# Evaluation of the SCICHEM Model for Applications Involving Single Source Ozone and Secondary PM2.5 Evaluations

**ENV-VISION**

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# Overview

- EPA has proposed a 2-tier approach to estimating secondary pollutant (ozone, PM2.5) formation due to increased emissions from a new source or source expansion.

- As described in available draft guidance and public presentations, Tier 1 generally will rely on existing information (PGM studies, other information) to make a case for non-significant contribution of a specific project.

- Tier 2, as contemplated, will rely on conducting a PGM study to determine the effect of the increased emissions.

- Numerous studies have been conducted and generally, EPA considers PGMs to be adequate and appropriate to determine single source impacts.

# What to Expect

- There are of course some gray areas
- Tiers 1 and 2 have not been built yet; the foundation is there, and the material that can be used for the construction is there.
- According to EPA, other "screening" approaches can include Lagrangian or other reduced form model(s) with chemistry which have not been specified although some have been mentioned.
- The approach will, as stated, rely on ozone/PM2.5 Significant Impact Levels (SILs) and Model Emissions Rates for Precursors (MERPs) to screen out and avoid the need to do any analysis.

# The Process

- Guidance on ozone SILs will be published first (timeframe: sometime in 2016, maybe July?)
- Once the SILs have been established, development of MERPs will start. User community should not expect a prescriptive approach to addressing secondary formation.
- Rather, MERPs will initially be "case by case" until experience is gained and lookup tables can be generated in some form.
- Key question: is there a role for a Lagrangian/reduced form model in this tiered system? SCICHEM is certainly a candidate; it has the features that will be required for a screening model for secondary ozone and PM25 impacts

# This Presentation

- PGM models and methodologies are available; if there is a place for other models to be used as screening techniques they would generally have to be easier to use and be demonstrably conservative.

- This presentation: giving SCICHEM a test drive from the perspective of an experienced modeler but one who is not a photochemical modeler, as an initial test of the suitability of SCICHEM to fit into the tiered system.

- In a sense, it already does!

# SCICHEM Overview

- Developed by the Electric Power Research Institute (EPRI); Publicly Available:
  https://sourceforge.net/projects/epri-dispersion/

- SCIPUFF + Chemistry = SCICHEM

- One of the difficulties with single source modeling using a puff model: determining the chemical environment into which the puffs are released and are transported and dispersed downwind.

- Developing (modeling) this chemical environment is at the heart of PGMs

# SCICHEM Overview (2)

- SCICHEM addresses this by providing ambient data files with the SCICHEM release that contain concentrations of oxidants and other species that are needed to drive conversion mechanisms for ozone (and PM2.5).
- Files were developed using CMAQ with 2005 CSAPR inputs
- Concentrations are provided for each hour of each month (i.e. 24 values per month) for 3 vertical layers: 0-300m, 300-1000m, and 1000-3000m.
- Files are provided for different geographic regions, mostly by state with some smaller states combined and some larger states split

# SCICHEM Overview (3)

- The chemical mechanisms for secondary formation of ozone (and PM2.5) are (needless to say) complex
- A multicomponent file is provided with the SCICHEM distribution containing all of the parameters to implement the full CB05 mechanism.
- The file contains characteristics of each species involved in the reactions, the set of equations used in CB05, and radiation-dependent rate constants needed in the transformation equations.
- The ambient and chemical mechanism files can be updated/modified (but with caution!)

# Model Setup: Source Parameters

- Hypothetical, combined cycle natural gas-fired combustion turbine ("CC", approx. 500 MW), typical of recently proposed and permitted generating units in the northeast U.S.
- Focused on NOx only, 20% = $NO_2$.
- Base case emissions represent advanced controls (SCR) resulting the equivalent of 130 tons NOx/year.
- A "stress test" was also conducted with the same stack characteristics, but increasing emissions to an equivalent of 500 and then 1000 tons per year. The stack, exhaust, and emissions parameters modeled are presented in Table 1

# Model Setup: Source Parameters

## Table 1 – Stack and Emissions Parameters

| | English Units | | Metric Units | |
|---|---|---|---|---|
| **Height** | 160.1 | ft | 48.79 | m |
| **Inner Diameter** | 22.6 | ft | 6.89 | m |
| **Stack Area** | 401.33 | ft^2 | 37.28 | m^2 |
| **Exhaust flow** | 1,376,994 | acfm | 649.87 | m^3/s |
| **Exhaust velocity** | 3431.10 | fpm | 17.43 | m/s |
| **Temperature** | 174.99 | F | 352.59 | K |
| **NOx Emissions** | 29.68 | lbs/hr | 3.74 | g/s |
| | 130.0 | TPY | | |
| **NOx Emissions** | 114.16 | lbs/hr | 14.38 | g/s |
| | 500 | TPY | | |
| **NOx Emissions** | 228.31 | lbs/hr | 28.77 | g/s |
| | 1000 | TPY | | |

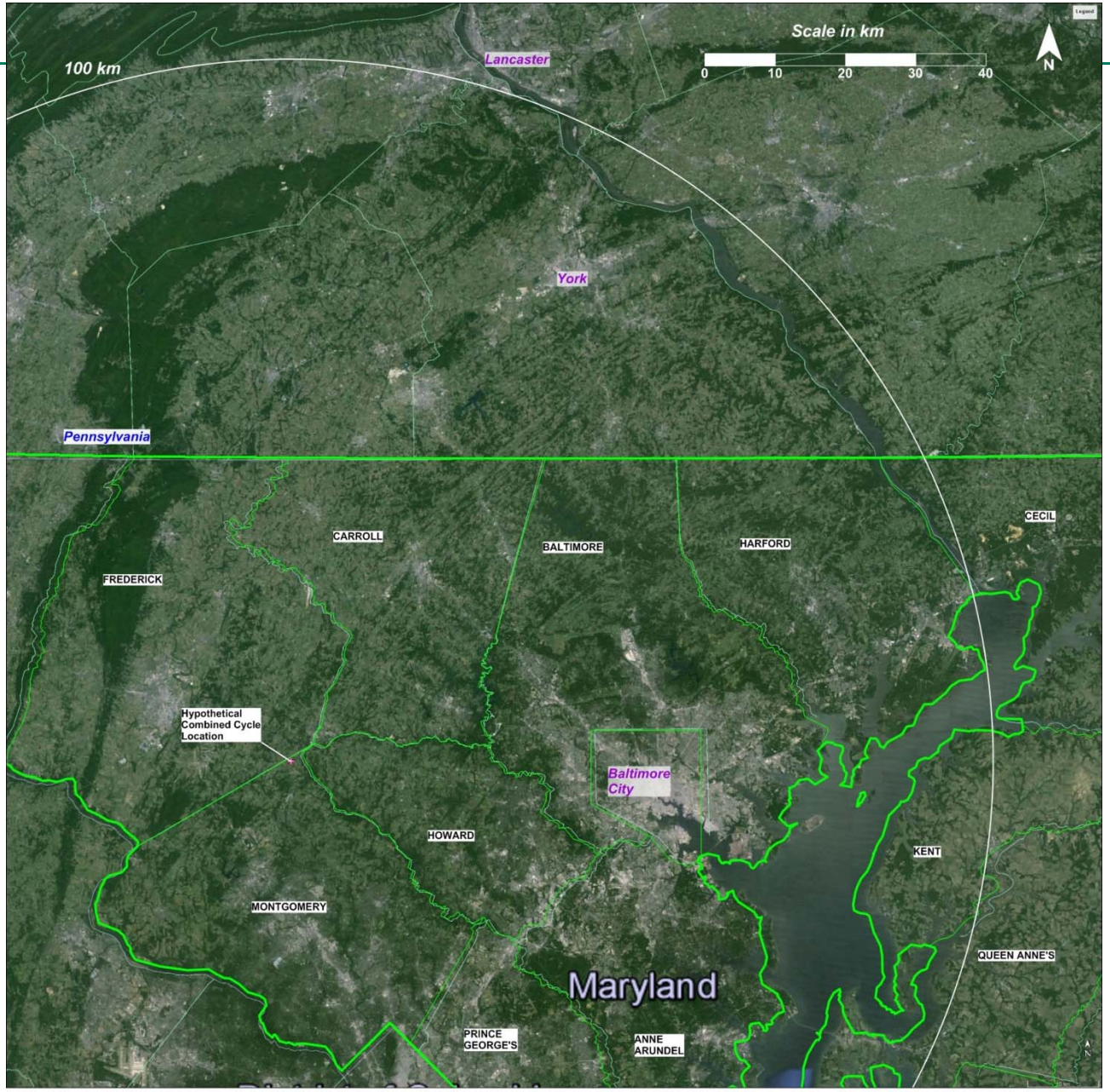
# Model Setup: Domain, Output

- SCICHEM produces several different types of output files, including concentration and deposition outputs on an "adaptive" grid and detailed puff files that contain information on each puff released.

- Output files can be read and processed by post-processors provided with the SCICHEM distribution.

- For the current effort, outputs were developed to represent near-field (1-5 km) and far-field (10-100 km) impacts. The focus was on capturing possible impacts to the east and northeast of the source, including the city of Baltimore.

# Model Setup: Source Location and Domain Extent



# Model Setup: Meteorology

- Meteorological inputs for SCICHEM were developed in two different ways.

- First the MET2SCI program was used to develop single-point surface and profile files for 2014, based on surface data from the BWI airport located between Baltimore, MD and Washington DC and upper air soundings from Dulles airport in Virginia.

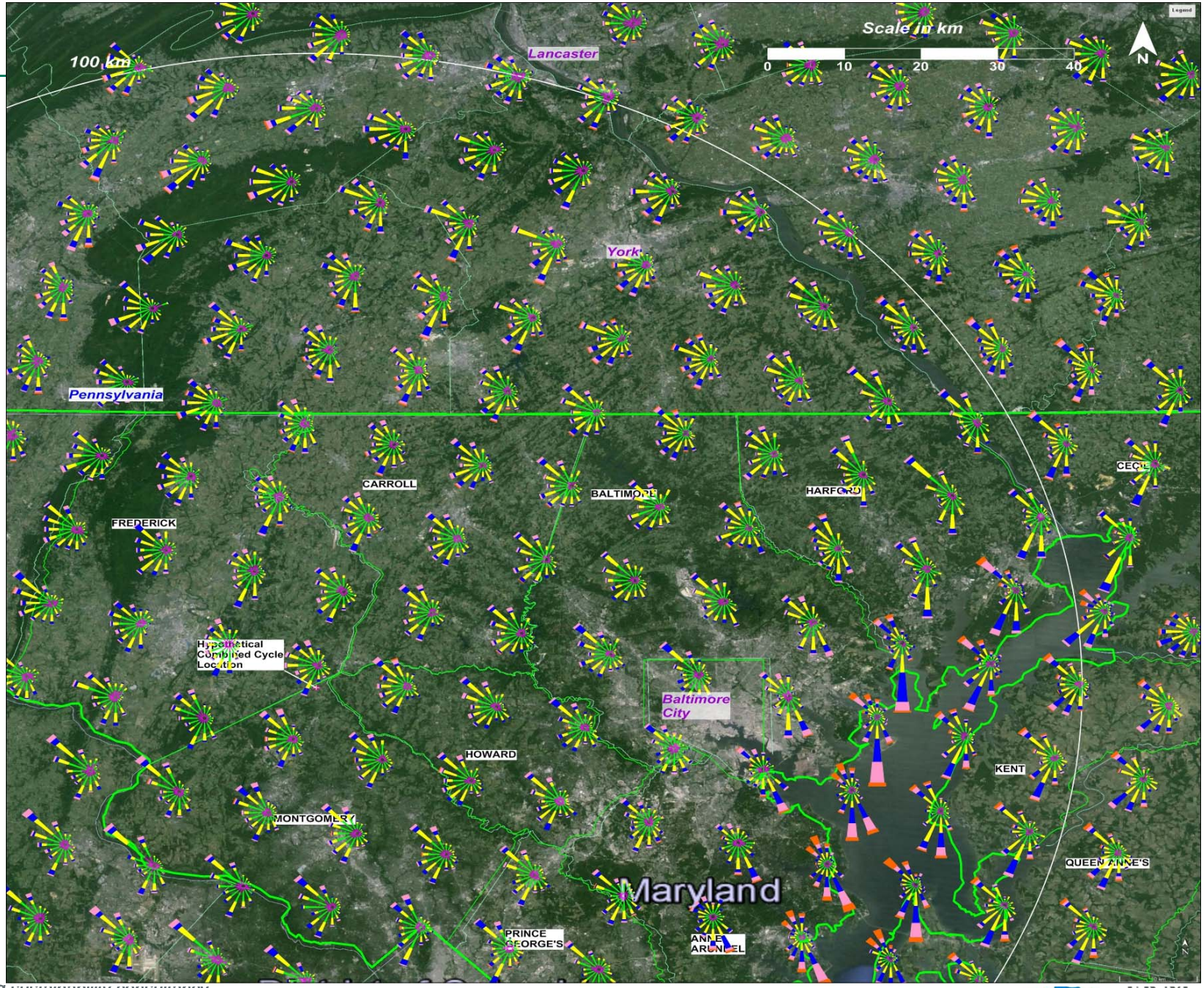
- MET2SCI produces surface (.scs) and profile (.prf) files for input to SCICHEM.

