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Evaluation of DUSTRAN Software System for Modeling Chloride Deposition on Steel Canisters

July 29, 2015

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U.S. DEPARTMENT OF ENERGY

Prepared for the U.S. Department of Energy
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ABSTRACT

The degradation of steel by stress corrosion cracking (SCC) when exposed to atmospheric conditions for decades is a significant challenge in the fossil fuel and nuclear industries. SCC can occur when corrosive contaminants such as chlorides are deposited on a susceptible material in a tensile stress state. The Nuclear Regulatory Commission has identified chloride-induced SCC as a potential cause for concern in stainless steel used nuclear fuel (UNF) canisters in dry storage. Modeling contaminant deposition is the first step in predictive multiscale modeling of SCC which is essential to develop mitigation strategies, prioritize inspection, and ensure the integrity and performance of canisters, pipelines, and structural materials. A multiscale simulation approach can be developed to determine the likelihood that a canister would undergo SCC in a certain period of time.

This study investigates the potential of DUSTRAN, a dust dispersion modeling system developed by Pacific Northwest National Laboratory, to model the deposition of chloride contaminants from sea salt aerosols on a steel canister. Results from DUSTRAN simulations run with historical meteorological data were compared against measured chloride data at a coastal site in Maine. DUSTRAN's CALPUFF model tended to simulate concentrations higher than those measured; however, the closest estimations were within the same order of magnitude as the measured values. The decrease in discrepancies between measured and simulated values as the level of abstraction in wind speed decreased suggest that the model is sensitive to wind speed. However, the influence of other parameters such as the distinction between open-ocean and surf-zone sources and the choice of source-term function needs to be explored further. Deposition values predicted by the DUSTRAN system were not in agreement with concentration values and suggest that the deposition calculations may not fully represent physical processes. Overall, results indicate that with parameter refinement, DUSTRAN has the potential to simulate atmospheric chloride dispersion on steel canisters.

1.0 INTRODUCTION

1.1 Background

Stress corrosion cracking (SCC) of susceptible materials is a long-standing problem for canisters, pipelines, and structures, especially in the fossil fuel and nuclear industries. This work considers SCC of steel canisters used to store used nuclear fuel (UNF) as a test case. The choice of UNF canisters was warranted by the availability of reliable experimental data for validation. In the absence of a national geological repository, UNF produced by nuclear power plants is stored at the reactor site or independent spent fuel storage installations (ISFSIs) for an indeterminate period of time. There is concern about the long-term structural integrity of UNF canisters. Through-wall cracking of stainless steel systems exposed to atmospheric conditions has been observed at currently operating nuclear power plants (U.S. Nuclear Regulatory Commission 2012), and it is hypothesized that UNF canisters in dry storage may undergo through-wall cracks initiated by SCC. In consideration of long term storage of up to 160 years beyond the licensed life of the reactor, the U.S. Nuclear Regulatory Commission (2014) has acknowledged that "one time replacement of the spent fuel canisters and cask" may be required. This process is expensive and it is difficult to experimentally characterize the progress of degradation due to the long time scales involved. Predictive modeling is thus essential to assist in the development of mitigation strategies, prioritize inspection, and ensure the integrity and performance of canisters. A multiscale simulation approach can be utilized to determine the likelihood that a steel canister would undergo SCC in a certain period of time. A key component of this approach is a reliable model of the effects of local climactic conditions such as wind speed, ambient temperature, and humidity on the deposition of contaminants (Jensen et al. 2015).

1.2 DUSTRAN

DUSTRAN is a comprehensive dispersion modeling system developed by Pacific Northwest National Laboratory with the intention of modeling dust emissions generated by Department of Defense activities (Shaw et al. 2015). The software system, which uses the open-source GIS software MapWindow and has the necessary terrain and meteorological preprocessors, has the capability to simulate particulate transport, diffusion, and deposition using one of three widely-used, regulatory dispersion models: CALPUFF, CALGRID, or AERMOD. Additionally, DUSTRAN integrates a diagnostic meteorological model known as CALMET (Scire et al. 2000), which supplies gridded meteorological fields to the chosen dispersion model. Previous evaluation with positive results has been done (Shaw et al. 2008) regarding DUSTRAN's CALGRID model, which is used for wind-blown dust emissions where the entire model domain is a potential emission source. No evaluation has been done regarding DUSTRAN'S CALPUFF processor, which is used for active dust emissions where explicit source types can be identified. Because DUSTRAN is not optimized for the modeling of chloride particulate matter, this project seeks to evaluate the potential of DUSTRAN's CALPUFF processor in modeling chloride concentration and deposition due to sea salt aerosols generated from the ocean.

