# Dispersion modeling of particulate matter containing hexavalent chromium during high winds in southern Iraq

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TECHNICAL PAPER

# Dispersion modeling of particulate matter containing hexavalent chromium during high winds in southern Iraq

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*The aim of this paper is to describe a scientific methodology (i.e., the combination of different well-established modeling techniques) and its application to a real case scenario of contaminated dust emissions in high winds. This scenario addresses potential air pollution problems at the water treatment plant (WTP) at Qarmat-Ali, Basra, Iraq, during 2003. Workplace practices at the WTP before 2003 resulted in sodium dichromate contamination in the area. Looting at the site in early 2003 also contributed to this contamination. Individuals who were assigned to provide security at the site in 2003 have claimed adverse health effects caused by exposure to dust containing hexavalent chromium [Cr(VI)]. This report presents our modeling study with respect to these claims in relation to (1) amount of Cr(VI) present in the soil, (2) wind erosion episodes, and (3) possible long-term (e.g., annual average) Cr(VI) concentrations inhaled by different people while at the site. Our modeling approach included (1) the analysis of Cr(VI) soil measurements to assess the degree of contamination in different areas of the plant at different times; (2) the use of DUSTRAN model equations to calculate the emission rate of particulate matter (PM) less than 10 μm in diameter ($PM_{10}$) during high-wind episodes; (3) the use of the U.S. Environmental Protection Agency (EPA) AERMOD modeling system to estimate Cr(VI) concentrations at the site; and (4) the calculation of modeling results in the form of both contour lines of average Cr(VI) concentrations at the site, and specific concentration values for selected individuals, based upon their recollection of their visits to the site.*

*Implications:* The assessment of individual exposure to contaminated dust during high-wind episodes requires a combination of modeling tools and the calculation of concentration impacts at precise locations and times. We have combined several state-of-the art simulation algorithms to provide a credible methodology for assessing individual exposure. The methodology has been applied to an actual case where exposure was claimed by individuals.

## Introduction and Background

This study addresses potential air pollution problems at the water treatment plant at Qarmat-Ali, Basra, Iraq, during 2003. The aim of the study is to describe a scientific methodology for determining breathing-zone outdoor ambient air concentrations, focusing on the combination of different well-established modeling techniques and its application to a real case scenario of contaminated dust emissions in high winds. It is not to assess possible health impacts resulting from these concentrations.

The region is depicted in Figure 1. In 2003, the facility was not operating due to the severe looting and damage that occurred during the Second Gulf War that began March 20, 2003.

In 2003, U.S. Army personnel were assigned to provide security for people working at the industrial-grade water treatment plant at Qarmat-Ali, Basra, Iraq. In mid-2003, contract work crews and safety personnel identified sodium dichromate as a potential occupational hazard in the work environment. Several U.S. Army soldiers reported to the supporting military medical facility and inquired about the potential health risks. Concurrently, containment

of the contaminated site was initiated and environmental sampling was conducted. In-theater military occupational and environmental health specialists addressed the health concerns of the military units at a local "town hall" meeting. Additionally, medical evaluations were conducted for all personnel present at that time (Defense Health Board [DHB], 2008).

Several U.S. Army soldiers alleged adverse health effects that they claim were caused by exposure to dust containing hexavalent chromium, Cr(VI), while on service at the Qarmat-Ali water treatment plant (WTP). This report presents our study with respect to these claims in relation to the physical aspects of the case, such as (1) amount of Cr(VI) present in the soil, (2) wind erosion episodes, and (3) possible long-term (e.g., annual average) Cr(VI) concentrations inhaled by soldiers while at the site.

## The Qarmat-Ali Water Treatment Plant

The Qarmat-Ali Water Treatment Plant, facility code "QARM," is located near Basra, Iraq (latitude 30.583° N and
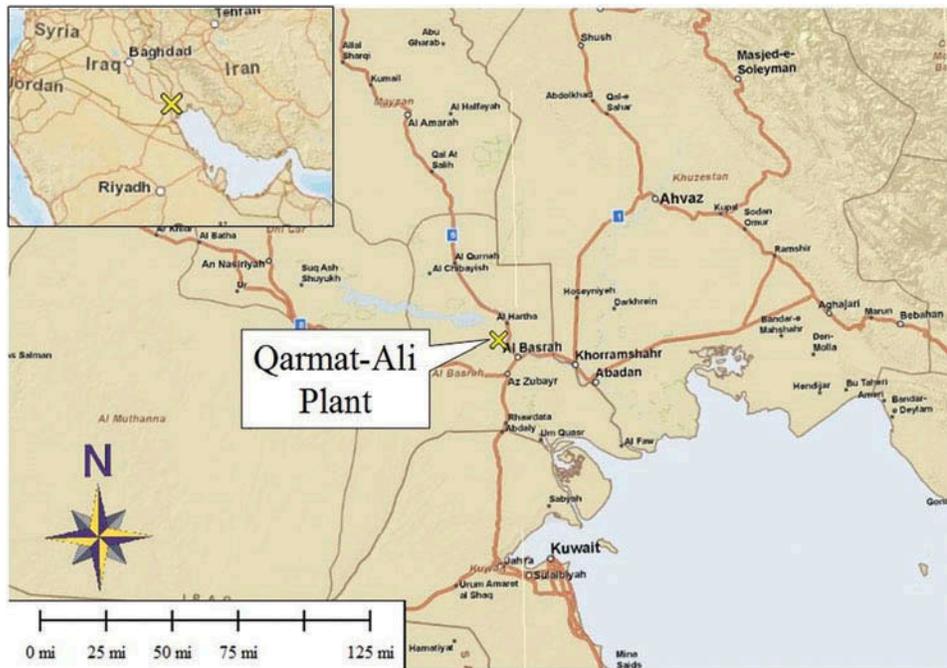
**Figure 1.** Region of interest.

longitude 47.69º E), and was designed to process raw river water from a tributary of the Tigris River for injection into the production wells in the North and South Rumalia and Al Zubair oil fields. When the plant was functioning before the 2003 war, water drawn from the Tigris River was treated at the facility and injected under pressure into the ground to drive oil to the surface and help prevent ground subsidence (Special Plans and Operations [SPO], 2010).

A detailed map of the facility is shown in Figure 2. As seen, the sodium dichromate soil contamination was predominantly
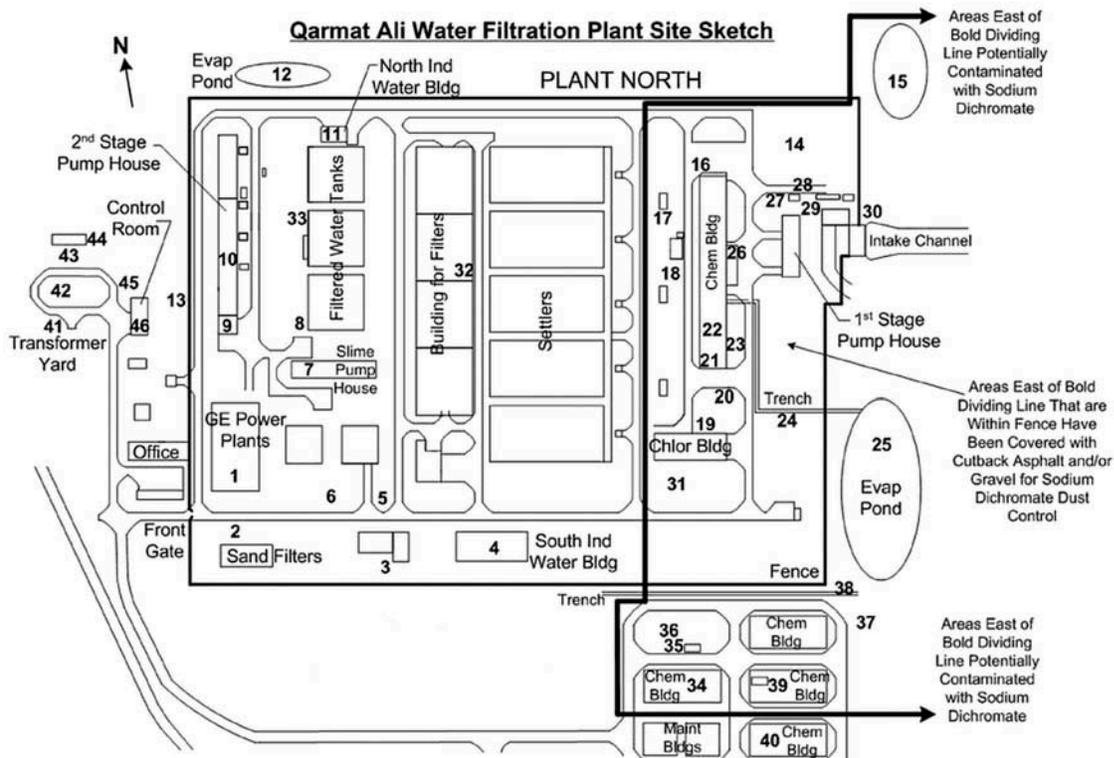


**Figure 2.** Map of Qarmat-Ali Water Treatment Plant.

restricted to the eastern part of the facility, around the areas of the chemical injection building ("Chem Bldg" on northeast of facility), first-stage pump house (northeast of facility), chlorination building ("Chlor Bldg," central east side of facility, just south of chemical injection building), and chemical warehouses (multiple "Chem Bldg" on far southeast of facility beyond fenceline). The contamination extended to areas east of the northeast fence line (around Location 15 on the map) and within the evaporation pond east of the southeast fence line (Location 25 on the map). Also noted on the map are areas within the eastern part of the facility that were treated with surface remediation material (liquid asphalt and gravel). This initial remediation was completed around August 22, 2003.

