Memo

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	Shell Global Solutions Inc..		Stantec Consulting Ltd.
File:	123513075	Date:	January 29, 2019

Reference: Condensate Spill Modelling (Privileged and Confidential)

INTRODUCTION

Between the dates of October 3 and October 7 2018, it is estimated that approximately 29 m^3 of condensate leaked into a canal in the vicinity of the NAM gas condensate storage facility (The Facility) located in Farmsum/Delfzijl, Netherlands.

This document is prepared by Stantec Consulting Ltd (Stantec) at the request of Shell Global Solutions Inc (Shell). This document summarizes the methodology, results and observations associated with source and dispersion modelling associated with the condensate spill and is divided into the following main sections:

- System Description,
- Hazard Identification,
- Source Characterization,
- Dispersion Modelling, and
- Results and Discussions.

The process group at the Facility has refined assumptions relating to the release event. This document intends to use this more refined information in conjunction with the weather conditions at the time to provide estimates of potential exposure in the vicinity of the release.

SYSTEM DESCRIPTION

It is currently understood that the condensate was released from the process into a rainwater sewer, and subsequently, into a canal to the northwest of the facility. The process group, associated with the facility, estimates that approximately 24 m^3 of condensate was released at a rate of 23 m^3/hr followed by the remaining 5 m^3 being released over approximately 72 hours. Additionally, it is estimated that the release started between 01:00 and 06:00 on October 4, 2018.

The surrounding area, approximate release point and locations of the containment booms are shown in Figure 1. The booms were placed in the canal on October 4 to support clean-up activities. The natural flow within the canal is typically to the north-east away from the release point and toward the outer main channel. In the event of back flow, the booms would serve to mitigate against flow of condensate to the south-west. The water surface area within the booms was estimated to be approximately 4,970 m^2. For the purposes of this assessment, the surrounding area is categorized as suburban and includes residential areas that are, at a minimum, approximately 60 m from the booms.

The composition of the natural gas condensate considered within the current assessment is provided in Table 1. Benzene is observed to be the largest constituent of the mixture. The parameters describing the system for modelling purposes are provided in Table 2. As there was uncertainty in the spill and water temperatures at the time of the release they were chosen to overstate the evaporation rates. Based on a review of ocean temperatures in the Netherlands, It is anticipated that the water in the canal would be below 20 ˚C in October.

Figure 1 **Aerial Image Indicating the Condensate Release Location Relative to Containment Booms and Populated Areas**

Table 1 Composition of Natural Gas Condensate Used in Modelling[1]

Component	Fraction (%)	
	Molar	Mass
Methane	0.007	0.001
Ethane	0.300	0.084
Propane	1.338	0.549
Isobutane	0.756	0.409
n-Butane	1.845	0.998
neoPentane	0.072	0.048
Isopentane	1.989	1.335
n-Pentane	2.948	1.979
Cyclopentane	0.167	0.109
n-Hexane	4.550	3.648
n-Heptane	3.917	3.652
Methylcyclopentane	1.052	0.824
Benzene	17.642	12.822
Cyclohexane	3.466	2.714
n-Hexane	5.304	4.253
n-Heptane	4.037	3.764
Methylcyclohexane	4.981	4.551
Toluene	5.569	4.774
n-Octane	9.193	9.771
Ethylbenzene	0.411	0.406
o-Xylene	2.833	2.798
n-Nonane	7.092	8.457
n-Decane	7.929	10.498
n-Undecane	4.302	6.257
n-Dodecane	2.615	4.145
n-Tridecane	1.851	3.176
n-Tetradecane	1.344	2.480
n-Pentadecane	0.893	1.765
n-Hexadecane	0.536	1.130
n-Heptadecane	0.366	0.819
n-Octadecane	0.277	0.657
n-Nonadecane	0.170	0.424
n-Eicosane	0.093	0.245
n-Heneicosane	0.058	0.160
n-Docosane	0.034	0.097
n-Tricosane	0.020	0.060

[1] Based on composition from Shell dated November 11, 2018 “CEMSETS model Results.”

Component	Fraction (%)	
	Molar	Mass
n-Tetracosane	0.024	0.076
n-Hexacosane	0.018	0.060
n-Triacontane	0.001	0.005

Table 2 Selected Modelling Parameters

Parameter	Units	Value
Area Within Booms	m^2	4,970
Ambient Temperature	˚C	Varying based on Observations
Water Temperature (2)	˚C	20
Spill Temperature	˚C	20
Spill Volume	m^3	29
Spill Rate	m^3/hr	23 and .07(1)
Event Start (Assumed for Modelling)		~October-04, 04:00
Spill Duration	hours	~73
Condensate Density (101.325 kPa, 20 ˚C)	kg/m^3	739.8
Notes: 1 24 m^3 spilled at a rate of 23 m^3/hr, 5 m^3 spilled at a rate of .07 m^3/hr 2 Uncertainty in temperature at time of release, anticipated to be lower and selected to overstate evaporation rate		

HAZARD IDENTIFICATION

The hazard considered for the current assessment is the potential toxicity of vapours evolved from the fluid during the release event. Based on a review of the condensate component partial pressures at ambient conditions and previous work completed by Shell, the compound of primary concern, from an inhalation perspective, was determined to be Benzene.

This assessment will delineate the hazard based on the extents of exposure guidelines put forward by regulatory agencies. The extents of the Dutch "Information Limit Value" and "Information Alarm Value" for Benzene are used to assess the hazard. These values are equivalent to the acute exposure guideline levels, the AEGL-1 and AEGL-2, respectively put forward by the United States Environmental Protection Agency (EPA). Descriptions of these levels are provided in Table 3.

Additionally, selected values associated with occupational exposure will be used to delineate the outer extents of the plume. Shell and many jurisdictions use a 15-minute average of 2.5 ppm Benzene as a short-term exposure limit. A value of 0.2 ppm is used in the Netherlands as a time-weighted-average (TWA) 8-hour concentration that a worker can be exposed to continuously during a normal work week.