1.3 Maine coastal site

Various environmental monitoring procedures were implemented at a coastal site in Maine (Maine Site) (Figure 1) from August 2012 to December 2014. Details regarding the site were not authorized for disclosure. However, the site is representative of a coastal ISFSI and is optimal for studying sea salt aerosols as a source of atmospheric chloride contaminants. Data from the Maine Site was used for comparison against results generated by DUSTRAN.

Figure 1. The approximate location of the Maine Site where environmental monitoring was done. Details regarding the site were not authorized for release.

2.0 METHODS

The study consisted of two phases of simulation, with the latter phase operating on parameters that were modified based on the results and analysis of the previous phase. The following sections detail the procedures and parameters that were consistent throughout the study.

2.1 Calculating emission rates

Particulate emission rates for area sources were calculated using an open-ocean source function derived by Monahan et al. (1986). The function calculates continuous particle number-size distributions (dF_N/dr, where F_N is the number flux and r is a characteristic radius; unit: number of particles/(m^2 s µm)).

$$\frac{dF_N}{dr_{80}} = 1.373\, U_{10}^{3.41}\, r_{80}^{-3}\, (1 + 0.057\, r_{80}^{1.05}) \times 10^{1.19\, exp(-B^2)}$$

where r_{80} is the droplet radius in microns at a reference relative humidity of 80%, U_{10} is the wind speed (m/s) at an elevation of 10 m from the water surface, and $B = (0.380 - \log r_{80}) / 0.650$. This function is applicable to $U_{10} < 10$ m s^{-1} and $0.8 < r_{80} < 10$ µm. For DUSTRAN input, the emission rate is converted to g/s. It is worth noting that de Leeuw et al. (2000) provides a source function for waves breaking in the surf zone; for this study, a distinction was not made between open-ocean and surf-zone sources.

Various emission rates were used throughout the modeling process and were generated from three sets of wind speed data inputted into Monahan's function. Data was drawn from two offshore buoys: buoy station 44032 (also known as "E01"), maintained by the Northeastern Regional Association of Coastal Ocean Observing Systems (NERACOOS), and buoy station 44007, maintained by the National Data Buoy Center. Data was also drawn from the land station KIWI at the Wiscasset Airport (Figure 2). For both buoy stations, hourly wind speeds were given in m/s from the NERACOOS historical data portal. The following adjustments were made on the buoy data:

1. Buoy 44007 reported data exactly on the hour while buoy 40032 reported data every ten minutes. For consistency, only data exactly on the hour was entered into Monahan's function.
2. Missing data values were interpolated by averaging the two adjacent recorded values.
3. Anemometers for buoys were placed at 4 m and not the standard 10 m required by Monahan's function. The logarithmic wind profile was utilized to adjust for the wind shear effect (DTI Noise Working Group, 1996). A roughness length of 0.0001 representing water, snow, and sand surfaces was used in calculations.

Data from the land station KIWI was provided through the National Oceanic and Atmospheric Administration's (NOAA) Quality Controlled Local Climatological Data (QCLCD) portal. The following adjustments were made on the land station data:

1. The airport data was recorded in Coordinated Universal Time (UTC) and converted to Eastern Standard Time (EST).
2. The airport data was recorded for the most part on the fifty-third minute of the hour with a few data points arbitrarily recorded at other minutes of the hour. For consistency, only the data on the fifty-third minute was entered. The data times were rounded up and entered for the nearest hour mark, e.g. data recorded at 5:53 was entered for hour 6.
3. Wind speeds were recorded in mph and converted to m/s.
4. Missing data values were interpolated by averaging the two adjacent recorded values.

Figure 2. The locations of buoys 44007 and 44032 and the KIWI land weather station at the Wiscasset Airport are shown. The Maine Site is in the vicinity of the KIWI station.

2.2 Simulation parameters

DUSTRAN is a system which has the capability to run three independent dispersion models: CALPUFF, CALGRID, and AERMOD. For this project, all simulations were run using CALPUFF, a multi-layer, multi-species non-steady-state Lagrangian puff dispersion model (Scire et al. 2000). CALPUFF is optimized for mid-sized domains of up to 200 km, models wind non-linearly, and is recommended by the U.S. Environmental Protection agency for the long-range transport characteristic of sea salt aerosol dispersion from the ocean.