- The MET2SCI surface (.scs) file contains hourly values of wind speed and direction, pressure, temperature, and relative humidity. The METSCI profile (.prf) file contains twice daily (0 and 12Z) vertical profiles of winds, temperature, and humidity up to approximately 5000 meters.

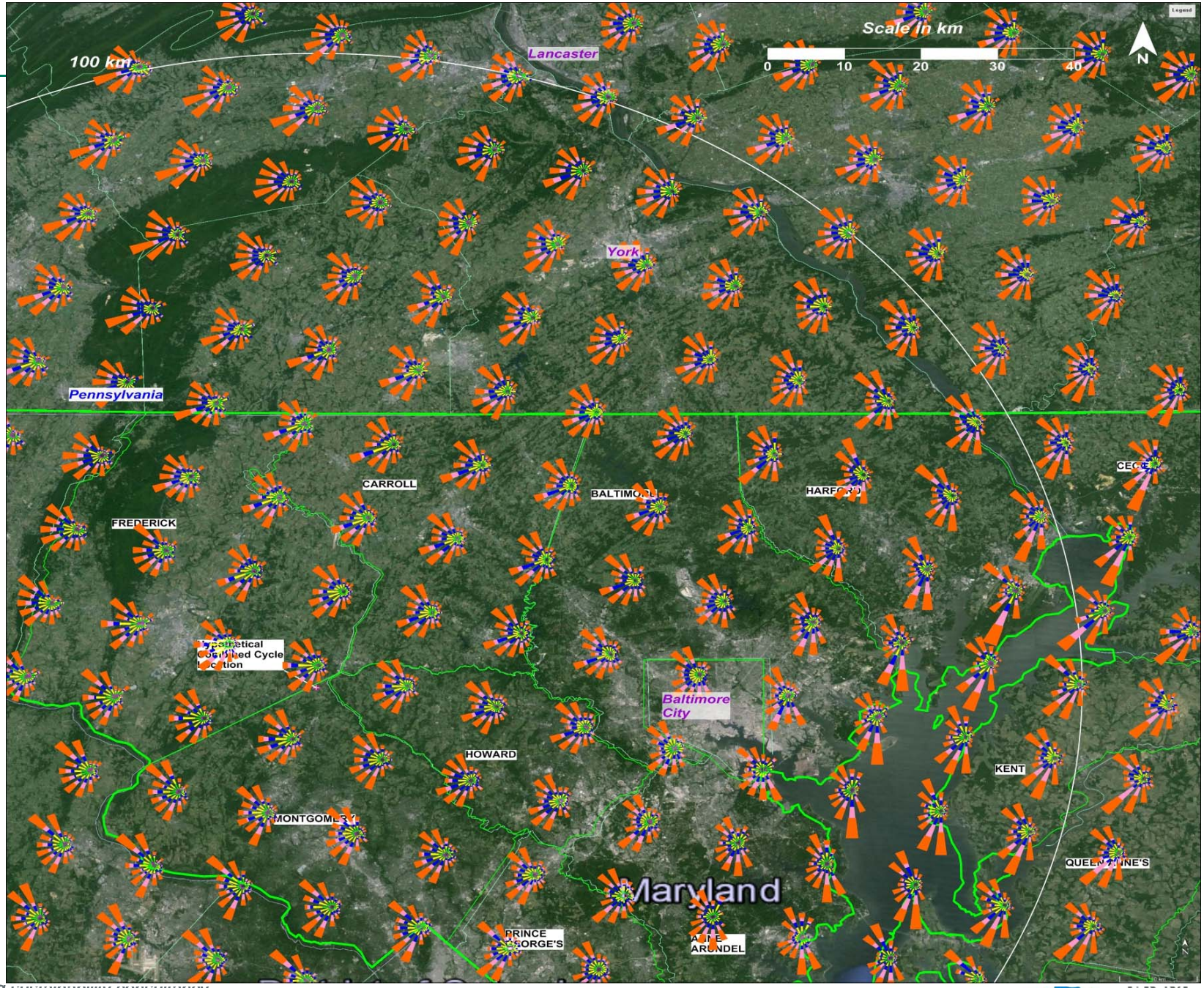
# Model Setup: Meteorology

- Next the MMIF program was used to extract data from 12-km WRF output files for 2014 to create a MEDOC file for input to SCICHEM.
- The MEDOC file contains gridded wind and temperature profiles, as well as micrometeorological parameters to characterize the boundary layer for each grid cell.
- Geographic and single point wind roses for July are presented.

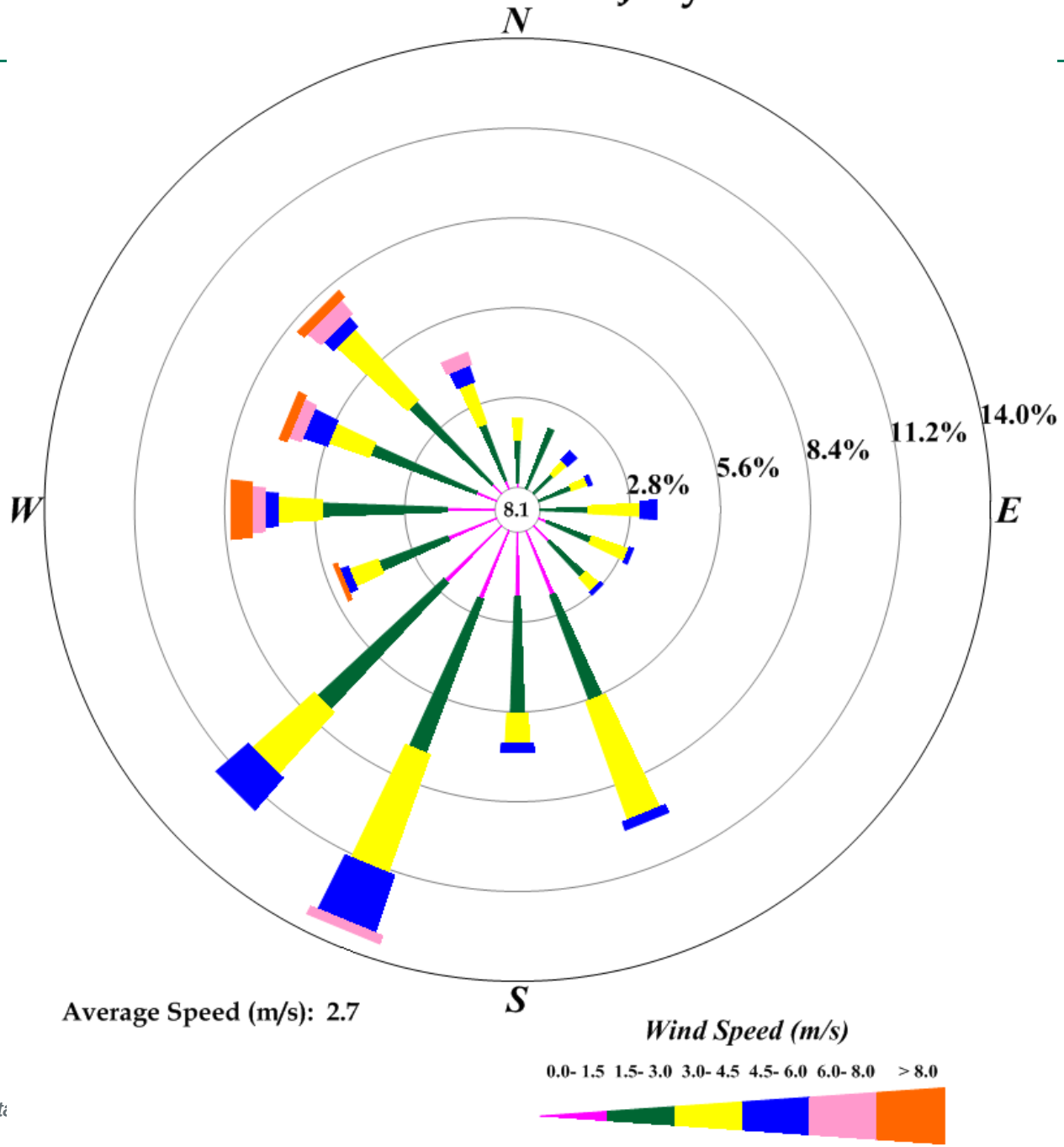
July
2014
10 m
(surface)



July
2014
240 m



# BWI WindRose: July 2014




Average Speed (m/s): 2.7

# Running SCICHEM

- All runs were conducted on a Windows machine with 8 quad-core processors.
- SCICHEM inputs can be entered in NAMELIST or KEYWORD (similar to AERMOD) formats. All runs for this study were conducted using the KEYWORD format.
- Several initial test runs were conducted with non-reactive pollutants and with the near-field NOx to $NO_2$ chemistry invoked, mostly to gain familiarity with SCICHEM operation.
- Single source runs took about 30/50 minutes for the near-field and far-field runs respectively (no chemistry), about twice as long with the NOx to $NO_2$ chemistry. SCICHEM results were generally higher than a similar AERMOD run; this analysis was not the focus of this study.

# Running SCICHEM (2)

- The primary set of runs was conducted using the full chemistry parameterization provided with the SCICHEM distribution package, in order to model secondary formation of ozone (and PM2.5).

- These runs used the fullchem_cb5_ae5.imc multi-component file that includes data to implement the full CB05 chemical transformation mechanism.

- The MD_DE.amb file was used which contains concentrations (that vary by hour of day and month) of constituents that participate in reactions that lead to the formation of ozone (and secondary PM2.5).