Table 3 Endpoint Description

Level	1-Hour /8-Hour (ppm)	Description [1]
Information Limit Value (AEGL-1)	52/9	Is the airborne concentration (expressed as ppm or mg/m^3) of a substance above which it is predicted that the general population, including susceptible individuals, could experience notable discomfort, irritation, or certain asymptomatic non-sensory effects. However, the effects are not disabling and are transient and reversible upon cessation of exposure.
Information Alarm Value (AEGL-2)	800/200	Is the airborne concentration (expressed as ppm or mg/m^3) of a substance above which it is predicted that the general population, including susceptible individuals, could experience irreversible or other serious, long-lasting adverse health effects or an impaired ability to escape.
Notes: 1 https://response.restoration.noaa.gov/oil-and-chemical-spills/chemical-spills/resources/acute-exposure-guideline-levels-aegls.html		

SOURCE CHARACTERIZATION

Source modelling was completed to estimate source parameters required for the subsequent dispersion modelling. Source parameters that can affect the dispersion modelling include:

- The emission rate,
- Source area,
- Source temperature, and
- Source density.

The modelling of the condensate spill was completed using a multicomponent pool spread and evaporation model. The pool size and constituent emission rates will be estimated by conducting mass, momentum and energy balances on the spreading pool.

The pool model uses a generally accepted empirical mass transfer coefficient correlation proposed by Mckay and Matsugi (Fernandez et al 2012). This relationship finds use within accepted hazard models and the EPA Water 9 model and characterizes the vapour phase resistance to mass transfer at a specified ambient wind speed. The current assessment assumes the vapour phase resistance to mass transfer is dominant and will neglect the liquid phase resistance. The vapour phase resistance controls the rate at which mass is transferred across the vapour/liquid interface. The liquid phase resistance controls the rate of mass transfer through the bulk fluid and to the vapour/liquid interface. It is anticipated that neglecting the liquid phase resistance will provide a reasonable and conservative (overstated) estimate of the benzene emission rate and the subsequent consequence extents. The correlations used to estimate the vapour phase resistance for a given component assume the mass transfer rate depends on parameters including the concentration of the component in the vapour at the interface, the diffusivity of the component in air, the size of the pool and the ambient wind speed.

The component concentration in the vapour at the vapour/liquid interface is estimated using the liquid phase fugacity coefficient and the component liquid phase concentration. This methodology is used in place of the often used Raoult's Law, which equates the liquid phase fugacity to the pure component vapour pressure. The methodology is dependant on the liquid pool composition, pool temperature and ambient pressure and allows for consideration of a wider range of component volatilities in the liquid phase than Raoult's Law. In the current assessment, the fugacity coefficient is obtained from the advanced Peng-Robinson equation of state (Peng&Robinson 1976) as implemented in a Virtual Materials Group (VMG) thermodynamic engine.

The pool temperature is estimated based on the heat and mass balance through consideration of heat transfer modes including:

- Incoming solar and long wave radiation,
- Free convection from the water, and
- Forced convection from the ambient surroundings.

In addition, the evaporation of vapour from the pool and spill of liquid into the pool contribute to the temperature change by further transferring energy to/from the pool. The composition of the pool is estimated by tracking the influx and evaporation of each component. Estimates of the temperature and composition of the liquid are used to estimate the concentration of each component in the air above the pool (vapour/liquid interface).

Concurrent estimates of the pool size through a mass and momentum balance in conjunction with the input ambient wind speeds allow the estimate of the overall vapour emission rate, the vapour composition and benzene emission rates used in the subsequent dispersion modelling.

The pool spread and evaporation modelling was completed with the following additional assumptions:

- Minimum condensate "slick" thicknesses of 1 mm, 3 mm, and 5 mm;
- Pool is confined to the 4,970 m^2 area (Table 2);
- Incoming solar radiation ranges from 0 W/m^2 to 700 W/m^2 (typical incoming solar radiation values for northern latitudes), assumed to depend on the estimated stability and the time of day, at each hour of the event;
- Water temperatures of 20 ˚C (Table 2);
- Ambient temperatures based on observations; and
- Wind speeds based on observations.

A brief review of oil spill observations indicated that spill minimum thicknesses ranging from a few 100 microns to tens of millimeters have been observed, with more observations in the range of a few millimeters. This brief review provided the basis for the minimum condensate "slick" thickness range considered (1 mm to 5 mm).

As indicated in the System Description section and for the purpose of providing information to be used in the assessment of potential health effects, the source modelling and subsequent dispersion modelling was completed assuming a 3-day release of 29 m^3 of condensate. Based on the information provided It was assumed that 24 m^3 was released at 23 m^3/hour, immediately followed by the remaining 5 m^3, which was released at a rate of 0.07 m^3/hr.

DISPERSION MODELLING

The SLAB dispersion model was used for the current assessment (Ermak 1990). The SLAB model is capable of modelling releases of buoyant and dense gases and contains algorithms to estimate the effects of phase change within the plume and reduced air entrainment resulting from stable density gradients between the plume and the ambient air. The SLAB model has been validated for a wide range of scenarios and is one of the U.S. EPA recommended models for hazard assessments. Additionally, the SLAB model is recognized by the Netherlands Organization for Applied Scientific Research (TNO) and described in the organization's "Yellow Book" which outlines methods for the calculation of physical effects due to hazardous releases (TNO 2005).

Based on the provided estimates of the release start, duration and profile, the SLAB dispersion model was applied for weather conditions observed during the event. The observations were obtained primarily from two weather stations:

- Nieuw Beerta (KNMI 2019)– Regional weather station located approximately 22 km south east of the release site and further inland;
- Delfzijl (Meteo Delfzijl 2019) – Weather station at a private residence, in a residential area located about 1 km from the release site.

The Nieuw Beerta station is further inland and there is a difference in the orientation of the water body when compared to Delfzijl which may impact the observed wind directions. The Delfzijl observation site is closer to the spill site but is located on a private residence in a residential area and the observations may be influenced by the structure it is attached to and the surrounding structures. For these reasons, predictions will be made using both sites to provide a range of potential impacts and review the sensitivity of the predictions to the choice of weather data.

