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Investigating ground-level ozone pollution in semi-arid and arid regions of Arizona using WRF-Chem v4.4 modeling

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Table S1. Ozone design values for the Phoenix-Mesa metropolitan area for the last two decades. Note: there were two concurred exceptional events in the 2017 design value (20 June 2015 and 7 July 2017). Without that the 2017 design value is 75 ppb.

Design Value years	Design Value (ppm)	NAAQS Value (ppm)	NAAQS Year
2020-2022	0.081	0.070	2015
2019-2021	0.080	0.070	2015
2018-2020	0.079	0.070	2015
2017-2019	0.077	0.070	2015
2016-2018	0.077	0.070	2015
2015-2017	0.076	0.070	2015
2014-2016	0.077	0.075	2008
2013-2015	0.076	0.075	2008
2012-2014	0.078	0.075	2008
2011-2013	0.081	0.075	2008
2010-2012	0.081	0.075	2008
2009-2011	0.077	0.075	2008
2008-2010	0.077	0.080	1997
2007-2009	0.076	0.080	1997
2006-2008	0.081	0.080	1997
2005-2007	0.083	0.080	1997
2004-2006	0.083	0.080	1997
2003-2005	0.084	0.080	1997

Table S2. EPA AQS sites selected for WRF-Chem evaluations.

City	AQS Site Number	Site Name	Latitude	Longitude	Measurements
Phoenix	40130019	West Phoenix	33.48378	-112.14256	O_3, CO, NO_x
Phoenix	40139997	JLG Supersite	33.503833	-112.095767	O_3, CO, NO_x
Phoenix	40133002	Central Phoenix	33.45797	-112.04659	O_3, CO, NO_x
Phoenix	40134003	South Phoenix	33.40314	-112.07526	O_3, CO
Phoenix	40133003	South Scottsdale	33.47968	-111.91721	O_3, CO, NO_2
Phoenix	40134005	Tempe	33.41123	-111.93471	O_3, CO
Phoenix	40131003	Mesa	33.41018	-111.86536	O_3, CO
Phoenix	40137022	Lehi (Fire Station)	33.474609	-111.805769	O_3
Phoenix	40137024	Salt River High School	33.508125	-111.83852	O_3
Phoenix	40137020	Senior Center	33.488131	-111.855443	O_3
Tucson	40191028	Children's Park	32.29515	-110.9823	O_3, CO, NO_2
Tucson	40191011	22nd and Craycroft	32.204411	-110.878067	O_3, CO, NO_2
Tucson	40191032	Rose Elementary	32.172995	-110.980134	O_3

Tucson	40190021	Saguaro National Park East	32.174538	-110.737116	O_3
Tucson	40191021	Cherry and Glenn	34.403052	-119.457914	CO
Tucson	40191034	Coachline	32.38082	-111.12716	O_3
Tucson	40191018	Tangerine	32.42526	-111.064	O_3
Yuma	40278011	Yuma Supersite	32.690278	-114.61444	O_3
Yuma	800268012	San Luis Rio Colorado Well	32.466389	-114.768611	O_3

Table S3. Evaluation of MDA8 O_3 over Phoenix, Tucson, and Yuma for individual years for WRF-Chem simulations. The datasets for evaluation include AQS observations, CMAQ reanalysis (2017-2018), and ADEQ forecasts (2019-2021).

