Training Materials and Best Practices for Chemical Weather/Air Quality Forecasting (CW-AQF)

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Outline

- Importance and Types of Application of RT CW-AQF
- Introduction to the CW-AQF Training Book
- History and Current Status
- Performance Evaluation
 - Evaluation Matrices and Protocols
 - Current RT CW-AQF Models' Skills
- Methods for Improvement of RT-AQF
 - Scientific Advancements
 - Numerical and Computational Techniques
- Major Research Challenges
 - Model Development and Improvement
 - Inputs, Outputs, and Community Outreach

Sources: Zhang et al. (2012a, b) and Zhang and Baklanov, 2019

Real-Time Chemical Weather-Air Quality Forecasting (RT CW-AQF) Importance and Types of Applications

- Air pollution levels are not decreased anywhere in anytime
 - Urban pollution levels decrease, but regional pollution has increased
 - Little or no improvement in AQ in some underdeveloped countries
- Public awareness of AQ increases despite decreased air pollution
 - Especially for sensitive subpopulations: children, elderly, asthmatics
 - Public reporting of observed AQ levels (e.g., AIRNow, news media)
- Emission reduction programs triggered by high pollutant levels
 - Rely on short-term forecasts of O₃, CO, PM_{2.5}, and visibility
- Climate change mitigation and integration with AQ management
 - Rely on long-term forecasts of greenhouse gases and PM species
- Types of Applications of RT CW-AQF Products
 - Public health notification
 - Episodic control programs (e.g., Ozone Action Days)
 - Scheduling specialized air monitoring programs
 - Deployed during major sport events (e.g., the 2008 Olympic Games in Beijing and the 2010 Commonwealth games in Delhi) and political summits (e.g., the G-20 in Hangzhou)

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Motivations and Objectives

Background

- Increasing numbers of reported human mortality rates due to ambient and indoor air pollution and associated human exposure in many regions where air quality remains poor
- Increasing needs for CW-AQF with increasing number of forecasters worldwide, increasing involvements of National Meteorological and Hydrological Services (NMHSs) and other federal and state-level environmental protection agencies in CW-AQF and Multi-Hazard Early Warning Systems (MHEWS)
- Increasing complexity of the 3-D numerical models for CW-AQF with recent scientific advancements in numerical weather prediction (NWP) and CW-AQF
- Common mistakes leading to unsuccessful implementation and application

Overarching goals

- Provide best existing experience from NMHSs and academic community to build scientific capacity of researchers and operational meteorologists in developing countries through bridging sciences into operations
- Make sustained contributions towards the implementation of relevant policy and decision support aimed at improving quality of life through enhancing the science-policy interface

• Specific Objectives

- Help forecasters worldwide, especially those in developing countries on using 3-D CW-AQF models for best practices and operations
- Provide practical information about the best CW-AQF practices and standardized procedures for the successful deployment and application
- Prepare materials that could be adapted for training by NMHSs, WMO training centers, and other users from environmental authorities and academic institutions



Training Materials and Best Practices for Chemical Weather/Air Quality Forecasting (CW-AQF)

Final Version

Scientific Editors: Yang Zhang and Alexander Baklanov

May 4, 2019

History and Overview

- •Initiated in May 2017 with Alex Baklanov and Yinka Adebayo
- •Sponsored by the WMO's Education and Training Office and the GAW Program, with support from GURME
- •Developed an outline, Jun-Dec, 2017
- Developed preliminary draft, Jan-May 2018
- •Developed final draft, Jun-Sep, 2018
- •Submitted final draft, May 2019
- Published online in Sep 2019, will be updated as an effective, long-lasting educational and outreach tool
- •12 Chapters, 539 pages, 49 tables, 111 figures
- •51 authors from 15 countries
- •17 Global and 51 regional CW-AQF models
- •24 demonstration cases over Global (3), Europe (4), North America (3), Asia (5), South America (2), Oceania (3), and Africa (4)

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Characteristics of the Training Book

- Describes basic principles, effective methods, and best practices important in the deployment and application of a 3-D model for CW-AQF on different scales: from global to urban. It focuses only on 3-D CW-AQF model, and it is not intended to be all-inclusive
- Summarize the current status, the state-of-the science CW-AQF models and their application and evaluation, special considerations for urban applications and extreme events, as well as advanced techniques for improved CW-AQF and uncertainty quantifications; Provides demonstration cases for representative regions in six major continents
- Provides practical recommendations for developing countries and urbanized regions how better to build a CW-AQF system on national, regional or city level
- Complement existing guidelines/reviews developed by governments/communities (e.g., 2003 guidelines by US EPA/NOAA/NWS; Zhang et al., 2012a,b, Stajner et al., 2016; Ryan, 2016)