The atmospheric stability is an indication of the level of turbulence and hence the dispersive capability of the atmosphere. A classification scheme which has six categories ranging from Class A (very unstable) to Class F (moderately stable) was considered to characterize atmospheric stability. The occurrence of these stability conditions can be summarized as follows:

- Unstable Conditions (Classes A through C) are characterized by strong to moderate incoming solar radiation and low to moderate wind speeds. These conditions typically occur on calm, warm, and sunny days where ground heating results in vertical motion of air within the layer of the atmosphere close to the surface. This vertical motion results in increased turbulence. Unstable conditions are restricted to daylight hours.
- Neutral Conditions (Class D) often occurs during overcast conditions or conditions with moderate to high wind speeds. Neutral stability can occur at any time during the day or night.
- Stable Conditions (Classes E and F) typically occur on calm cool clear nights where radiative cooling of the ground relative to the layer of air above it results in a stable temperature gradient (increasing temperature with altitude). This stable gradient dampens vertical motion and results in a reduction in the level of turbulence. Stable conditions generally occur during nighttime hours.

The atmospheric stability was estimated using the simplified STAR (stability array) methodology which requires the following:

- Horizontal wind speed,
- Cloud cover,
- Ceiling height, and
- Time of day.

As cloud cover observations were not available at the Nieuw Beerta station, they were obtained from the Eelde station (located 30 km south-west of the spill area). The ceiling height was not available, but a large value was conservatively assumed as this predicts more stable conditions. (and thus, higher ground-level concentration predictions).

A surface roughness parameter of 10 cm was used as the winds in the directions from the pool to the surrounding residents are observed to come from a region that would be anticipated to result in less turbulence than would be typically attributed to urban or sub-urban land use. Additionally, the ambient temperatures observed at the stations were used in the dispersion and source modelling. The water temperature is anticipated to have more of an impact than the ambient temperature on the source modelling (higher water temperature promotes evaporation) and a temperature of 20 ˚C was assumed.

For the purposes of the dispersion modelling an effective source with the same crosswind and downwind dimensions was assumed. This will provide the largest downwind extents from the downwind edge of the assumed pool. The pool was always assumed to be attached to the upstream boom and the pool source center was positioned at a downstream location, at a distance equal to a half-width of the pool.

The source and dispersion modelling were completed for the duration of the event with consideration of the time varying weather conditions (including the wind direction). The results were processed and presented for selected averaging times and compared to the criteria discussed in the Hazard Identification section. As an example, the observed and estimated weather conditions when the wind is blowing from the pool to the nearby residences, are provided in Table 4.

Table 4 Sample of Observed Weather and Estimated Stability Conditions in the Vicinity Based on the Nieuw Beerta Monitoring Station[1]

Date	Hour of Day	Cloud Cover [2] (eighths)	Wind Speed (m/s)	Temperature (deg C)	Stability	Wind Direction [3] (Degrees)
06/10/2018	22	8	8	12.4	D	350
06/10/2018	23	8	10	11.3	D	360
07/10/2018	24	8	10	10.9	D	10
07/10/2018	1	8	9	10.5	D	20
07/10/2018	2	8	8	10	D	10
07/10/2018	3	8	7	9.7	D	20
07/10/2018	4	8	5	9	D	30

Notes:
1 https://www.knmi.nl/nederland-nu/klimatologie/uurgegevens
2 Cloud cover data obtained from Eelde weather station.
3 Wind direction blowing from.

RESULTS

SOURCE MODELLING

Review of the initial sensitivity run results indicated that varying the pool minimum thickness produced less than a 0.1% difference in predicted peak benzene emission rate, for the cases reviewed. As a result, the results will be presented for a condensate pool minimum thickness of 3 mm.

For the purpose of estimating the potential health effects in the vicinity of the spill, the provided release rate profile was assumed, and the source modelling was completed with consideration of the time varying weather conditions. The estimated pool area and benzene emission rate over the first 8 hours of the release are shown for the two weather condition assumptions in Figure 2 and Figure 3, respectively. The following observations are made related to the source modelling results:

- The benzene emission rate is predicted to decay rapidly once the high initial release rate phase has ended,
- The peak emission is higher when the Nieuw Beerta weather observations are used,
- The average emission rate for the second and third hour are higher when the Delfzijl observations are used, and
- The estimated pool area is predicted to reach the maximum boomed area (4970 m^2) when the Delfzijl observations are used.