	Phoenix					Tucson					Yuma				
Year	2017	2018	2019	2020	2021	2017	2018	2019	2020	2021	2017	2018	2019	2020	2021
AQS	67.9	66.6	64.1	62.0	67.8	60.1	54.9	54.8	54.6	57.2	54.3	53.8	56.1	48.2	52.1
WRF Chem	66.8	62.6	58.9	59.2	62.6	60.2	55.3	52.8	54.3	56.8	60.5	61.8	58.5	57.8	57.7
CMAQ /ADEQ	58.4	57.5	67.7	65.1	68.5	53.7	51.1	55.6	55.6	57.1	64.1	64.7	53.8	50.8	50.4
R (W)	0.81	0.69	0.61	0.56	0.62	0.79	0.70	0.68	0.68	0.26	0.85	0.50	0.72	0.40	0.83
R (C/A)	0.87	0.66	0.44	0.66	0.19	0.71	0.78	0.55	0.77	0.22	0.44	0.30	0.82	0.31	0.71
MB (W)	-1.09	-3.94	-5.21	-2.76	-5.16	0.14	0.37	-1.98	-0.35	-0.40	6.16	7.95	2.32	9.62	5.62
MB (C/A)	-9.5	-9.1	3.1	1.2	0.0	-6.4	-3.8	0.7	-1.1	-0.5	9.8	10.9	-2.7	2.8	0.6
ME (W)	6.3	6.6	7.0	6.6	8.1	4.7	4.7	4.3	4.8	7.0	9.1	11.8	5.5	10.1	6.8
ME (C/A)	9.9	10.1	5.1	4.2	9.9	7.4	5.1	3.9	4.0	6.0	13.8	14.2	4.1	6.8	6.8
RMSE (W)	7.6	8.5	8.3	8.3	10.4	5.7	5.9	4.9	6.2	9.0	11.9	15.5	6.6	13.2	9.5
RMSE (C/A)	11.1	12.7	7.4	5.4	12.6	8.8	6.6	4.9	4.9	6.9	16.6	17.5	5.5	8.0	8.3
NMB (W, 100%)	-1.6	-5.9	-8.1	-4.5	-7.6	0.2	0.7	-3.6	-0.6	-0.7	11.3	14.8	4.1	20.0	10.8
NMB (C/A, 100%)	-14.0	-13.6	4.8	1.9	-0.1	-10.7	-6.9	1.3	-2.0	-0.8	18.0	20.2	-4.9	5.8	1.1
NME (W, 100%)	9.2	10.0	10.8	10.7	12.0	7.8	8.6	7.8	8.7	12.3	16.8	22.0	9.8	21.0	13.0
NME (C/A, 100%)	14.6	15.2	8.0	6.7	14.6	12.3	9.3	7.2	7.3	10.6	25.3	26.3	7.3	14.2	13.0
MNB (W, 100%)	-2.0	-6.0	-7.7	-4.3	-7.0	0.3	1.0	-3.2	0.2	0.0	11.6	18.5	5.0	21.3	12.3
MNB (C/A, 100%)	-14.5	-13.9	5.9	2.1	1.8	-10.5	-7.1	2.1	-1.5	0.1	25.8	25.9	-4.4	7.8	4.1
MNE (W, 100%)	9.4	10.0	11.0	10.6	11.4	7.8	8.7	8.0	8.7	12.5	16.9	24.6	10.1	22.1	14.2
MNE (C/A, 100%)	14.9	15.3	8.9	6.6	13.7	12.2	9.4	7.6	6.9	10.7	31.0	30.5	7.0	14.9	14.1
FB (W, 100%)	-2.7	-6.9	-8.6	-5.3	-8.0	-0.2	0.4	-3.6	-0.4	-1.3	9.5	14.2	4.3	17.9	10.5
FB (C/A, 100%)	-16.1	-16.1	5.0	1.8	0.4	-11.7	-7.9	1.6	-1.8	-0.7	19.3	19.7	-4.8	6.4	2.6
FE (W, 100%)	9.6	10.7	11.7	11.3	12.2	7.7	8.8	8.1	8.7	12.7	15.3	21.0	9.7	18.8	12.4
FE (C/A, 100%)	16.5	17.5	8.1	6.4	13.9	13.2	10.2	7.3	7.0	10.7	24.9	24.6	7.3	14.1	13.4