Outline of the CW-AQF Document

- Chapter 1. Introduction
- Chapter 2. History and Characteristics of CW-AQF
- Chapter 3. Fundamentals of CW-AQF
- Chapter 4. Model Deployment and Application
- Chapter 5. Special Considerations for Urban Applications
- Chapter 6. Special Considerations for Extreme Events
- Chapter 7. Model Input and Preparation
- Chapter 8. Model Output and Data Management
- Chapter 9. Model Evaluation
- Chapter 10. Bias Correction and Forecast Skill Improvement Methods
- Chapter 11. Uncertainty Quantification and Probabilistic Forecasting
- Chapter 12. Demonstration Cases for Real-Time CW-AQF
- Acknowledgements
- List of Tables
- List of Figures
- Nomenclature

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Milestones of RT CW-AQF (Zhang et al., 2012a)

Time	Milestone
1954	Heavy smog shut down schools and industry in LA in the US
1955	A three-stage smog alert system was established by LA County Air Pollution Control District (LACAPCD)
1960s	US provided the first forecasts of air stagnation or pollution potential
1966	The First International Clean Air Congress held in London with weather officials from 25 nations
1970	The US established national air pollution potential forecast program
1970s-1980s	Development and application of RT CW-AQF based on empirical approaches and statistical models
1990s	Application of 3-D AQMs for short-term forecasting of O ₃ in Germany, Japan, Australia, Canada, US, etc
1994-1995	The first application by U.K. to support the stratospheric field studies
1997	The U.S. EPA revised the AQI and established AIRNow; the first application by the Norway to support the tropospheric field studies
1999	MSC, Canada initiated an AQF program for eastern Canada;
	The US EPA developed Guideline for Developing an O ₃ forecasting
2000	WRF was developed to serve as the backbone of the US public NWP. A decision to develop WRF/Chem was made at an NCAR
	workshop
2001	MSC launched the national AQF; France reported first ensemble O ₃ AQF; the 1 st application of chemical data assimilation (CDA) for
	AQFs
2002	US congress mandated NOAA to develop nationwide RT-AQF for O ₃ ; US's first pilot AQF of O ₃ for the New England; WRF/Chem version 1 released
2003	US held 1st workshop and issued an MOA to develop national AQF
2004	NOAA's first pilot AQF of O ₃ and PM _{2.5} for the New England using 6 AQF models; the U.S. EPA/NOAA's NAQFC was deployed.
2007	CFD models coupled with 3-D AQF models over urban areas at 1-10 m in Spain
2005-2010	Ensemble forecast based on sole sequential aggregation (SA); the ensemble forecast of analyses (EFA) approach to combine SA and CDA
	in France; bias correction/data-fusion algorithm, data assimilation of satellite observations in ECMWF IFS-CTMs and GEOS-5 ESM
2010-present	Multi-model ensemble CW-AQF on global scale and regional scales (e.g., the CAMS (7 models) in Europe and the MarcoPolo – Panda (9
	models) in China, ICAP MME (7 global models)).

Major Differences between Air Quality Backcasting and Forecasting

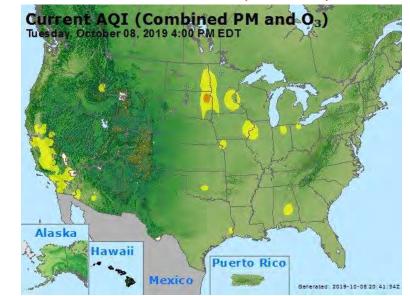
Attribute	Air Quality Backcasting	Air Quality Forecasting
Driving force	Regulatory guidance and compliance	Societal pressures to minimize the human, environmental and
		economic impacts
Input datasets	Best available historical dataset	Real-time or near-real time dataset
Format of input datasets	Pre-processed archived files	Automatic downloading and pre-processed RT or near RT dataset
Model mechanisms and treatments	Best available options	Simplified, optimized options to meet time requirements
Model option tuning and adjusting	Yes	No
Special techniques for accuracy and efficiency	None or rarely use	Bias correction, ensemble forecasting, data fusion
Typical application	Simulations of past high pollution events	Predictions of poor AQ days for public health notification and episodic control programs; planning air field studies
Products	Concentrations and deposition fluxes of chemical species	O ₃ , NO ₂ , PM _{2.5} , and PM ₁₀ , customized products, and post-calculated AQI and color codes
Time requirement for products	No time window requirements	Next-day's forecast must be available before 2 pm today
Evaluation of products	Temporal and spatial overlay; discrete statistical evaluation; uses the best available historic observational data	+ categorical evaluation; uses real-time or near real-time observational data
End users	Researchers, regulators, decision makers,	+ the public, the media, and the commercial sector
Goals and societal/economic benefits	Advancement in sciences, regulatory analyses and policy-making	Warnings for sensitive groups; actions to timely reduce exposure and emissions; cost-saving for large field campaigns
IT infrastructure	No special requirements	Web-based, interactive, and user-friendly interfaces