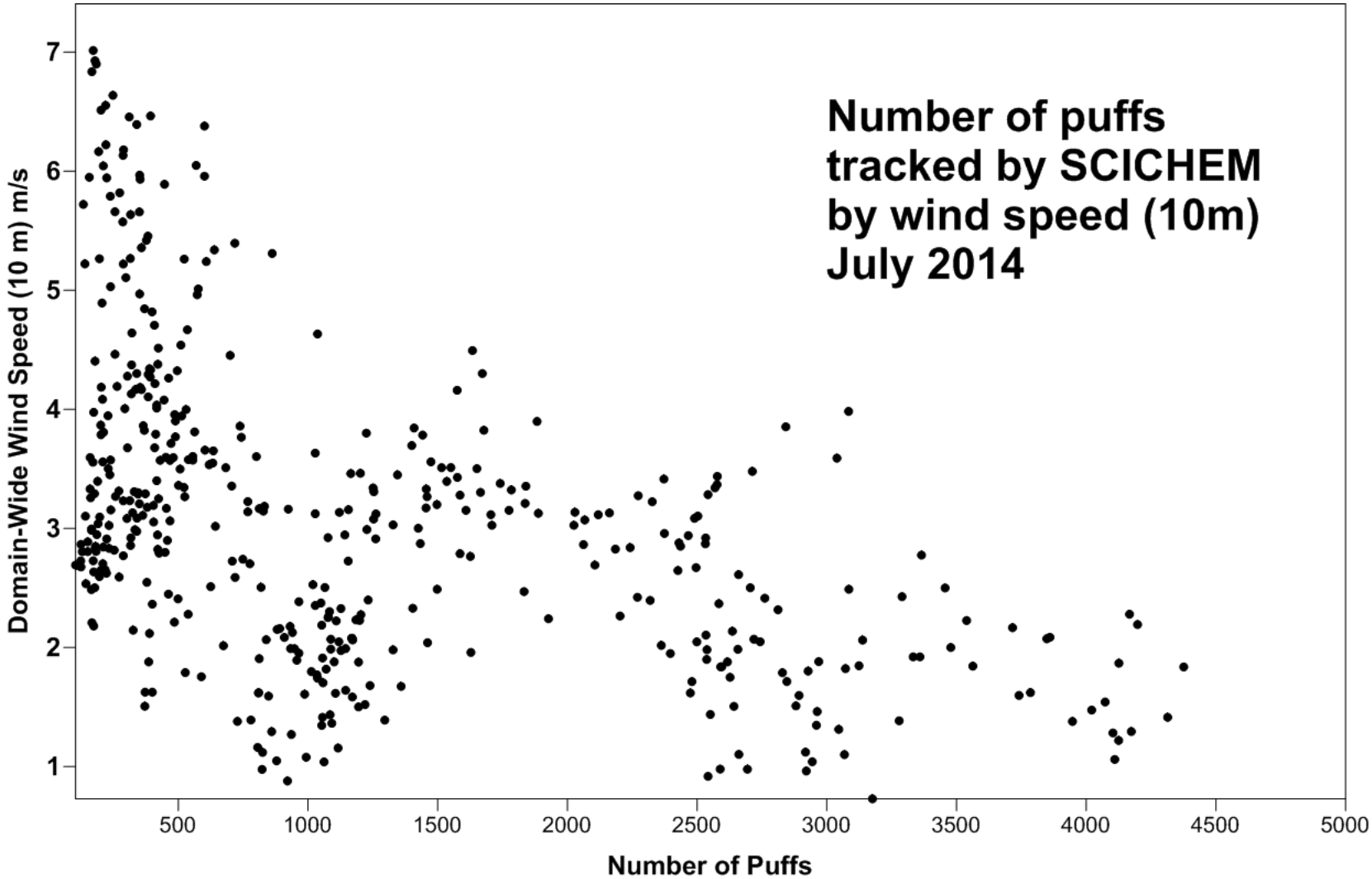
# Running SCICHEM (3)

- To help manage total modeling time, the runs were divided into monthly runs where each month was configured with a 2-day spin-up time.

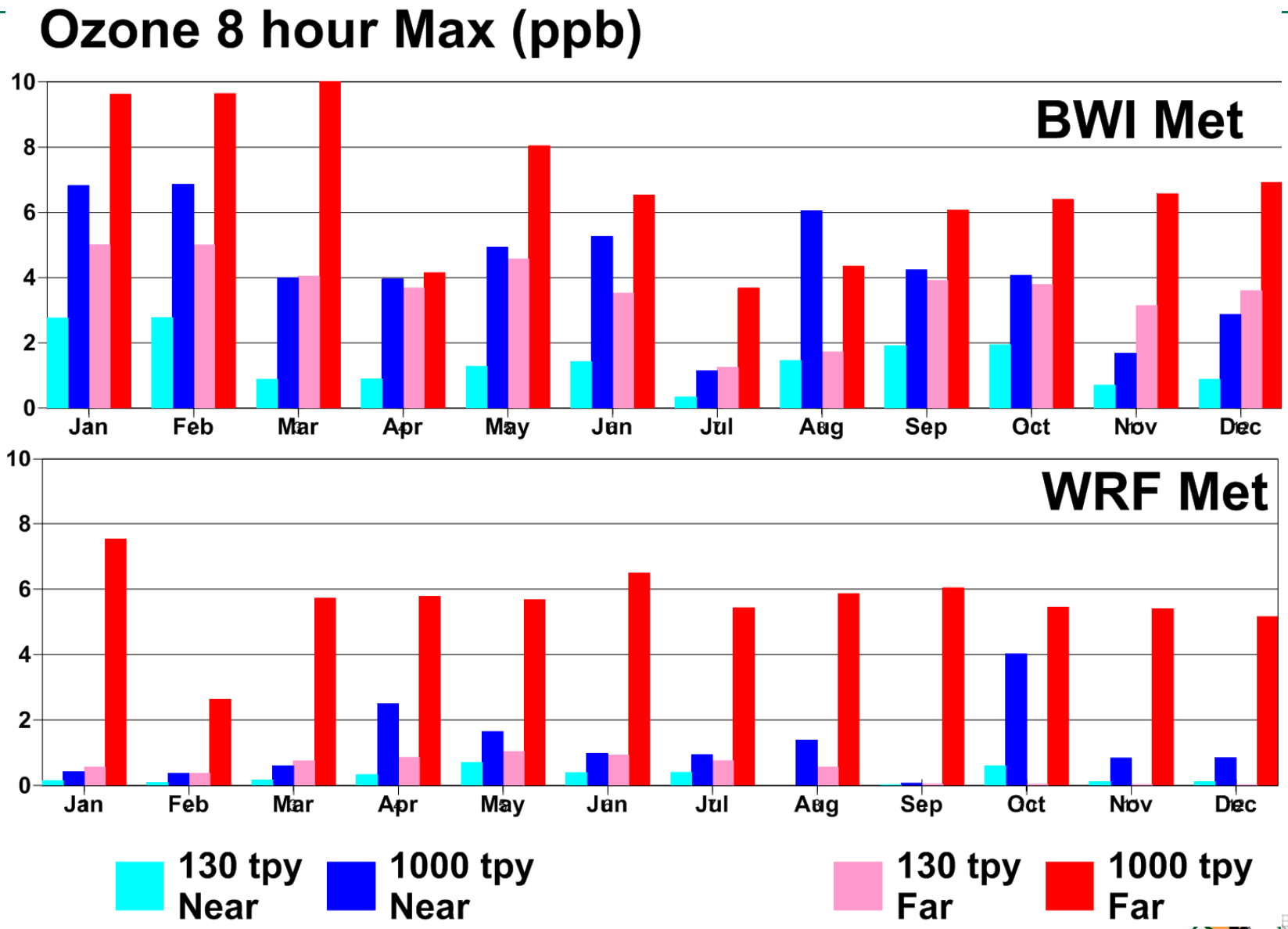
- The near-field and far-field receptor runs were run simultaneously on a total of 24 processors.

- Most monthly runs finished within about 3-4 hours. July took longer – nearly 10 hours. Preliminary investigation revealed that the number of active puffs was greater than any other month. It is hypothesized that frequent low wind speeds during July led to the puff accumulation on the grid.