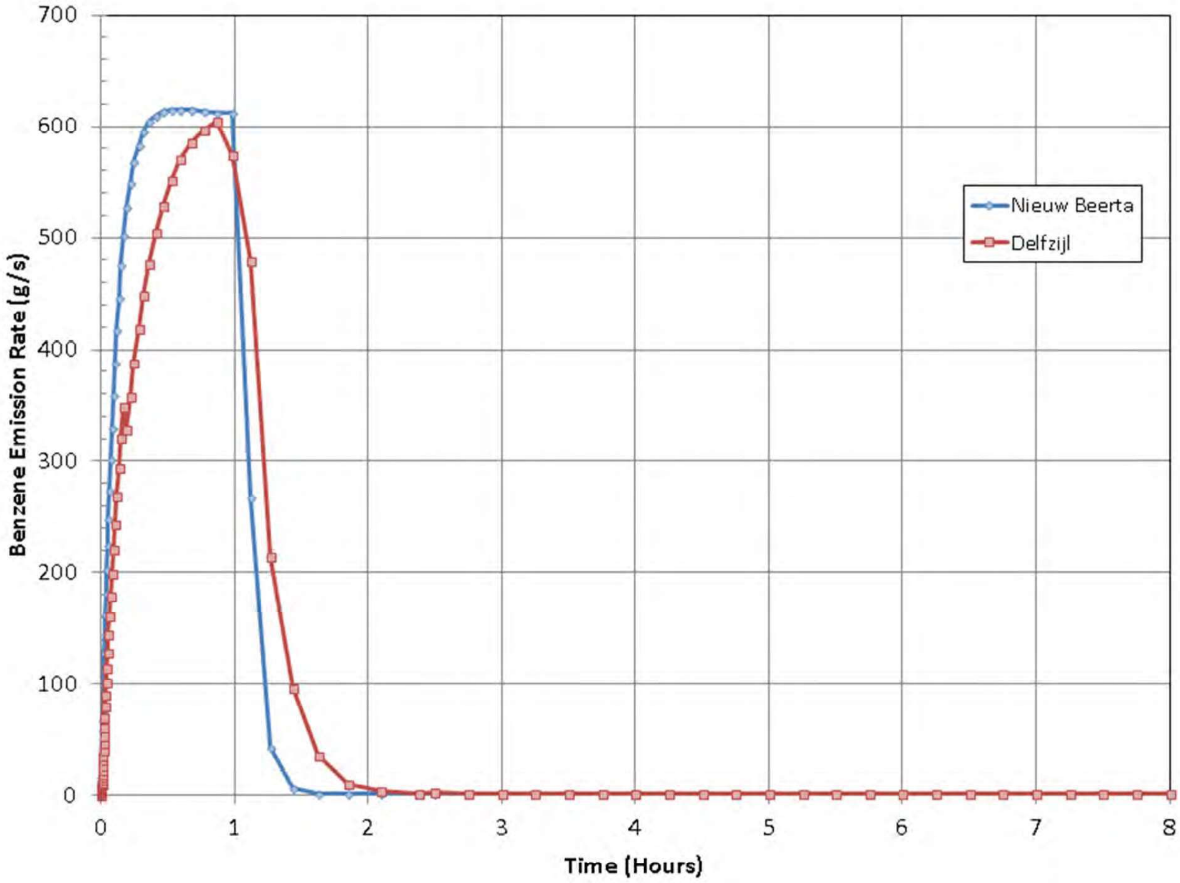

Figure 2 **Predicted Benzene Emission Rate, For the First 8 hours of the Release**

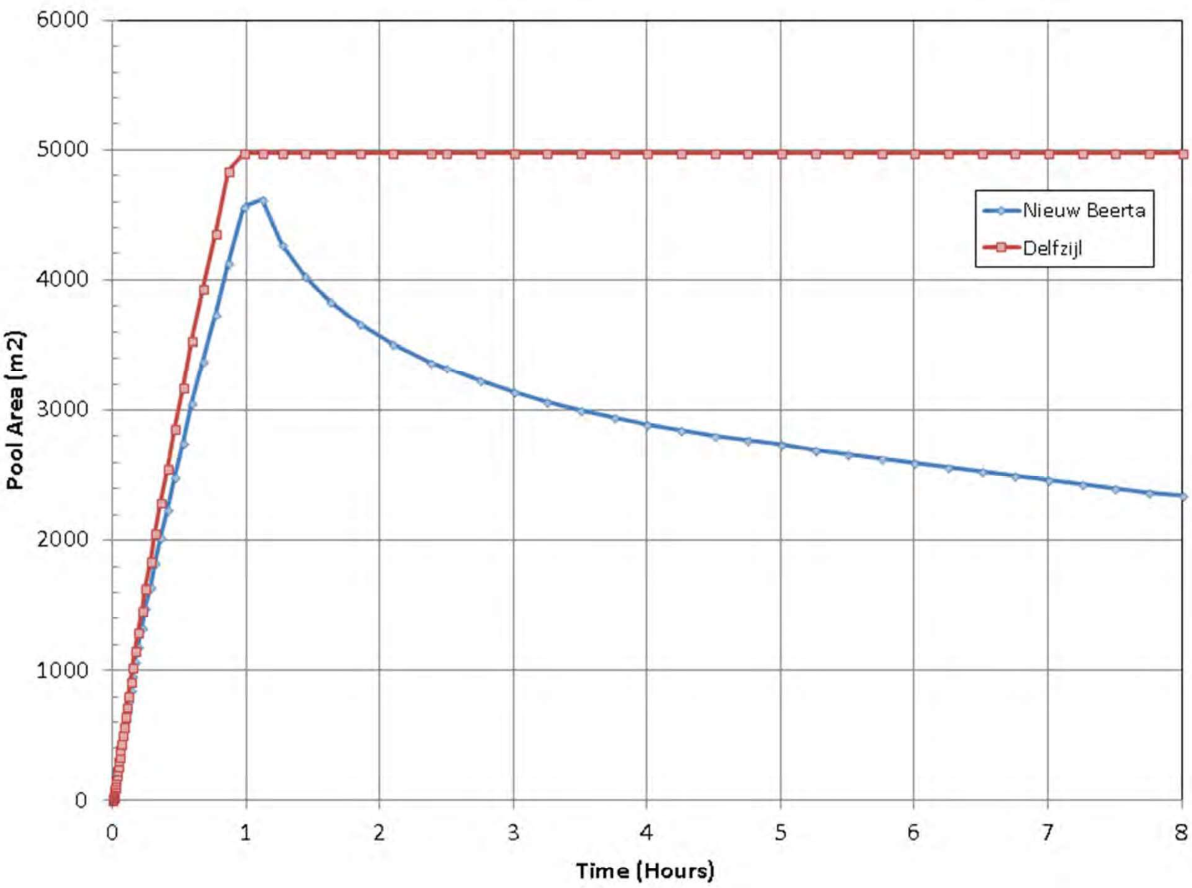

Figure 3 **Predicted Spill Area for the First 8 Hours of the release**

DISPERSION MODELLING

The dispersion modelling was completed for the time varying source and weather conditions. The maximum predicted 1-hour average and 8-hour average concentrations, at each receptor in the domain and over the ~73-hour event, are provided in Figures 4 to 7. The results are presented as contours showing the spatial extents of the 1-hr and 8-hr, “Information” and “Alarm” criteria. In contrast to the above presentation the 1-hour average concentrations for the first hour of the release are shown in Figure 8 and Figure 9 for the Nieuw Beerta and Delfzijl weather observations respectively.

The following observations are made relating to the figures:

- There are no predictions of concentrations at either the 1-hour or 8-hour “Alarm Value” for the cases considered and the assumptions made

- For the weather conditions used, there are no predictions of the “Information Value” in the residential areas.
- The overall spatial extents to the selected criteria are predicted to be greater when the Nieuw Beerta weather observations are used.
- The occupational exposure limits considered as a possible bound for the plume extents are predicted to extend into the residential area to the northwest of the canal.