Prior to the 2003 war, the facility was capable of operating at between 60 to 75% of its 70,000 U.S. gallons per minute (GPM) (140 million m$^3$/year) designed upstream capacity. Capacity was limited by normal backwash, losses to poor valve seating, maintenance, and unrecovered backwash water. At 70% capacity, or 49,000 GPM (98 million m$^3$/year), the facility was capable of displacing 1.2 million barrels of oil per day at a 0.7:1 oil/water ratio. The controls were out of date even by 1979 standards, with the use of large electromechanical relays, switches, and mechanical local instruments. The plant was automatic block valve intensive; almost all were motor-operated valves (MOVs) (U.S. Army Corps of Engineers [COE], 2003).

Also prior to the 2003 war, the Qarmat-Ali WTP provided industrial-grade water as a critical step in southern Iraq's oil production process. Water for this purpose was treated with an inexpensive corrosion inhibitor, sodium dichromate, to reduce corrosion of the oil production facility's pipes and other equipment. Workplace practices at the WTP resulted in sodium dichromate contamination within and on the soils surrounding the sodium dichromate mixing building and storage area. The U.S. Army Center for Health Promotion and Preventive Medicine (CHPPM) reported that looting at the site in early 2003 contributed to this contamination when roofing and siding materials were taken from certain buildings and warehouses at the compound (U.S. Army CHPPM, 2003).

## The Region and Its Weather

The climate of Iraq (*CIA Factbook*, 2011) is mostly desert with mild to cool winters and dry, hot, cloudless summers. The northern mountainous regions that border Iran and Turkey experience cold winters with occasionally heavy snows that melt in early spring. This snowmelt sometimes causes extensive flooding in central and southern Iraq.

For the summer period, the Basra region of Iraq is very hot and dry. Daytime temperatures usually exceed 110°F with nighttime temperatures only reaching about 80°F. The Basra area is mostly barren land except for some vegetation and irrigated croplands that surround local rivers. Figure 3 shows an aerial picture of the Qarmat-Ali site from November 9, 2003.

## Meteorological Measurements

We selected the period of April 15, 2003, through October 15, 2003 for our modeling calculations. We believe this period covers all the principal times of alleged exposure of soldiers in this case. Figure 4 shows the local weather stations that have reliable data for the modeling period. We collected surface weather data measured at the Kuwait International Airport and weather data for the upper atmosphere measured by stations in both Kuwait and Iran.

Figure 5 shows wind roses for the wind data at the Kuwait Airport for April 15, 2003, through October 15, 2003. The prevailing winds for this period come from the north-northwest and northwest, especially strong winds. Unfortunately, local weather data (collected at the Basra airport) were mostly missing during this time period. However, we have verified, during periods in which both Basra and Kuwait wind stations were in operation, that winds at the two stations are similar and concluded that the Kuwait station can be used to represent air flow in the study area in our modeling. For example, when comparing the climatological wind roses (5 years, 2005–2009) for Basra and Kuwait, Basra has prevailing winds from WNW to NW, while Kuwait has prevailing winds from NW to NNW.



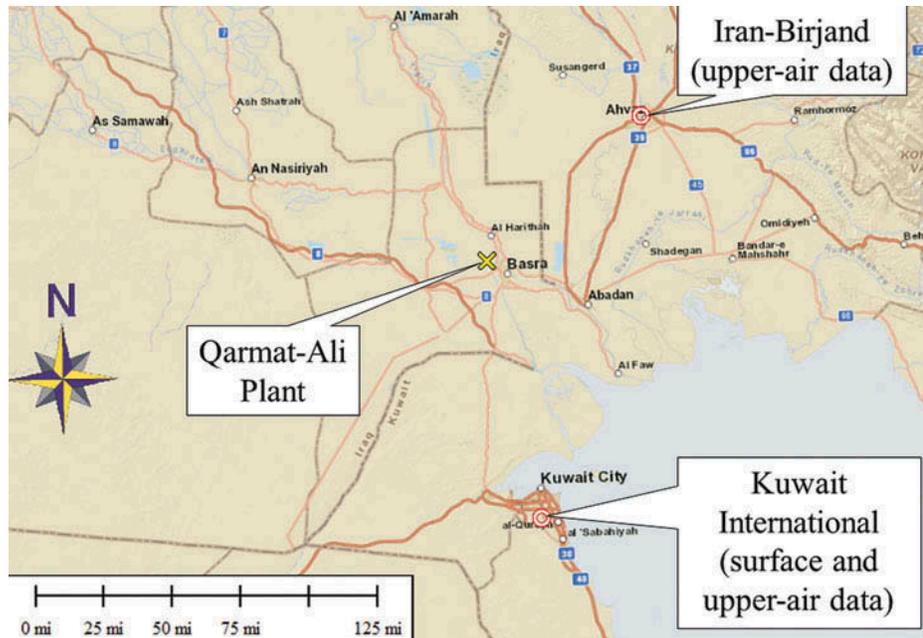**Figure 3.** Qarmat-Ali WTP, November 9, 2003.

**Figure 4.** Weather stations (marked by circle) with data used for modeling simulations, along with the Qarmat-Ali plant.
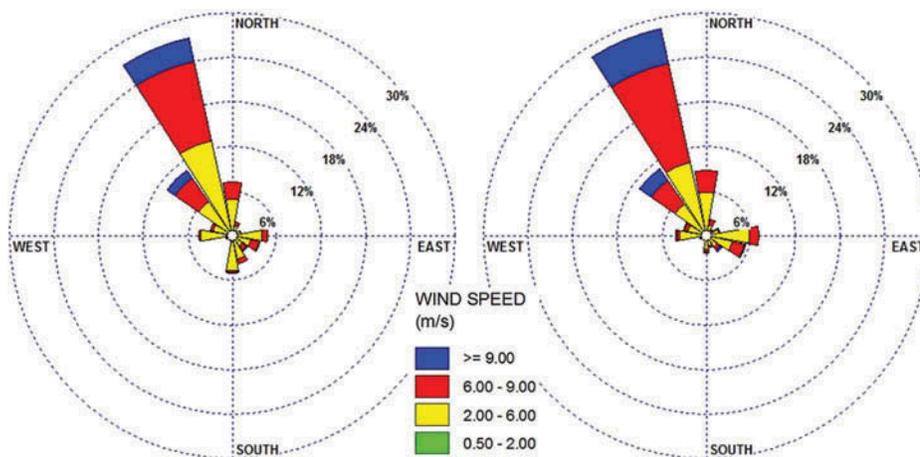


**Figure 5.** Wind Roses showing prevailing winds for Kuwait Airport from April 15, 2003, through October 15, 2003. These hourly measurements are taken at 10 m above the ground. Wind rose on left (total hours = 4,416) is for all hours of day, with average wind speed of 4.1 m/sec, and 17% of hours are calm winds. Wind rose on right (total hours = 2,808) is for "daytime" hours (6:00 a.m. to 9:00 p.m. local time), with average wind speed of 4.9 m/sec, and 10% of hours are calm winds.

The average wind speed for Basra is 9.3 knots, which is close to the Kuwait average wind speed of 8.3 knots.

Also, we downloaded from Lakes Environmental Software (2014) gridded wind fields from the 5th Generation Penn State University/National Center for Atmospheric Research Mesoscale Model (MM5). The 6-month average wind speed at the grid box containing Basra (lat/lon = +30.5838, +47.6905) was similar to that measured at Kuwait during our modeling period: 4.1 m/sec for Kuwait Airport versus 4.2 m/sec for the Basra MM5 grid. The prevailing winds are from NW at the Basra grid and from NNW at Kuwait Airport.

