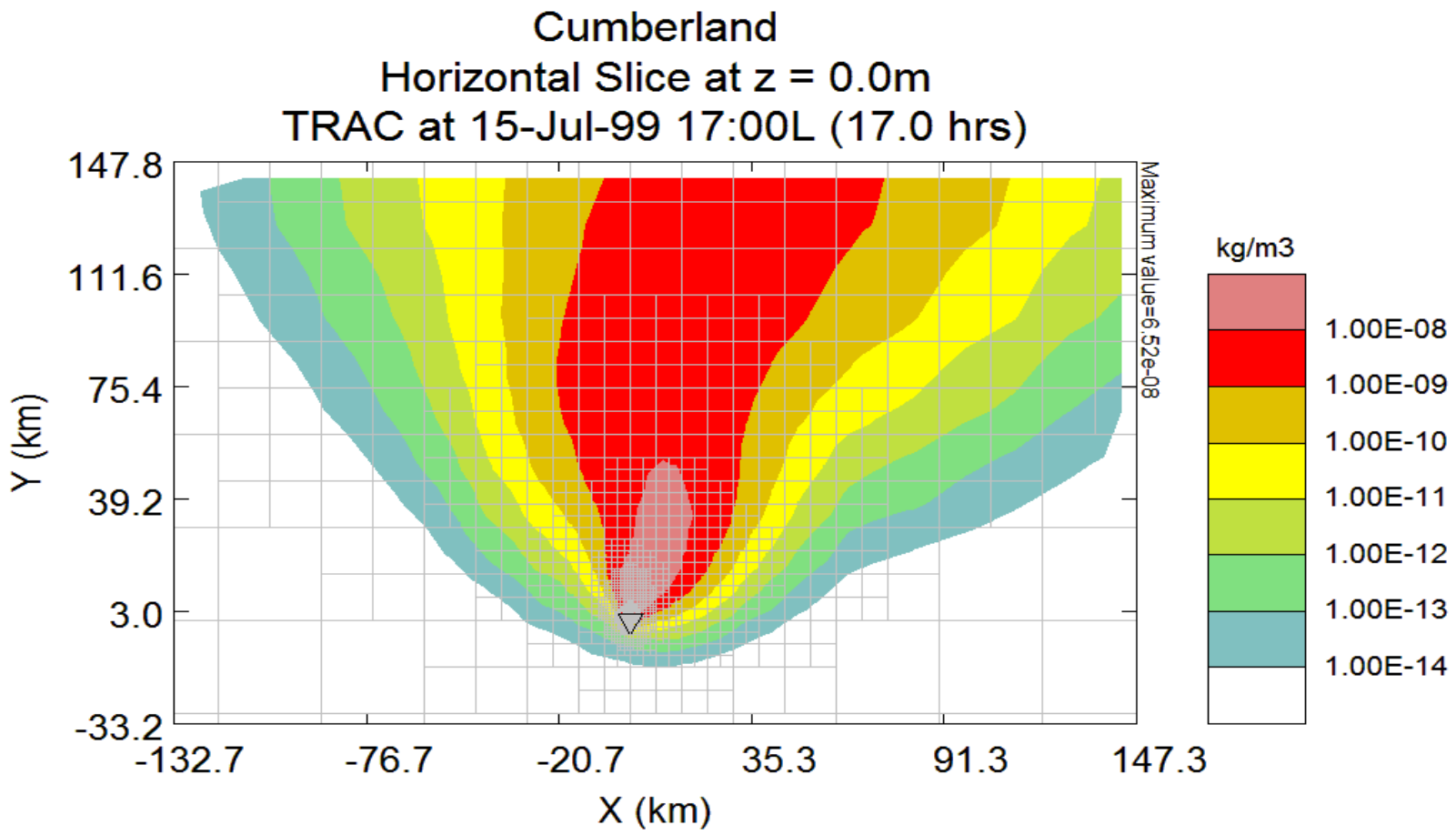
| Date | $SO_2$ (tonnes/hr) | $NO_x$ (tonnes/hr) |
|---|---|---|
| 8/25/98 | 2.5 | 15.2 |
| 7/15/99 | 2.1 | 11.5 |

- Profiler met data from Cumberland (8/25/98) and Dickson (7/15/99)