All simulations were run on a 200 km by 200 km domain (Figure 3) within Universal Transverse Mercator zone 19.

All DUSTRAN simulation start times must be before sunrise because of the explicit use of the surface energy balance method in CALMET (Shaw et al. 2008). As a result, the start time for the run was set at the default 4:00 AM EST. The software allowed for the release period to start at a different time than the run period; the start time for the release period was set at 9:00 AM EST on the same day as the start of the run period. The run duration was therefore five hours longer than the release duration. Only data calculated during the release duration was analyzed.

DUSTRAN applies a single set of hourly meteorological data denoted “Single Observation” across the entire domain and run duration. For all simulations, the meteorological data from the Wiscasset Airport weather station KIWI was used as input. The data was provided through NOAA’s QCLCD portal. The same adjustments were made on the Wiscasset Airport data for DUSTRAN input as were made for input into Monahan’s function for calculation of emission rates. Additionally, the mixing height and atmospheric stability parameters were left constant at 1000 m and D-Neutral, respectively.

DUSTRAN has the capability to run point sources, line sources, and area sources. Area sources were determined to most accurately represent open-ocean and were the only sources assigned nonzero emission rates. In both phases of simulation, a single trapezoidal area source was defined (Figure 3). The parameters required by area sources can be seen in Figure 4. The following parameters were left at default values: effective height above ground (0 m), effective rise velocity (1 m/s), effective radius (1 m), and initial vertical spread (1 m). The air temperature for area sources was entered as the average air temperature over the run duration and given by NERACOOS historical data. At the start of this study, DUSTRAN had the capability to run a single set of emission rates, one rate per species, over the entire run duration. This capability was later expanded. The emission rates in mass per area-time were calculated by Monahan’s function as noted previously and converted into mass per time by the source term area. Additionally, the software allocates a polar grid of receptors to point sources; though point sources were not considered in this study as a source of sea salt aerosols, a point source was assigned to the Maine Site and given emission rates of zero to increase the concentration of receptors near the site.

DUSTRAN provides four default species defined by particulate diameter in microns: $PM_{2.5}$, PM_{10}, PM_{15}, and PM_{30}. Only $PM_{2.5}$ and PM_{10} were modeled to remain inside the applicability limits of Monahan’s function.

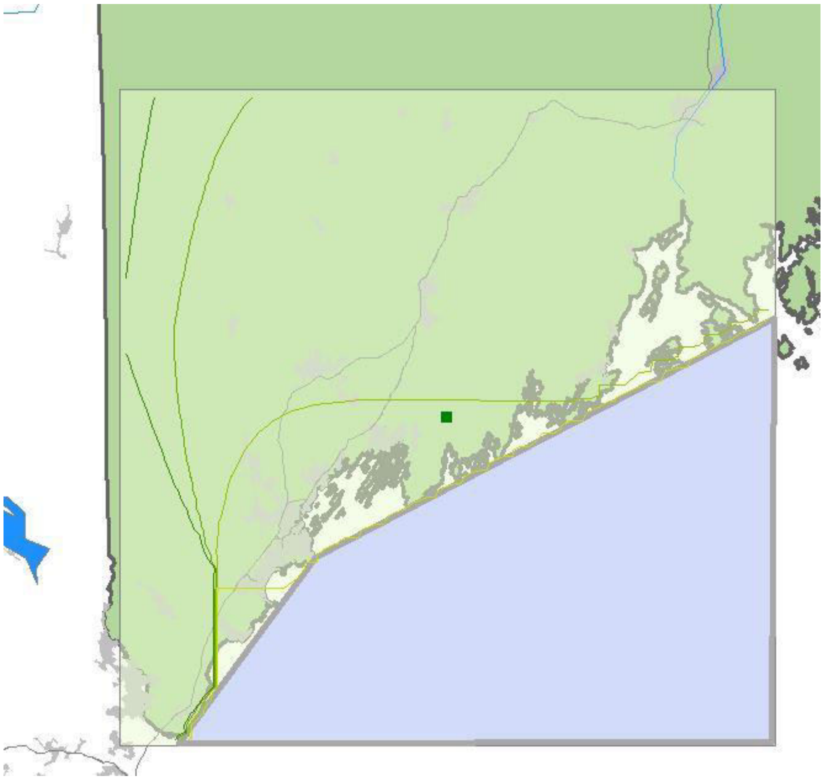

Figure 3. The opaque rectangle represents the domain and the blue trapezoid represents the user-defined area source used for all DUSTRAN simulations. The green marker represents the Maine Site.