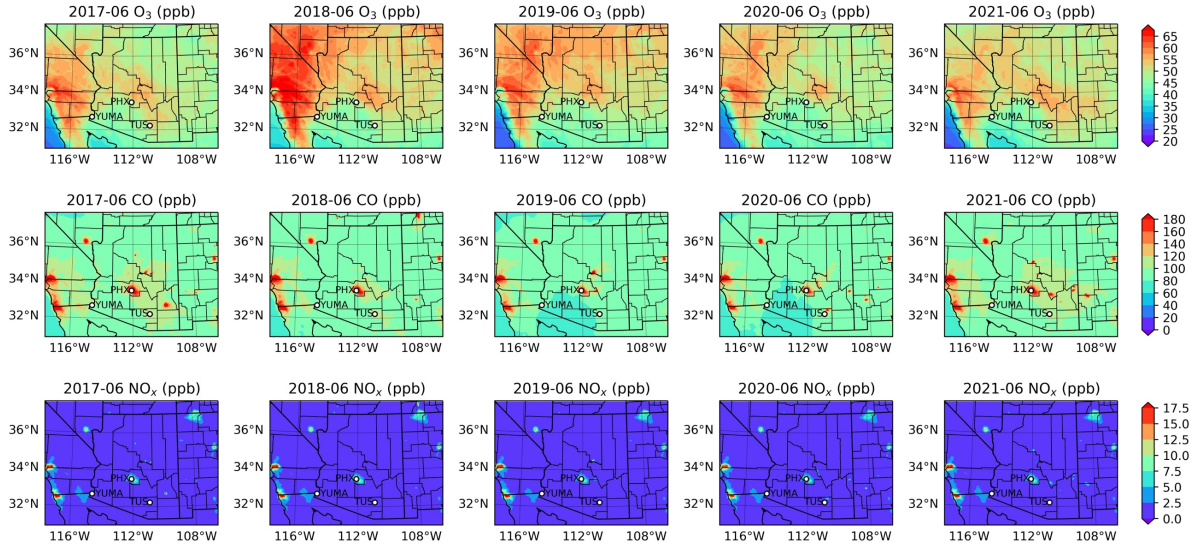

Figure S1. June monthly mean O_3, CO, and NO_x from WRF-Chem simulations for 2017 to 2021.

