PHOTOCHEMICAL MODELING OF AN INDUSTRIAL CITY IN QATAR

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INTRODUCTION

The Ras Laffan Industrial City (RLIC) is located 80 km north of Doha and forms the heart of Qatar's natural gas industry **(Figure 1)**. Covering 106 km^2, RLIC is home to major companies such as RasGas and Qatargas and is assigned to host additional companies in the future. In recent years, monitoring has indicated that ozone concentrations in communities downwind of RLIC are exceeding standards set by the State of Qatar. Therefore, as a permit condition for expansion at RLIC, Qatar's Supreme Council for the Environment and Natural Reserves (SCENR) required that a photochemical grid modeling analysis be performed to assess RLIC's contributions to ozone concentrations in the region.

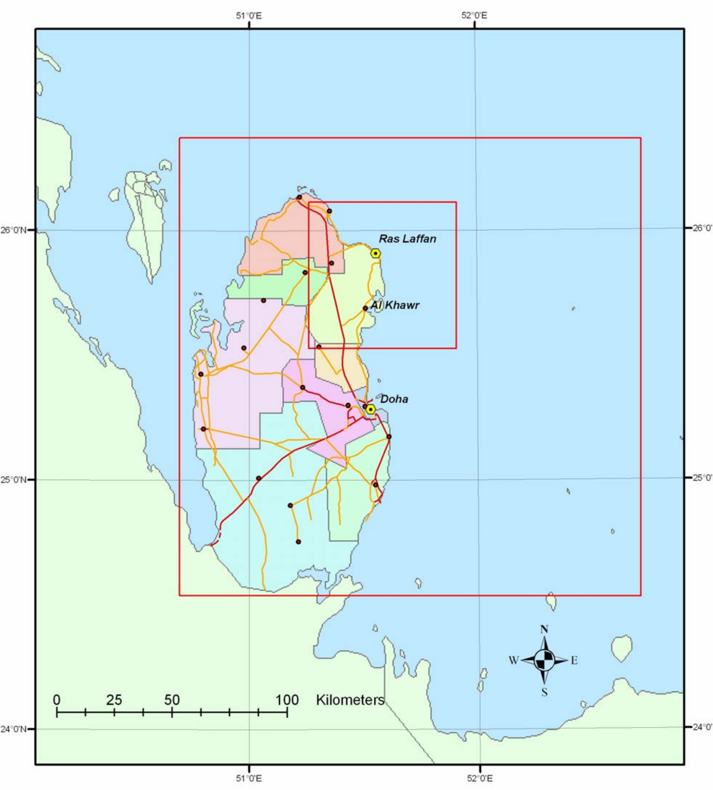

Figure 1. Map of Qatar.

METHODOLOGY

Two periods were selected for analysis. The first period selected was August 23-30, 2004, which included two days on which peak observed 1-hr ozone concentrations approached the state standard of 120 ppb at Ras Laffan City site (RLAC) — 113 ppb on August 26 and 119 ppb on August 29. The second period was November 25-28, 2004 with a peak 1-hr ozone concentration at the Al Khawr site (ALKH) of 108 ppb on November 27.

Air quality data from two sites in the Ras Laffan region, RLAC and ALKH, were available for the August 23-30, 2004, period. The RLAC site is located in the southeastern portion of the RLIC. The ALKH site is located on the north side of the city of Al Khor at the edge of a housing community. The data were initially provided from these sites for August and September 2004. However, data from the first week of August were suspect.

The ALSH site is located in the park at Al Shamal. Data became available for this site in the last week of November 2004 and was available for the second period investigated. These data along with available meteorological data were analyzed to gain a better understanding of high ozone days in the Ras Laffan area.

Meteorological modeling was performed with the Pennsylvania State University/National Center for Atmospheric Research Mesoscale Model, Version 5 (MM5) with the three domains shown in **Figure 2**. The outer domain consisted of 93 x 63 36-km cells. The intermediate domain consisted of 79 x 79 12-km cells. The inner domain consisted of 73 x 79 4-km cells. Each domain had 34 vertical levels extending from the surface to approximately 14 km.