# Puff Accumulation

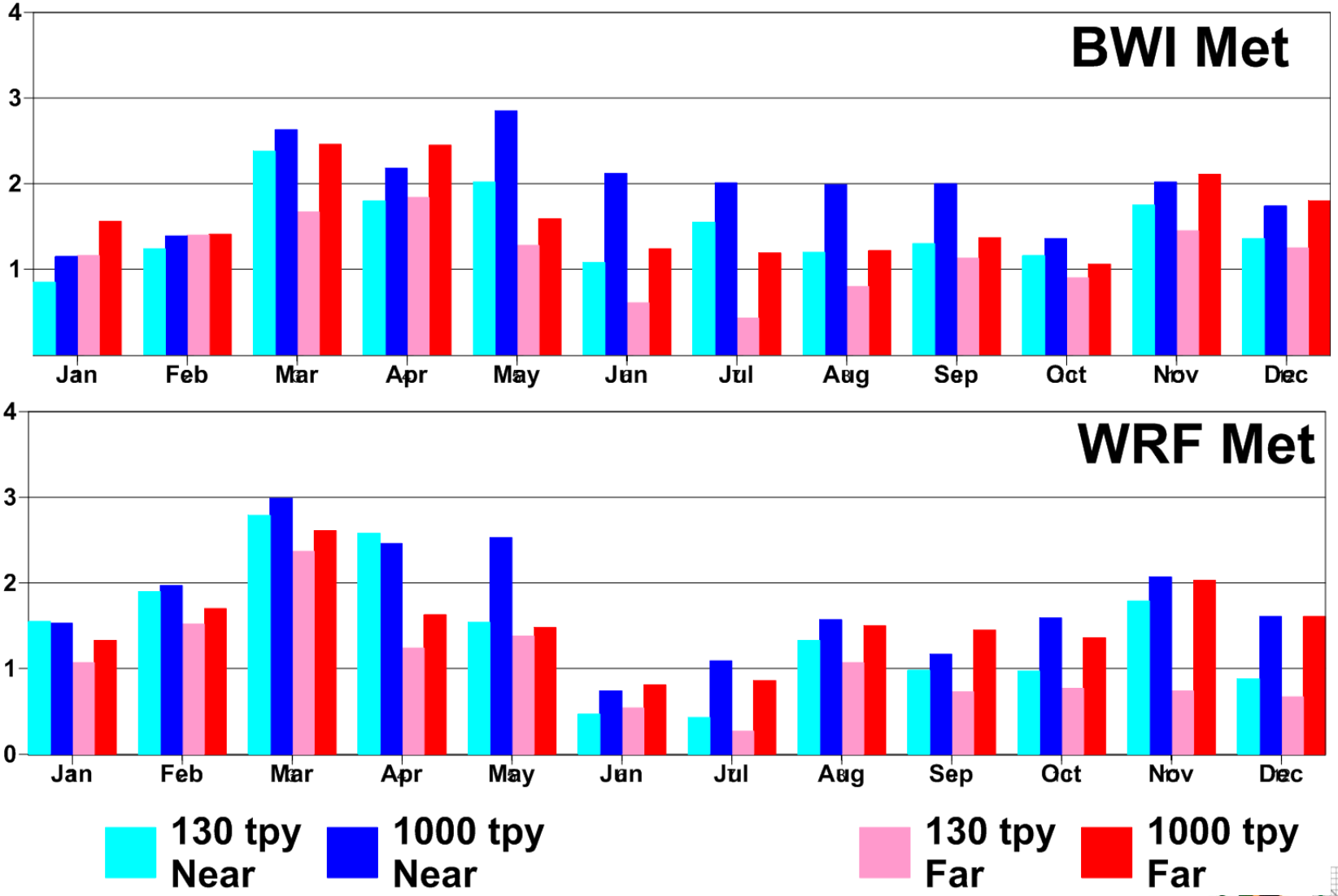


# Results - Ozone



# (Results PM2.5)

## (PM2.5 24-hr Max)



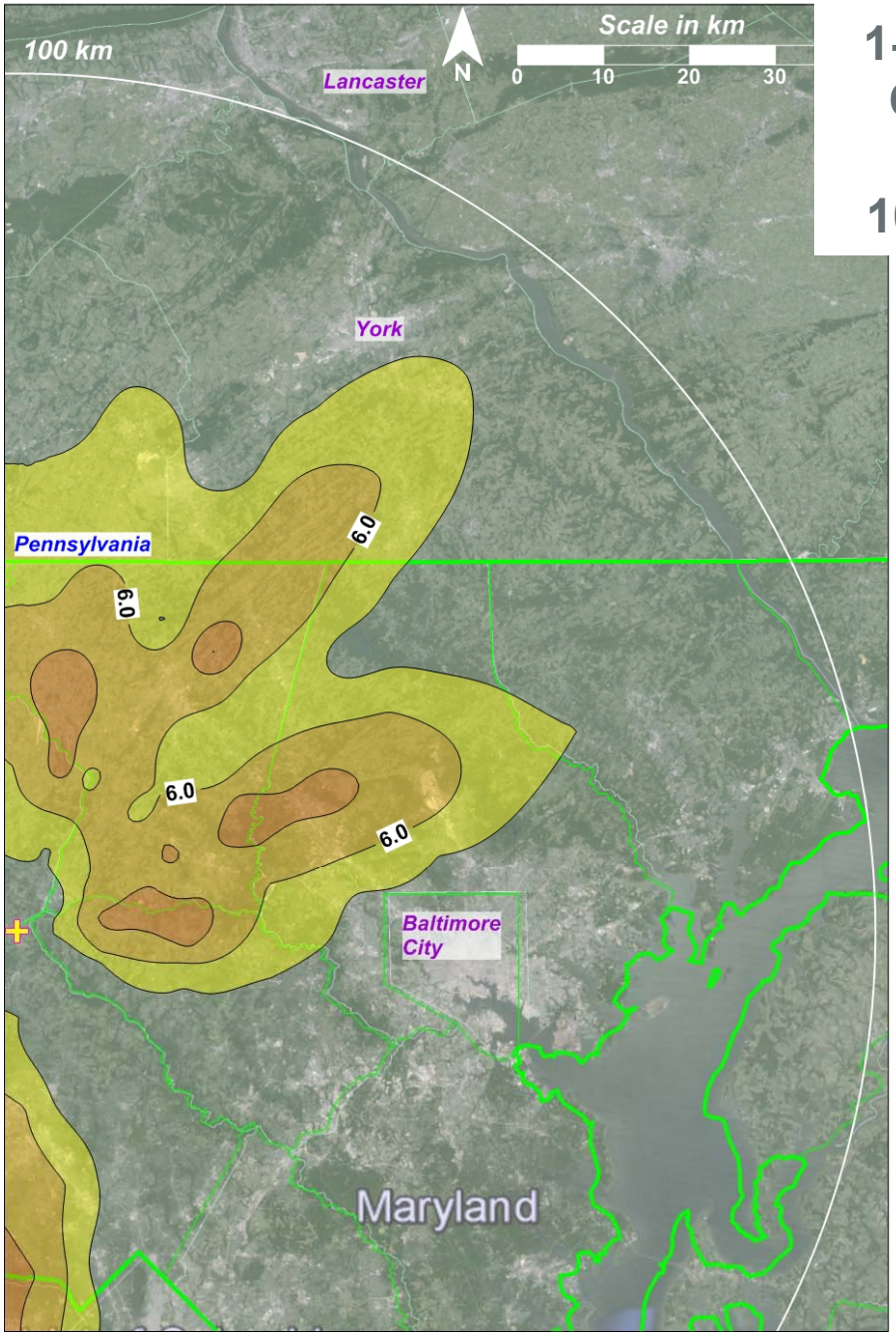
# Results Summary

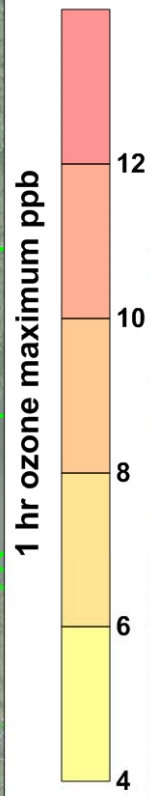
| Pollutant/Avg | Units | Met | Max_Near | | Max_Far | |
|---|---|---|---|---|---|---|
| | | | 130 TPY | 1000 TPY | 130 TPY | 1000 TPY |
| Ozone 1 hr Max | ppb | BWI | 9.33 | 19.82 | 6.96 | 31.58 |
| | | WRF | 2.39 | 11.15 | 3.86 | 29.08 |
| Ozone 8 hr Max | ppb | BWI | 2.77 | 6.86 | 2.34 | 10.26 |
| | | WRF | 0.70 | 4.02 | 1.04 | 7.53 |
| Ozone 8 hr 3d High by Month | ppb | BWI | 0.92 | 2.92 | 0.82 | 4.06 |
| | | WRF | 0.15 | 0.29 | 0.56 | 2.70 |
| | | | | | | |
| PM2.5 24 hr Max | ug/m3 | BWI | 2.38 | 2.85 | 1.84 | 2.46 |
| | | WRF | 2.79 | 2.99 | 2.37 | 2.61 |
| HNO3 24 hr Max | ug/m3 | BWI | 2.03 | 6.52 | 1.26 | 2.08 |
| | | WRF | 3.09 | 8.52 | 1.57 | 3.31 |
| Particulate Nitrate 24 hr Max | ug/m3 | BWI | 1.98 | 2.56 | 1.57 | 2.05 |
| | | WRF | 2.37 | 2.46 | 2.00 | 2.22 |
| | | | | | | |
| NO2 1hr Max | ug/m3 | BWI | 4.66 | 34.56 | 1.83 | 14.07 |
| | | WRF | 4.52 | 33.29 | 1.91 | 15.78 |
| NO 1hr Max | ug/m3 | BWI | 1.84 | 18.10 | 0.32 | 2.75 |
| | | WRF | 3.12 | 27.37 | 0.41 | 3.60 |