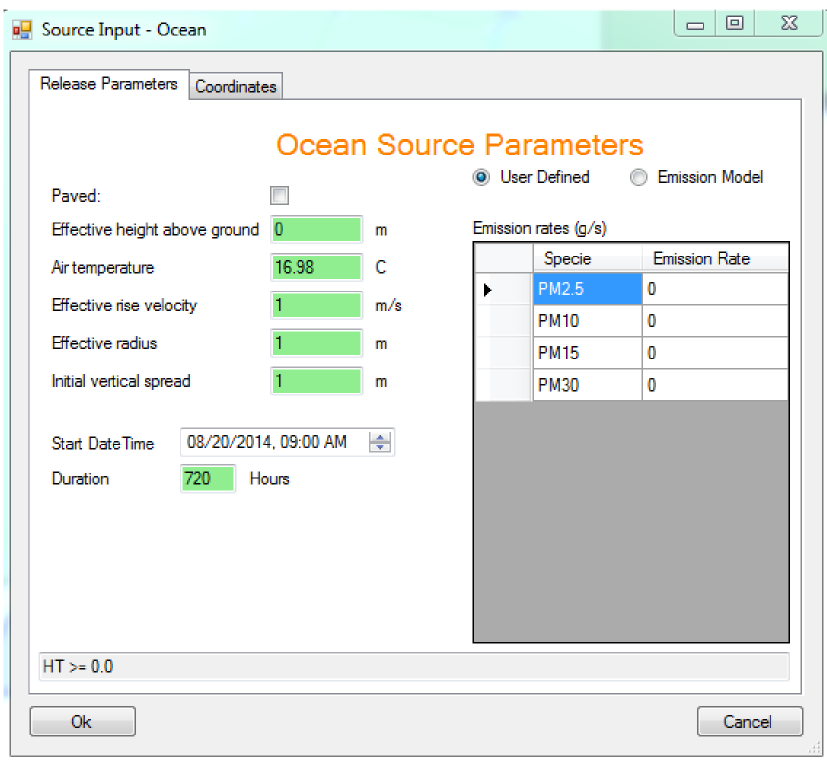

Figure 4. The parameters required for a DUSTRAN area source. Sample input is shown.

2.3 Time periods used in simulation

At the onset of this study, DUSTRAN was capable of running one set of emission rates across the entire run duration. The first phase of simulation used a single set of emission rates. For each species, the average hourly rate was calculated for each buoy and those two average rates were then averaged again to produce a final rate. Time periods to be studied thus had to be chosen during relatively stable wind speed patterns to prevent outliers from biasing the average emission rates. The study was also constrained by available data from the Maine Site; data collection methods and durations at the site were not consistent across the period of environmental monitoring. The following time periods were chosen for study:

1. April 21, 2014 – April 22, 2014 (24-hour release duration)
2. April 22, 2014 – April 23, 2014 (24-hour release duration)
3. May 20, 2014 – May 27, 2014 (7-day release duration)
4. August 20, 2014 – September 19, 2014 (30-day release duration)
5. October 13, 2014 – October 20, 2014 (7-day release duration)

The specific start and end times were as discussed previously. For comparison with available Maine Site data, the two 24-hour periods and two 7-day periods were modeled for concentration while the 30-day period was modeled for deposition.

2.4 Parsing and manipulation of output for comparison against measured data

DUSTRAN's CALPUFF model creates a 50 by 50 grid of receptors over the domain regardless of the type or number of sources used. Since a domain of 200 km was uniformly used, the spacing between grid receptors was 4 km. As noted previously, a single point source with emission rates of zero was used in each simulation to generate a polar grid of receptors around a point within the Maine Site (Figure 5). DUSTRAN does not provide the ability to precisely place a point source; the center of the polar grid coincided with the center of the simulation domain which was within the Maine Site but did not coincide exactly with the locations of the monitoring equipment used onsite. The polar grid consists of 360 discrete receptors placed 10 degrees apart at radial distances of 200, 400, 800, 1500, 2500, 3500, 4500, 5500, 6500, and 7500 m from the center point. The output file contains concentration data and dry flux (also known as deposition rate or deposition) data for every hour of the run duration. Four different Java applications were written to parse through and organize the output data.