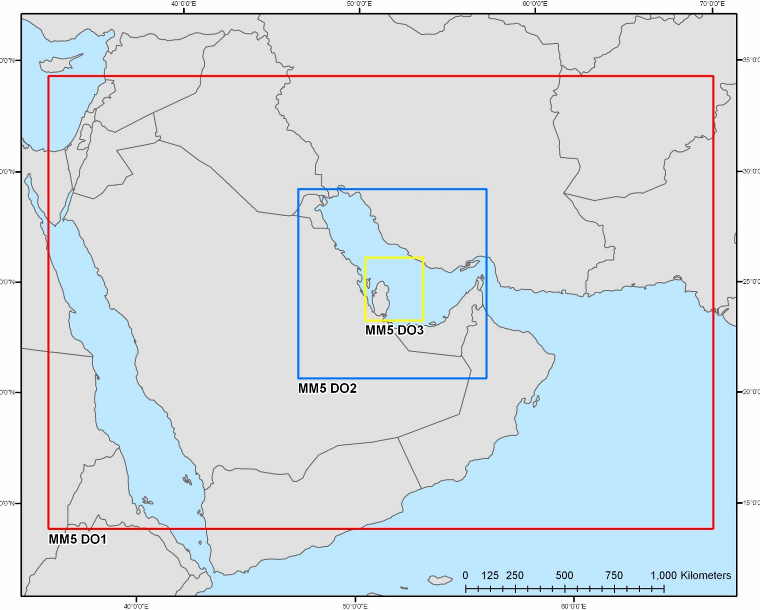

Figure 2. Meteorological modeling grids for the Ras Laffan modeling study.

Stationary source emissions data were obtained from the inventory developed by URS Corporation. URS provided an emission inventory spreadsheet designed to calculate atmospheric emissions from stationary sources in the region surrounding RLIC and Al Khawr. The spreadsheet was populated with existing information about stationary sources and allowed users to enter new sources, modify existing sources, and generate graphical and tabulated emissions summaries from a selection of sources, facilities, and regions. The inventory included current and planned emissions sources.

URS also prepared a mobile source emission inventory for RLIC. The mobile source inventory was intended to estimate emissions from mobile sources in the Ras Laffan air shed. The air shed generally covers the area between Al Khor and RLIC. The majority of the mobile sources identified in this study were believed to be associated with operations inside RLIC. However, other sources were included if their activity data could be characterized and estimated.

Photochemical modeling was performed with the Comprehensive Air Quality Model with Extensions (CAMx) . The photochemical domain covered the entire State of Qatar as shown in Figure 1 and was defined to cover an area of 248 km x 264 km with 49,104 4-km cells. The domain included a large portion of the Arabian Gulf and was made as large as possible without extending into other countries. The domain was defined in Lambert Conformal coordinates to ensure compatibility with the MM5 meteorological model. The CAMx domain had 12 vertical layers

RESULTS

A scatterplot of oxides of nitrogen (NO_x) concentrations by wind direction at the ALSH monitor for the second model-ing period was prepared and four clusters of NO_x concentrations were seen. The lowest NO_x concentrations are as-sociated with winds from the northwest (315 degrees). Three other clusters show higher NO_x concentrations: when the winds were from (1) the west-northwest (285 degrees), (2) the southwest (210 degrees), and (3) the southeast (140 degrees). These clusters are annotated on **Figure 3** When vectors are drawn to ALSH from these directions, as shown in **Figure 4**, the relationships between known source regions and NO_x concentrations measured at ALSH become apparent: cluster 1 is associated with sources in Bahrain (and possibly sources in Saudi Arabia), cluster 2 is associated with sources in the industrial city of Dukhan, and cluster 3 is associated with sources in the RLIC.

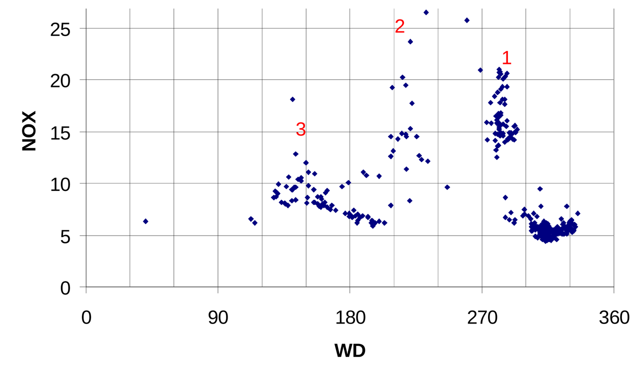

Figure 3. Scatterplot of NO_x concentrations (ppb) at the ALSH monitor by wind direction (WD).

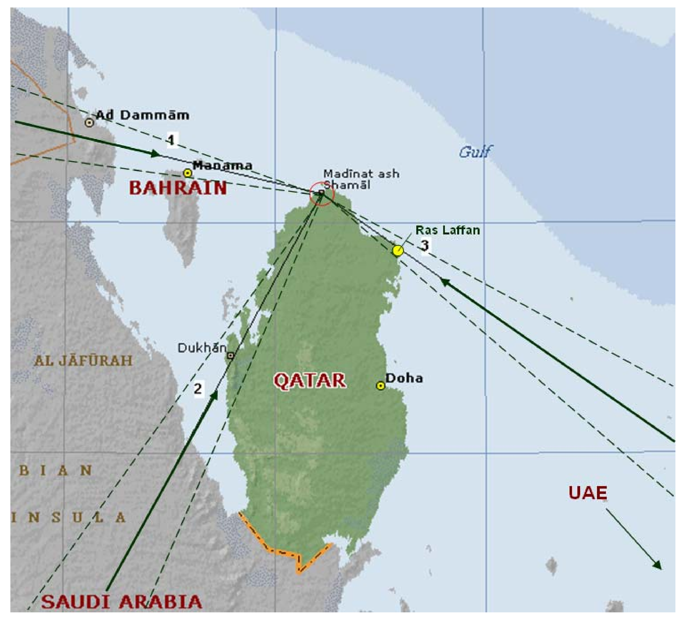

Figure 4. Source-receptor relationships in northern Qatar.