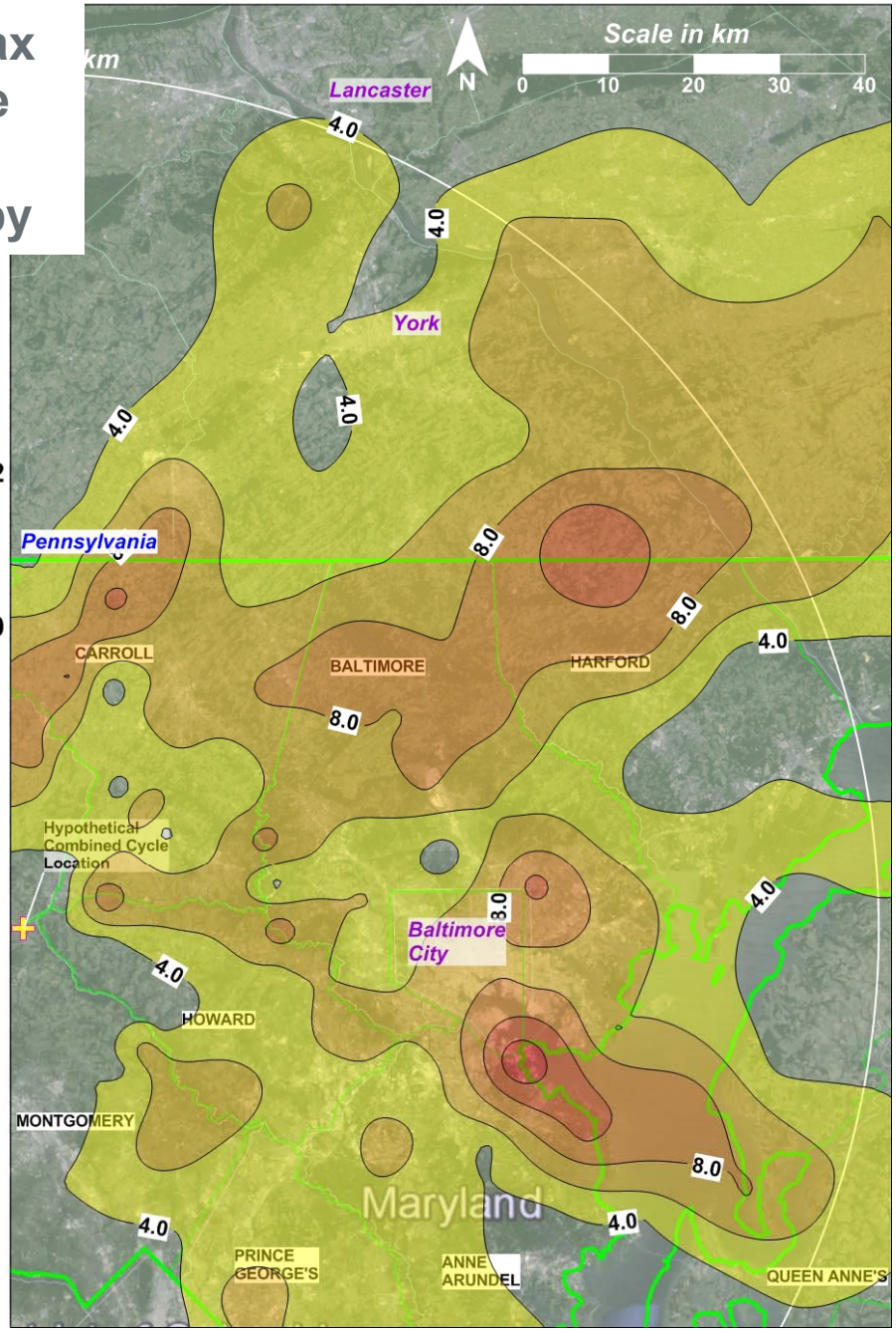
## BWI Meteorology

## WRF Meteorology

# 1-hr Max Ozone July 1000 tpy

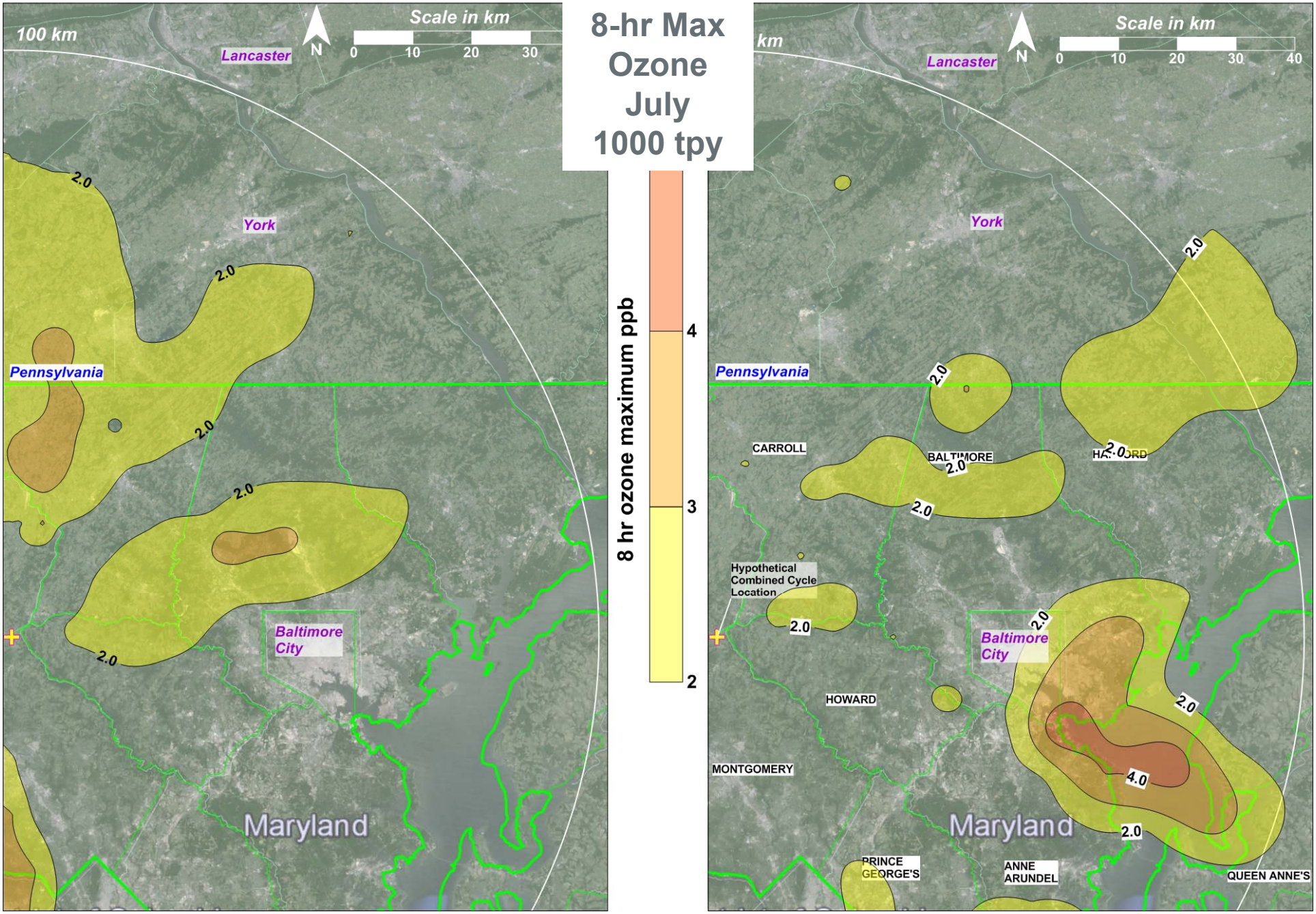


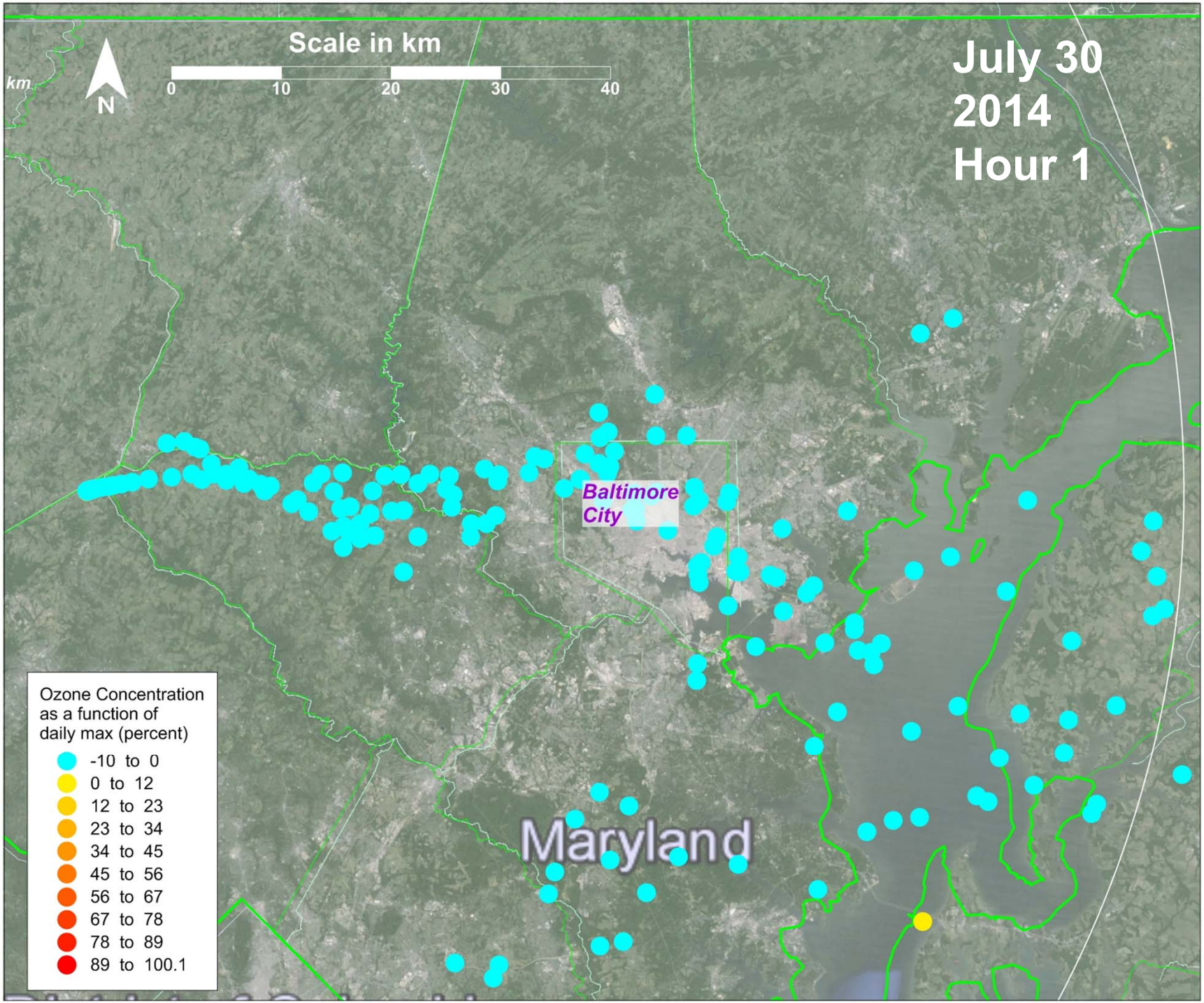



## BWI Meteorology

## WRF Meteorology




Scale in km
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July 30
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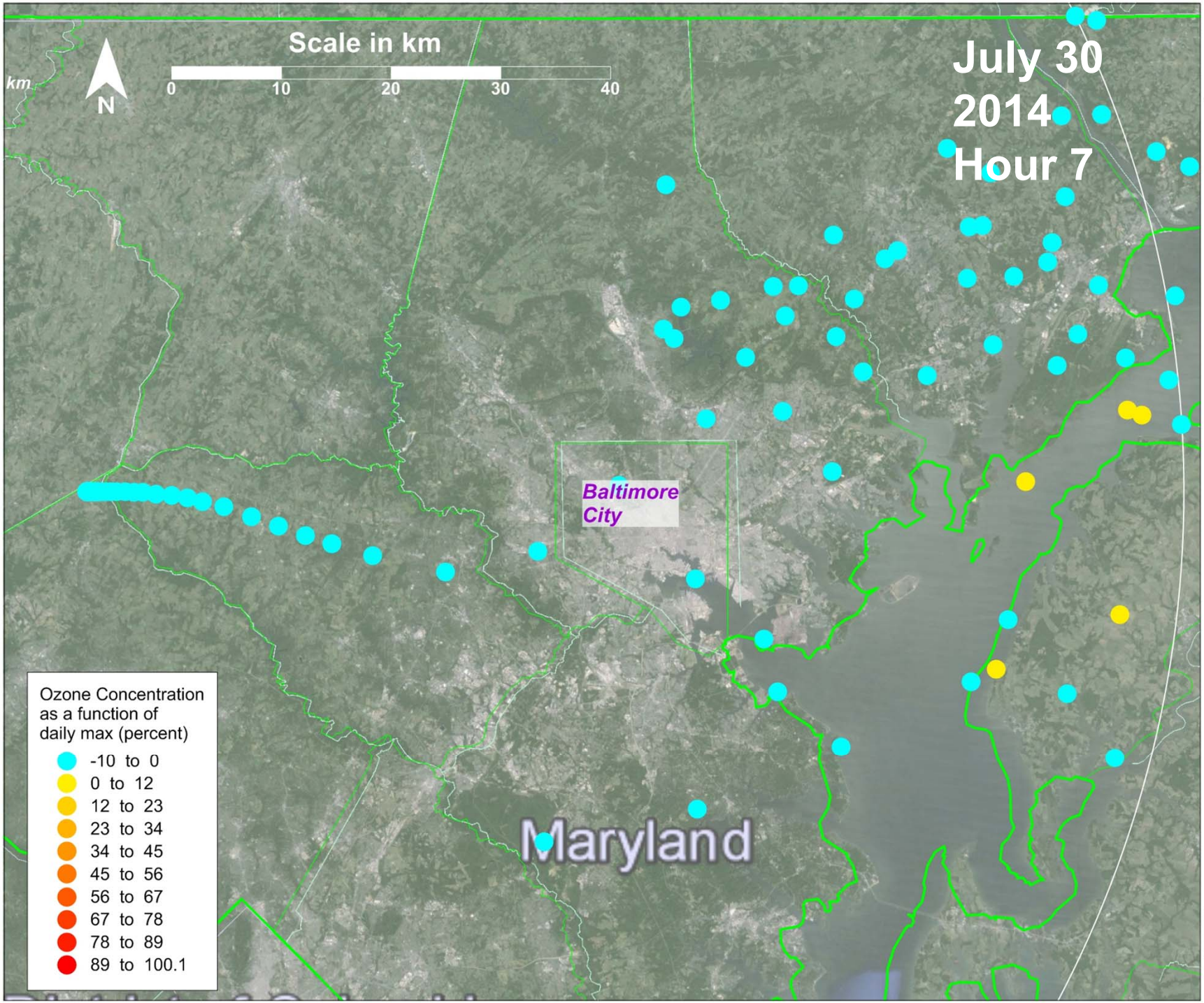
Hour 1
Baltimore
City
Maryland
Ozone Concentration
as a function of
daily max (percent)
-10 to 0
0 to 12
12 to 23
23 to 34
34 to 45
45 to 56
56 to 67
67 to 78
78 to 89
89 to 100.1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Ozone Concentration
as a function of
daily max (percent)
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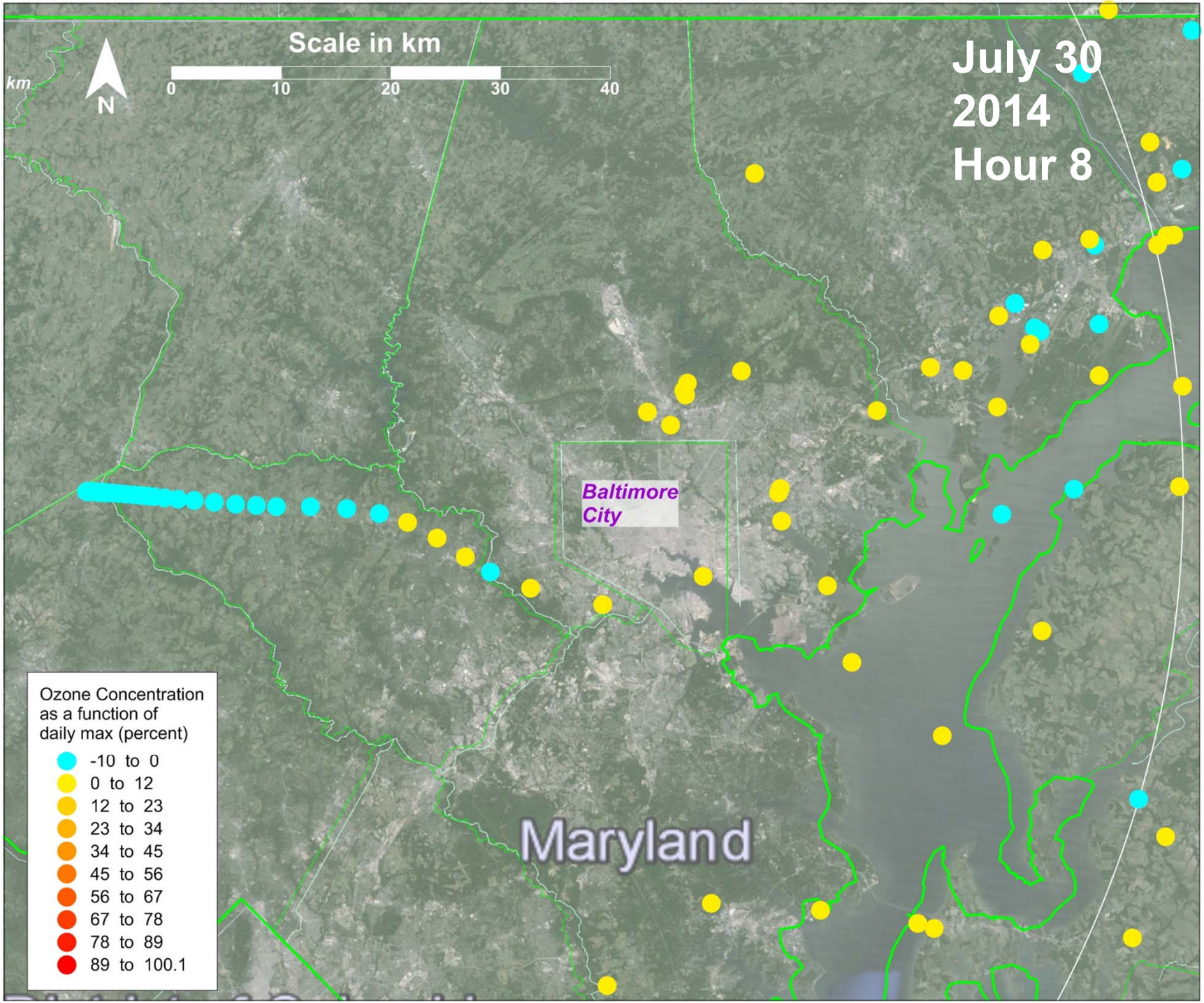
34 to 45
45 to 56
56 to 67
67 to 78
78 to 89
89 to 100.1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Ozone Concentration
as a function of
daily max (percent)