Many of our analyses presented in the following sections deal with daytime hours because that covers the time of day that the vast majority of soldiers allege they were at the plant and because daytime typically is more windy than nighttime in Southern Iraq. Therefore, presented in Figure 5 are wind roses for two cases: (1) all hours and (2) "daytime" hours from 6:00 a.m. to 9:00 p.m.

We believe that winds measured at the Kuwait Airport are representative for the region around Basra, Iraq, because the region is flat and, in our modeling calculations, we are only concerned about strong winds, potentially capable of causing soil erosion. In fact, the strong northwesterly winds apparent in the wind roses just presented are part of a larger scale wind pattern over the Persian Gulf area called the "Summer Shamal" (U.S. Marine Corps [USMC], 1990). The persistent strong northwesterly winds characteristic of the Summer Shamal are well captured in the Kuwait City wind roses.

# Modeling Approach

In this study, our main goal was to calculate the potential ambient concentrations of Cr(VI)-containing $PM_{10}$ particulate matter that could have been inhaled by people working at or visiting the site (Qarmat-Ali WTP) during the period April 15, 2003, through October 15, 2003. We assumed that wind erosion processes at the site were the most significant cause of soil disturbance causing exposure via air pathway. Vehicle traffic at the site was very limited because the site was not in operation.

In this project, the chemical of concern is hexavalent chromium [Cr(VI)]. Our approach was to examine available soil measurements of chromium and extract information on the soil concentration of Cr(VI) in different surface areas around the plant at different times. Then, by knowing the Cr(VI) concentration in soil, our $PM_{10}$ calculations can be expressed in Cr(VI) ambient concentrations that possibly could have been inhaled by people at the site.

We selected the U.S. Environmental Protection Agency (EPA) recommended model AERMOD to calculate the ambient concentrations of $PM_{10}$/Cr(VI) at the site. According to the EPA, AERMOD is the "preferred/recommended" model for short-range dispersion studies, such as the case under examination here. This model is fully accepted in the scientific community as a reliable method for simulating atmospheric transport of pollutants, including particulate matter and any material attached to particles. Models like AERMOD have been developed, accepted, and recommended by the EPA after decades of extensive peer-reviewed research, testing, validation, and calibration with actual measurements in many sites. The AERMOD model is routinely used, without any additional recalibration with local data, in the United States and abroad for regulatory studies, urban and industrial planning, permitting, and research. The application of AERMOD in this study is of interest because, as described later, it will be used in combination with equations from the DUSTRAN module that determines wind erosion emissions from the site. Traditionally, DUSTRAN has been coupled to CALPUFF; however a "beta" version of the DUSTRAN software coupled to AERMOD is forthcoming (Pacific Northwest National Laboratory, 2014). The concentration results provided in this paper are a useful precedent in anticipation of this software release.

Using AERMOD, we simulated $PM_{10}$/Cr(VI) concentrations in the area caused by emissions due to wind erosion for all the hours when the wind speed exceeded an erosion threshold, which happened about half of the time during the period of interest. AERMOD simulations provide ambient hourly concentrations of Cr(VI) in all points of interest, as presented in the following. Our simulation period includes the month of October 2003, when some atmospheric measurements of total chromium (TCr) and Cr(VI) were taken at the site. Therefore, as discussed in the following, we were able to perform a partial validation of our modeling results by comparing them to actual measurements at the site.

# Emission Calculations

Sodium dichromate was present at Qarmat-Ali due to its prior use as a water treatment agent. Sodium dichromate contains Cr(VI), and therefore the presence of Cr(VI) in soils at and around the facility was likely a result of workplace practices at the plant spreading this sodium dichromate contamination within and on the soils surrounding the facility. Looting at the site in 2003 likely contributed to additional spreading when the sodium dichromate storage bags were vandalized and all of the roofing and siding materials were taken from the compound's buildings and warehouses, thus allowing the natural elements to deteriorate storage containers and further spread the contamination. The main areas of this contamination were in the eastern part of the facility, in the area around the chemical injection building. All of the contamination at issue occurred before soldiers ever arrived at Qarmat-Ali.

The soil contamination made as a result of workplace practices created conditions in which liquid sodium dichromate solution spills contaminated the ground during normal operations. Sodium dichromate is soluble and, as part of the operations at the site, was mixed with water prior to injection into the oil fields. We believe that most of the visible contamination of yellow soils outside the injection building was probably the result of these liquid spills. We also believe that the looting of the facility and any damage to the bags containing crystals of sodium dichromate created a different type of soil contamination, more localized, and characterized by the presence of larger particles released from the bags.

The spreading of the sodium dichromate by liquid spills outdoors likely resulted in some amounts of Cr(VI) becoming attached to soil particles. This contaminated soil showed up around the site as areas of yellow-stained soils. Wind erosion of the surface soils provides a pathway by which Cr(VI) would have been transported downwind, potentially exposing some people at the facility. In particular, we look only at the $PM_{10}$ portion of this airborne Cr(VI) in soil dust, since it is of sizes 10 μm or less that can be inhaled into the lungs. In fact, pure sodium dichromate material spread as a result of looting would be granular, of size much larger than 10 μm (e.g., 2,000 μm), and therefore would not be directly subject to airborne transport across the site and could not be inhaled into lungs.

We therefore aimed in our emission representation to account for the amount of Cr(VI) contained in the outdoor surface soil that at least possibly could have been uplifted to the air due to wind erosion. We based our estimation of this amount on measurements of Cr(VI) in outdoor surface soil made by various groups at the site over the summer and fall 2003. Measurements made of Cr(VI) in soils indoors, in piles, in trenches, and/or below grade were excluded as nonrepresentative in our analysis because these measurements were (1) highly localized, (2) small in area, (3) located in areas that would not have been readily exposed to ambient surface winds, and (4) in the cases of piles and trenches, were likely made of material in which the Cr(VI) was not in an erodible $PM_{10}$ form. We do not believe that these measurements are useful in characterizing the concentration of erodible Cr(VI) in surface soil across outdoor areas of the site, which would be the largest source area of Cr(VI) subject to wind erosion.

We estimated the emission rate of Cr(VI) in windblown $PM_{10}$ dust from Qarmat-Ali hourly over the period April 15, 2003, through October 15, 2003. The amount of Cr(VI) in

airborne $PM_{10}$ was estimated by calculating the time-varying rate of $PM_{10}$ windblown dust emission (grams per square meter per hour), and then multiplying this by our estimate of the fraction of Cr(VI) in the $PM_{10}$ in soil surface—a fraction that varied with time and location. This is termed the "dust loading" methodology (Walsh, 2002). By simply multiplying the $PM_{10}$ emission rate by the Cr(VI) concentration in the soil, the methodology does not account for differences between the size distribution of Cr(VI) and the soil itself. While concentration measurements were made of Cr(VI) in soil, no measurements were made of its size distribution, and therefore we had no basis to assign a different size distribution to the Cr(VI) content of the soil. Further, we feel application of the dust loading methodology is more appropriate in this case than the alternative "resuspension factor" approach described in Walsh (2002), which is most appropriate in the days immediately following soil contamination in an emergency response context. In our case, soldiers arrived at the site in the summer of 2003, a couple months after the looting and site damage that occurred during the preceding spring.

## Calculation of the $PM_{10}$ Emission Rate

Using the equations of the DUSTRAN model (Allwine et al., 2006), we calculated over the period April 15, 2003, through October 15, 2003, the emission rates of $PM_{10}$ due to wind erosion from surfaces at the Qarmat-Ali WTP. DUSTRAN is a dust emission and transport model developed for the U.S. Department of Energy (Shaw et al., 2008). In DUSTRAN, dust is emitted from a source area if the wind speed exceeds a threshold value, which depends on the soil moisture, soil composition, and the surface roughness. When the wind speed exceeds the threshold, the amount of dust emitted is proportional to almost the fourth power of the wind speed, so emissions of dust increase very rapidly with wind speed.

After calculating the amount of dust that is emitted, DUSTRAN has formulas that estimate the particle size distribution in the airborne dust based on the particle size distribution in the soil. From this, DUSTRAN can estimate the amount of $PM_{10}$ contained in the overall dust emission.

We applied to the DUSTRAN formulas the hourly wind speeds measured at Kuwait City International Airport over the period of interest. In addition, the following inputs were provided:

- Roughness length = 0.05 m.
- Soil composition = 82% coarse sand, 6% large silt, 6.7% small silt, 5.3% clay.
- Soil moisture content = 2%.

