### Application of WRF/Chem-MADRID for real-time air quality forecasting over the Southeastern United States

Ming-Tung Chuanga, Yang Zhanga,\*, Daiwen Kangb

Reporter: Liu Di

2014-5-9

### Outline

- 1 Background
- 2 Objective
- 3 Method
- 4 Analysis
- 5 Conclusion

## Background

- A Real-Time Air Quality Forecast (RT-AQF) system that is based on a three-dimensional air quality model provides a powerful tool to forecast air quality and advise the public with proper preventive actions.
- This model exits the overpredictions of O<sub>3</sub> and underprediction of PM2.5are likely due to uncertainties in emissions, inaccuracies in simulated meteorological variables such as 2-m temperature, 10-m wind speed, and precipitation, and uncertainties in the boundary conditions.
- WRF/Chem-MADRID demonstrates good forecasting skill that is consistent with current RT-AQF models

### Objectives

 The objectives of this study are to evaluate the forecasting skill of WRF/Chem-MADRID in RT-AQF applications and to identify likely causes of model biases as well as the areas of the improvement.

### Methods

- Existing AQF tools include simple rules of thumb in which thresholds of forecasted meteorological variables can indicate future high pollutant concentrations based on their correlation derived from observed and forecasted meteorological and air quality data,
- An RT-AQF system based on an online-coupled meteorology-chemistry model has a potential to better represent the real atmosphere and thus provides more accurate AQF.
- WRF/Chem for RT-AQF is based on the modal approach, MADRID uses a sectional representation for particle size distribution and more advanced model treatments.

## Analysis

 Fig. 1 Flowchart of the RT-AQF system based on WRF/Chem-MADRID

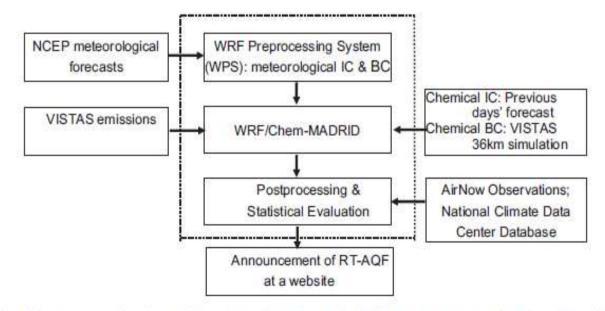


Fig. 1. Flowchart of the RT-AQF system based on WRF/Chem-MADRID (VISTAS denotes the Visibility Improvement State and Tribal Association of the Southeast).

 Fig. 2. Simulated domain for RT-AQF. Numbers of 1-9 indicate geographical regions(separated by dash lines) to be evaluated.

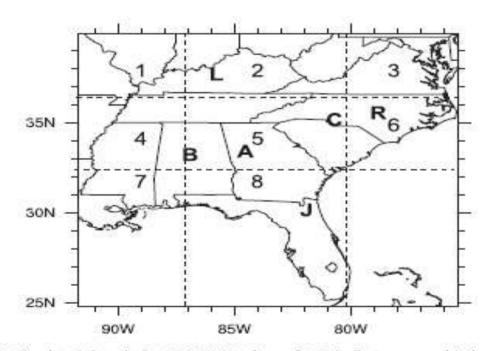


Fig. 2. Simulated domain for RT-AQF. Numbers of 1—9 indicate geographical regions (separated by dash lines) to be evaluated; letters indicate the locations of the selected six urban sites for detailed analyses: A-Atlanta city in Georgia; B-Birmingham city in Alabama; C-Charlotte city in North Carolina; J-Jacksonville city in Florida; L: Louisville city in Kentucky, and R: Raleigh city in North Carolina.