Peak 1-hr ozone concentrations predicted by CAMx are compared to observed concentrations in **Table 1**. It is clear from these comparisons that peak 1-hr ozone concentrations are significantly underpredicted on the days with the highest observed concentrations.

For the three highest ozone concentration days modeled, contour plots of peak predicted ozone concentrations were prepared. **Figure 5** shows the spatial distribution of ozone at 1400 LST on August 26. The peak predicted ozone was 64.2 ppb in the northeast corner of the modeling domain. **Figure 6** shows the predicted pattern of ozone at 1400 LST on August 29. The peak predicted ozone was 66.8 ppb just northeast of RLIC. **Figure 7** shows the spatial distribution of ozone at 1500 LST on November 27, when the predicted peak ozone was 48.1 ppb approximately 135 km east of RLIC.

Table 1. Comparison of observed and predicted peak 1-hr ozone concentrations for the days modeled.

Date	Peak 1-hr Ozone Concentrations (ppb)				
	Observed	Hour	Site	Predicted	
				At Site	Hour
8/23/2004	43.6	10	RLIC	33.6	9
8/24/2004	66.9	21	RLIC	44.4	10
8/25/2004	58.2	9	RLIC	45.5	9
8/26/2004	112.5	14	RLIC	47.3	11
8/27/2004	45.2	12	RLIC	48.5	9
8/28/2004	22.3	9	RLIC	47.1	9
8/29/2004	119.1	17	RLIC	50.7	9
8/30/2004	83.2	10	RLIC	44.5	11
11/25/2004	50.6	16	ALKH	36.7	13
11/26/2004	61.6	14	ALKH	43	15
11/27/2004	108.8	14	ALKH	38.7	14
11/28/2004	47.9	12	ALKH	36.8	13

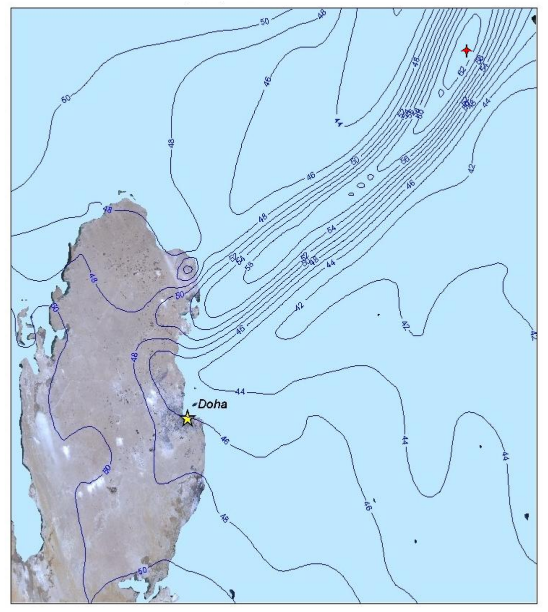

Figure 5. August 26, 2004, at 1400 LST.

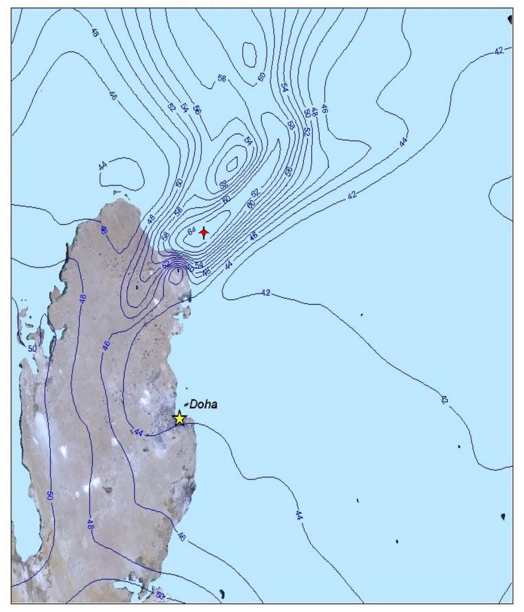

Figure 6. August 29, 2004, at 1400 LST.