The roughness length is used with the wind speed input to the DUSTRAN formulas to arrive at a parameter called the "friction velocity." The value for roughness length must therefore be consistent with the location where the wind measurements come from. Since the winds come from Kuwait City airport, a roughness length of 0.05 m (5 cm) is therefore chosen since this is an appropriate value to characterize airport areas (Arya, 2001).
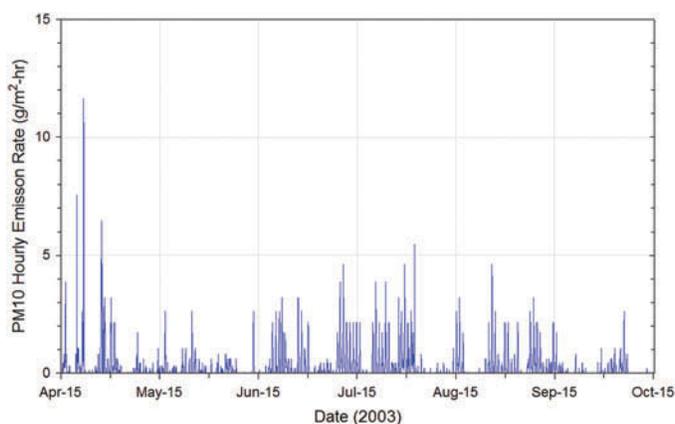


**Figure 6.** Hourly $PM_{10}$ Emission Rates during April 15, 2003 through October 15, 2003.

The soil composition is taken from measurements in the Basra desert (McDonald and Caldwell, 2004). Because we are dealing with summer desert conditions, we expect extremely dry soils. For the soil composition inputs, the DUSTRAN formulas compute a minimum value for soil moisture of around 1%. We do not expect, however, absolute minimum soil moisture conditions at the site because of the adjacent sources of water in the area (i.e., the river, intake canal, and evaporation pond). In fact, it was observed by the U.S. Army CHPPM that the evaporation pond, although dry, had soils "within the center portion that were extremely wet and soft." We therefore chose a value of 2%, still very dry but elevated slightly above minimum to reflect these adjacent sources of water. The value of 2% is in the low end of observations of soil moisture in desert soils reported in the literature (Scanlon, 1994; Agam (Ninari) and Berliner, 2004).

From these inputs, the threshold wind speed for dust emission was calculated by the DUSTRAN equations as 4.0 m/sec (~9 mph). We note that, because of our conservative assumptions, we ended up using a low wind speed threshold of about 9 mph, while in many studies in the scientific literature, values between 11 and 22 mph have been used instead (Hannesen and Weipert, 2003). Our choice of threshold is conservative because a lower threshold generates higher $PM_{10}$ emission rates.

The computed hourly emission rates of $PM_{10}$ over the period of April 15, 2003, through October 15, 2003, are shown in Figure 6. The largest value (11.7 $g/m^2$-hr) occurred on April 22, 2003, with a sustained wind speed of 32 mph.

## Estimates of Cr(VI) Concentrations in Soils

Our estimation of the Cr(VI) concentration in surface soil at Qarmat-Ali was based on 121 samples of Cr(VI) in surface soil taken at various locations around the site from August to October of 2003; 41 samples from Kellogg, Brown, and Root (KBR), 60 samples by the U.S. Army CHPPM (2003), and 20 samples by the British Army Medical Directorate Environmental Monitoring Team (2003). The KBR samples include the "Yellow Lid," "White Lid," and "BS" samples indicated in Figures 8 and 9
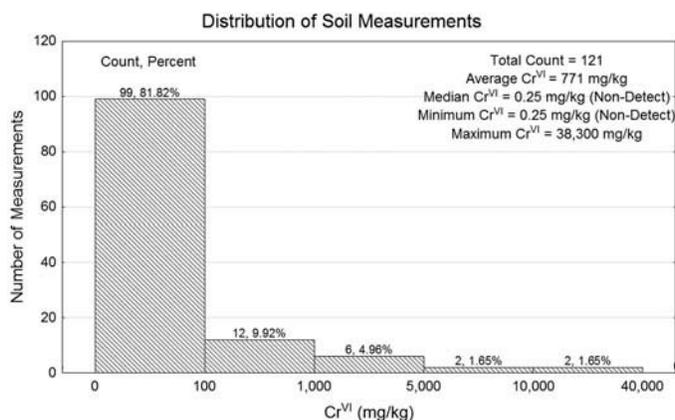
**Figure 7.** Soil samples taken at Qarmat-Ali WTP (including samples we consider nonrepresentative).

(shown in the following). A statistical summary of these measurements, which includes those that we discarded as non-representative, is shown in Figure 7. The samples were of loose surface soil, filtering out coarse gravel and any remediation material. The U.S. Army CHPPM sample material corresponding to a reported measurement was a composite of material collected at five points: a central point and four surrounding points about 6 ft from the central point.

As seen from the Figure 7, around 80% of the measurements are below 100 mg/kg, similar to values reported in uncontaminated areas around the world (WHO, 2013). These are generally found on the west side of the site, where contamination was not visibly evident, although some of these

measurements occurred on the east side as well. Several of the values within the remaining 20% are higher than 1,000 mg/kg, with the maximum representative value being 8,290 mg/kg on the northeast of the facility. These values are comparable to those reported in other contaminated areas around the world (World Health Organization [WHO], 2013). These high values were measured in August prior to surface remediation completed on or around August 22, 2003. No noticeable concentration trends other than pre- versus postremediation were clearly evident from the data provided, and therefore we applied constant average values for pre- and postremediation conditions to affected areas, as described in the following.

We present, in Figure 8 (eastern area) and Figure 9 (western area), maps with locations of the soil samples we used in our analyses. Based on the distribution of these measurements in time and space, we divided the site into seven areas for our modeling, as shown in Figure 10. In defining our emission areas, we included the areas covered by buildings as sources, even though this choice overestimates the actual emission rates of Cr(VI)-containing dust.

## Area 1

Area 1 is the northeast portion of Qarmat-Ali.

Area 1 initial surface remediation (by application of liquid asphalt) was completed by August 22, 2003. Therefore, we characterized average surface Cr(VI) soil concentrations over Area 1 as:

- A "preremediation" value before August 22, 2003, calculated as the average of surface Cr(VI) measurements in Area 1 before this date.
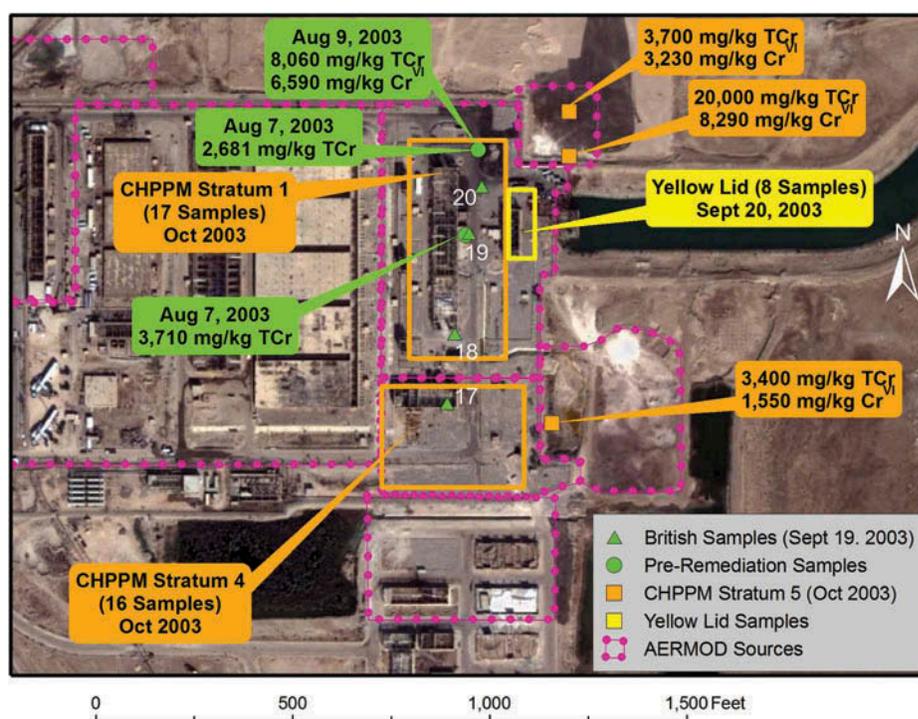