RT CW-AQF Current Status: Participants

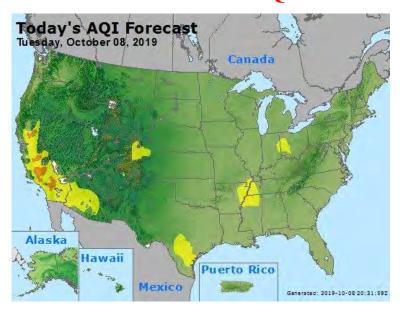
(http://www.airnow.gov)

- Current Status: O₃ and PM_{2.5} forecast with statistical models (most states in U.S. and some countries), or CTMs or both (increasing numbers of states)
- Participants in US: Daily forecast in > 400 cities by 146 state and local partners in 50 states and by 6 federal partners (USDA, NPS, NOAA-NWS, NOAA-ERSL, NASA, CDC)
- International Participants: > 37 countries
- Annual National Air Quality Conference sponsored by the U.S. EPA and its co-sponsor, the National Association of Clean Air Agencies (NACAA)

Current AQI (Airnow)



Forecasted AQI



Action Day

Good

Moderate

Unhealthy

USG – Unhealthy for Sensitive Groups

Air Quality Index (AQI) in the USA

(https://www.airnow.gov/aqi/aqi-basics)

Air Quality Index (AQI) Table

Air Quality Index Levels of Health Concern	Numerical Value	Meaning					
Good	0-50	Air quality is considered satisfactory, and air pollution poses little or no risk.					
Moderate	51-100	Air quality is acceptable; however, for some pollutants there may be a moderate health concern for a very small number of people who are unusually sensitive to air pollution.					
Unhealthy for Sensitive Groups	101-150	Members of sensitive groups may experience health effects. The general public is not likely to be affected.					
Unhealthy	151-200	Everyone may begin to experience health effects; members of sensitive groups may experience more serious health effects.					
Very Unhealthy	201-300	Health alert: everyone may experience more serious health effects.					
Hazardous	> 300	Health warnings of emergency conditions. The entire population is more likely to be affected.					

AQI Color Code Guide in the USA

(http://www.landofsky.org/cleanair/aqindex.htm)

Air Quality	Weather Conditions	Recommended Actions	Health Effects
Good AQI: 0-50 (Green)	 Cool summer temperatures Windy conditions Significant cloud cover Heavy or steady precipitation 	 Keep cars and boats tuned up Use environmentally safe paints and cleaning products Conserve electricity-set A/C to highest comfortable level 	No health effects are expected.
Moderate AQI: 51-100 (Yellow)	 Temperatures in the upper 70's to lower 80's Light to moderate winds Partly cloudy or mostly sunny skies Chance of rain or afternoon thunderstorms 	 Keep cars and boats tuned up Use environmentally safe paints and cleaning products Conserve electricity-set A/C to highest comfortable level 	 Unusually sensitive people should consider limiting prolonged outdoo exertion.
Unhealthy for Sensitive Groups AQI: 101-150 (Orange)	 Temperatures in the 80's and 90's Light winds Mostly sunny skies Slight chance of afternoon thunderstorms 	 Limit daytime driving Limit vehicle idling Refuel vehicles after dusk Don't "top off" your gas tank Avoid congested periods Use water-based paints Use transit or carpool Bike or walk for short trips Use newest or best maintained car Combine trips and share rides Postpone using gasoline mowers Barbeque without starter fluid 	 Active children and adults, and people with respiratory disease, such as asthma, should limit prolonged outdoor exertion.