DISCUSSIONS

Uncertainties in the modelling assessment include the following:

- Release rate profile,
- Weather observations,
- Canal water temperature,
- Site specific spreading of the hydrocarbon within the canal
- Impact of mixing within the sewer
- The effect of assuming a spatially uniform hydrocarbon pool composition, and
- Vapour loss within the sewer

Throughout the assessment the attempt has been made to overstate the predicted concentrations to help address uncertainty. The following assumptions are intended to overstate the predicted concentrations:

- Crosswind and downwind dimensions of the pool assumed to be the same, this produces largest centerline concentrations;
- Source location assumed closer to residences than would be anticipated,
- Canal water temperature set constant at 20 ˚C;
- No weathering within the sewer system, vapour space in sewer assumed saturated based on the condensate tank liquid composition
- Hydrocarbon assumed to sit on top of water, no consideration of turbulence and potential mixing at sewer outlet.

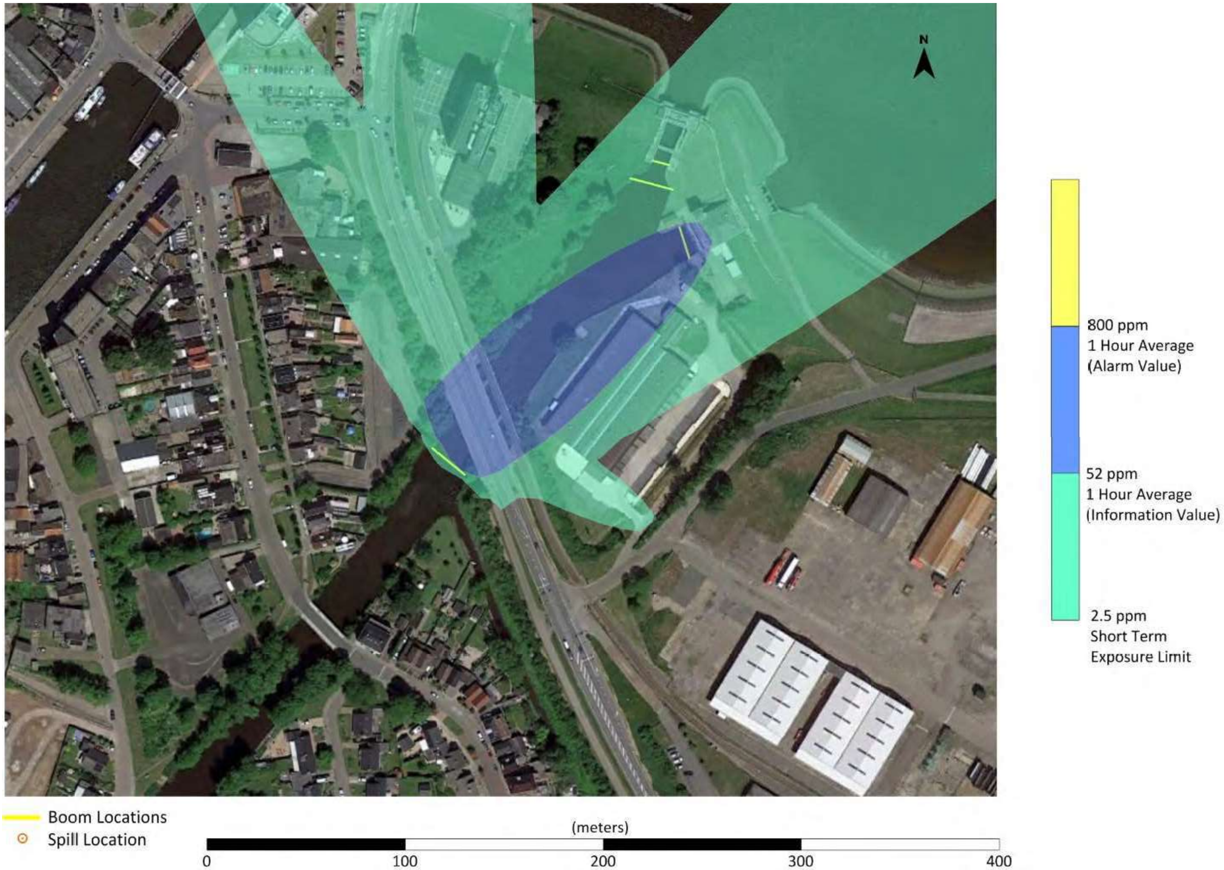

Figure 4 **Predicted Extents to the 1-hour average Alarm and Information Criteria for the 73-hour Event, Based on Nieuw Beerta Weather Observations**

