pennsylvania
DEPARTMENT OF ENVIRONMENTAL PROTECTION
BUREAU OF AIR QUALITY

MEMO

TO Mark Gorog JMRG
Environmental Engineer Manager
Southwest Regional Office

FROM Craig Evans, Chief CE 9/21/2020
Air Toxics and Risk Assessment Section
Division of Permits
Bureau of Air Quality

THROUGH Viren Trivedi, Chief VT 9/21/2020
Division of Permits
Bureau of Air Quality

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RE As Built Air Quality Modeling and Inhalation Risk Evaluation
Shell Chemical Appalachia LLC, Potter and Center Townships,
Beaver County, Pennsylvania

Background

Shell Chemical Appalachia LLC (Shell) is constructing a petrochemicals complex in Potter and Center Townships in Beaver County. The petrochemicals is being built on approximately 400 acres on the site of the zinc smelter previously owned by the Horsehead Corporation. The complex will be comprised of an ethene manufacturing plant with an average capacity of 1,500,000 metric tons per year. The ethene that is produced will be used to supply feed to three polyethylene production units with a combined annual production of approximately 1,600,000 metric tons of polyethylene. Steam and electricity required for the process will be supplied by natural gas-fired combined cycle (NGCC) cogeneration units (Cogen Units). The project will also include all of the ancillary units needed to support a new standalone complex including effluent treatment, storage, logistics, cooling water facilities, emergency flares, buildings, and warehouses. Excess electricity produced by the Cogen Units will be sold for distribution within the PJM grid for regional use.

The project's seven cracking furnaces "crack" hydrogen (H_2) out of the ethane (C_2H_6) found in natural gas to produce ethene (C_2H_4). "Tail gas", a byproduct from the cracking furnaces that contains methane and a high concentration of hydrogen, will be used to fuel the process, along with natural gas used to supplement the energy requirements of the process. The ethene that is produced in the cracking furnaces will be used to feed the two gas phase polyethylene manufacturing units and one slurry technology unit. The two gas phase units are each designed to produce 550,000 metric tons per year while

the slurry unit is designed to produce 500,000 metric tons per year. Both technologies employ catalysts but use different process equipment and operating conditions to produce each specific grade of polyethylene.

To support the plant operations, three on-site natural gas-fired combustion turbines with duct burners and heat recovery steam generators (HRSGs) will be used to generate the required steam and electricity. These are the NGCC Cogen Units that were previously mentioned. Other ancillary equipment will include six emergency diesel generators and two diesel-driven firewater pumps, cooling towers, numerous storage tanks and pressure vessels for raw materials and by-products, and a wastewater treatment facility.

In February 2020, the Department of Environmental Protection (DEP) received a revised report titled “Inhalation Risk Assessment For Shell Polymers Monaca Site Shell Chemical Appalachia LLC Beaver County, Pennsylvania”. This report was prepared for Shell by RTP Environmental Associates to support Shell’s plan approval application. Subsequently, on September 3, 2020, the DEP received a revised risk assessment report. The DEP’s Air Quality Modeling Section then performed an independent air quality analysis in order to calculate the COPC ambient air concentrations for a risk assessment on the facility. The DEP’s Air Toxics and Risk Assessment Section then performed an independent risk assessment and found no unacceptable risks from the operations. The purpose of this memo is to discuss the results of the risk assessment analysis.

Inhalation Risk Assessment

The risk assessment process includes four primary steps: hazard identification, exposure assessment, toxicity assessment, and risk characterization. The hazard identification step involves identifying the compounds of potential concern (COPC) expected to be emitted from the project considering factors such as fuel type, emissions control equipment, feedstock characteristics, etc. COPC emissions data from similar facilities were used in conjunction with manufacturers’ specifications and engineering calculations to estimate emission rates from the facility.

These emission rates, in conjunction with the results from the dispersion modeling conducted by the DEP for this facility, were used to estimate the maximum hourly and annual ground level ambient concentrations of the COPC over a defined grid outside the plant perimeter. The DEP’s risk assessment analysis includes two inhalation pathway risk scenarios: acute risk and chronic risk for the maximum exposed individual. The COPC identified for the risk assessment are found in Table 1.