AQI Color Code Guide in the USA

(http://www.landofsky.org/cleanair/aqindex.htm)

			•
Unhealthy AQI: 151-200 (Red)	 Hot, hazy, and humid Stagnant air Sunny skies Little chance of precipitation 	 Limit daytime driving Limit vehicle idling Refuel vehicles after dusk Don't "top off" gas tank Avoid congested periods Use water-based paints Use transit or carpool Bike or walk for short trips Use newest or best maintained car Combine trips and share rides Postpone using gasoline mowers Barbeque without starter fluid 	 Active children and adults, and people with respiratory disease such as asthma, should avoid prolonged outdoor exertion; everyone else, especially children, should limit prolonged outdoor exertion.
Very Unhealthy AQI: 201-300 (Purple)	 Hot and very hazy Extremely stagnant air Sunny skies No precipitation 	 Limit daytime driving Limit vehicle idling Refuel vehicles after dusk Don't "top off" gas tank Avoid congested periods Use water-based paints Use transit or carpool Bike or walk for short trips Use newest or best maintained car Combine trips and share rides Postpone using gasoline mowers Barbeque without starter fluid 	 Active children and adults, and people with respiratory disease such as asthma, should avoid all outdoor exertion; everyone else, especially children, should limit outdoor exertion.

AQI vs. Concentrations

(http://daq.state.nc.us/airaware/ozone/codecalc.shtml)

AQI Category		O ₃ (ppm) 8-hour Max	O ₃ (ppm) 1-hour Max	PM _{2.5} 24-hour Avg (μg m ⁻³)	PM ₁₀ 24-hour Avg (μg m ⁻³)
0-50 Good	Green	0.000-0.059	-	0.0-15.4	0-54
51-100 Moderate	Yellow	0.060-0.070	-	15.5-35.4	55-154
101-150 Unhealthy for sensitive groups	Orange	0.076-0.095	0.125-0.164	35.5-65.4	155-254
151-200 Unhealthy	Red	0.096-0.115	0.165-0.204	65.5-150.4	255-354
201-300 Very Unhealthy	Purple	0.116-0.374	0.205-0.404	150.5-250.4	355-424
>301 Hazardous	Maroon	-	> 0.404	> 250.4	> 424

AQI Equation:

$$AQI = \frac{I_{HI} - I_{LO}}{BP_{HI} - BP_{LO}} X (C_{03} - BP_{LO}) + I_{LO}$$

where:

AQI = **Air Quality Index**

 I_{LO} = Index value at the lower limit of the AQI category

 I_{HI} = Index value at the upper limit of the AQI category

 BP_{LO} = Break-point concentration at lower limit of AQI category

 BP_{HI} = Break-point concentration at upper limit of AQI category

 C_{03} = 8-hour ozone concentration

Yellow

$$I_{LO} = 51$$
 $I_{HI} = 100$
 $BP_{LO} = 0.060 \text{ ppb}$
 $BP_{HI} = 0.070 \text{ ppb}$

$$C_{O3} = 0.074 \text{ ppb}$$

 $\Rightarrow AQI = 119$

CW-AQF Numerical Model Systems and Applications in the U.S.

Model System	Met. Model	CTM	Forecasting Areas/Periods	AQF Products
NOAA/NWS NAQFC (Eta-CMAQ or WRF-CMAQ or FV3-CMAQ) modeling system	Eta or WRF (NMM) or FV3	Community Multiscale Air Quality (CMAQ) modeling system; SMOKE (off-line); in- line biogenics and mobile source emissions	E. U.S. (operational); CONUS (experimental); 12-km grid cells; 12 UTC – 48-hr run (next-day forecast)	O ₃ (operational); PM _{2.5} (developmental)
Baron Advanced Meteorological Systems (BAMS) MM5-MAQSIP/RT modeling system	NCAR/PS U MM5	Multiscale Air Quality Simulation Platform- Real Time (MAQSIP/RT); SMOKE (online)	CONUS – 45-km; Regional – 15-km; Metro-area – 5- km; 18 UTC – 120-hr run (next-day guidance)	O ₃ and PM _{2.5}
NOAA/ESRL WRF/Chem	WRF (ARW)	Online coupled WRF/Chem; offline static anthro. emissions and online biogenic emissions	CONUS – 40-km; E. U.S. – 27-km; 00 UTC – 36-hr run: (next-day forecast)	O ₃ and PM _{2.5}
NCSU WRF-Chem/MADRID	WRF (ARW)	Same as above except for WRF/Chem- MADRID	S.E. U.S. – 12-km; 00 UTC – 60-hr run: (next 2-day forecast)	O ₃ , PM _{2.5} , and PM ₁₀

CW-AQF Numerical Model Systems and Applications Beyond U.S.