Summary of discrete evaluation for meteorological and chemical variables in May-September of 2009,

|   |               | Mean<br>Obs | Mean<br>Sim | MB   | RMSE | NMB<br>(%)  | NME<br>(%) |
|---|---------------|-------------|-------------|------|------|---|------------|
| hourly T2 (* C)                               | May           | 19.8        | 20.1        | 0.3  | 2.7  | 1.8   | 7.6        |
|   | June          | 23.9        | 24.2        | 0.3  | 2.5  | 1.5   | 5.9        |
|   | July          | 24.1        | 24.4        | 0.3  | 2.4  | 1.4   | 5.5        |
|   | August        | 24.4        | 25.0        | 0.6  | 2.4  | 2,6   | 6.         |
|   | September     | 21.5        | 21.6        | 0.1  | 2.3  | 0.3   | 6.         |
|   | May-September | 22.7        | 23.1        | 0,4  | 2.5  | 1.5   | 6.         |
| hourly WS10 (m s <sup>-1</sup> )              | May           | 5.6         | 4.3         | -1.3 | 3.4  | -23.9   | 35.        |
|   | lune          | 4.7         | 3.6         | -1.1 | 3.1  | -22.6   | 38         |
|   | July          | 4.5         | 3.5         | -1.0 | 2.9  | -21.8   | 42.        |
|   | August        | 4.1         | 3.3         | -0.8 | 2.9  | -20.4   | 41.        |
|   | September     | 4.5         | 3.5         | -1.0 | 3.3  | -22.5   | 42         |
|   | May-September | 4.7         | 3.7         | -1.0 | 3.2  | -22.3   | 40         |
| Total daily Precip<br>(mm day <sup>-1</sup> ) | May           | 3.5         | 4.5         | 1.0  | 16.1 | 29.4  | 175.       |
|   | June          | 2.4         | 2.3         | -0.1 | 11.7 | -5.7  | 161.       |
| 0.550.00095                                   | July          | 2.8         | 3.8         | 1.0  | 15.5 | 35.7  | 197.       |
|   | August        | 2.5         | 2.9         | 0.4  | 14.3 | 15.5  | 184.       |
|   | September     | 3.1         | 3.3         | 0.2  | 16.2 | 7.9   | 166.       |
|   | May-September | 2.9         | 3.4         | 0.5  | 14.9 | 18,7  | 178.       |
| Max 1-h O3                                    | May           | 45,9        | 49.7        | 3.8  | 17,4 | 8,4   | 28.        |
| (ppb)   | June          | 52,8        | 53.7        | 0.9  | 17.5 | 1.6   | 25         |
|   | July          | 48.5        | 54.3        | 5,8  | 16.9 | 3   0.3     5   1.5     4   -23.9     1   -22.6     9   -21.8     9   -20.4     3   -22.5     2   -22.3     1   29.4     7   -5.7     3   15.5     2   7.9     9   18.7     4   8.4     5   1.6     9   12.0     4   8.4     5   1.6     9   12.0     4   8.4     5   1.6     9   2.7     9   1.7.0     4   8.4     5   9.2     8   9.4     9   5.7     9   0.4     10.2   5     5   -10.7     3   -16.2     0   -8.8 | 25,        |
|   | August        | 46.3        | 54.2        | 7.9  | 16.4 | 17.1  | 26,        |
|   | September     | 43.2        | 47.3        | 4.0  | 15.6 | 9.2   | 27.        |
|   | May-September | 47.3        | 51.8        | 4.4  | 16.8 | 9,4   | 26,        |
| Max 8-h average O3                            | May           | 41.5        | 43.9        | 2.4  | 13.9 | 5.7   | 26,        |
| (ppb)   | June          | 47.4        | 47.6        | 0,2  | 13.9 | 0,4   | 23.        |
|   | July          | 43.5        | 47.9        | 4.4  | 13.3 | 10.2  | 23.        |
|   | August        | 41.2        | 48.2        | 7.0  | 13.6 | 17.0  | 25.        |
|   | September     | 38.7        | 42.7        | 4.0  | 13.5 | 10,3  | 27.        |
|   | May-September | 42.5        | 46,0        | 3.5  | 13.6 | 8,5   | 25         |
| 24-h average PM25                             | May           | 9,2         | 8,2         | -1.0 | 4.5  | -10,7   | 36         |
| (µg m <sup>-3</sup> )                         | June          | 13.5        | 11.3        | -2,2 | 6.3  | -16.2   | 34         |
| NGC - AL                                      | July          | 12.5        | 11,4        | -1.1 | 6.0  | -8.8  | 35         |
|   | August        | 12.4        | 12,0        | -0.4 | 6.4  | -3.2  | 36.        |
|   | September     | 10.2        | 11.8        | 1.7  | 5.9  | 16.5  | 42.        |
|   | May-September | 11.5        | 10.0        | -0.6 | 5.9  | -5.2  | 37.        |