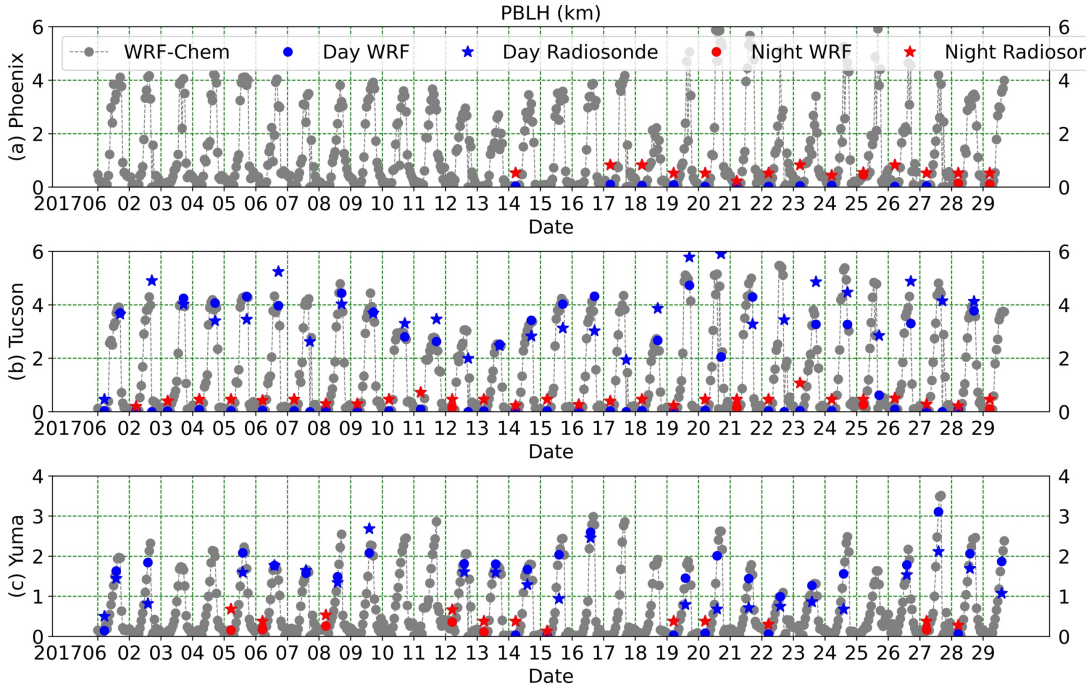

Figure S2. Radiosonde observed and WRF-Chem simulated PBLH in June

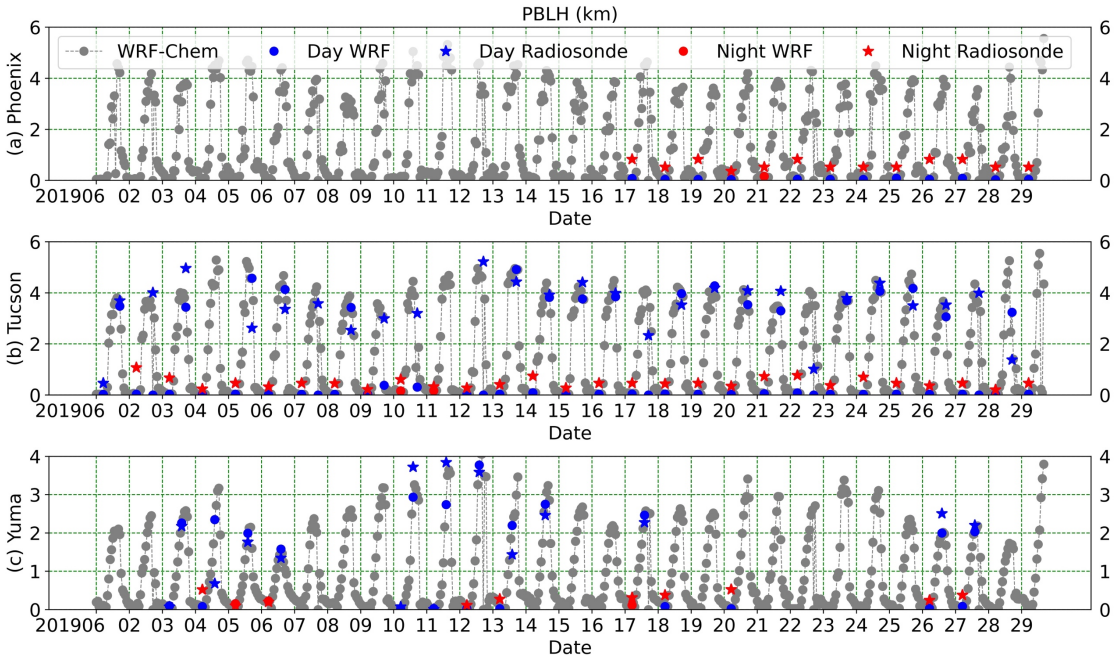

Figure S3. Radiosonde observed and WRF-Chem simulated PBLH in June 2019.