Model System	Met. Model	CTMs	Forecasting Areas/Periods	AQF Products
Australian AQF system	LAPS	Australian CTM; with static emissions inventory	Sydney and Melbourne; Nested domains with 1-5 km grid cells	O ₃ , urban aerosol, wind-blown dust, wildfire impacts
Germany EURAD modeling system	Univ. of Cologne MM5	European RADM model; with static emissions inventory	European continent domain with nested 125/25 km grid cells; 5 km over parts of Germany	O ₃ , CO, PM ₁₀
French PREVAIR modeling system	Meteo France Ministry for Ecology MM5	CHIMERE or other models; with static emissions inventory	European continent with 0.5° grid cells; 0.1° over France	O ₃ , NO _x , PM _{2.5} , PM ₁₀
Canadian GEM- CHRONOS modeling system, now online- coupled GEM-MACH	Meteorological Service of Canada (MSC) Global Environ. Model (GEM) Weather Forecasting model	Canadian Hemispheric and Regional O ₃ and NO _x System (CHRONOS or MACH); SMOKE (off-line); in-line biogenics emissions	North American domain – 21-km; 00 UTC – 48-hr run: once per day forecast	O ₃ and PM _{2.5}

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AQF Products and Evaluations

CW-AQF Products

- O₃ (initial focus) and PM_{2.5} (recent expansion)
- CO, SO₂, NO, NO₂, VOCs, PM_{2.5} composition, PM₁₀, and AOD

CW-AQF Lead Time

- 1-4 days for RT CW-AQF
- 8-24 hrs for field study planning

CW-AQF Evaluation

- Most evaluations focus on O₃, fewer include its precursors
- Limited evaluation of PM_{2.5} AQF, fewer for coarse particles
- Most evaluations focus on summer and very few include winter or full year

Evaluation of AQF Model Skills

Discrete Evaluation

Mean bias (MB)

$$MB = \frac{1}{N} \sum_{1}^{N} (Model - Obs)$$

Mean normalized bias error (MNBE)

$$MNBE = \frac{1}{N} \sum_{1}^{N} \left(\frac{\text{(Model-Obs)}}{\text{Obs}} \right) \times 100\%$$

Mean fractionalized bias (MFB)

$$MFB = \frac{1}{N} \sum_{1}^{N} \left(\frac{\text{(Model-Obs)}}{\text{(Model+Obs/2)}} \right) \times 100\%$$

Mean absolute gross error (MAGE)

$$MAGE = \frac{1}{N} \sum_{1}^{N} |Model - Obs|$$

Mean normalized gross error (MNGE)

$$MNGE = \frac{1}{N} \sum_{1}^{N} \left(\frac{|Model-Obs|}{Obs} \right) \times 100\%$$

Normalized mean error (NME)

$$NME = \frac{\sum_{1}^{N} |Model - Obs|}{\sum_{1}^{N} Obs} \times 100\%$$

Normalized meanbias (NMB)

$$NMB = \frac{\sum_{1}^{N} (M \text{ odel-Obs})}{\sum_{1}^{N} (Obs)} \times 100\%$$

Root mean square error (RMSE)

$$RMSE = \sqrt{\frac{1}{N} \sum_{1}^{N} (Model - Obs)^2}$$

Unpaired peak accuracy (UPA)

$$\text{UPA} = \frac{\text{Model}_{\text{max}} - \text{Obs}_{\text{max}}}{\text{Obs}_{\text{max}}} \times 100\%$$

Evaluation of AQF Model Skills Categorical Evaluation

• Accuracy (A)

Percentage of forecasts that correctly predict an exceedance or a nonexceedance

- Critical Success Index (CSI)
 Indicate how well actual exceedances are predicted, accounting for both missed events and false alarms
- Probability Of Detection (POD)
 Percentage of actual exceedances that are forecasted, accounting for only missed events
- Bias (B)
 Judges if forecasts are underpredicted (< 1)
 or overpredicted (> 1)
- False Alarm Ratio (FAR)