**Figure 8.** Soil Samples taken in the eastern area of the Qarmat-Ali WTP.
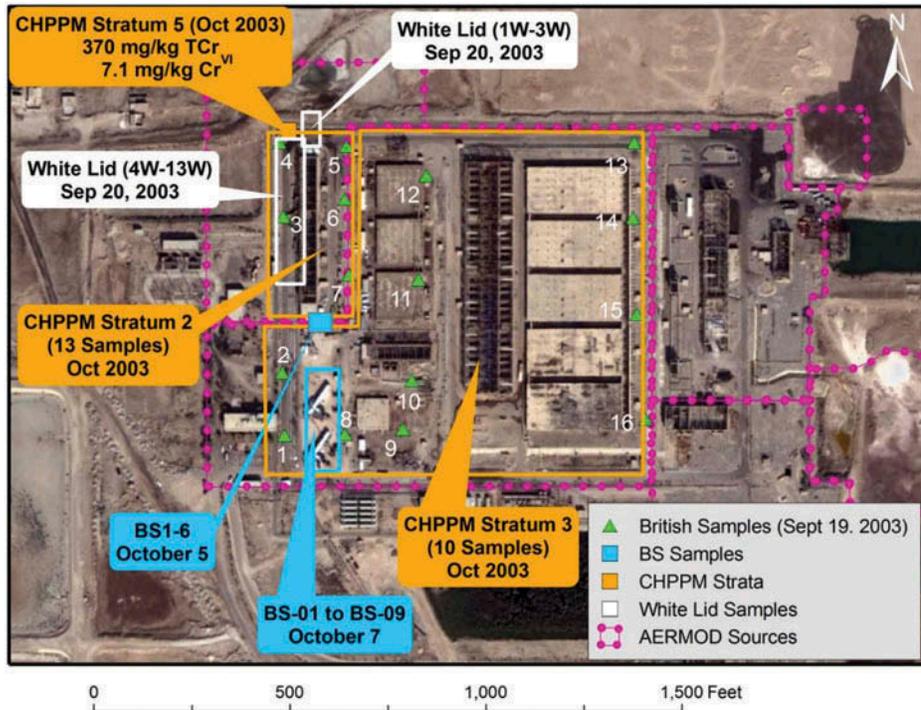
**Figure 9.** Soil samples taken in the western area of the Qarmat-Ali WTP.
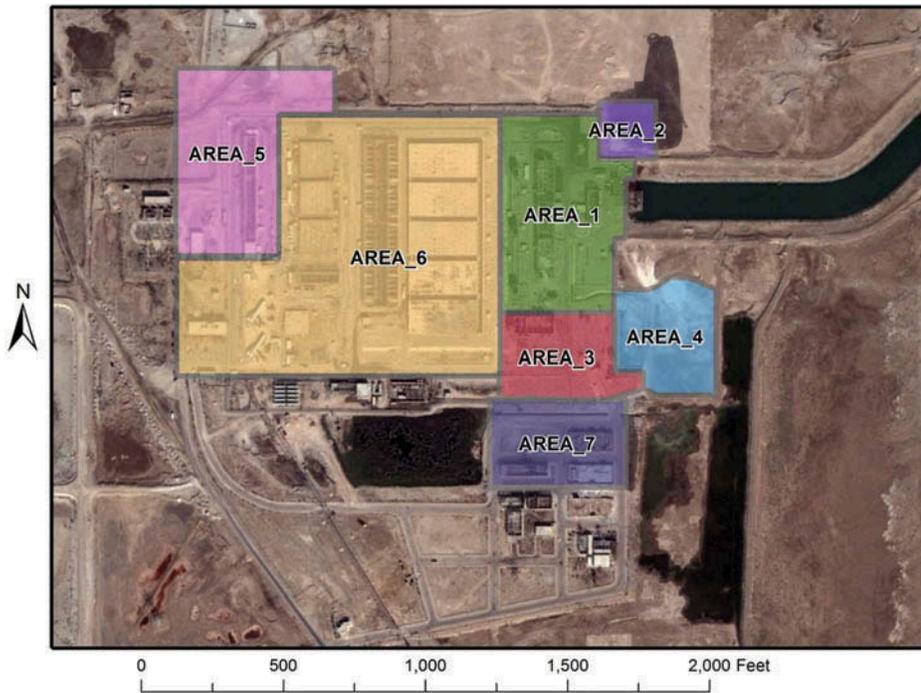


**Figure 10.** Seven areas across the Qarmat-Ali WTP used to characterize average Cr(VI) soil concentrations and associated Cr(VI) air emissions in modeling.

- A "postremediation" value starting on August 22, 2003, calculated as the average of surface Cr(VI) measurements in Area 1 after this date.

There were three samples taken preremediation with values 6,590, 2,192, and 3,033 mg/kg. We take the average of these

three samples, 3,940 mg/kg, for the preremediation Area 1 value. There were 28 samples taken postremediation, ranging from close to zero to 2,500 mg/kg. The average of these 28 samples is 346 mg/kg, which we take for the postremediation Area 1 value. Table 1 shows the individual soil measurements used for Area 1 calculations.

**Table 1.** Area 1, soil concentrations

| TCr (mg/kg) | Cr(VI) (mg/kg) | Date | Location |
|---|---|---|---|
| 8060 | 6590 | Aug. 9, 2003 | KBR Parking Area |
| 2681 | 2192 | Aug. 7, 2003 | KBR Parking Area |
| 3710 | 3033 | Aug. 7, 2003 | KBR Generator Area |
| | 3938 | Area 1 Average (Preremediation) | |

*Note*: Aug. 7, 2003 Cr(VI) values were estimated based on the Aug. 9, 2003 ratio of Cr(VI) to TCr.

| TCr (mg/kg) | Cr(VI) (mg/kg) | Sample and date | Sample ID |
|---|---|---|---|
| 2350.0 | 732.0 | Yellow lid 9/20 | 001Y |
| 4950.0 | 2190.0 | Yellow lid 9/20 | 002Y |
| 1460.0 | 310.0 | Yellow lid 9/20 | 003Y |
| 4730.0 | 2490.0 | Yellow lid 9/20 | 004Y |
| 153.0 | 1.4 | Yellow lid 9/20 | 005Y |
| 469.0 | 3.9 | Yellow lid 9/20 | 006Y |
| 71.9 | 0.25 | Yellow lid 9/20 | 007Y |
| 20.7 | 0.25 | Yellow lid 9/20 | 009Y |
| 200.0 | 102.0 | CHPPM Stratum 1 10/2003 | IRA-QAR-S01-03280 |
| 920.0 | 559.0 | CHPPM Stratum 1 10/2003 | IRA-QAR-S02-03280 |
| 810.0 | 257.0 | CHPPM Stratum 1 10/2003 | IRA-QAR-S03-03280 |
| 460.0 | 34.6 | CHPPM Stratum 1 10/2003 | IRA-QAR-S04-03280 |
| 100.0 | 6.4 | CHPPM Stratum 1 10/2003 | IRA-QAR-S05-03280 |
| 4900.0 | 823.0 | CHPPM Stratum 1 10/2003 | IRA-QAR-S06-03280 |
| 350.0 | 80.0 | CHPPM Stratum 1 10/2003 | IRA-QAR-S07-03280 |
| 230.0 | 25.0 | CHPPM Stratum 1 10/2003 | IRA-QAR-S08-03280 |
| 840.0 | 334.0 | CHPPM Stratum 1 10/2003 | IRA-QAR-S09-03280 |
| 260.0 | 4.6 | CHPPM Stratum 1 10/2003 | IRA-QAR-S10-03280 |
| 910.0 | 196.0 | CHPPM Stratum 1 10/2003 | IRA-QAR-S11-03280 |
| 830.0 | 350.0 | CHPPM Stratum 1 10/2003 | IRA-QAR-S12-03280 |
| 560.0 | 10.7 | CHPPM Stratum 1 10/2003 | IRA-QAR-S13-03280 |
| 150.0 | 4.1 | CHPPM Stratum 1 10/2003 | IRA-QAR-S14-03280 |
| 64.0 | 3.1 | CHPPM Stratum 1 10/2003 | IRA-QAR-S15-03280 |
| 69.0 | 2.6 | CHPPM Stratum 1 10/2003 | IRA-QAR-S16-03280 |
| 340.0 | 91.0 | CHPPM Stratum 1 10/2003 | IRA-QAR-S17-03280 |
| 2550.3 | 834.5 | British 9/19 | 18 |
| 249.2 | 81.5 | British 9/19 | 19 |
| 476.7 | 156.0 | British 9/19 | 20 |
| 1052.6 | 345.8 | Area 1 Average (Postremediation) | |

Hourly emission rates of Cr(VI) for Area 1 (and the other areas below) were obtained by multiplying the average fractional soil concentrations by the hourly $PM_{10}$ emission rates, as discussed before.