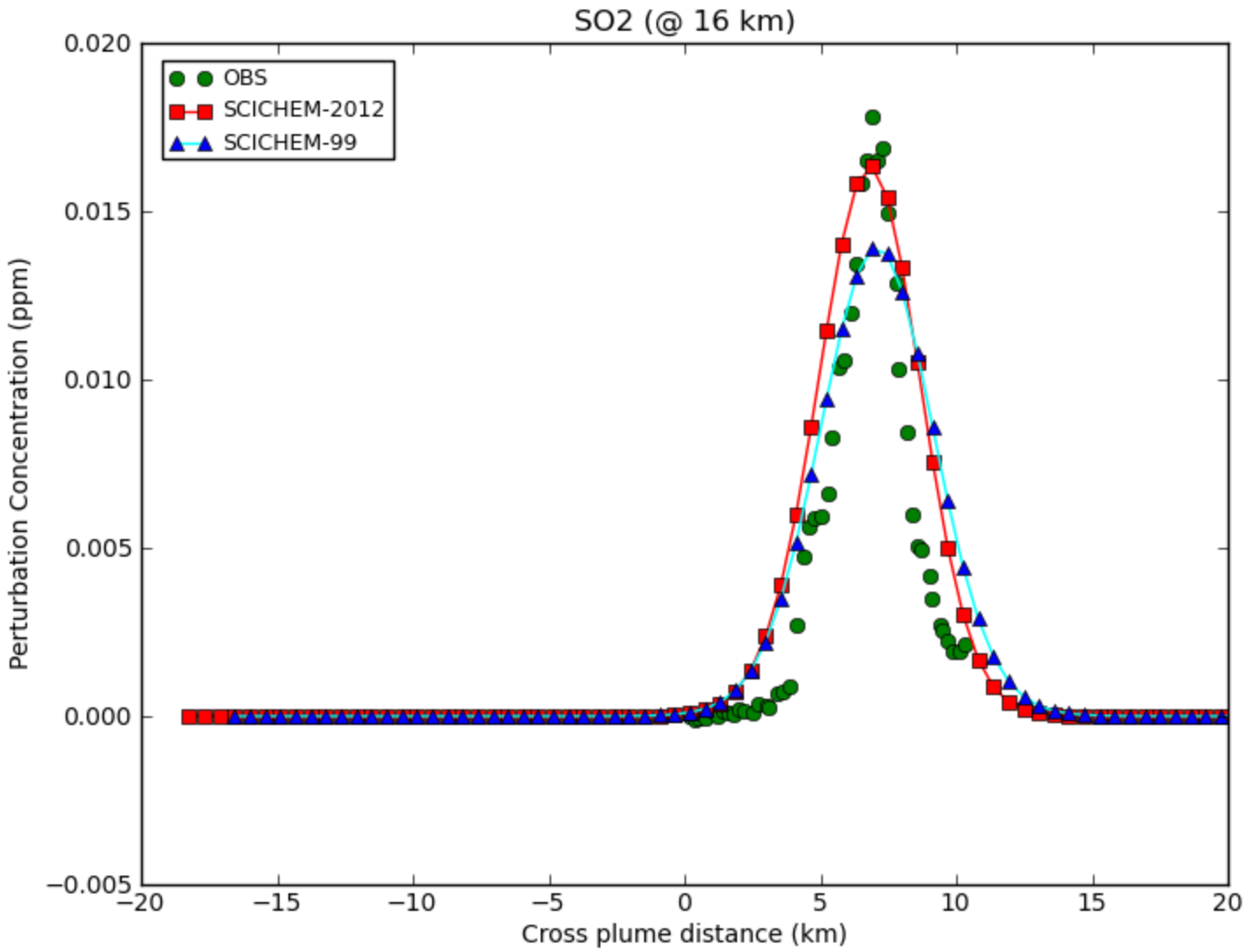
# Simulations

- Started at 00:00
- Run for $\geq$ 15 hours
- Compared with measurements ~ 12:00
- Gases: NO, $NO_2$, $NO_y$, $O_3$, $SO_2$