 Measures the percentage of times an exceedance was forecasted when none occurred

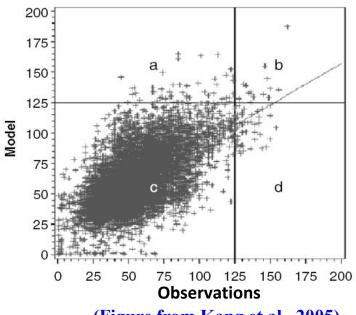
$$A = \left(\frac{b+c}{a+b+c+d}\right) \times 100\%$$

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

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

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

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



(Figure from Kang et al., 2005)

Evaluation of Max 8-hr O₃ Forecasting Skill

Table 10.1. Discrete and categorical evaluation of RT-AQF results for O₃ predictions (modified from Zhang et al., 2012).

Pollutants	Area	Period	MB	RMSE	NMB (%)	NME (%)	Threshold	A (%)	CSI (%)	POD (%)	В	FAR (%)	model
maximum 8-h	NE US	8/1-10,2001	1	70.3.7			85	80.0	34.0	49.0	1.1	13.0	MM5/MAQSIP RT
average O ₃	NE US.	8/5-29,2002	8.3	18.2	15.1	25.4	85	85.8	18.1	26.7	0.7	64.0	MAQSIP-RT
5.45. B. M.	NE US	8/5-29,2002	2.8	13.0	5.0	18.6	85	76.2	17.6	36.4	1.4	74.6	MM5/Chem
	NE US	6/1-9/30,2004	10.2	15.7	22.8	28.1	85	98.9	14.2	41.0	2.3	82.1	Eta/CMAQ
	EUS	7/1-8/15,2004	10.4	16.6	22.6	28.8	-	\exists	20			-	Eta/CMAQ
	NY	7/1-9/30,2004	6.5	12.8	-		-		8	-	-	-	Eta/CMAQ
	NY	7/1-9/30,2004	_	<u> </u>			65	84.0-95.2	31.4-53.2	46.5-84.8		32.9-55.2	Eta/CMAQ
	NE US	7/14-8/17,2004	10.0	14.0	-	-	-	\rightarrow	-	-	-		7-model ensemble b
	PN	8/1-9/30,2004	2.7	2	6	17	F-1		-		=	-	MM5/CMAQ
	EUS	8/12,2005		-	-		85	90.4	24.3	37.5	0.9	59.1	Eta/CMAQ
	CONUS	8/12,2005	\Rightarrow	A	-	\rightarrow	85	87.4	26.0	54.2	1.6	66.7	Eta/CMAQ
	EUS	6/1-9/30,2005 2006, 2007	7.9-10.9	14.5-16.3	16.5-22.4	24.1-27.1	4	ē.		8		8	WRF-NMM/CMAQ
	CONUS	6/1-8/31,2007	4.3	13.0	8.7	20.4	75	92.4	23.2	42.5	1.2	66.3	WRF-NMM/CMAQ
	CONUS	6/1-8/31,2007		_	-	0	85	96.9	15.4	32.2	1.4	77.3	WRF-NMM/CMAQ
	E. Texas	8/31-10/12,2006	6.0	13.1			75 85		18.0 6.0	32.0 10.0		59.0 70.0	7-model ensemble c
	SUS	5/1-9/30, 2009	3.5	13.6	8.3	25.0	65 75	91.5 97.2	9.2 3.9	28.4 25.5	2.4 5.8	88.0 95.6	WRF/Chem-MADRID
							85	99.0	0.9	15.6	17.0	99.1	
		5/1-9/30,2009-2011	-2.2 -6.1	10.5-13.9	4.5 –14.6	17.8-26.1	60	81.4-85.7	14-24.9	29.1-33.3	0.6-1.7	48.6-80.6	WRF/Chem-MADRID
		5/1-9/30,2012-2014	-0.8 -8.8	10.3-15.1	-2.0 -22.0	21.0-29.0	60	98.7-100	9.9-25.3	26.6-46.7	0.8-4.2	54.9-88.9	WRF/Chem-MADRID

Evaluation of Max 24-hr PM_{2.5} Forecasting Skill

Table 10.2. Discrete and categorical evaluation of RT-AQF results for PM_{2.5} predictions (modified from Zhang et al., 2012).