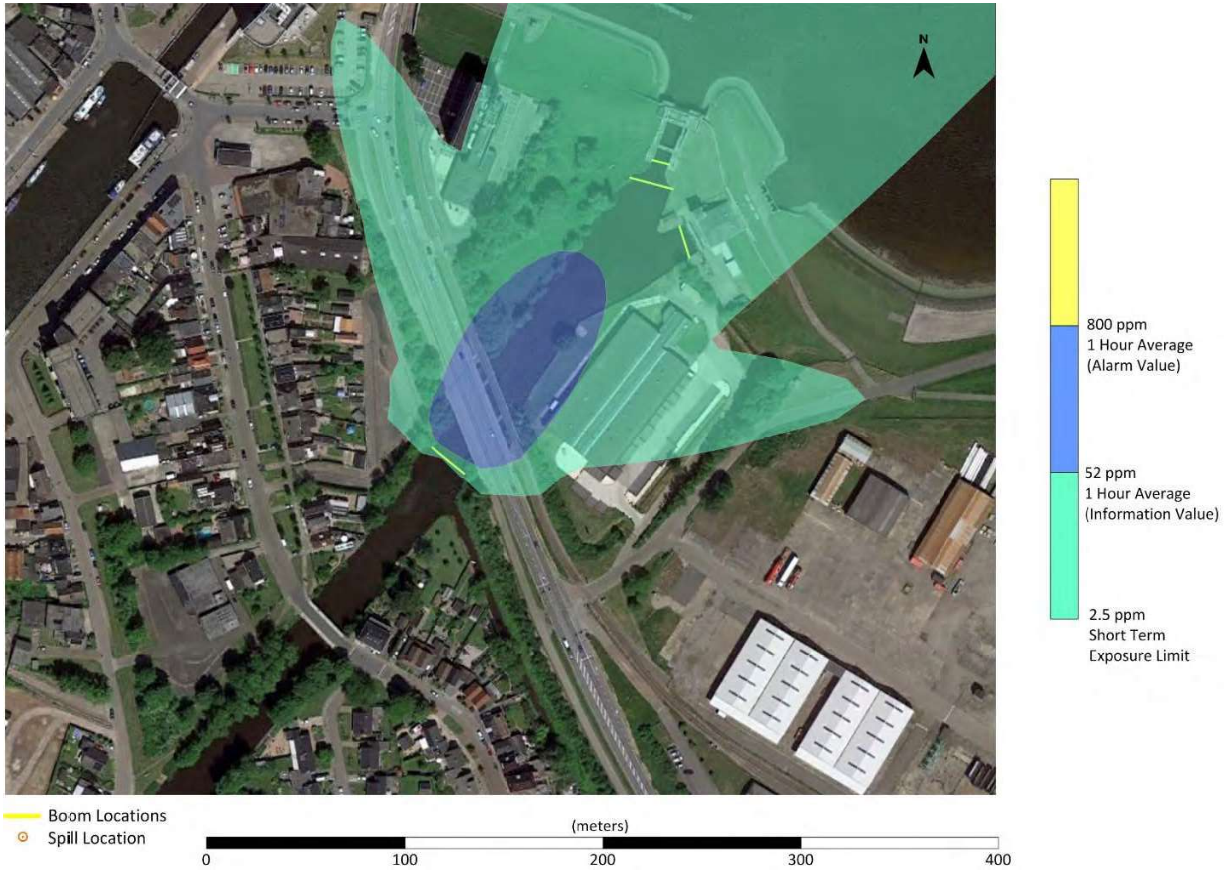

Figure 5 **Predicted Extents to the 1-hour average Alarm and Information Criteria for the 73-hour Event, Based on Delfzijl Weather Observations**

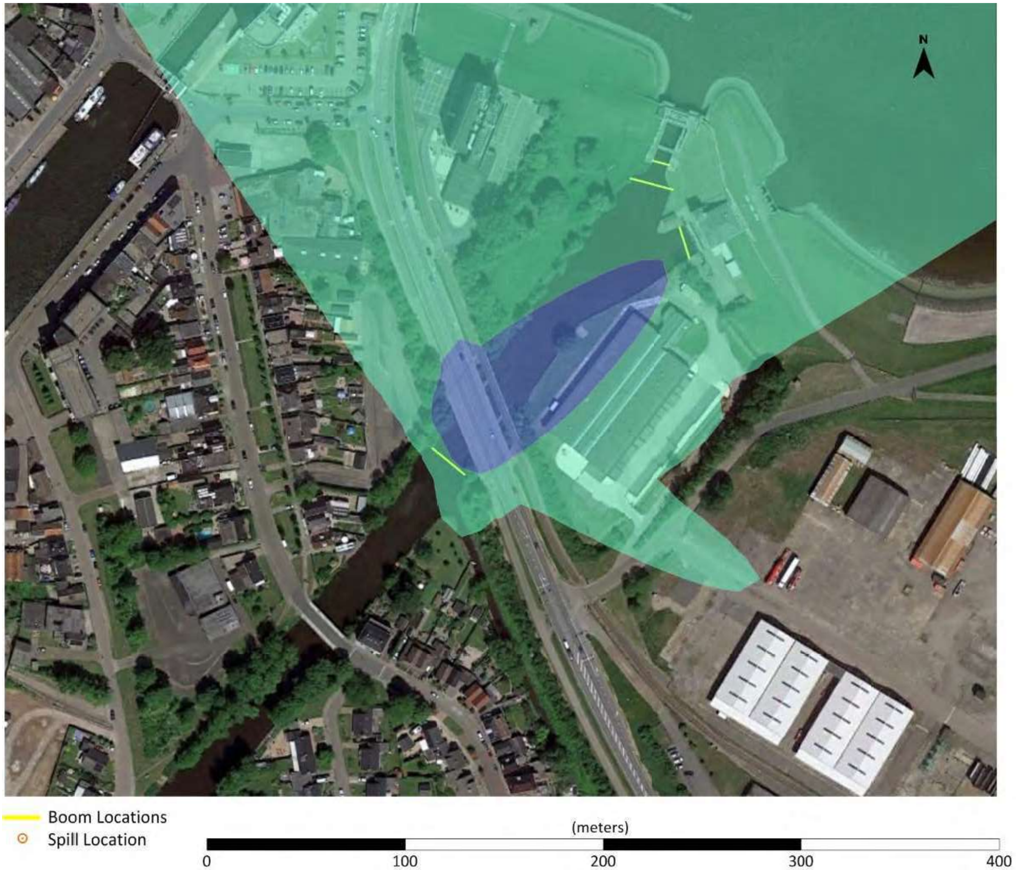

Figure 6 **Predicted Extents to the 8-hour average Alarm and Information Criteria for the 73-hour Event, Based on Nieuw Beerta Weather Observations**