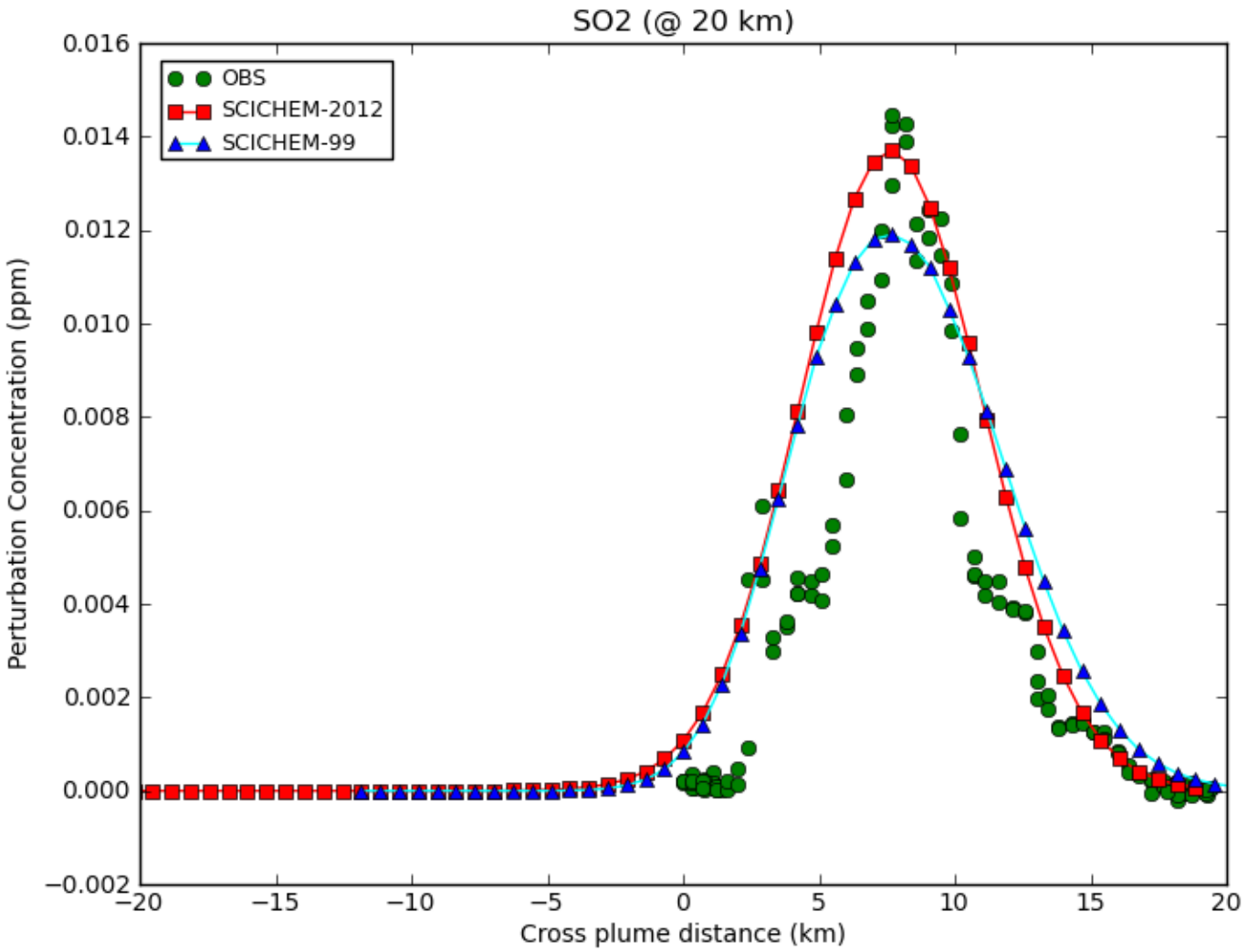
# Horizontal Slice



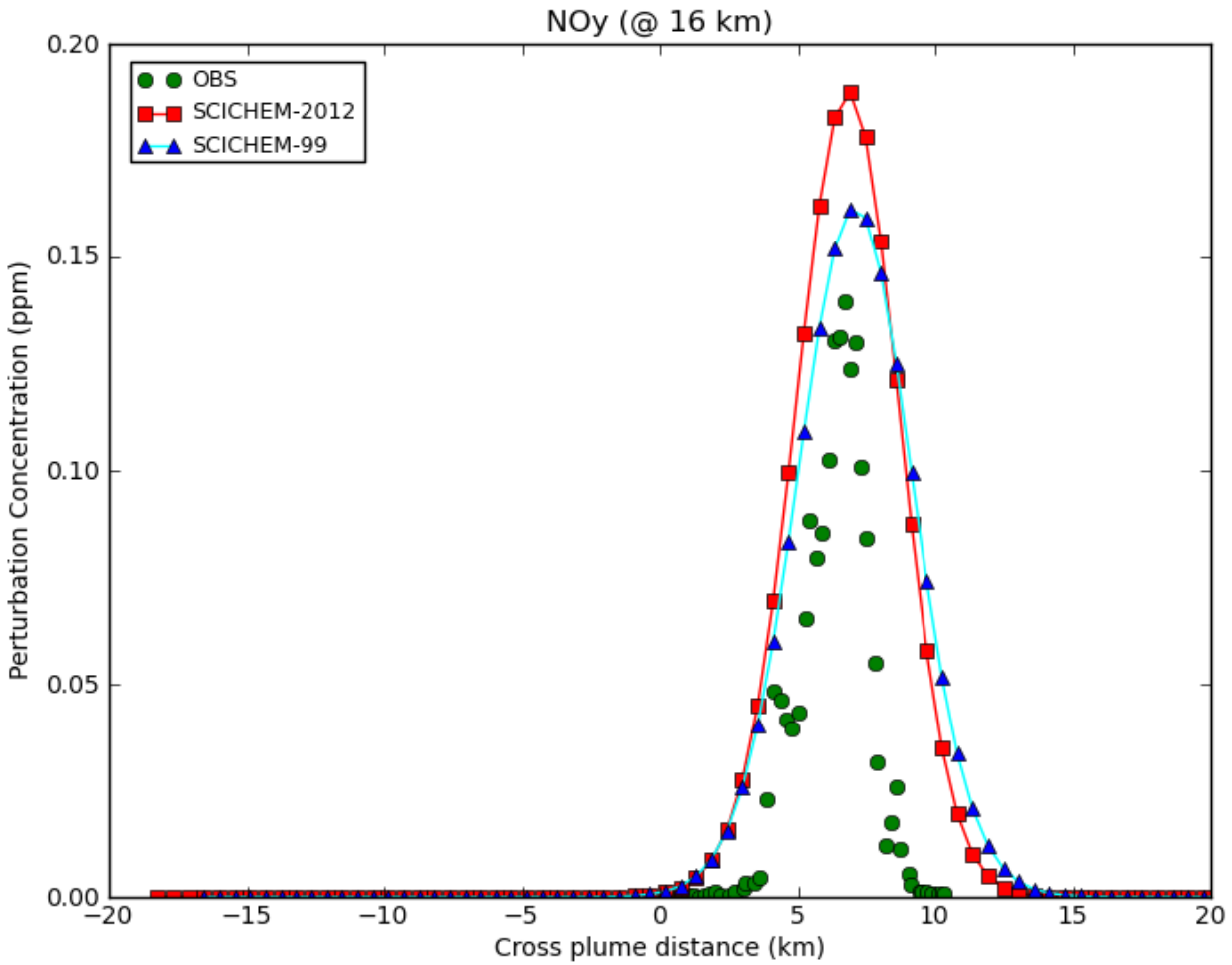
# 16 KM Downwind on 07/15/99



# 20 KM