Pollutants	Area	Period	MB	RMSE	NMB (%)	NME (%)	Threshold	A (%)	CSI (%)	POD (%)	В	FAR (%)	model
24-h	NY	7/1-9/30,2004	5.4	13.2	-	-	-	_	_	\Rightarrow	-	-	Eta/CMAQ
average	NY	1/1-3/31,2005	6.2	14.5	=	-	0-	-	-	-	-	-	Eta/CMAQ
PM _{2.5}	NY	6/1-7/31,2005	4.4	13.6	-	-	-	=	8	8	-	-	Eta/CMAQ
	NY	7/1-9/30,2004		\rightarrow	-	\vdash	15.5	60.8-89.7	22.5-53.7	24.3-90.9		25.0-55.0	Eta/CMAQ
		1/1-3/31, 6/1- 7/31,2005			1	-	45.5	91.4-99.7	0-3,6	0-44.7	=	N/Aª, 96.2-100	Eta/CMAQ
	EUS	7/14-8/17, 2004		1.69									6-model ensemble a
	PN	8/1-11/30,2004	2.1-2.2	-	17-32	70-81	ė	-	-	-	-	-	MM5/CMAQ
	E US	7/14-8/18,2004	-3.2	8.8	-21.0	41.2	_	=	-	-	-	-	Eta/CMAQ
	eastern	8/31-10/12,2006	-1.3	5.5	0.00		31.5		0.0	0.0		100	7-model ensemble b
	Texas						16.5		8.0	14		80	
	NA	Summer 2008	-2.08	12.8									GEM-CHRONOS
	NA	Winter 2008	0.86	14.1									GEM-CHRONOS
	NA	Summer 2009	-0.70	12.9									GEM-CHRONOS
	NA	Summer 2008	0.69	13.5									GEM-MACH15
	NA	Winter 2008	-0.18	15.9									GEM-MACH15
	NA	Summer 2009	2.08	13.6	Poly.	1.40	Nain.		CRACK!	Section .		71.00	GEM-MACH15
	SUS	5/1-9/30,2009	-0.6	5.9	-5.6	37.0	15.5	78.0	20.6	29.1	0.7	58.8	WRF/Chem-MADRID
	202	No. of the State of China	Aller Trops	200	500	0.50 000	45.5	99.5	0.0	0.0	1.9	100.0	
		5/1-9/30,2009-2011		4.8 - 20.1	-10.1 - 34.3		15.0	70.7-76.2	22.3-27.9	31.5-36	0.6-0.7	44.6-56.7	WRF/Chem-MADRID
		5/1-9/30,2012-2014		3.8-10.8	2.0 - 53.0	33.0 - 74.0	15.0	77.5-83.2	10.3-21.3	15.3-40.1	0.6-1.3	68.3-75.9	WRF/Chem-MADRID
		winter,2009-2012	-2.9 - 3.1	4.9 - 9.3	-20.6 - 36.6		15.0	82.2-85.9	14.8-22.2	27.7-38.3	0.7-1.2	61.3-76.6	WRF/Chem-MADRID
		winter,2012-2015	0.1 - 5.2	4.9-10.5	4.9 - 68.4	37.3 - 89.0	15.0	83.5-85.3	14.7-17.1	25.5-31.8	1.0-1.2	72.1-74.1	WRF/Chem-MADRID

Outline

- Importance and Types of Application of RT CW-AQF
- Introduction to the CW-AQF Training Book
- History and Current Status
- Performance Evaluation
 - Evaluation Matrices and Protocols
 - Current RT CW-AQF Models' Skills
- Methods for Improvement of RT-AQF
 - Scientific Advancements
 - Numerical and Computational Techniques
- Major Research Challenges
 - Model Development and Improvement
 - Inputs, Outputs, and Community Outreach

Sources: Zhang et al. (2012a, b) and Zhang and Baklanov, 2019

Scientific Advancements to Improve RT-AQF

Improvement of Meteorological Forecasts

- Representations of episodes that typically have very weak dynamical forcing (PBL schemes under strongly stable conditions and for nocturnal mixing layers)
- Mesoscale circulations (e.g., land-sea breeze, topographic induced circulations, sea-breeze circulations, and their interactions with synoptic flows)
- Meteorological forecasts at 1-km or smaller (stable/stagnation conditions, turbulence and vertical mixing, deep convection, low-level jets, land-surface processes, and precipitation)