## Area 2

Area 2 is a 200 ft × 200 ft area outside the northeast Qarmat-Ali fence line.

Three measurements of surface soil Cr(VI) were taken in areas outside the eastern fence line by the U.S. Army CHPPM, with values 1,550, 3,230, and 8,290 mg/kg. We used these to characterize soil concentrations in both Area 2 and Area 4, our

modeling areas that are outside the eastern fence line. Averaging these three measurements, we calculated an average surface Cr(VI) concentration for Area 2 of 4,360 mg/kg—a value that we used for the entire simulation period since there was no remediation outside the facility. Table 2 shows the individual soil measurements used for Area 2 calculations.

## Area 3

Area 3 is around the "Chlorination Building" of Qarmat-Ali.

Measurements of surface soil Cr(VI) were taken in this area by the British Army and by the U.S. Army CHPPM. Initial surface remediation by application of liquid asphalt over this

**Table 2.** Area 2, soil concentrations

| TCr (mg/kg) | Cr(VI) (mg/kg) | Sample and date | Sample ID |
|---|---|---|---|
| 3400 | 1550 | CHPPM Stratum 5 10/2003 | IRA-QAR-S57-03280 |
| 20000 | 8290 | CHPPM Stratum 5 10/2003 | IRA-QAR-S58-03280 |
| 3700 | 3230 | CHPPM Stratum 5 10/2003 | IRA-QAR-S59-03280 |
| | 4357 | Area 2 Average | |

area was apparently completed by August 22, 2003. We therefore characterized average surface Cr(VI) concentrations over Area 3 using a "preremediation" value before August 22, 2003, and a "postremediation" value starting on August 22, 2003. There were no samples taken in the area prior to the remediation data, so the preremediation soil concentration for Area 3 was assumed to be the same as the preremediation value for Area 1 (3,940 mg/kg). The postremediation value was calculated by averaging 17 samples, ranging in value from close to zero to a maximum of 365 mg/kg, taken by the U.S. Army CHPPM and British Army measurements over the area after August 22, 2003. Doing this, an average postremediation surface soil Cr(VI) concentration for Area 3 of 30 mg/kg was applied. Table 3 shows the individual soil measurements used for Area 3 calculations.

## Area 4

Area 4 is a 3-acre area around the "Evaporation Pond," outside the southeast Qarmat-Ali fence line. We assumed the average surface soil Cr(VI) concentration in this area was the same as for Area 2, an area also outside the eastern fence line. As

described earlier, this value is 4,360 mg/kg for the entire simulation period.

## Area 5

Area 5 is the northwestern portion of Qarmat-Ali, comprising the area around the second-stage pump house and extending slightly outside the northwestern and western fence line. Measurements of either or both Cr(VI) and TCr were taken by KBR, the British Army, and the U.S. Army CHPPM.

There were 47 samples taken in the area, all of which showed detectable for TCr but most of which showed nondetectable for Cr(VI). Values of TCr range from close to zero to around 200 mg/kg. To calculate average surface Cr(VI) in Area 5 from these data, we first replaced nondetect measurements of Cr(VI) with a value of 0.25 mg/kg, which is half the detection limit of these Cr(VI) measurements (0.5 mg/kg). Even though several new methods have been proposed for handling nondetect measurements (Alaska Department of Environmental Conservation [ADEC], 2008), for this study we believe that the most commonly used method (substitution of one-half of the detection limit) remains very appropriate.

**Table 3.** Area 3, soil concentrations (postremediation)

| TCr (mg/kg) | Cr(VI) (mg/kg) | Sample and date | Sample ID |
|---|---|---|---|
| 77.0 | 6.8 | CHPPM Stratum 4 10/2003 | IRA-QAR-S41-03280 |
| 489.0 | 365.0 | CHPPM Stratum 4 10/2003 | IRA-QAR-S42-03280 |
| 47.0 | 3.5 | CHPPM Stratum 4 10/2003 | IRA-QAR-S43-03280 |
| 50.0 | 4.6 | CHPPM Stratum 4 10/2003 | IRA-QAR-S44-03280 |
| 190.0 | 33.0 | CHPPM Stratum 4 10/2003 | IRA-QAR-S45-03280 |
| 140.0 | 1.7 | CHPPM Stratum 4 10/2003 | IRA-QAR-S46-03280 |
| 480.0 | 4.2 | CHPPM Stratum 4 10/2003 | IRA-QAR-S47-03280 |
| 1300.0 | 10.3 | CHPPM Stratum 4 10/2003 | IRA-QAR-S48-03280 |
| 490.0 | 9.6 | CHPPM Stratum 4 10/2003 | IRA-QAR-S49-03280 |
| 33.0 | 7.2 | CHPPM Stratum 4 10/2003 | IRA-QAR-S50-03280 |
| 340.0 | 5.6 | CHPPM Stratum 4 10/2003 | IRA-QAR-S51-03280 |
| 130.0 | 3.7 | CHPPM Stratum 4 10/2003 | IRA-QAR-S52-03280 |
| 51.0 | 1.7 | CHPPM Stratum 4 10/2003 | IRA-QAR-S53-03280 |
| 210.0 | 44.7 | CHPPM Stratum 4 10/2003 | IRA-QAR-S54-03280 |
| 140.0 | 3.4 | CHPPM Stratum 4 10/2003 | IRA-QAR-S55-03280 |
| 130.0 | 3.4 | CHPPM Stratum 4 10/2003 | IRA-QAR-S56-03280 |
| 70.2 | 8.7 | British 9/19 | 17 |
| | 30.4 | Area 3 Average (postremediation) | |

*Notes:* Area 3 preremediation Cr(VI) soil concentration set to Area 1 preremediation value of 3,940 mg/kg, as described in Subsection "Area 3" of Section "Estimates of Cr(VI) Concentrations in Soils."

We then estimated the surface soil Cr(VI) concentrations at points where only TCr was measured by multiplying the measured TCr at these points by the ratio of the average Cr(VI) to TCr at points in Area 5 where both were measured. Carrying out this procedure, our average surface soil concentration of Cr(VI) for Area 5 is 0.85 mg/kg. No known remediation was conducted in this area, so this concentration is used throughout the modeling period. Table 4 shows the individual soil measurements used for Area 5 calculations.

### Area 6

Area 6 is the middle and southwestern portion of Qarmat-Ali.

Measurements of surface soil TCr and Cr(VI) were taken by the British Army and the U.S. Army CHPPM. The U.S. Army CHPPM measurements were all nondetect, and therefore we set the Cr(VI) soil concentration for these samples to 0.25 mg/kg, half the detection limit of 0.5 mg/kg. The British samples were only of total chromium and were of values similar to the total chromium measured by the U.S. Army CHPPM. We therefore also set the soil Cr(VI) concentrations to 0.25 mg/kg. An average value of 0.25 mg/kg was therefore applied for Area 6. No known remediation was conducted in this area, so this concentration is used throughout the modeling period. Table 5 shows the individual soil measurements used for Area 6 calculations.

### Area 7

Area 7 is around the chemical warehouses south of the southeast fence line of Qarmat-Ali. This area contained chemical warehouses, where damage to the facility and resultant spills of sodium dichromate from bags occurred. Visual evidence indicates that the damage and spills were contained within the warehouses themselves, not reaching areas outside exposed to ambient winds. Since our study focuses on ambient concentrations due to wind erosion, we did not consider exposure to dichromate from spills inside the warehouses in our analysis.

No measurements of outdoor soil Cr(VI) were taken in this area. We therefore applied the average of Area 1 and Area 3 soil concentrations described earlier: 3,940 mg/kg preremediation and 227 mg/kg postremediation, the result of averaging the postremediation samples from Area 1 and Area 3.

## AERMOD Inputs

AERMOD requires input data for emissions and meteorology. The Cr(VI) emission inputs were explained earlier. Meteorological inputs were supplied by running the AERMET preprocessor for AERMOD (EPA, 2011), which generates the required hourly meteorological inputs for AERMOD given observed hourly meteorological inputs. AERMET (version 11059) outputs the wind speed, wind direction, temperature, and various atmospheric stability-dependent turbulence quantities required by AERMOD (version 11103) to characterize pollutant mixing as it blows downwind. Surface meteorological data were

obtained from hourly measurements at the Kuwait City International Airport (International Civil Aviation Organization [ICAO] call sign "OKBK," World Meteorological Organization [WMO] code 40582). Upper air meteorological data, also required for AERMET, were obtained from both the Kuwait City Airport and from the Birjan, Iran, upper air sites (ICAO call sign "OIMB," WMO code 40809). We used two upper air sites because of the large amount of missing data in each of these upper air data individually. Combining data from these two sites reduces the amount of missing data. In fact, only approximately 3% of the hours were missing, and these missing data are scattered more or less uniformly over the 6-month period of interest and do not appear to be biased toward any particular time of day. Note that EPA regulatory modeling requires less than 10% missing data (EPA, 2000). The Kuwait City site is 55 m above sea level and the Birjan site is 22 m above sea level.