1. Single point in time. This program took in a location given by latitude and longitude coordinates and an hour during the run duration and outputted the concentration or deposition for each species at that hour as given by the closest grid receptor and closest discrete receptor.
2. Average over time. This program took in a location given by latitude and longitude coordinates and outputted the average concentration or deposition for each species across the release duration as given by the closest grid receptor and closest discrete receptor.
3. Average across space. This program outputted the average concentration or deposition across each of the ten radial rings of discrete receptors on an hourly basis.
4. Average across space and time. This program outputted the average concentration across a given radial ring of discrete receptors over the release duration.

Because Maine Site data was reported as averages over the data collection period, DUSTRAN results were also analyzed as averages across the release duration. Additionally, a statistical analysis of concentrations and depositions from sample runs showed low variability across the rings of the polar grid and only a slight increase in variance as radial distance increased. It was decided that an average over both space and time would provide the best comparison against Maine Site data.

The Maine Site reported that the majority of sodium chloride particles were between three and five microns in diameter. The DUSTRAN results for $PM_{2.5}$ and PM_{10} were added together for comparison for both concentration and deposition.

In summary, for each species, the average concentration or deposition was calculated across the receptors in the 7500 m ring on an hourly basis. All the hourly averages were then averaged over the release duration. These averages across both space and time, one for each species, were then added together. The numbers reported as DUSTRAN results represent this sum. Henceforth the terms “concentration” or “deposition” represent the values calculated as such.

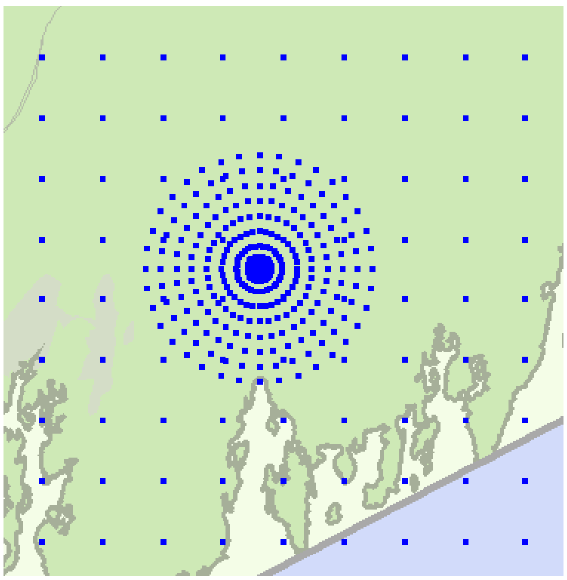

Figure 5. A polar grid of discrete receptors created around a point source and a uniform grid created across the modeling domain in DUSTRAN.

3.0 RESULTS AND DISCUSSION

3.1 Single emission rates

The first phase of simulation used a single set of emission rates throughout the run duration. For each buoy, hourly emission rates for each species were calculated. These hourly rates were averaged to produce a rate for each species for each buoy. The sets from the two buoys were then averaged together to produce a single set used for simulation. Table 1 displays the concentration results generated by DUSTRAN’s CALPUFF processor and the measured values at the Maine Site.

Time Period	DUSTRAN (μg/m³)	Maine Site (μg/m³)
4/21/14 – 4/22/14	192	2.53[1, 3]
4/22/14 – 4/23/14	4.47E8	1.80[1, 4]
5/20/14 – 5/27/14	33.5	0.173[2]
10/13/14 – 10/20/14	188	0.585[2]

Table 1. Chloride concentration values modeled using single emission rates and as measured at the Maine Site.

1. A 5-micron filter was used during the 24-hour time periods.
2. A 2-micron filter was used during the 7-day time periods.
3. The mass of the loaded filter was less than the tare weight of the filter, resulting in a negative particulate mass.
4. The loaded filter mass is nearly two times the tare weight of the filter, indicating an unlikely amount of particulate loading.