Improvement of Chemical Inputs

- Initial and boundary conditions (outputs from a global CTM, assumed climatological profiles, and adaptation of satellite and surface data for chemical profiles)
- Emissions (offline emissions; online emissions (e.g., mobile, biogenic, pollen, electric power generation, surface coating, wildfires, dust, sea-salt, and re-emissions))

Improvement of Physical, Dynamic, and Chemical Treatments

- Parameterizations of the urban environment (e.g., heterogeneity of building disposition, rough surface, anthropogenic heat fluxes the streets geometry)
- Gas-phase chemistry representations (e.g., SAPRC2011/2007, CB05-TU, CB6)
- Heterogeneous chemistry (e.g., HONO, reactions on sea-salt, photochemistry on soot)
- Aerosol dynamics and chemistry (e.g., new particle formation and subsequent growth processes, SOA formation, mixing states)

Numerical/Computational Techniques to Improve RT-AQF

- Improvement in Initial Conditions (ICONs)
- Simple approaches to improve model ICONs (e.g., the climatology of concentration profiles, satellite data with a broad spatial coverage)
- Advanced approches based on chemical data assimilation (e.g., 3DVAR, 4DVAR)
- Meteorological forecasts at 1-km or smaller (stable/stagnation conditions, turbulence, deep convection, low-level jets, land-surface processes, precipitation)
- Improvement of Emissions, Boundary Conditions, or Model Parameters
- Inverse modeling using data assimilation
- Multiscale data assimilation method
- Ensemble Forecasting
- Types (one model but with different inputs or multiple models)
- Methods (e.g., Monte Carlo simulations, multimodel ensembles, ensembles calibrated for uncertainty estimation, sequential aggregation, coupled sequential aggregation and classical data assimilation)
- Other Types of Techniques
- Simple bias correction methods
- Data fusion methods
- Combination of several bias-correction methods

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Sources: Zhang et al. (2012a, b) and Zhang and Baklanov, 2019

Major Challenges Model Development and Improvement

- Improve Accuracy of Meteorological Forecasting
- Improve Representations of Urbanization
- Improve Representations of Other Atmos. Processes
- Develop/improve online-coupled met. and chem. models
- Apply Techniques for Accuracy Improvements
- Develop various bias correction approaches
- Improve/expand various CDA techniques to reduce uncertainty in inputs
- Develop ensemble forecasting to reduce error and estimate uncertainties
- Apply Techniques for Comp. Efficiency Improvements
- Develop efficient parameterizations/representations
- Optimize model schemes/algorithms and data interpolation algorithms
- Ensure a high level of automation and parallelism
- Use refinement techniques such as the dynamic adaptive grids techniques

Major Challenges: Inputs, Outputs, and Community Outreach

Improve Accuracy of Model Inputs

- Develop better quantification of spatial/temporal emissions
- Develop/improve online modules for weather-dependent emissions
- Develop/improve methods for inversion modeling with data assimilation
- Adapt observations to specify initial and boundary chemical profiles
- Develop global-through-urban online-coupled models for ICs/BCs

Expand Model Outputs

- Include other pollutants (visibility/haze, air toxics, deposition)
- Extend the lead time to 3-7 days

Promote Community/Stateholder Outreach and Increase of Awareness

- Develop consistent forecast guidance documents
- Establish effective education and training programs
- Develop and strengthen community outreach and public awareness programs
- Support/coordinate centralized RT-AQF efforts region-, country-, and world-wide

References

- Zhang, Y., C. Seigneur, M. Bocquet, V. Mallet, and A. Baklanov, 2012, Real-Time Air Quality Forecasting, Part I: History, Techniques, and Current Status, *Atmospheric Environment*, 60, 632-655, doi:10.1016/j.atmosenv.2012.06.031.
- Zhang, Y., C. Seigneur, M. Bocquet, V. Mallet, and A. Baklanov, 2012, Real-Time Air Quality Forecasting, Part II: State of the Science, Current Research Needs, and Future Prospects, *Atmospheric Environment*, 60, 656-676, doi:10.1016/j.atmosenv.2012.02.041.
- Zhang, Y. and A. Baklanov, 2019, Best Practices and Training Materials for Chemical Weather/Air Quality Forecasting (CW-AQF), pp 560, The first edition is available on: https://elioscloud.wmo.int/share/s/WB9UoQ5kQK-dmgERjSAqIA.