For surface characteristic inputs, we assigned a roughness length of 0.05 m (consistent with Kuwait City Airport wind observation inputs), a noontime surface albedo of 0.3 (a suitable value for desert areas), and 3 for Bowen Ratio (suitable for desert areas).

We used area sources in our AERMOD runs with an initial vertical standard deviation of 10 m, in order to account for the initial turbulent eddies created by the frictional forces of the high winds on the surface. This choice is in agreement with most previous studies in the literature, where dust storms are simulated by grid models (Liu et al., 2003; Nickovic et al., 2001; Shaw et al., 2008; Song et al., 2001; Spyrou et al., 2010) and the dust is initially mixed in the first grid layer.

We ran AERMOD without plume depletion so that a conservative estimate of air concentrations could be obtained. By eliminating plume depletion, the reduction of air concentrations due to dry deposition and gravitational settling of particulate during downwind travel is not accounted for. By making this choice, we also do not need to account for particulate resuspension.

## AERMOD Partial Validation

During the period August 16–October 12, 2003, 29 air quality samples were collected at the site. These measurements were taken on the eastern side of the site, where the majority of soil contamination had occurred. Fourteen of the measurements were taken using the NIOSH 7300 technique, with a detection limit ranging between 1 and 3 $\mu g/m^3$ depending on the sample. The other 15 utilized high-volume air sampling with a detection limit ranging between 0.04 and 0.1 $\mu g/m^3$ depending on the sample. The samples were over multiple hours during daytime, and some were explicitly reported to be 8-hr samples.

These measurements of ambient concentrations of Cr(VI) and TCr were all below the detection limit, which unfortunately does not allow us to perform a full modeling validation. However, a comparison can still be made by conservatively assuming that (1) the measurements are half of the detection limit, and (2) measured TCr is all made of Cr(VI). The comparison is a partial validation in the sense that it can indicate

**Table 4.** Area 5, soil concentrations

| TCr (mg/kg) | Measured Cr(VI) (mg/kg) | Sample and date | Sample ID | Note | Final Cr(VI) (mg/kg) with fills for "NO Cr (VI)" or "ND" |
|---|---|---|---|---|---|
| 38.0 | 0.50 | CHPPM Stratum 2 10/2003 | IRA-QAR-S18-03280 | ND | 0.25 |
| 37.0 | 0.50 | CHPPM Stratum 2 10/2003 | IRA-QAR-S19-03280 | ND | 0.25 |
| 36.0 | 0.50 | CHPPM Stratum 2 10/2003 | IRA-QAR-S20-03280 | ND | 0.25 |
| 49.0 | 0.50 | CHPPM Stratum 2 10/2003 | IRA-QAR-S21-03280 | ND | 0.25 |
| 47.0 | 0.50 | CHPPM Stratum 2 10/2003 | IRA-QAR-S22-03280 | ND | 0.25 |
| 34.0 | 0.50 | CHPPM Stratum 2 10/2003 | IRA-QAR-S23-03280 | ND | 0.25 |
| 38.0 | 0.50 | CHPPM Stratum 2 10/2003 | IRA-QAR-S24-03280 | ND | 0.25 |
| 50.0 | 0.50 | CHPPM Stratum 2 10/2003 | IRA-QAR-S25-03280 | ND | 0.25 |
| 41.0 | 0.50 | CHPPM Stratum 2 10/2003 | IRA-QAR-S26-03280 | ND | 0.25 |
| 46.0 | 0.50 | CHPPM Stratum 2 10/2003 | IRA-QAR-S27-03280 | ND | 0.25 |
| 28.0 | 0.50 | CHPPM Stratum 2 10/2003 | IRA-QAR-S28-03280 | ND | 0.25 |
| 49.0 | 10.60 | CHPPM Stratum 2 10/2003 | IRA-QAR-S29-03280 | | 10.60 |
| 46.0 | 0.50 | CHPPM Stratum 2 10/2003 | IRA-QAR-S30-03280 | ND | 0.25 |
| 31.0 | 1.23 | October 5, 2003 | BS1 | | 1.23 |
| 20.4 | 0.61 | October 5, 2003 | BS2 | | 0.61 |
| 25.6 | 0.50 | October 5, 2003 | BS3 | ND | 0.25 |
| 213.0 | 0.50 | October 5, 2003 | BS4 | ND | 0.25 |
| 56.3 | 0.50 | October 5, 2003 | BS5 | ND | 0.25 |
| 115.0 | 0.50 | October 5, 2003 | BS6 | ND | 0.25 |
| 8.7 | | October 7, 2003 | BS-01 | NO Cr(VI) | 0.25 |
| 9.4 | | October 7, 2003 | BS-02 | NO Cr(VI) | 0.25 |
| 18.4 | | October 7, 2003 | BS-03 | NO Cr(VI) | 0.31 |
| 8.2 | | October 7, 2003 | BS-04 | NO Cr(VI) | 0.25 |
| 5.5 | | October 7, 2003 | BS-05 | NO Cr(VI) | 0.25 |
| 5.7 | | October 7, 2003 | BS-06 | NO Cr(VI) | 0.25 |
| 8.8 | | October 7, 2003 | BS-07 | NO Cr(VI) | 0.25 |
| 5.3 | | October 7, 2003 | BS-08 | NO Cr(VI) | 0.25 |
| 9.6 | | October 7, 2003 | BS-09 | NO Cr(VI) | 0.25 |
| 13.2 | 0.50 | White lid 9/20 | 006W | ND | 0.25 |
| 16.5 | 0.50 | White lid 9/20 | 007W | ND | 0.25 |
| 16.2 | 0.50 | White lid 9/20 | 008W | ND | 0.25 |
| 20.9 | 0.50 | White lid 9/20 | 009W | ND | 0.25 |
| 20.4 | 0.50 | White lid 9/20 | 010W | ND | 0.25 |
| 24.0 | 0.50 | White lid 9/20 | 011W | ND | 0.25 |
| 25.8 | 0.50 | White lid 9/20 | 012W | ND | 0.25 |
| 23.0 | 0.50 | White lid 9/20 | 013W | ND | 0.25 |
| 32.8 | 0.50 | White lid 9/20 | 001W | ND | 0.25 |
| 33.7 | 0.50 | White lid 9/20 | 002W | ND | 0.25 |
| 34.0 | 0.50 | White lid 9/20 | 003W | ND | 0.25 |
| 33.4 | 0.50 | White lid 9/20 | 004W | ND | 0.25 |
| 38.6 | 0.50 | White lid 9/20 | 005W | ND | 0.25 |
| 370.0 | 7.10 | CHPPM Stratum 5 10/2003 | IRA-QAR-S60-03280 | | 7.10 |
| 62.0 | | British 9/19 | 3 | NO Cr(VI) | 1.05 |
| 100.3 | | British 9/19 | 4 | NO Cr(VI) | 1.70 |
| 65.9 | | British 9/19 | 5 | NO Cr(VI) | 1.12 |
| 70.3 | | British 9/19 | 6 | NO Cr(VI) | 1.19 |
| 67.3 | | British 9/19 | 7 | NO Cr(VI) | 1.14 |
| 54.4 | | Averages (excluding "NO Cr(VI)" data) | | | 0.81 |
| | | Area 5 Average (mg/kg) | | | 0.85 |

**Table 5.** Area 6, soil concentrations

| TCr (mg/kg) | Cr(VI) (mg/kg) | Sample and date | Sample ID |
|---|---|---|---|
| 25.0 | 0.25 | CHPPM Stratum 3 10/2003 | IRA-QAR-S31-03280 |
| 17.0 | 0.25 | CHPPM Stratum 3 10/2003 | IRA-QAR-S32-03280 |
| 140.0 | 0.25 | CHPPM Stratum 3 10/2003 | IRA-QAR-S33-03280 |
| 16.0 | 0.25 | CHPPM Stratum 3 10/2003 | IRA-QAR-S34-03280 |
| 32.0 | 0.25 | CHPPM Stratum 3 10/2003 | IRA-QAR-S35-03280 |
| 37.0 | 0.25 | CHPPM Stratum 3 10/2003 | IRA-QAR-S36-03280 |
| 21.0 | 0.25 | CHPPM Stratum 3 10/2003 | IRA-QAR-S37-03280 |
| 28.0 | 0.25 | CHPPM Stratum 3 10/2003 | IRA-QAR-S38-03280 |
| 39.0 | 0.25 | CHPPM Stratum 3 10/2003 | IRA-QAR-S39-03280 |
| 38.0 | 0.25 | CHPPM Stratum 3 10/2003 | IRA-QAR-S40-03280 |
| 41.7 | | British 9/19 | 1 |
| 139.6 | | British 9/19 | 2 |
| 87.6 | | British 9/19 | 8 |
| 41.1 | | British 9/19 | 9 |
| 39.0 | | British 9/19 | 10 |
| 48.9 | | British 9/19 | 11 |
| 40.7 | | British 9/19 | 12 |
| 26.1 | | British 9/19 | 13 |
| 58.3 | | British 9/19 | 14 |
| 45.4 | | British 9/19 | 15 |
| 34.1 | | British 9/19 | 16 |
| | 0.25 | Area 6 Average | |

model overprediction, but not underprediction (since observations were nondetectable).