Downwind on 08/25/98



# 16 KM Downwind on 07/15/99



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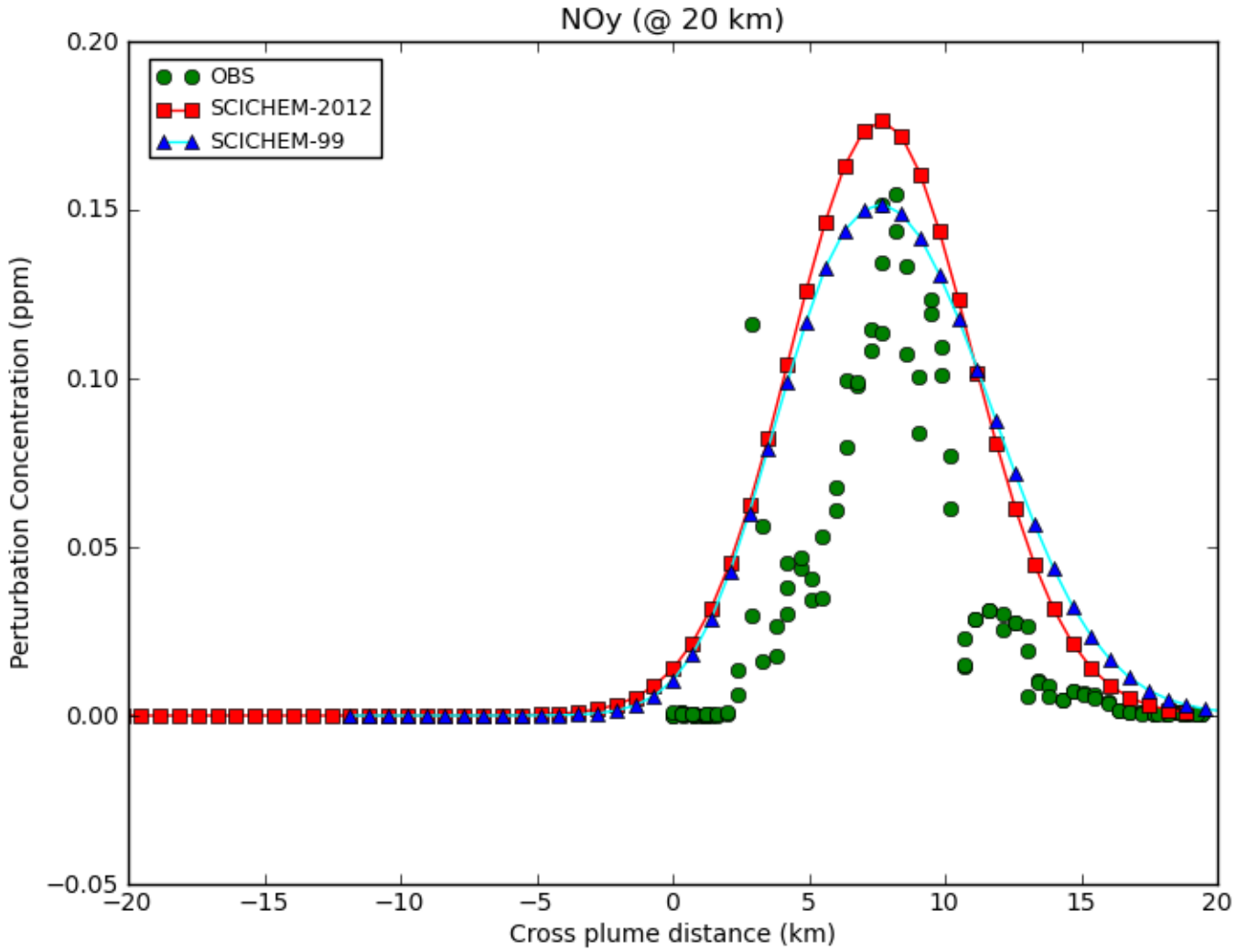