The modeled concentrations ranged from two orders of magnitude to eight orders of magnitude greater than those measured at the Maine Site. It was suspected that the emission rates were biased high because they were calculated from offshore wind speeds. It has been observed that wind speeds decrease as distance to shore decreases; the emission rates were perhaps an unfair representation of the entire area source. Notably, the simulated concentration during the period of April 22 to April 23 is eight orders of magnitude from the measured concentration. It was theorized that a few hours of high wind speeds had led to unusually high emissions rates which caused a significant raise in the average emission rate.

A sensitivity analysis was done to pinpoint the factors that needed to be more carefully considered to improve the accuracy of the model. The following regression plots and time-series plots were generated for the two 7-day periods: concentration vs. wind direction, concentration vs. time, concentration vs. buoy wind speed, buoy wind speed vs. time, concentration vs. temperature, and concentration and wind speed vs. time (Figure 6).

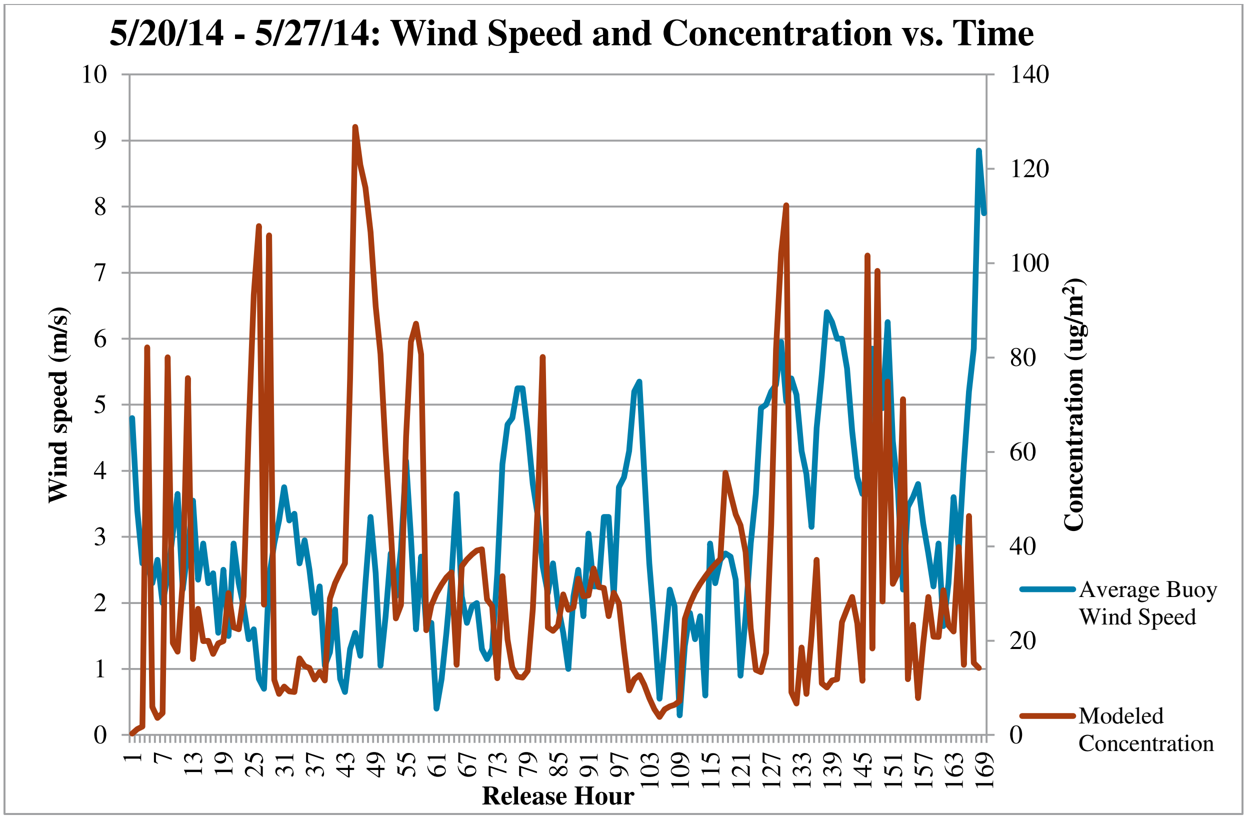

Figure 6. A plot of the average wind speed between buoys 44007 and 44032 and modeled concentrations throughout the release duration during the 5/20/14 – 5/27/14 time period.