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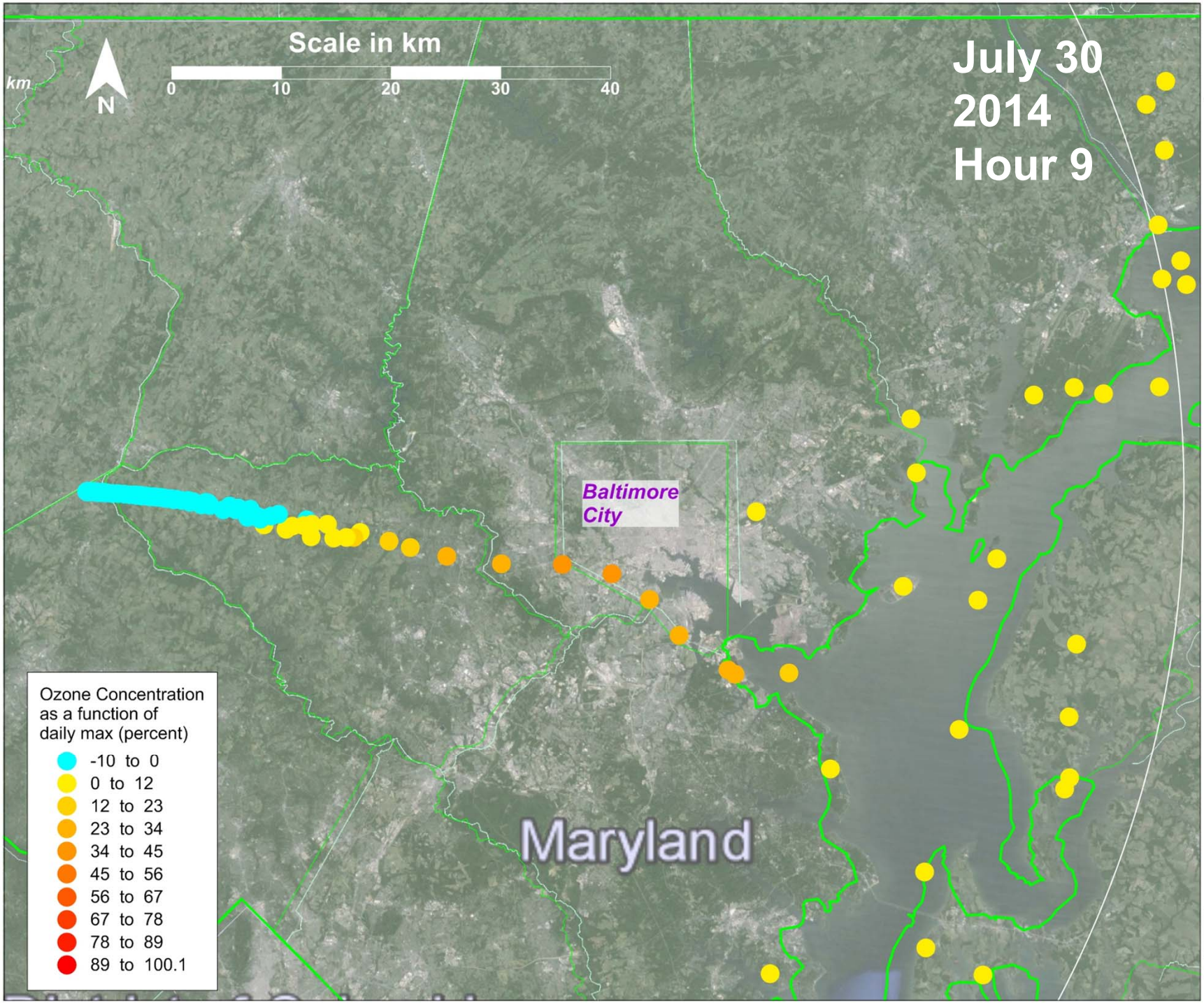
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Ozone Concentration
as a function of
daily max (percent)
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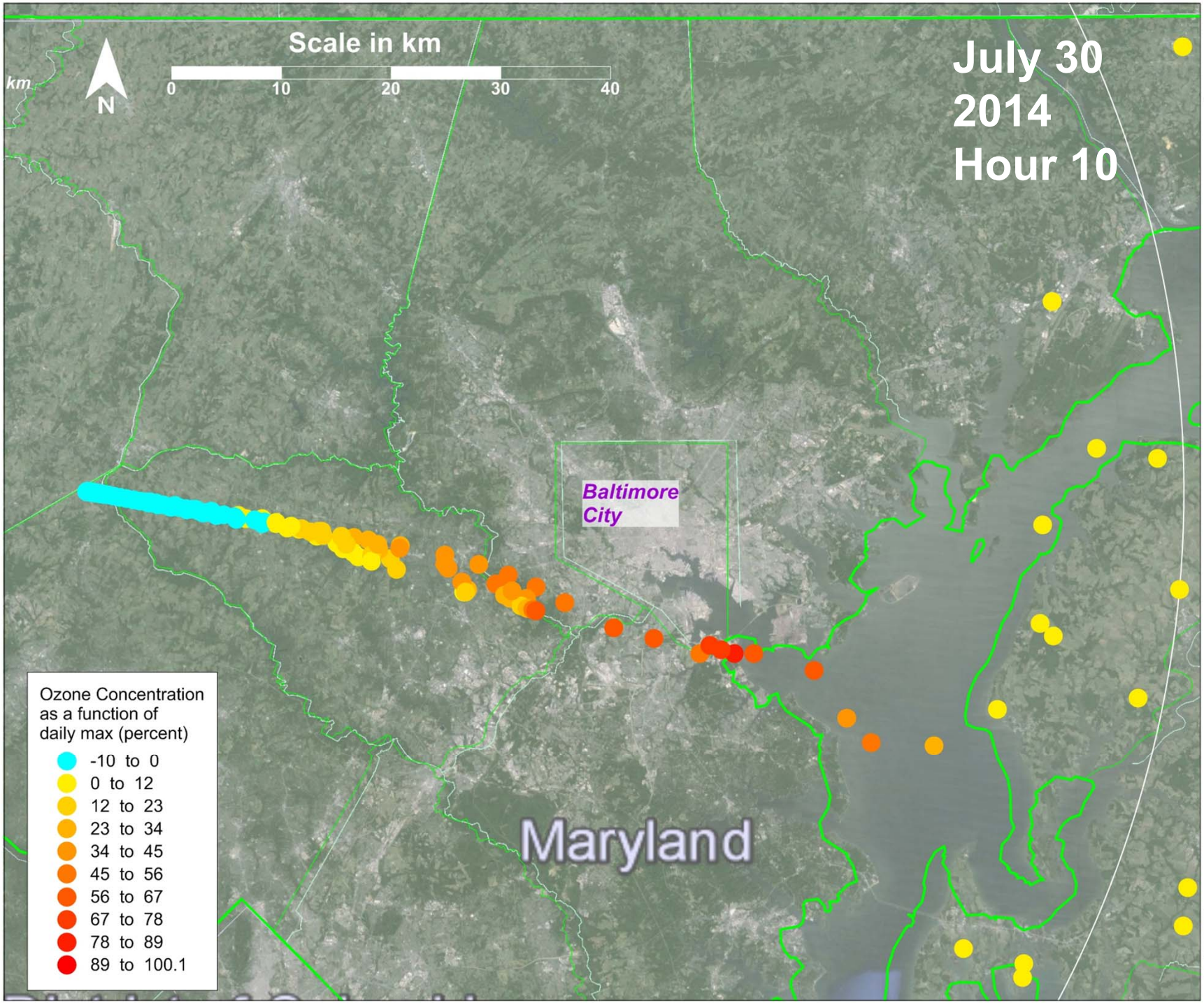
78 to 89
89 to 100.1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Ozone Concentration
as a function of
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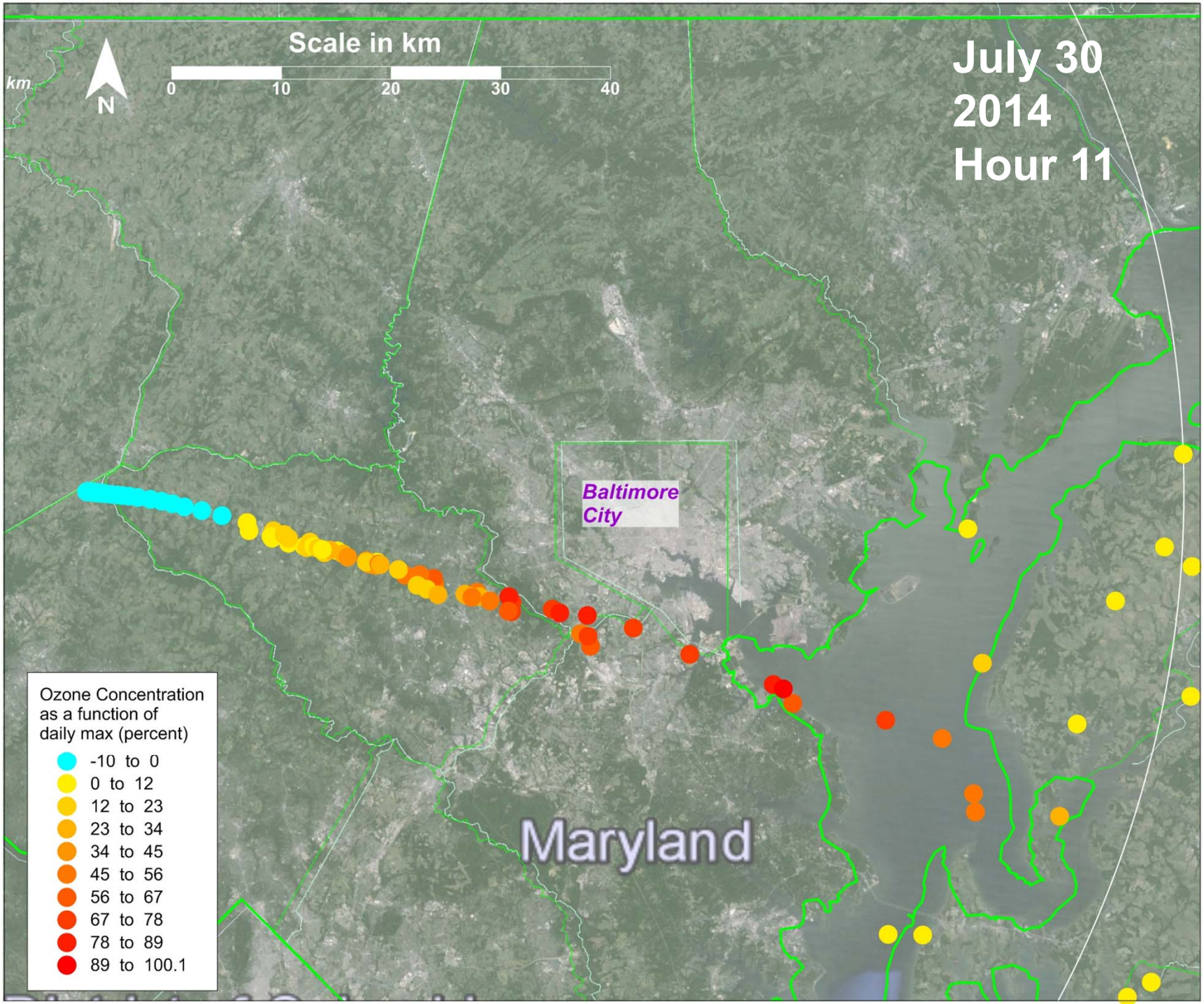
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Ozone Concentration
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daily max (percent)
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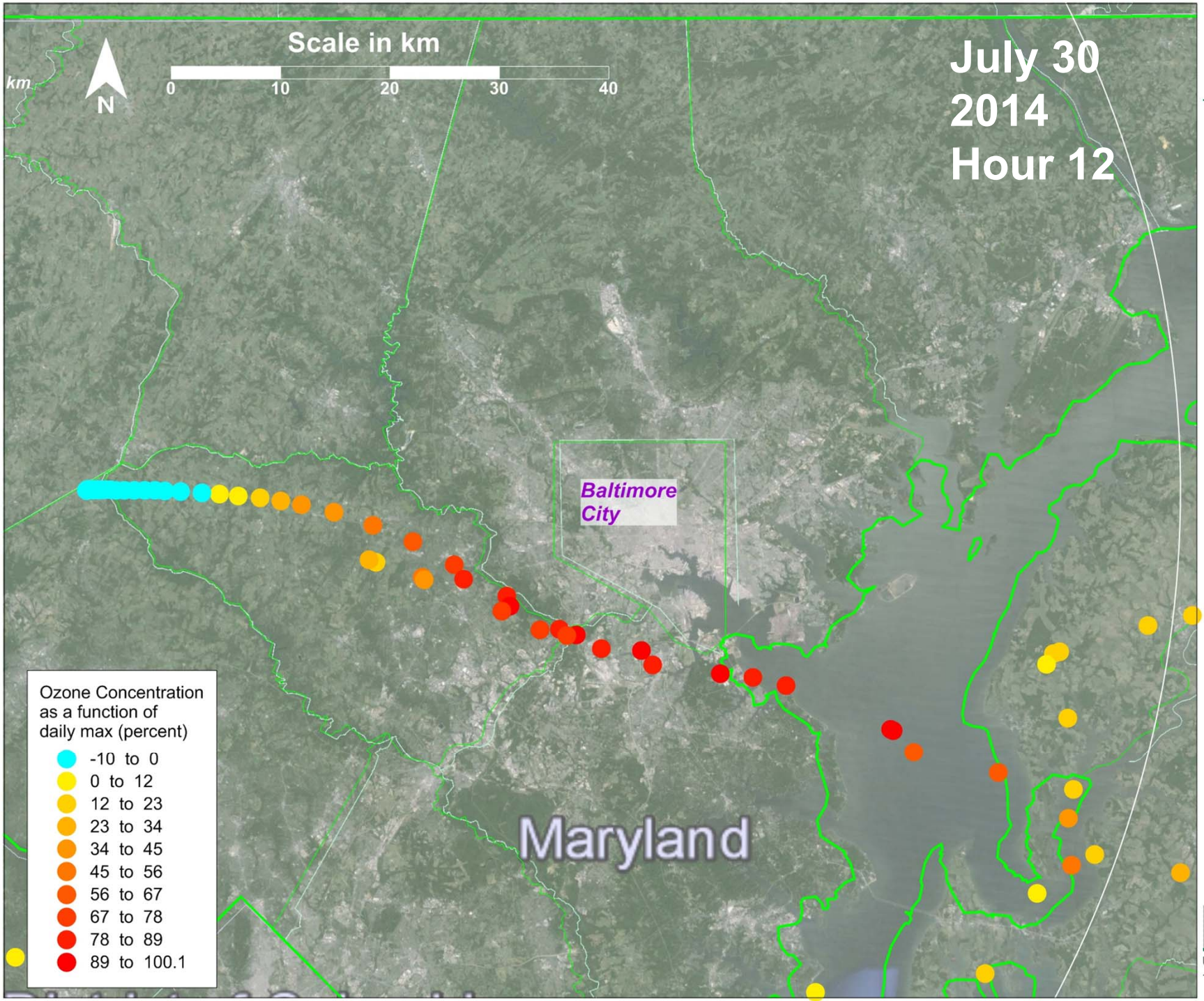
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Ozone Concentration
as a function of
daily max (percent)
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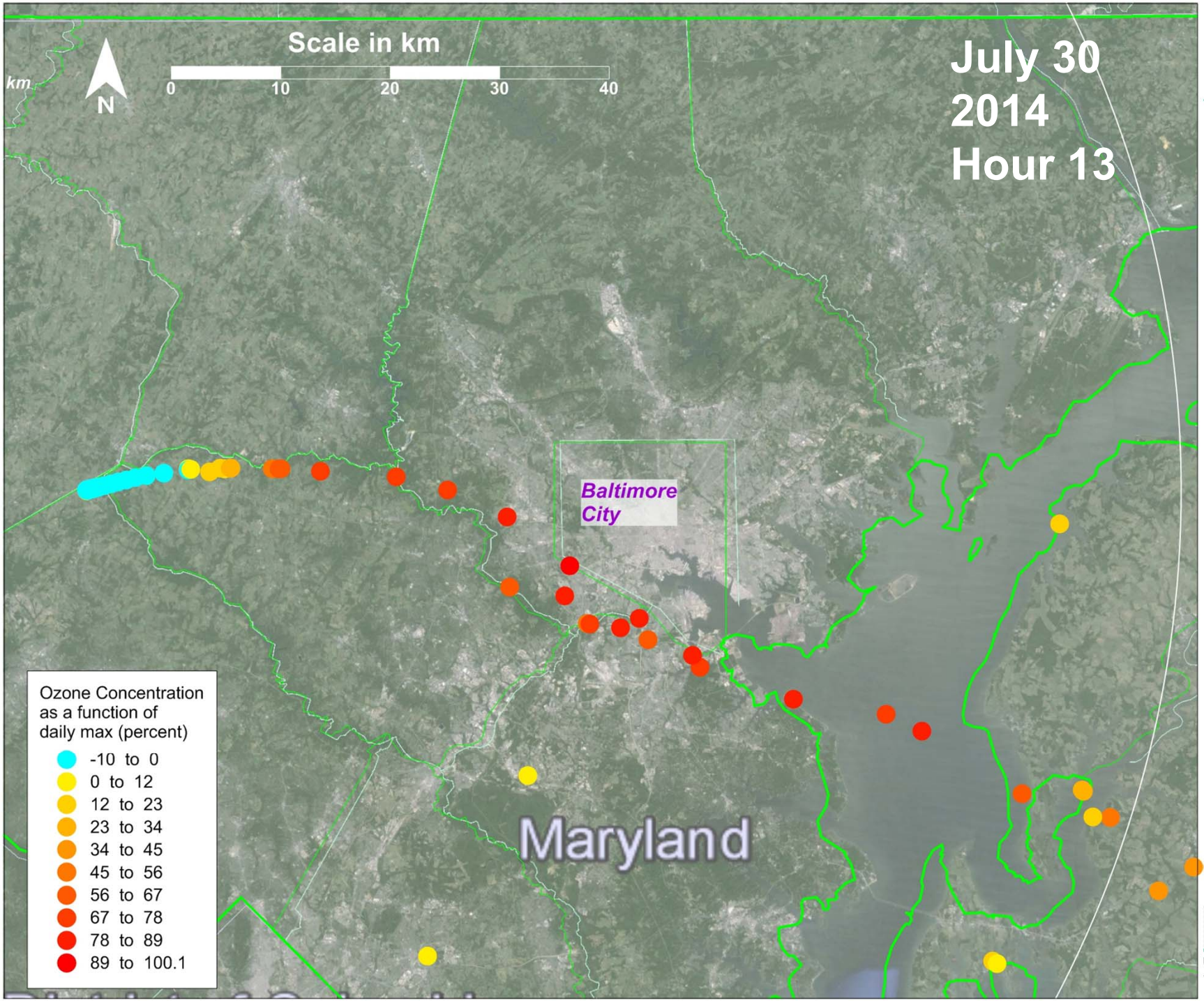