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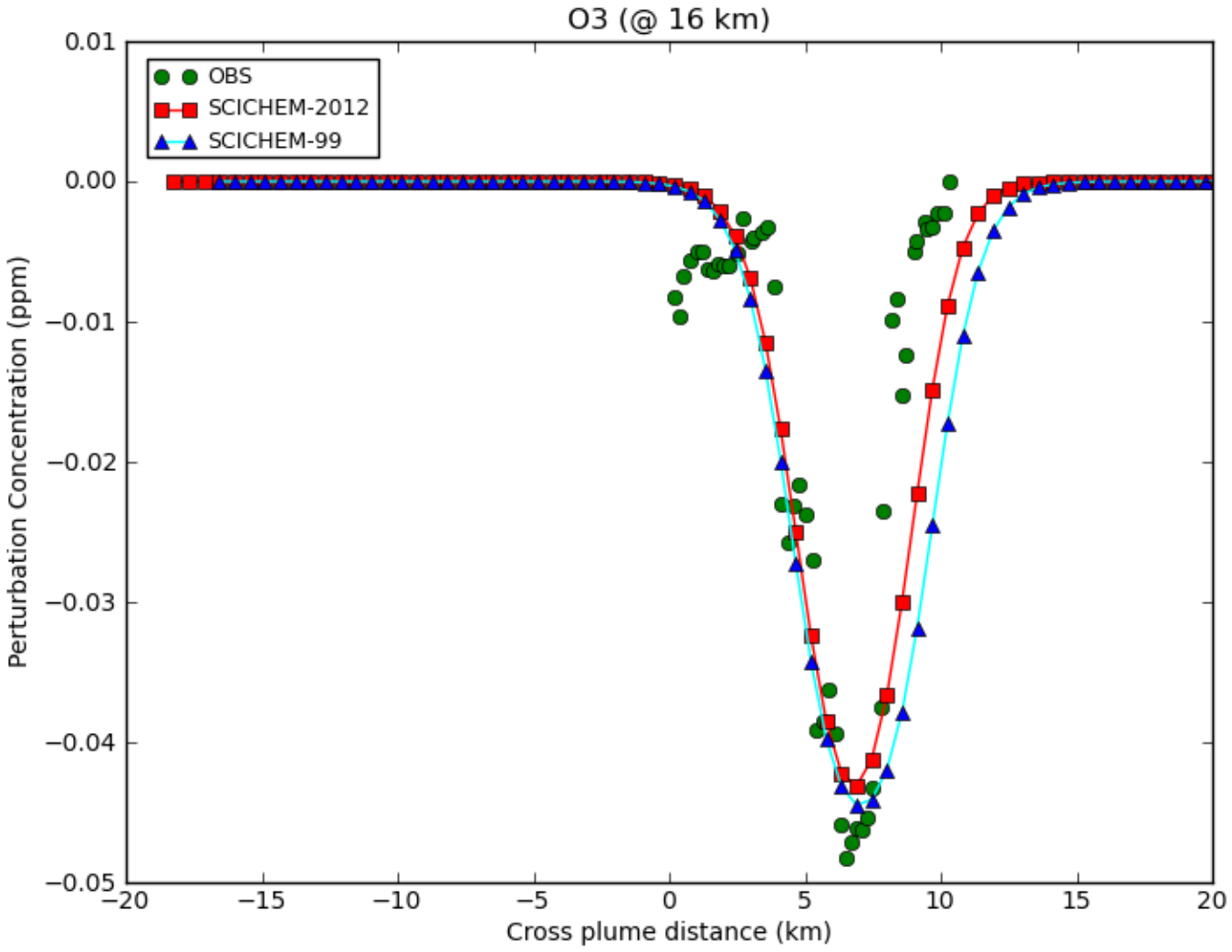