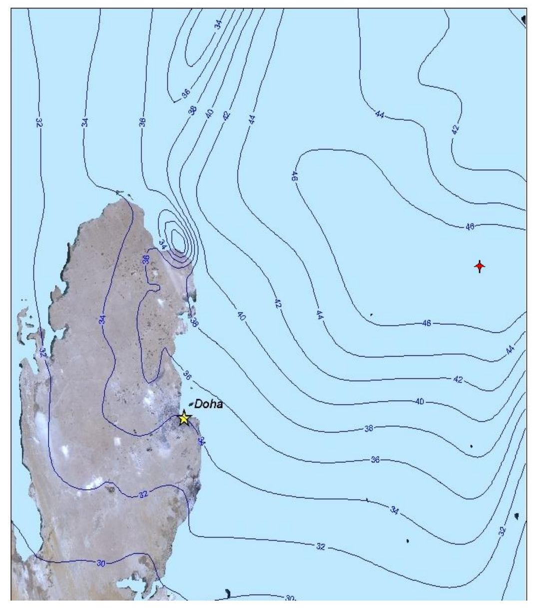

Figure 7. November 27, 2004, at 1500 LST.

FINDINGS

Data Analysis Findings

- Both the 1-hr and 8-hr ozone standards are exceeded in the Ras Laffan area. The 8-hr standard appears to be exceeded more often than the 1-hr standard. During the periods reviewed (which unfortunately did not include July 2004), one 1-hr and eight 8-hr ozone standard exceedances occurred.
- Background ozone concentrations (when winds are persistently from the north) measured at the ALSH monitoring site can exceed the 8-hr standard, which implies that there may be significant regional contributions to observed ozone concentrations. During February 2005, a 1-hr ozone concentration of 103 ppb and an 8-hr concentration of 99 ppb were observed at ALSH.
- NO_x concentrations at ALSH were often above 5 ppb under northerly winds, which indicated that air upwind of Qatar is not clean.
- NO_x concentrations at ALSH show a correlation with wind direction. The highest concentrations were observed when the winds were from the direction of Dukan but, on average, the concentrations were higher when the winds were from northern Bahrain and Ad Dammam. The third highest concentrations were observed when the winds were from the direction of Ras Laffan. The correlation between NO_x concentrations in northern Qatar and transport from known emission source areas highlights the importance of expanding the emission inventory for photochemical modeling.
- Transport distances of 100 to 200 km per day were observed during ozone episodes; thus, the potential for regional contributions to ozone is significant. Based on analysis of observed winds, transport distances of 100 km or more per day were likely during the August episodes and more than 200 km per day were likely during the November episode.

Photochemical Modeling Findings

- Ras Laffan area emissions alone contribute only a small portion of total observed ozone. Photochemical modeling of the RLIC emissions only produced peak concentrations that were 12 to 15 ppb above background (boundary) concentrations.
- Modeling to date does not account for the total observed ozone. The modeling system was only able to predict concentrations that were about 56% of those observed.
- Ozone is underpredicted by the modeling system, in part, because of the domain size. On several of the days modeled, it was evident that emissions reached the modeling domain boundary before winds reversed and brought emissions and ozone back to the RLIC area.
- Ozone is underpredicted by the modeling system, in part, because not all emissions sources in the domain are included in the model. It is evident from the modeled transport that emissions from areas outside RLIC may contribute to the formation of ozone that eventually affects the RLIC area.
- Ozone is underpredicted by the modeling system, in part, because transport of ozone and ozone precursors were not modeled completely and could not be addressed through boundary conditions alone. Without specific measurements at many locations along the modeling domain boundary, adjusting boundary conditions to represent sources outside the domains tends to result in under- or overpredictions.
- Emission sensitivity simulations with the photochemical model indicate that doubling NO_x emissions will usually decrease peak ozone concentrations and doubling volatile organic com-pound (VOC) emissions will increase peak ozone concentrations.
- Based on the RLIC emission inventory, the Ras Laffan area would appear to be VOC-limited, and VOC reductions will likely be most effective in reducing ozone concentrations. The response of the modeling system to VOC and NO_x reductions indicates that the modeled atmosphere is VOC-limited, which is consistent with the large NO_x emissions in the RLIC inventory.
- NOx reductions will likely increase ozone unless very high levels of NO_x reduction are obtained. However, smaller NO_x reductions may be effective at reducing regional ozone concentrations downwind of RLIC. In VOC-limited atmospheres, NO_x reductions tend to increase ozone near the source area due to reduced ozone titration. However, NO_x provides the "building blocks" for ozone, and NO_x reductions, even under VOC-limited conditions, will reduce ozone concentrations at some distance downwind of the source.
- Inclusion of other regional sources may significantly change the conclusions of this study. It is apparent that significant amounts of NO_x are being transported into northern Qatar. If NO_x is the only ozone precursor being transported into the region, we expect that the conclusions about emission controls will prevail. However, if significant amounts of VOCs are being transported into the region, the conclusions may differ.