89 to 100.1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Ozone Concentration
as a function of
daily max (percent)
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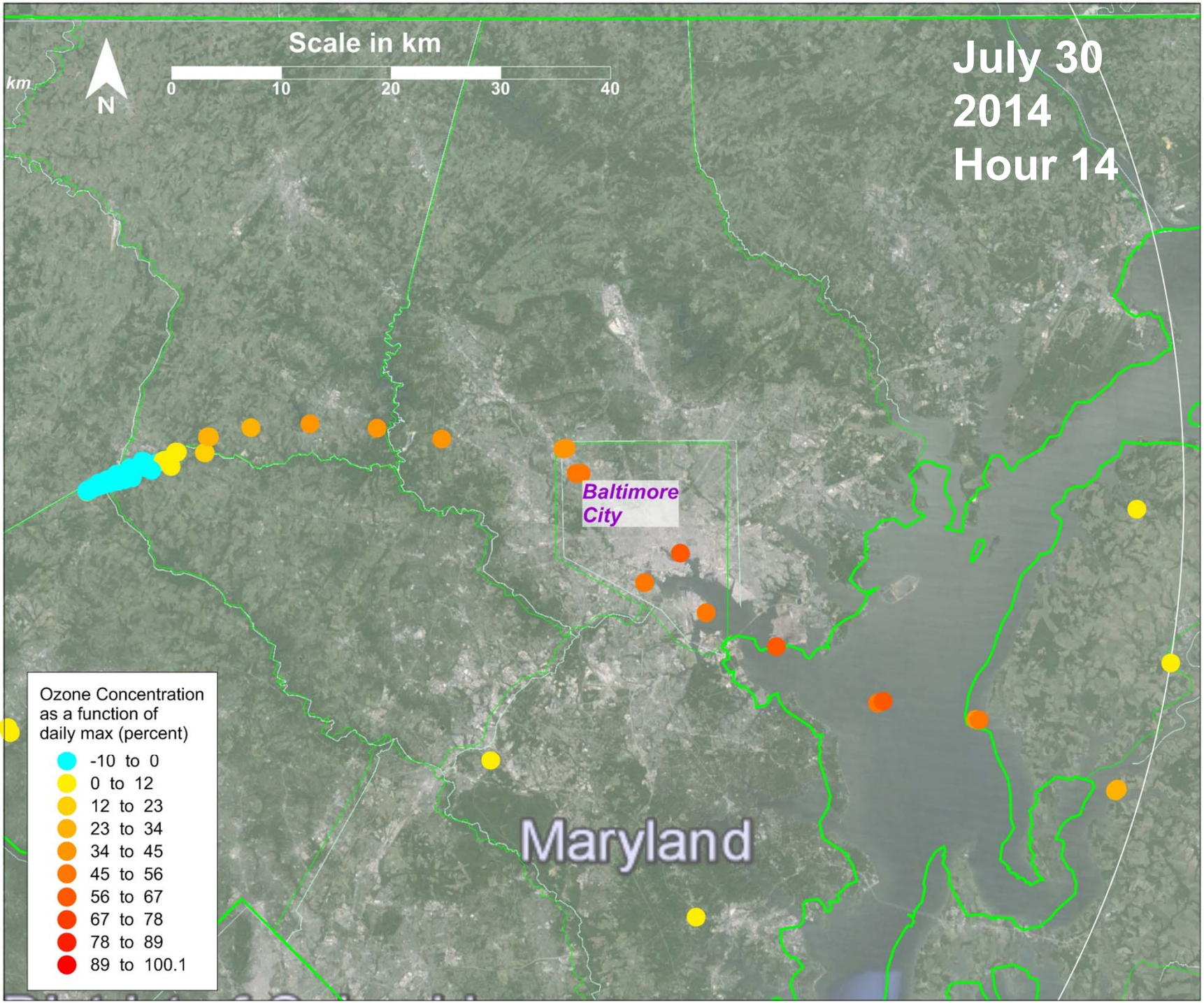
67 to 78
78 to 89
89 to 100.1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Ozone Concentration
as a function of
daily max (percent)
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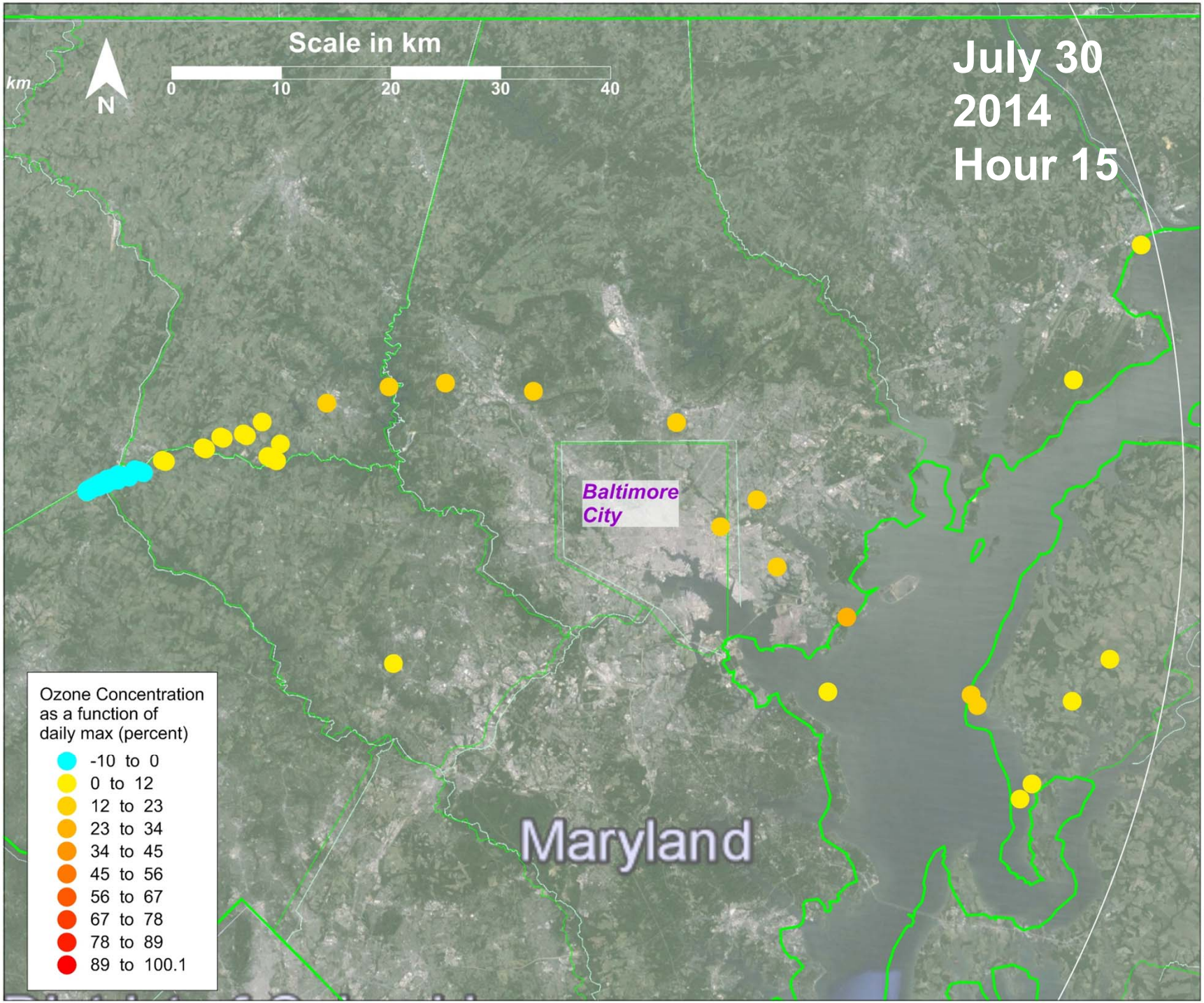
67 to 78
78 to 89
89 to 100.1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Ozone Concentration
as a function of
daily max (percent)
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78 to 89
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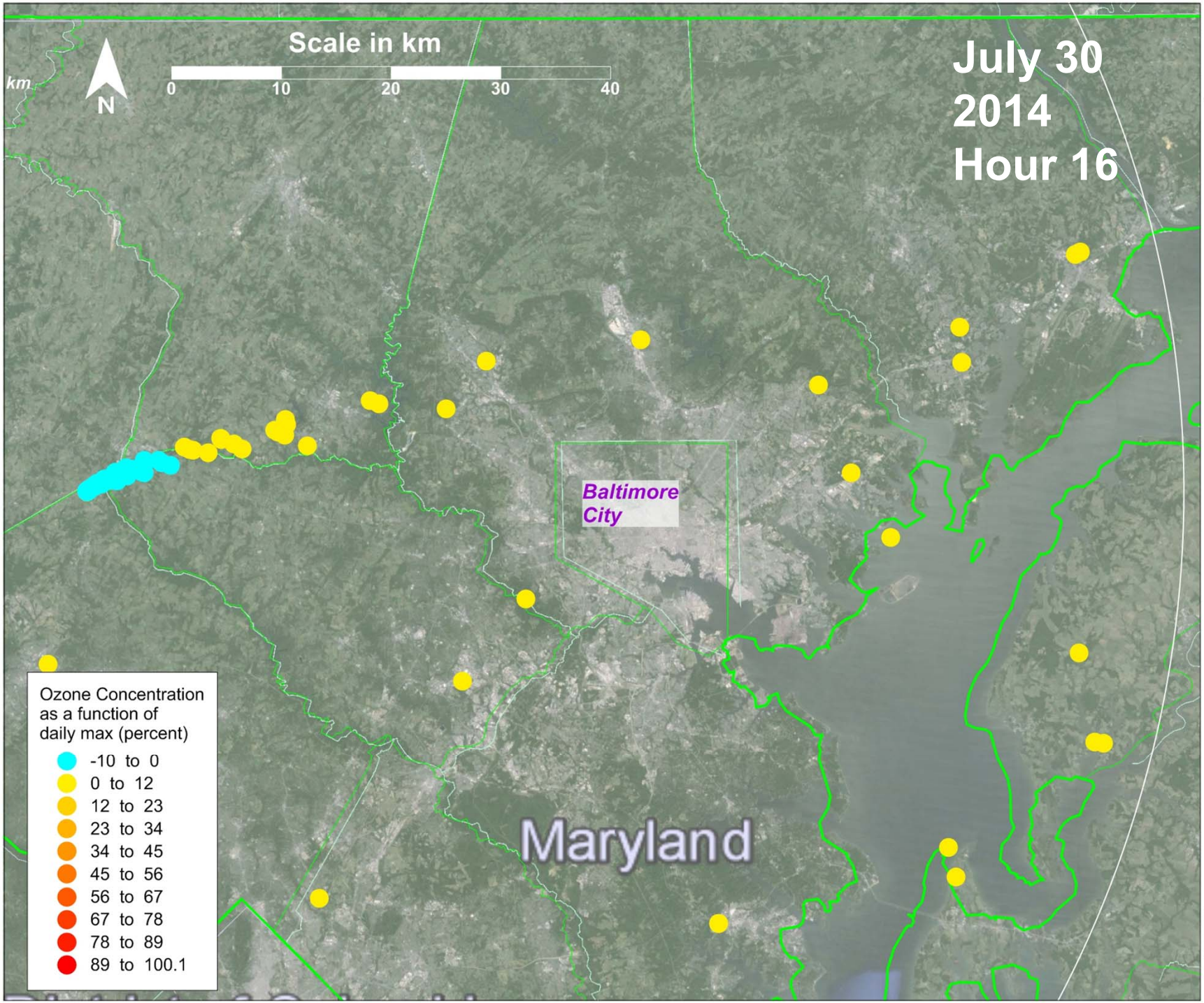
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Ozone Concentration
as a function of
daily max (percent)
-10 to 0
0 to 12
12 to 23
23 to 34
34 to 45
45 to 56
56 to 67
67 to 78
78 to 89
89 to 100.1