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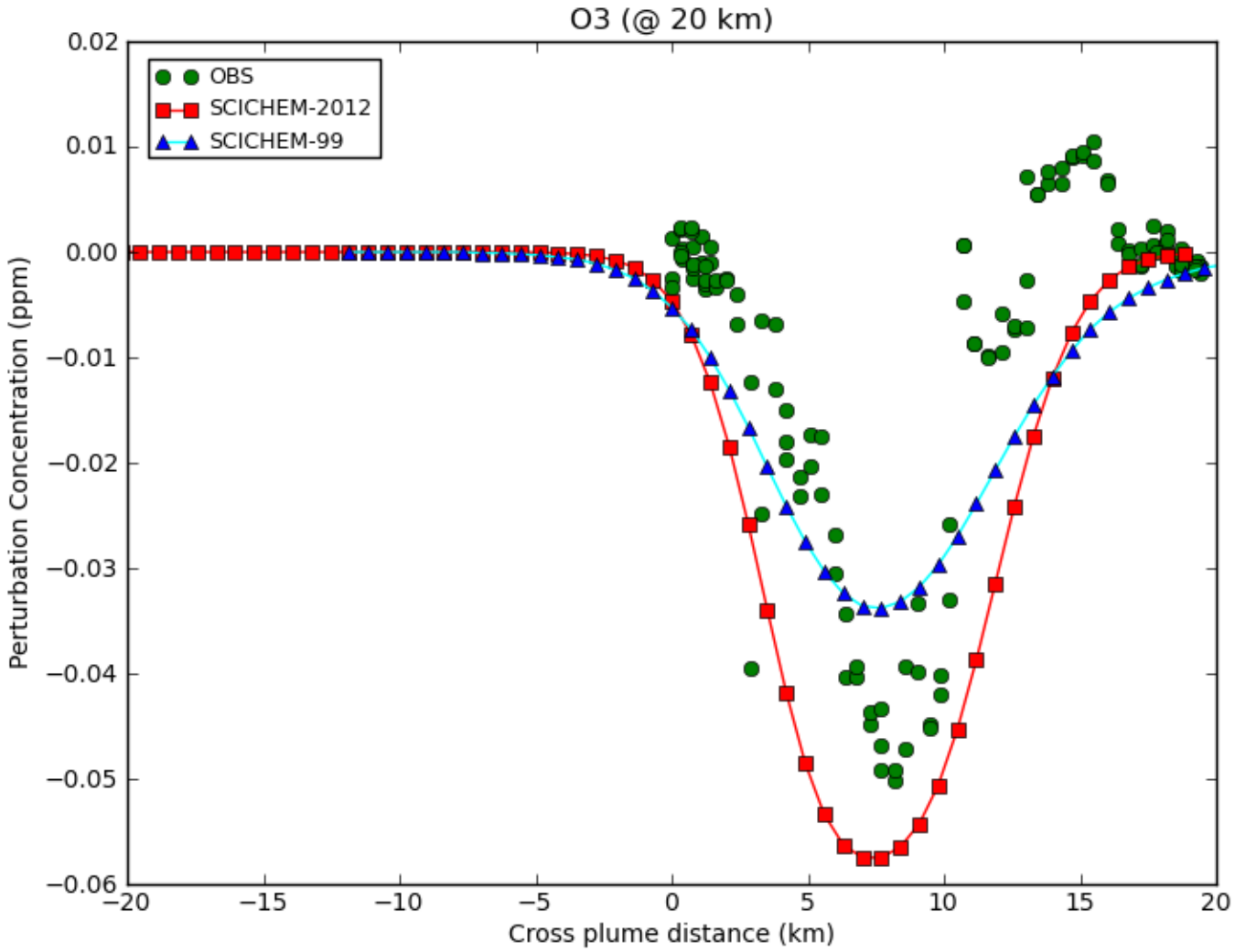
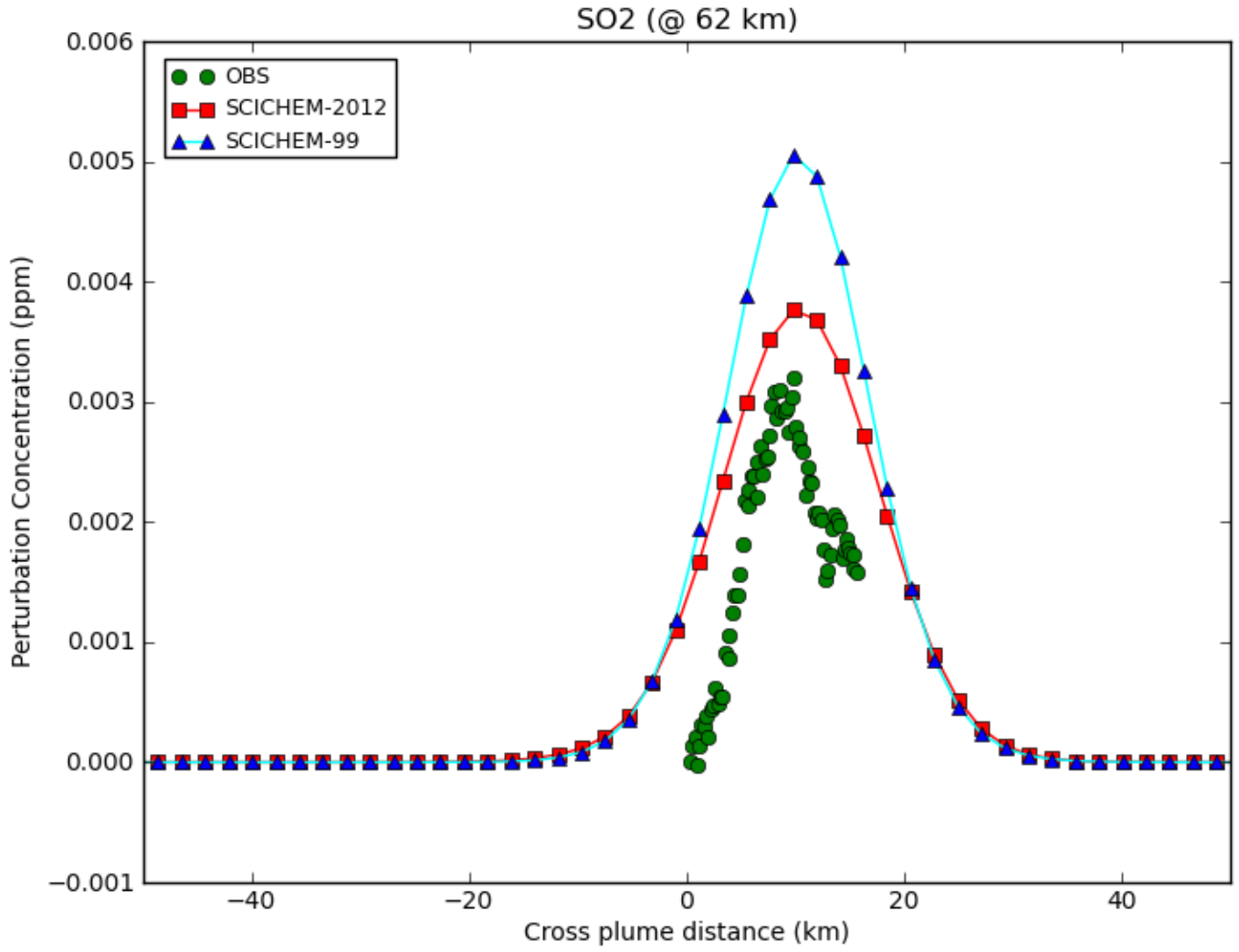
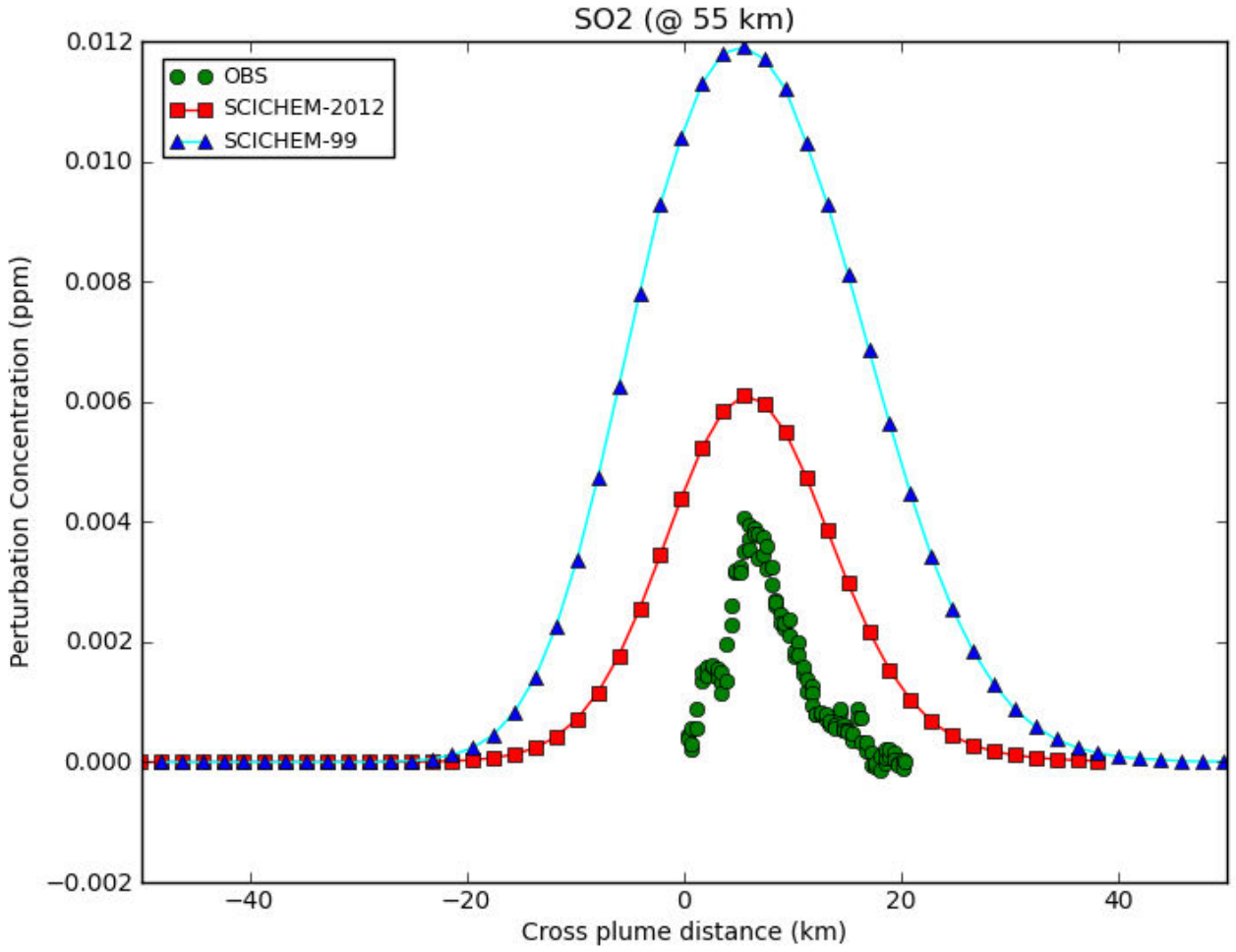