With these assumptions, we compared the measurements with our AERMOD Cr(VI) simulations of the daytime concentrations on the days of the measurements. In all but a few cases, the modeling results are consistent with the measurements; this is because the model also predicts a concentration that is less than the detection limit. Only for three days did the model predict a value greater than the detection limit, but still within a factor of two. The average daytime wind speeds measured at the Kuwait City airport (used in the model) and at the Basra station (close to Qarmat Ali) for the days of air monitoring were approximately 10 mph, above the threshold of 9 mph determined by DUSTRAN for this case for wind erosion emissions. Approximately 25% of the hourly winds during the daytime hours of the measurement days were above 15 mph, and in only two days were daytime winds less than threshold throughout the day. Modeled and actual Cr(VI) air concentration from wind erosion emissions from the site were therefore likely nonzero on the days of most of the air monitoring—just not above the measurement thresholds.

## Modeling Results and Discussion

### Area results

We present in Figure 11 the results of our AERMOD runs. Colored regions represent the atmospheric concentrations of Cr(VI) near the surface calculated by AERMOD over an averaging period of 6 months (April 15, 2003, through October 15, 2003). Figure 11 shows the 6-month average concentration at the site using only daytime hours (i.e., 15 hours from 6 a.m. to 9 p.m. each day). In this simulation, the emissions include the effects of initial remediation measures starting on August 22, 2003, as discussed before. Peak values are on the southeast side of the facility, extending beyond the fenceline, and downwind of the most contaminated areas on the northeast side of the facility. Peak values are just above 0.5 $\mu g/m^3$, similar to high values reported in industrial and urban areas of the United States (WHO, 2013).

Air concentration results are very similar if we ignore remediation and do not decrease emissions after August 22, 2003, with the peak concentration values in the southeast area of the facility increasing to around 0.7 $\mu g/m^3$. Although soil concentrations are much different pre- versus postremediation, as discussed earlier, the modest increase in air concentrations in the two situations is a consequence of the relatively short time period (around 1 month of the total 6 simulated) where remediated soil conditions are accounted for in our simulations. Concentration results are also very similar (slightly lower) if emissions are computed over all the 24 hr of each day and concentration averages include all 24 hr (because high winds are less likely at nighttime).

### Individual results

In our study, we selected individual soldiers to investigate their frequency, locations, and dates of visits. This information was used to provide conservative estimates of the their total exposure to Cr(VI) via atmospheric pathway and inhalation.
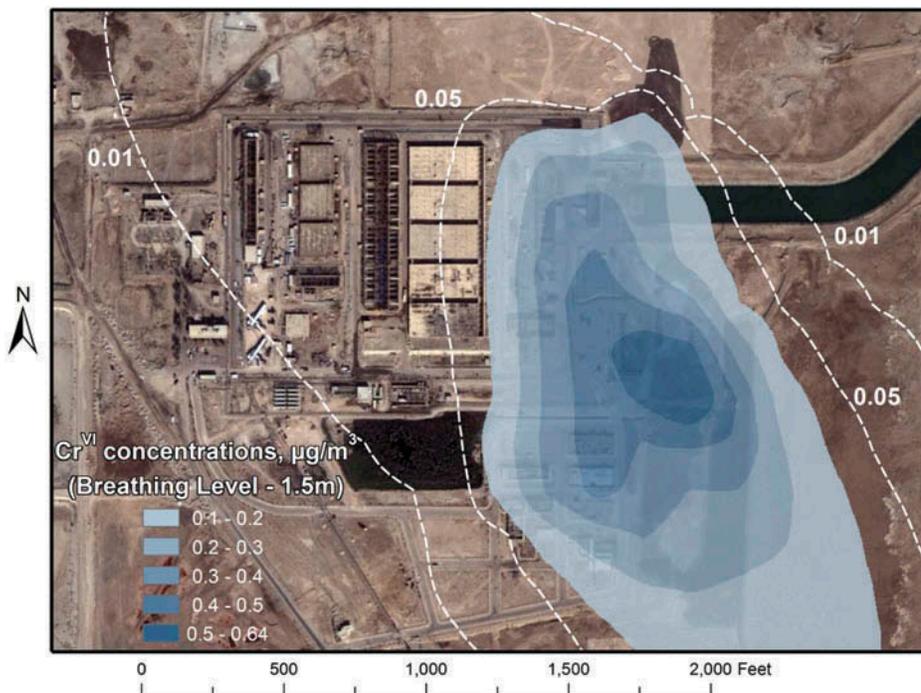
**Figure 11.** Six-month average daytime concentrations of Cr(VI) for daytime emissions (15 hr per day only) with inclusion of initial remediation measures from August 22, 2003.

We selected below one individual ("Soldier X") to illustrate our additional investigation and data analysis from modeling runs. For this person, some details were known about his visits. This analysis is applicable to, and informative about, other people who spent similar or less time at Qarmat-Ali.

*"Soldier X."* After reviewing available documents and testimonies, we concluded that this soldier's highest possible exposure was outdoors even during high-wind episodes raising dust when soldiers would typically be indoors (this conservative assumption is made by us for all soldiers). We assumed 20 visits of 12 hr each to the site during the months of June, July, and August located at a point in the northeast of the site where the soldier reported he spent the majority of time while at the site. The average inhaled Cr(VI) concentration utilizing the 15-hr daytime average concentrations during these three months was 0.43 µg/m$^3$ and the 90th percentile of the 15-hr daytime average concentrations for the 20 visits was 1.25 µg/m$^3$ If we normalize this soldier's highest alleged 240-hr exposure over a full year, we obtain this average annual concentration:

$$0.43 \ \mu g/m^3 \ \times \ \left[ \frac{240}{365 \times 24} \right] \ = \ 0.012 \ \mu g/m^3 \qquad (1)$$

Similar calculations were performed for other soldiers, giving similar (generally lower) concentration results.

## Conclusion

We have examined a large set of documents and data, in relation to the soil contamination of Cr(VI) found at the Qarmat-Ali Water Treatment Plant (WTP), near Basra, Iraq, during different periods in 2003, when soldiers visited the site. We analyzed soil measurements and established the degree of soil contamination at the site. We also used an EPA-approved model (AERMOD) to simulate PM$_{10}$ wind erosion phenomena and calculate Cr(VI) inhalable concentrations at the site for different locations and periods of time. We were able to perform a partial validation of our modeling runs, by successfully comparing models outputs with air quality measurements at the site.

Our modeling effort provided results in the form of both contour lines of average Cr(VI) concentrations at the site, and specific concentration values for selected soldiers.

We have made several conservative assumptions in the development of our work and in our choices of data and parameterizations. In particular:

- In defining our emission areas, we included the areas covered by buildings as sources, even though this choice overestimates the actual emission rates of Cr(VI)-containing dust.
- We chose a low wind threshold of about 9 mph, even though higher values are generally reported in the literature.
- In calculating the concentrations possibly inhaled by the selected soldiers, we made conservative assumptions by locating people in points of maximum exposure and/or calculating exposure for the entire duration of their visit to the site.

## Disclaimer

The research and preparation of this paper relate to work done by the authors in a litigation project. Dr. Zannetti served

as an expert witness and testified about his expert work on behalf of the KBR defendants. The responsibility for the preparation and content of this paper rests with the authors, and the opinions and interpretations expressed reflect the views of the authors and not of any company.

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