Though there was no one-to-one correlation, the time-series plot revealed a cyclic pattern in wind speeds as is consistent with meteorological observation. A similar cyclic pattern was observed in concentration, suggesting that the concentration model was sensitive to wind speed. It was theorized that the usage of single emission rates across the entire run duration was not sufficient. A statistical analysis of average emission rates calculated for both buoys revealed standard deviations greater than the mean in all cases, further suggesting that the set of single emission rates did not accurately represent the time periods. Other plots did not appear to show significant trends.

Table 2 displays the deposition results generated by DUSTRAN and the measured values at the Maine Site.

Time Period	DUSTRAN (µg/(m^2 s))	Maine Site (µg/(m^2 s))
8/20/14 – 9/19/14	0.089	0.050

Table 2. Chloride deposition values modeled using single emission rates and as measured at the Maine Site.

Compared to concentration, there was less discrepancy between the simulated deposition value and the measured deposition value. As discussed previously, simulated concentration values were not in agreement with measured concentration values and it would be expected that consequently, simulated deposition values would not agree. This suggests the algorithm used by DUSTRAN's CALPUFF model may not adequately characterize chloride deposition, since as simulated concentration values decrease towards measured values with refinements in the model, simulated deposition values will decrease non-linearly away from measured values. This may be explained by the way CALPUFF handles deposition. CALPUFF calculates a deposition velocity, defined to be the rate at which particulate mass is ejected from a plume, based on surface roughness and wind speed. This deposition velocity is a bulk rate used for the entire plume; as mass is ejected from the plume, the deposition on the ground increases while the concentration in the plume decreases. If the surface roughness and wind speed parameters are not accurate, this may result in a low deposition velocity, which means the concentration calculated in the plume will be higher than the deposition calculated on the ground as a result of low rate of mass depletion. There may also be a cancellation of errors effect in the deposition model. This issue was not explored further in the study. Future work will incorporate a more robust deposition model into DUSTRAN.

3.2 Hourly emission rates

In response to the sensitivity analysis, the modeling procedure was altered to more accurately integrate variable wind speeds. The DUSTRAN software was revised to run with hourly emission rates as input. Additionally, the wind speeds from the two buoys were averaged with those from the land station at the Wiscasset Airport to produce a set of wind speeds more representative of the entire area source. Before averaging, the Wiscasset Airport wind speeds were adjusted to 4 m height using the logarithmic wind profile. This averaged set was then inputted into Monahan's function to produce a set of hourly emission rates. Table 3 displays the concentration results generated by DUSTRAN and the measured values at the Maine Site.

Time Period	DUSTRAN (μg/m^3)	Maine Site (μg/m^3)
4/21/14 – 4/22/14	29.0	2.54[1, 3]
4/22/14 – 4/23/14	2.13	1.80[1, 4]
5/20/14 – 5/27/14	4.27	0.173[2]
10/13/14 – 10/20/14	33.1	0.585[2]

Table 3. Chloride concentration values modeled using hourly emission rates and as measured at the Maine Site.

1. A 5-micron filter was used during the 24-hour time periods.
2. A 2-micron filter was used during the 7-day time periods.
3. The mass of the loaded filter was less than the tare weight of the filter, resulting in a negative particulate mass.
4. The loaded filter mass is nearly two times the tare weight of the filter, indicating an unlikely amount of particulate loading.

The results generated by DUSTRAN ranged from within an order of magnitude to two orders of magnitude greater than those measured at the Maine Site. It is apparent that modifying DUSTRAN to use hourly emission rates and using the averages of buoy and land wind speeds improved the agreement between measured and modeled chloride concentrations. However, it is unclear at this time why there is a variation in differences between simulated and measured results: the 24-hour period from April 22 to April 23 produced a value that differed from the measured value by a factor of less than two while the 7-day period from October 13 to October 20 produced a value two orders of magnitude greater than the measured value.

There are a variety of possible factors causing the discrepancy between simulated and measured results. The DUSTRAN parameters left at default value (effective height above ground, effective rise velocity, effective radius, initial vertical spread, mixing height, and atmospheric stability) may have a greater influence on dispersion and deposition than previously thought. Though temperature is not used in Monahan's function for calculating emission rates and the sensitivity analysis did not appear to show a strong correlation between temperature and concentration, the usage of a single average temperature across the release duration may also be contributing to an inaccurate model.