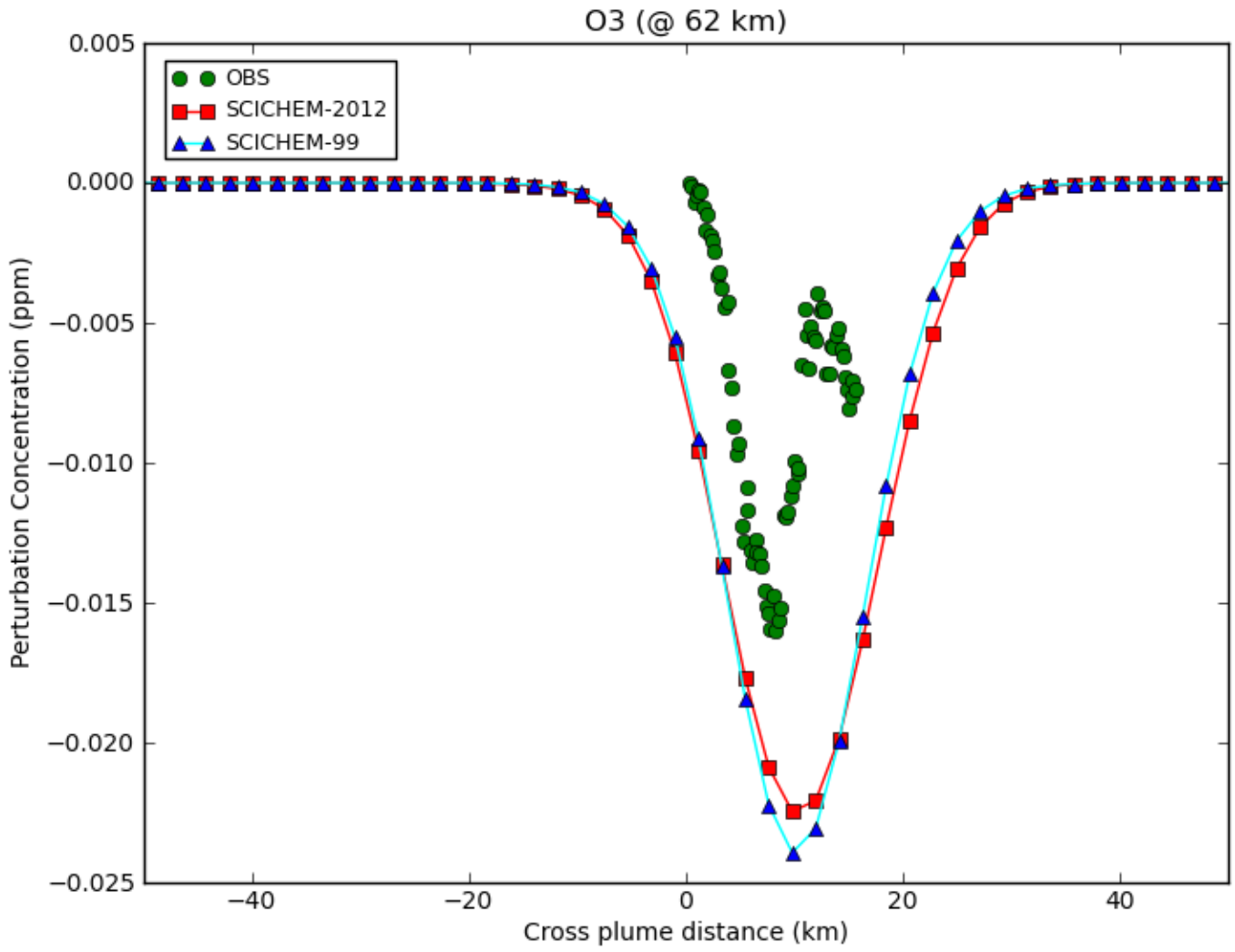
# 62 KM Downwind on 07/15/99



# 55 KM Downwind on 08/25/98



# 62 KM Downwind on 07/15/99



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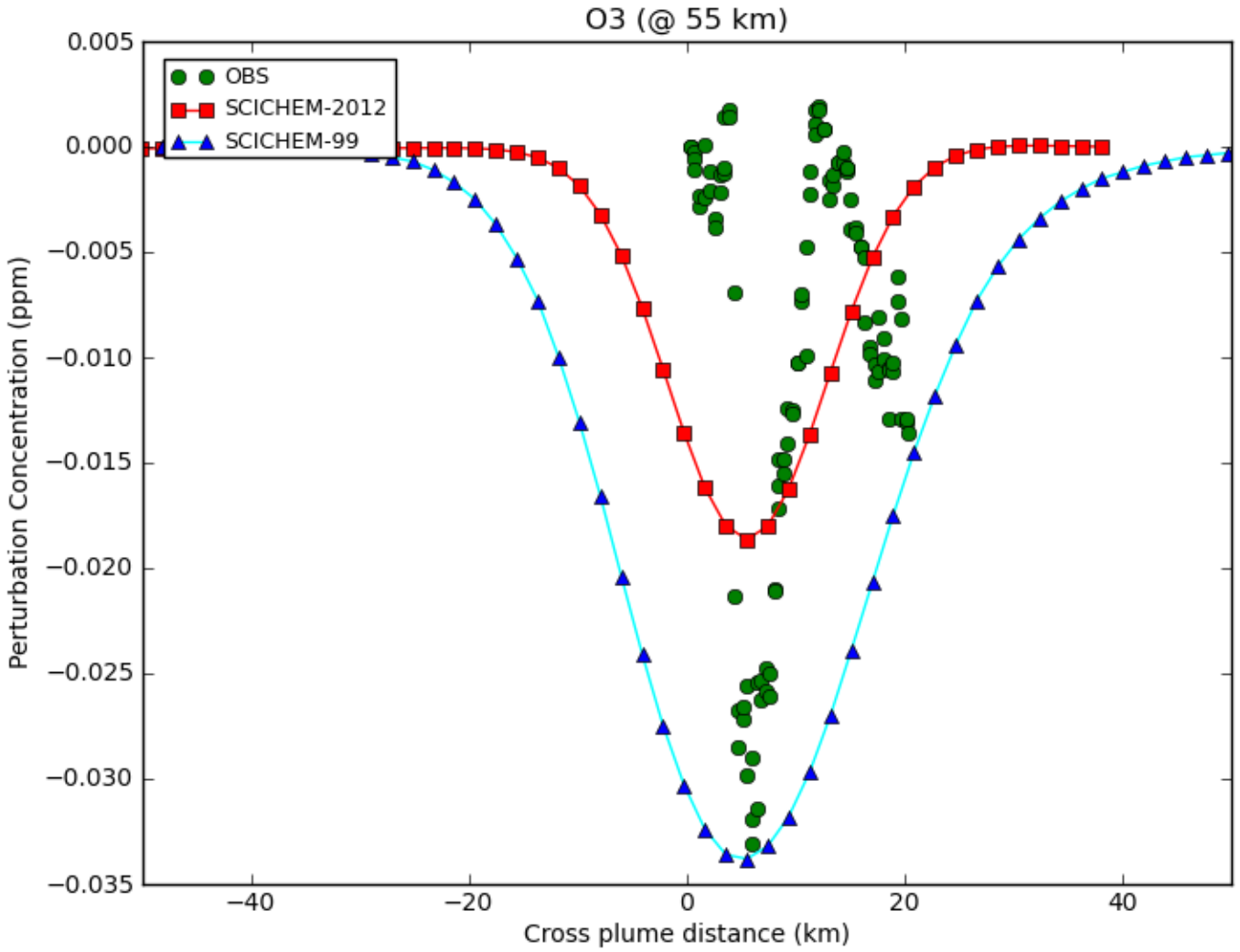

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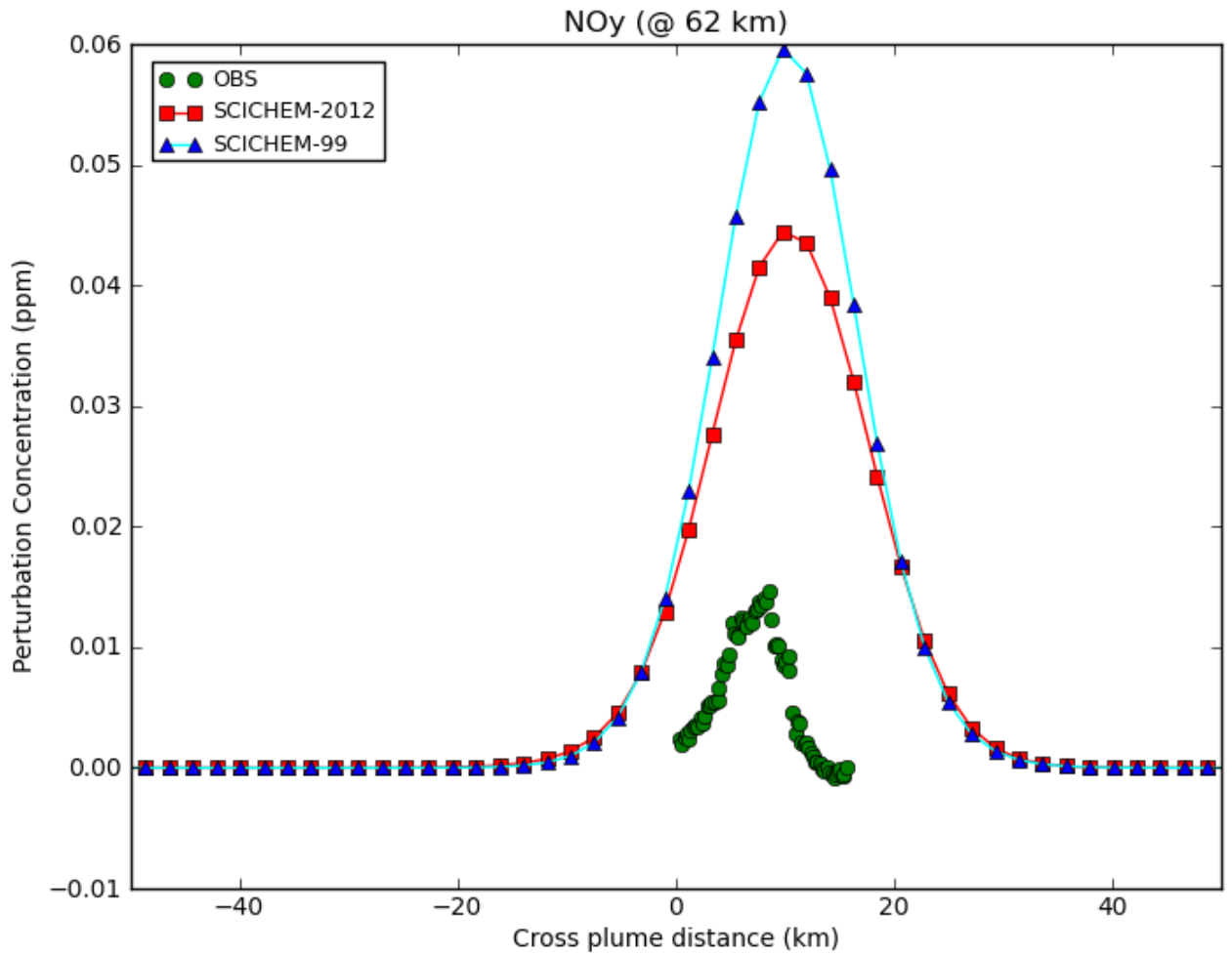