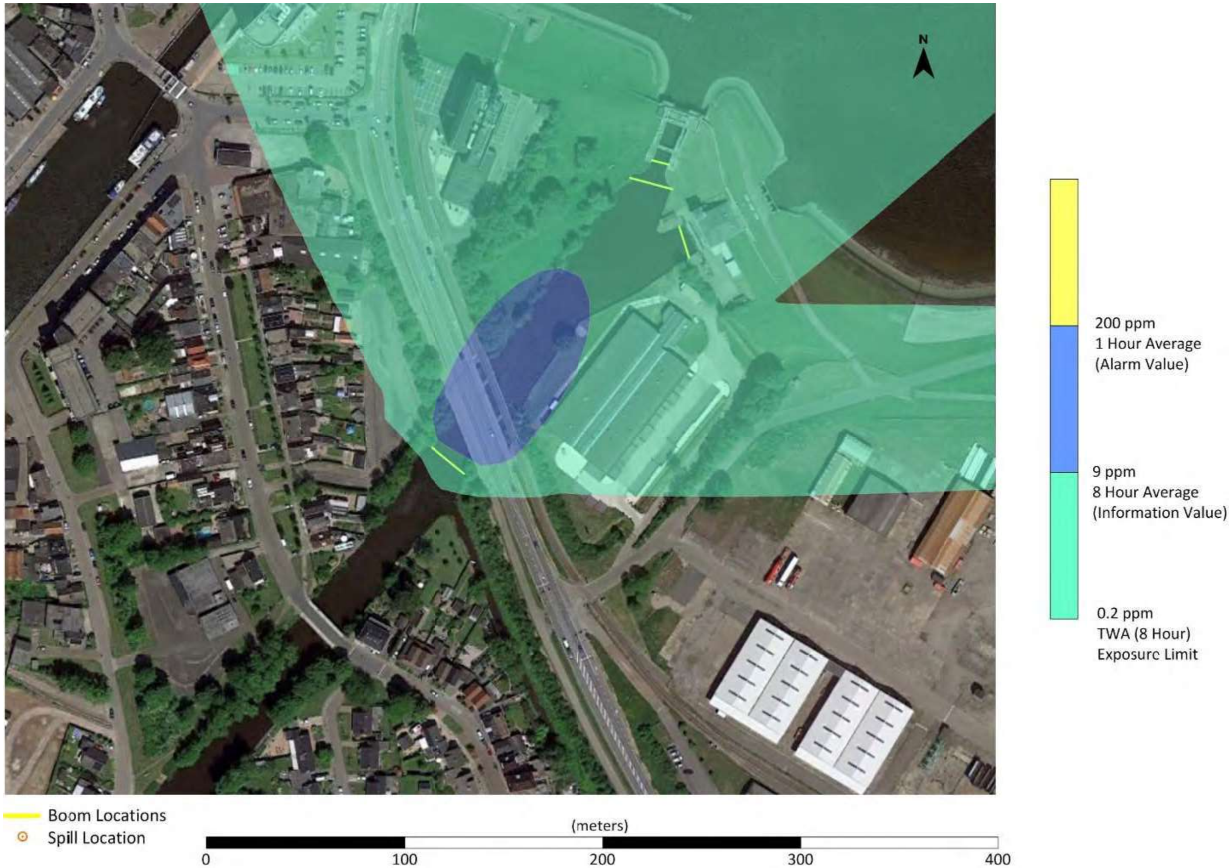

Figure 7 **Predicted Extents to the 8-hour average Alarm and Information Criteria for the 73-hour Event, Based on Delfzijl Weather Observations**

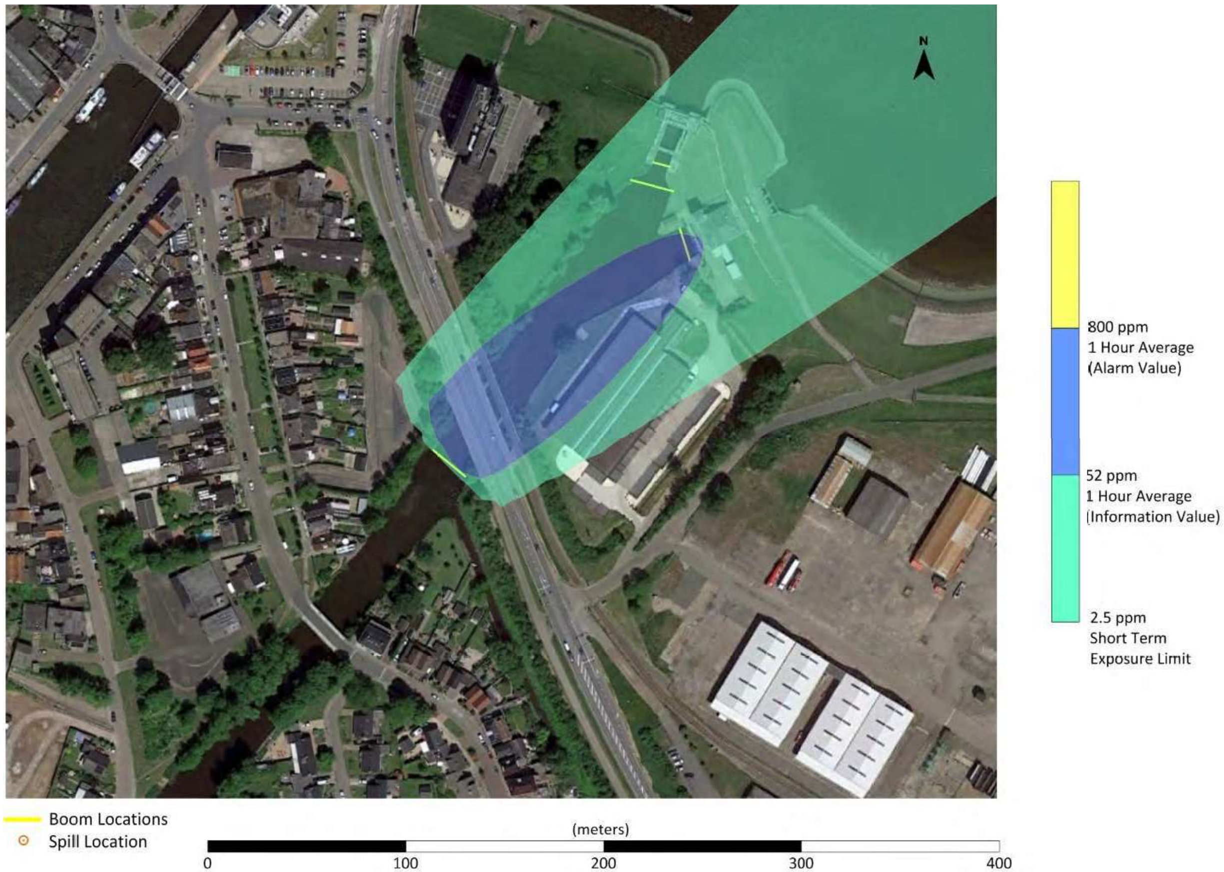

Figure 8 **Predicted Extents to the 1-hour average Alarm and Information Criteria for the First Hour of the Release Event, Based on Nieuw Beerta Weather Observations**