Additionally, it is likely that DUSTRAN's capability to model using a single set of meteorological data is not sufficient in accurately modeling local climactic conditions across the whole domain. Data from the KIWI land station was used in all simulations; in most cases, weather conditions recorded on land would be milder than those recorded offshore. If this factor was to be a cause for error, it would underestimate concentrations relative to those measured. The choice of single observation meteorological data therefore must not have had a substantial influence on the overestimated concentrations. However, the input of meteorological data at a single point and CALPUFF's subsequent extrapolation of that data across the 200 km domain is a likely source of discrepancy. If DUSTRAN is to be used in creating an accurate model of steel canister degradation, it is recommended that the modeling system be revised to integrate multiple meteorological data sets. This is an existing function within CALMET.

Furthermore, receptor location and height could have contributed to the discrepancy between simulated and measured concentrations. For the Maine Site it was unclear where equipment was placed in regards to nearby structures and natural barriers. If filters were placed behind a wind-blocking structure, measured concentrations could have been less than characteristic of the area. Receptor height also has a possible influence. The discrete receptors in the polar grid used to calculate simulated results were placed at ground level. However, the gridded receptors were placed at a height of 10 m and there was not a significant difference between concentrations calculated at discrete and gridded receptors. The Maine Site filter height was also ambiguous. If it is to be assumed that filters were placed at ground level, then receptor height could not have contributed to the discrepancies. If filters were placed above ground level, then the measured concentrations would be lower after adjustments were made for height and the discrepancy between simulated and measured concentrations would then be greater. It would appear that receptor height did not influence overestimation, though it is recommended that a sensitivity analysis on receptor height be performed. It may also be worthwhile to use other experimental data sets for validation to make the model generally applicable.

Emission rates were calculated using Monahan's function. Because the model is a power law, emission rates and thus concentrations will grow exponentially with wind speed. Because Monahan's function is only applicable for wind speeds up to 10 m/s, the meteorological data used in simulation was a likely factor in yielding high results because wind speeds were included that were outside of the applicability range. However, other source term functions may improve DUSTRAN's predictive power. Andreas (1998) notes Monahan's function is the best function for predicting the production of film and jet droplets but tends to predict too many droplets. Additionally, Monahan's function was derived from observations in a windless wave tank and thus may not accurately represent "spume" droplets, produced by wind blowing across wave crests. Andreas uses Monahan's function to amplify a function derived by Smith et al (1993) to produce a spray generation function applicable for wind speeds up to 32 m/s. Exploration of Andreas' function may yield results more in agreement with experimental values.

Finally, the analysis of ocean waters near the Maine Site as a single area source likely had a great influence in the discrepancy. It is known that the surf-zone, defined to be location of wave breaks, has a greater contribution to the production of sea salt aerosols than open-ocean. The lack of distinction between surf-zone and open-ocean sources most likely obscured the true behavior of sea salt aerosols: emission rates would be overestimated in areas far offshore with no wave-break action and underestimated in areas nearshore where waves are known to break. It is theorized that the averaging of wind speeds in the second iteration of the model decreased the discrepancies between measured and simulated concentrations for this reason. The averaging process eliminated high wind speeds from open-ocean and likely produced wind speeds more representative of the surf-zone. It is recommended that future models consider separately open-ocean and surf-zone sources to account for wave-breaking behavior.

4.0 CONCLUSION

Comparisons of simulated and measured data have provided encouragement as to the potential practical value of DUSTRAN in predicting the dispersion of atmospheric chloride from sea salt aerosols. Though modeled concentrations tended to be greater than measured concentrations, the decrease in error as the level of data abstraction decreased suggest that both further refinement in the software system and more detailed input would result in more accurate predictions. It was shown that revisions to run hourly emission rates resulted in a decrease in discrepancies between measured and simulated values.

In future research, refinements to the modeling system will be made. The extent of the influence of other parameters such as receptor height, meteorological data, and particularly the distinction between open-ocean and surf-zone sources may need to be explored further. A switch to a grid-based transport model such as CALGRID would allow for a more refined gridded emission source term compared to the plumes modeled by CALPUFF, and different source term functions may better incorporate physical processes and yield more reasonable estimates. The refinement of models with consideration to more experimental data sets may also improve predictive power. The significance of this work is that DUSTRAN has been validated against experimental data, deficiencies in the models have been identified, and areas for improvement are discussed. Overall, results demonstrate DUSTRAN's potential in the application of atmospheric chloride dispersion and transport modeling for stress corrosion cracking of steel canisters.

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