Note: T2: Temperature at 2 m; WS: Wind Speed; Precip: Precipitation; MB: Mean Bias; RMSE: Root Mean Square Error; NMB: Normalized Mean Bias; NME: Normalized Mean Error,

Normalized Mean Error (MSE) =  $\sqrt{1/N \sum_{1}^{N} (\text{Sim} - \text{Obs})}$ , Root Mean Square Error (RMSE) =  $\sqrt{1/N \sum_{1}^{N} (\text{Sim} - \text{Obs})^2}$ , Normalized Mean Bias (NMB) =  $\sum_{1}^{N} (\text{Sim} - \text{Obs}) / \sum_{1}^{N} (\text{Obs}) \times 100\%$ , Normalized Mean Error (NME) =  $\sum_{1}^{N} |\text{Sim} - \text{Obs}| / \sum_{1}^{N} (\text{Obs}) \times 100\%$  where Sim, Obs, and N are simulated values, observated values, and the number of observations, respectively.

 Table 1 Summary of discrete evaluation for meteorological and chemical variables in May-September of 2009.

Accuracy (A) = 
$$\left(\frac{b+c}{a+b+c+d}\right) \times 100\%$$
 (1)

Critical Success Index (CSI) = 
$$\left(\frac{b}{a+b+d}\right) \times 100\%$$
 (2)

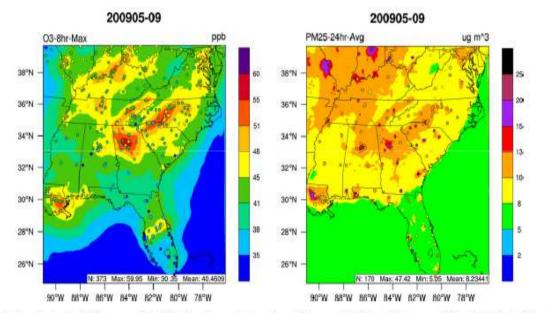
Probability Of Detection (POD) = 
$$\left(\frac{b}{b+d}\right) \times 100\%$$
 (3)

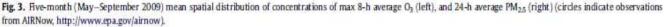
Bias 
$$(B) = \left(\frac{a+b}{b+d}\right)$$
 (4)

False Alarm Ratio (FAR) =  $\left(\frac{a}{a+b}\right) \times 100\%$ (5)

where a, b, c, and d, are the numbers of simulated and observed data pairs at one site at a specific time in the four regions (see Fig. S1 in the supplementary material). They represent forecast

 Fig. 3 shows the overlay plots of 5-month mean daily max 8-h average O<sub>3</sub> and 24-h average PM<sub>2.5</sub> with AIRNow observations.





 $O_3$  overpredictions are most apparent in most areas of Kentucky and Tennessee, southern areas of Indiana, Illinois, and Ohio, and the Appalachian Mountains region.

 Fig. 5 shows simulated and observed daily max 8-h average O<sub>3</sub> mixing ratios at the six urban sites.

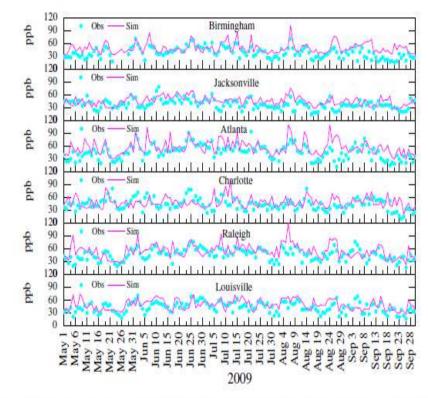


Fig. 5. Simulated and observed daily max 8-h average O<sub>3</sub> mixing ratios at representative urban sites during May–September 2009 (see site locations in Fig. 2). The observational data were obtained from AIRNow, http://www.epa.gov/airnow. Louisville is in Region 2, Atlanta, Birmingham, and Charlotte are in Region 5, Raleigh is in Region 6, Jacksonville is in Region 8.