# Results Comparisons

- An initial comparison is made between the maximum ozone predictions presented here, and the results presented in a paper by Baker, et. al.
  - Baker, K.R.; Kotchenruther, R.A.; Hudman, R.C. *Estimating ozone and secondary PM2.5 impacts from hypothetical single source emissions in the central and eastern United States*. Atmospheric Pollution Research (2015) pages 1-12.

- Figure 2 of the Baker, et.al. paper displays "Annual peak daily maximum 8-hr average O3 contribution (ppb) from 24 different hypothetical sources of 1000 TPY of NOx emissions with an elevated [90 m] release point." The 24 sources refer to 24 different locations in the central and eastern U.S. The reported increases in

- O3 concentrations range from 1.3 to 7.3 ppb depending on the location. This study: 10.3 ppb (BWI), 7.5 (WRF)

# Summary

- This preliminary work suggests that SCICHEM is a good candidate for use in evaluating the impacts of single sources on ozone (and PM25) concentrations, and to play a role in the Tiered system proposed by EPA

- Computer requirements are not excessive, documentation is thorough, and the model appears to be well-adapted to a Windows as well as a Linux platform.

- It appears that the use of WRF provides better estimates based on a review of spatial and temporal patterns, but this should be the subject of further review and understanding.

- Further review and understanding is also necessary to develop guidance on the proper use of this model for the purpose of estimating single source impacts, and to avoid potentially anomalous predictions.

# Observations/Future Work

- SCICHEM estimates the maximum impacts from a single source – very different than estimating the effect on the design value in a given area or at a given monitor
- Current use of SILs for non-reactive pollutants involves comparing maximum predictions to SIL level independent of location/time of occurrence
- Further thought should be given to considering spatial distribution and frequency in judging significance of secondary impacts

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