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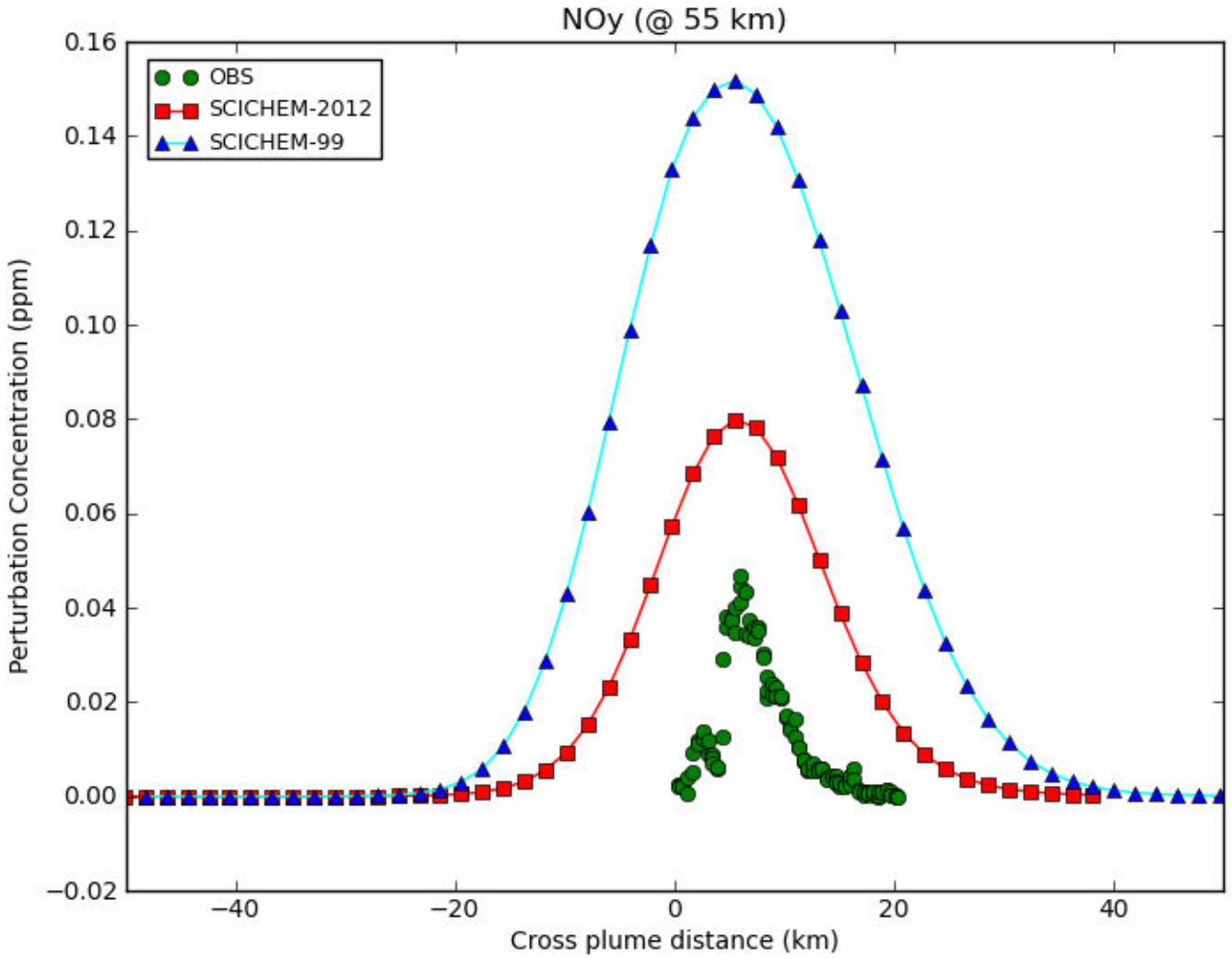

# Summary

## AERMOD Test Cases (Max P/O)

| Model | Exp. | 1hr | 3hr | 24hr | Period |
|---|---|---|---|---|---|
| SCICHEM-2012 | Baldwin | 1.07 | 1.12 | 1.22 | 1.14 |
| AERMOD | Baldwin | 1.43 | 2.14 | 1.26 | 0.96 |
| SCICHEM-2012 | Kincaid(SO2) | 0.81 | 1.29 | 2.06 | 1.44 |
| AERMOD | Kincaid(SO2) | 0.62 | 1.02 | 1.11 | 0.3 |

# Summary

## TVA Test Cases (Max P/O)

| Date | Distance (Km) | Species | SCICHEM 2012 | SCICHEM 99 |
|---|---|---|---|---|
| 08/25/98 | 20 | SO2 | 0.93 | 0.86 |
| 07/15/99 | 16 | SO2 | 0.83 | 0.72 |
| 08/25/98 | 55 | SO2 | 1.5 | 2.4 |
| 07/15/99 | 62 | SO2 | 1.15 | 1.56 |

# Future Work

- Initial results of AERMOD and TVA test cases using SCICHEM-2012 (Beta) model are promising.
- After carrying out further testing we plan to release the code in the public domain.

# Acknowledgement


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# Questions?