### Fig. 6 shows simulated and observed 24-h average PM<sub>2.5</sub> concentrations at urban sites.

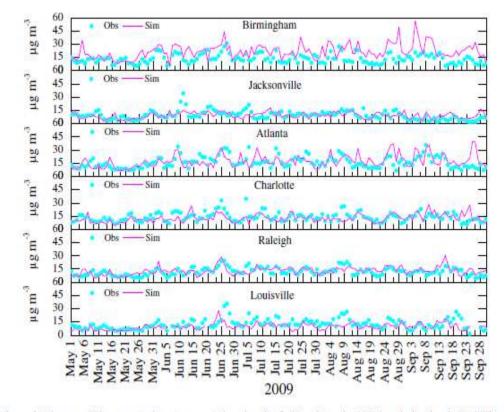


Fig. 6. Simulated and observed 24-h average PM<sub>2.5</sub> concentrations at representative urban sites for May–September 2009 (see site locations in Fig. 2). The observational data were obtained from AIRNow, http://www.epa.gov/airnow. Louisville is in Region 2, Atlanta, Birmingham, and Charlotte are in Region 5, Raleigh is in Region 6, Jacksonville is in Region 8.

#### Table 2 summarizes categorical evaluation results.

#### Table 2

Summary of categorical evaluation for O3 and PM25 in May-September of 2009.

|  | Threshold             | Period        | A (%) | CSI(%) | POD (%) | В    | FAR (%) | a    | Ь    | c      | d    |
|--|-----------------------|---------------|-------|--------|---------|------|---------|------|------|--------|------|
| Max 1-h O <sub>3</sub> (ppb)                         | 80 ppb                | May           | 94,6  | 2,0    | 22.0    | 10.0 | 97.7    | 576  | 13   | 10,914 | 46   |
|  |                       | June          | 92.3  | 7.7    | 25.5    | 2.5  | 90.0    | 658  | 73   | 10,332 | 213  |
|  |                       | Jul           | 92.9  | 6.0    | 40.8    | 6,2  | 93,4    | 754  | 53   | 10,766 | 77   |
|  |                       | August        | 92.2  | 4.8    | 43.0    | 8,3  | 94.8    | 844  | 46   | 10,707 | 61   |
|  |                       | September     | 97.9  | 0.4    | 5.6     | 11.9 | 99.5    | 218  | 5    | 11,024 | 22   |
|  |                       | May-September | 94.0  | 5.2    | 31.3    | 5,3  | 94.1    | 3050 | 190  | 53,743 | 419  |
| Max 8-h average O3 (ppb) 60 ppb                      | 60 ppb                | May           | 88.3  | 12.5   | 29.1    | 1.6  | 82.0    | 863  | 189  | 9813   | 460  |
|  |                       | June          | 80.0  | 15.1   | 26.0    | 1.0  | 73.5    | 1100 | 395  | 8470   | 1123 |
|  |                       | Jul           | 83.9  | 14.8   | 41.7    | 22   | 81.4    | 1389 | 318  | 9278   | 444  |
|  |                       | August        | 84.5  | 17.5   | 56.8    | 2.8  | 79.7    | 1474 | 374  | 9179   | 285  |
|  |                       | September     | 91.8  | 2.5    | 7.2     | 1,9  | 96.2    | 594  | 27   | 9901   | 300  |
|  |                       | May-September | 85.6  | 14.0   | 33.3    | 1.7  | 80.6    | 5420 | 1303 | 46,641 | 2612 |
| 24-hraverage PM <sub>2.5</sub> (µg m <sup>-3</sup> ) | 15 µg m <sup>-3</sup> | May           | 91.9  | 10.8   | 16.0    | 0.6  | 74.7    | 160  | 54   | 4655   | 284  |
|  | 清沉的                   | June          | 69.9  | 26.7   | 32,1    | 0.5  | 38.6    | 341  | 541  | 2904   | 1143 |
|  |                       | Jul           | 70,8  | 19.2   | 27.1    | 0.7  | 60.1    | 539  | 358  | 3282   | 965  |
|  |                       | August        | 69.9  | 21.1   | 30.0    | 0.7  | 58.2    | 571  | 409  | 3137   | 955  |
|  |                       | September     | 78.8  | 25.8   | 47.8    | 1.3  | 64.1    | 643  | 362  | 3482   | 395  |
|  |                       | May-September | 76.2  | 22.3   | 31.5    | 0,7  | 56.6    | 2254 | 1724 | 17,460 | 3742 |

1. A: Accuracy; CSI: Critical success index; POD: probability of detection; B: bias: FAR: False alarm ratio.

2. a, b, c, d, are the number of simulated and observed data pairs at one site for a specific time in the four regions shown in Fig. S1.