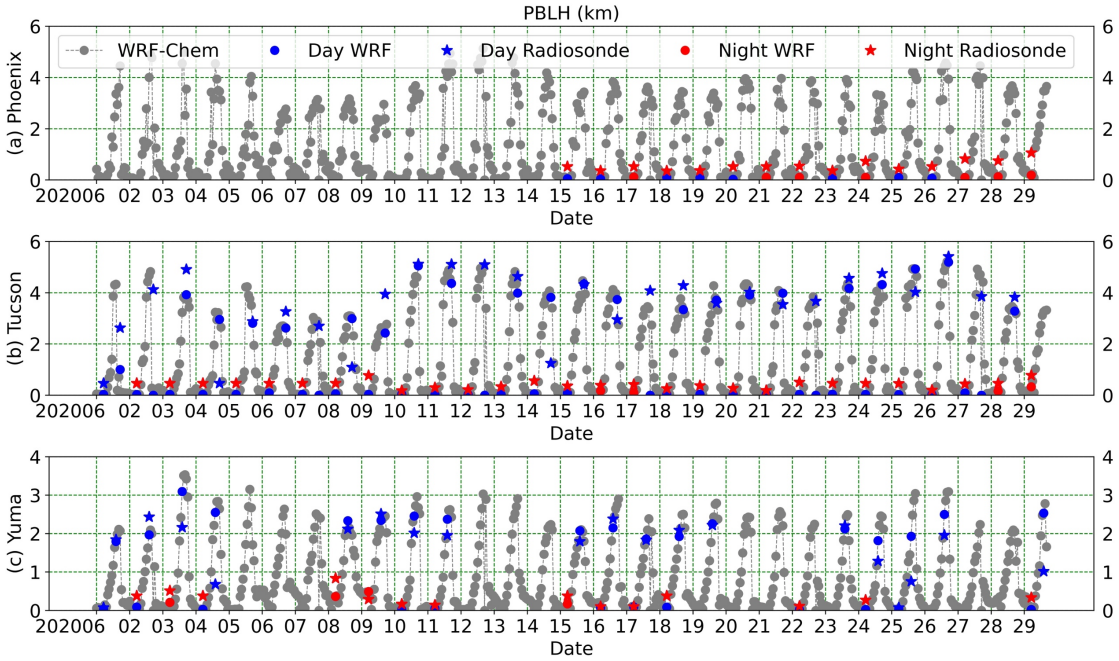

Figure S4. Radiosonde observed and WRF-Chem simulated PBLH in June 2020.

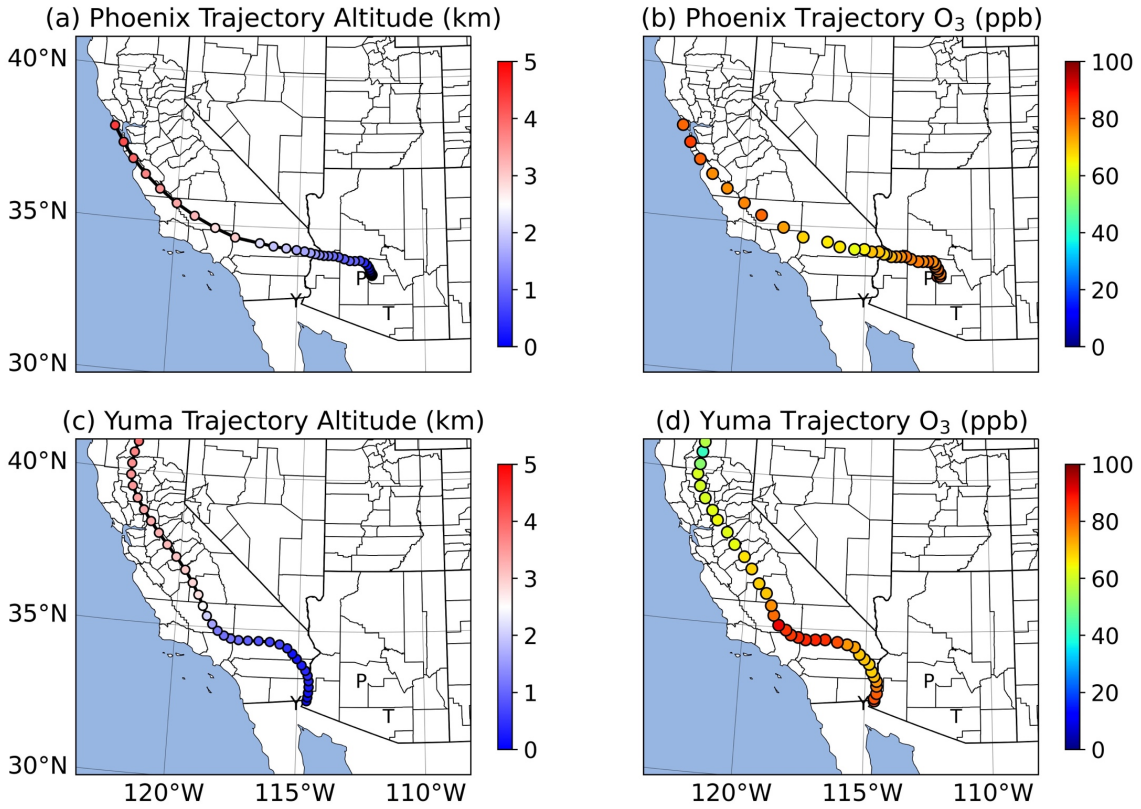

Figure S5. 48-hour HYSPLIT back trajectories for the observed O_3 exceedance event on 13 June 2017 in both (a) Phoenix and (c) Yuma, and the corresponding O_3 concentrations along the trajectories.