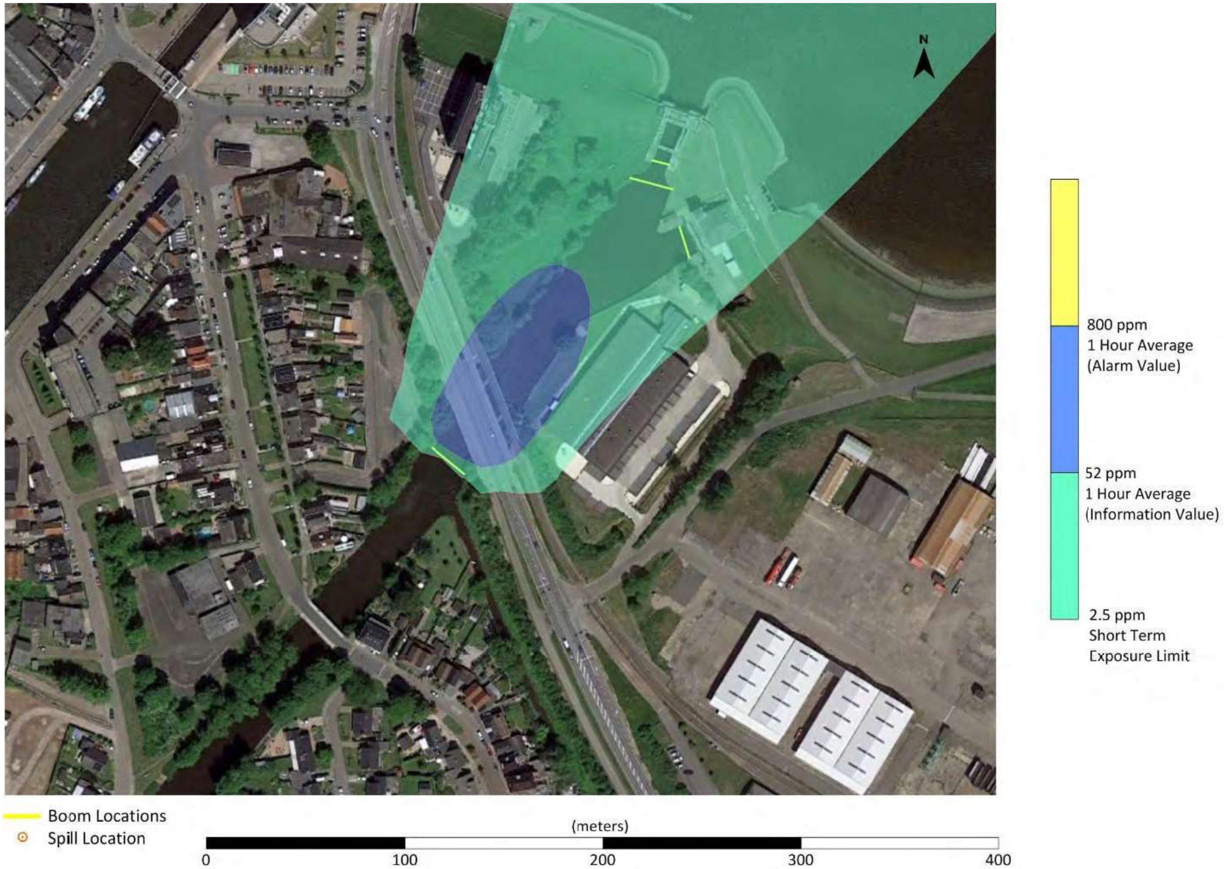

Figure 9 **Predicted Extents to the 1-hour average Alarm and Information Criteria for the First Hour or the Release Event, Based on Delfzijl Weather Observations**

CONCLUSIONS

Source and dispersion modelling were completed to estimate the consequences associated with the leak of condensate into a canal in the vicinity of the NAM gas condensate storage facility located in Farmsum/Delfzijl, Netherlands. The leak was estimated to be 29 m^3 and occurred over about 73 hours between Starting on October 4 between 01:00 and 06:00 and running until October 7, 2018.

Source modelling was completed over the duration of the event with consideration of the time varying weather conditions including the wind speed, atmospheric stability (turbulence levels), and ambient temperature. The modelling was completed assuming selected minimum hydrocarbon slick thickness levels and a single pool temperature. The following observations were made relating to the source modelling:

- The source modelling was not predicted to be sensitive to the hydrocarbon slick thickness,
- The source modelling was predicted to show some sensitivity to the weather observations selected
- Using the Delfzijl weather observations the pool is predicted to reach and maintain the maximum area of the canal.
- Using the Nieuw Beerta weather the pool was not predicted to cover the full area prior to the area starting to decay.
- The hydrocarbon and benzene emission rates were predicted to decay "rapidly" after the initial 23 m^3/hr release event was completed.

The Information and Alarm values for benzene, equal to 52 (1-hour) and 9 (8-hour) ppm and 800 (1-hour) and 200 (8-hour) ppm respectively, were used to predict consequence extents associated with the release. The following observations were made relating to the dispersion modelling:

- There are no predictions of concentrations at either the 1-hour or 8-hour "Alarm Value" for the cases considered and the assumptions made
- For the weather conditions used, there are no prediction of the "Information Value" in the residential areas.
- The overall spatial extents to the selected criteria are predicted to be greater when the Nieuw Beerta weather observations are used.
- The occupational exposure limits considered as a possible bound for the plume extents are predicted to extend into the residential area to the northwest of the canal.

The assessment herein was conducted to assess the potential consequences associated with the release event and associated weather conditions. As there is still uncertainty in aspects of the event including the timing of the release and the weather, conservative assumptions were made to trend towards larger estimates of downwind concentrations:

- Crosswind and downwind dimensions of the pool assumed to be the same, this produces largest centerline concentrations;
- Source location assumed closer to residences than would be anticipated,
- Canal water temperature set constant at 20 °C;
- No weathering within the sewer system, vapour space in sewer assumed saturated based on the condensate tank liquid composition
- Hydrocarbon assumed to sit on top of water, no consideration of turbulence and potential mixing at sewer outlet.

CLOSURE

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This memo represents the best professional judgment of Stantec personnel at the time of its preparation. Stantec reserves the right to modify the contents of this memo, in whole or in part, to reflect the any new information that becomes available. If any conditions become apparent that differ significantly from our understanding of conditions as presented in this memo, we request that we be notified immediately to reassess the conclusions provided herein.

Regards,

Stantec Consulting Ltd.

[redacted]

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