### Table 3 compares model performance using offline and online BVOC emissions in July 2009.

#### Table 3

Comparison of discrete evaluation of the baseline RT-AQF with offline biogenic emissions and the sensitivity simulations with online biogenic emissions based on the modified Guenther scheme, and modified boundary conditions in July 2009.

|   |               | Mean<br>Obs | Mean<br>Sim  | MB   | RMSE | NMB<br>(%)   | NME<br>(%) |
|---|---------------|-------------|--|------|------|--|------------|
| Max 1-h O3 (ppb)  | Offline BVOCs | 48.5        | 54.4   | 5.9  | 16.9 |  | 25.9       |
|   | Online BVOCs  |             | 54.4   | 5.9  | 16.9 | 12.1   | 26.0       |
|   | Modified LBCs |             | 50,3   | 1.8  | 15,6 | 3.7  | 24.3       |
| Max 8-h average 03                                      | Offline BVOCs | 43.5        | 47.9   | 4.4  | 13.3 | 10.2   | 23.6       |
| (ppb)   | Online BVOCs  |             | 54.4 5.9 1   54.4 5.9 1   50.3 1.8 1   47.9 4.4 1   48.1 4.6 1   44.4 0.9 1   11.4 -1.1 1   12.3 -0.3 -0.3 | 13.4 | 10.5 | 23.9   |            |
| 020400  | Modified IBCs |             | 44.4   | 0.9  | 12.6 | 12.1<br>12.1<br>3.7<br>10.2<br>10.5<br>2.0<br>-8.9<br>-1.7 | 22.3       |
| 24-h average PM <sub>2.5</sub><br>(µg m <sup>-3</sup> ) | Offline BVOCs | 12.5        | 11.4   | -1.1 | 6.0  | -8.9   | 35.9       |
|   | Online BVOCs  |             | 12.3   | -0.3 | 6,0  | -1.7   | 35.4       |
| 202 1   | Modified LBCs |             | 12.8   | 0.3  | 6,1  | 2.8  | 36.5       |

Obs: Observation; Sim: Simulation; MB: Mean Bias; RMSE: Root Mean Square Error; NMB: Normalized Mean Bias; NME: Normalized Mean Error; BVOCs: Biogenic Volatile Organic Carbons; LBCs: Lateral Boundary Conditions.

Fig. 7. July 2009 monthlymean bias of concentrations of daily max 8-h average O3 (upper) and 24-h average PM2.5 (lower) from simulations with offline (baseline) and online (Guenther scheme) biogenic volatile compound emissions, and modified boundary condition

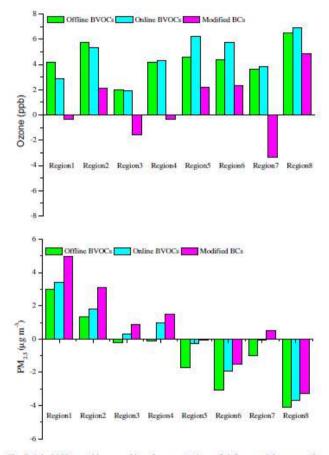


Fig. 7. July 2009 monthly-mean bias of concentrations of daily max 8-h average  $O_3$  (upper) and 24-h average PN<sub>2.5</sub> (lower) from simulations with offline (baseline) and online (Guenther scheme) biogenic volatile compound emissions, and modified boundary condition (labeled as offline BVOCs, online BVOCs, and modified BCs, respectively).

## Conclusion

- 1. Even though this system exists lots of uncertainties and inaccuracies, the RT-AQF model based on WRF/Chem-MADRID demonstrates a promising forecasting skill that is consistent with current RT-AQF models.
- 2. These bias correction approaches may be explored to further improve the model's forecasting skill.

# Thank you