The acute risk assessment compares the estimated one hour modeled maximum concentration to an acceptable one hour reference concentration. The maximum exposed individual (MEI) is assumed to live a 70 year lifetime at the point on the receptor grid where the exposure concentration is the highest. However, the EPA assumes a 30 year exposure duration for an adult resident.[1]

[1] Human Health Risk Assessment Protocol for Hazardous Waste Combustion Facilities, Chapter 6, Quantifying Exposure, September 2005 https://archive.epa.gov/region6/6pd/rcra_c/pd-o/web/html/protocol.html

The DEP's Air Quality Modeling Section used the AERMOD air dispersion model to perform their analysis. The maximum ground level concentrations (at the MEI location) were determined using the estimated COPC emission rates. This procedure was performed for both the acute and the chronic exposure scenarios. More detail pertaining to the air dispersion modeling is available in the memorandum written by the DEP's Air Quality Modeling Section. The results of the DEP's air quality analysis were used for the risk assessment.

Toxicity assessment involves the identification of the adverse health effects posed by an individual compound and relates the development of these effects to the level of exposure. The toxic potential of a chemical may depend on exposure route and duration as well as the mode of action. In an inhalation risk assessment the health risk value potentially posed by each COPC is mathematically applied to the modeled exposure concentration to provide the estimated risk level.

Risk Factors and Their Application

For cancer risk, the risk value is determined using an inhalation unit risk factor (URF) expressed as risk per unit concentration ($m^3/\mu g$). The URF is multiplied by the modeled exposure concentration to derive the individual cancer risk for each carcinogenic COPC which is then summed along with all other individual COPC cancer risks to calculate a total excess lifetime cancer risk (ELCR). The Department's acceptable total ELCR level is one-in-one hundred thousand (1×10^{-5}).

For noncancer risk, the risk value is determined using a reference concentration (RfC) expressed in mass per cubic meter of air (typically mg/m^3). An RfC is "an estimate of a continuous inhalation exposure for a given duration to the human population (including susceptible subgroups) that is likely to be without an appreciable risk of adverse health effects over a lifetime."[2] The RfC is divided into the modeled exposure concentration of the COPC (expressed in the same units of concentration) to derive the hazard quotient (HQ) which is then summed along with all other individual COPC HQ's to calculate a total hazard index (HI). The Department's acceptable total HI level is 0.25.

The acute health risk benchmark is the short term (one hour) exposure inhalation reference concentration. An HQ of 1.0 or less indicates that a compound poses no threat of an adverse effect on a one hour exposure basis rather than a chronic basis. The acute RfC for each COPC should not be exceeded by its respective modeled maximum hourly concentration - the predicted maximum one hour hazard quotient (the modeled acute exposure concentration divided by the acute RfC) should be no greater than 1.0.

Risk Factor References

As a reference for chronic human health inhalation risk values for the COPC, DEP follows the hierarchy provided by EPA's Office of Solid Waste[3] in the "Human Health

[2] EPA IRIS Glossary, http://www.epa.gov/iris/gloss8_arch.htm (accessed 8/21/12).
[3] Human Health Risk Assessment Protocol, Appendix A-2, EPA530-R-05-006, September 2005. p. A-2-33. https://epa-prgs.ornl.gov/radionuclides/2005_HHRAP.pdf

Risk Assessment Protocol" (HHRAP), Appendix 2-A. This list is recommended by EPA "for acquiring human health toxicity data to be used in performing risk assessments of hazardous waste combustion facilities" and is ranked as follows:

1. EPA's Integrated Risk Information System (IRIS)
2. EPA's Provisional Peer Reviewed Toxicity Values (PPRTVs)
3. Other Toxicity Values (including California Environmental Protection Agency (Cal EPA) Reference Exposure Levels (RELs), Agency for Toxic Substances and Disease Registry (ATSDR) Minimal Risk Levels (MRLs), and Health Effects Assessment Summary Tables (HEAST) toxicity values

The Department uses the following hierarchy of acute risk values[4] for the acute risk assessment:

1. Short-Term Exposure Limit/40
2. Ceiling/10
3. 3 x Time-Weighted Average/20
4. Immediately Dangerous to Life or Health/20

Results

There is one chronic scenario and one acute scenario that have been assessed for the COPC. The chronic scenario is:

1. Maximum Exposed Individual (MEI) Non-Cancer Risk

   Hazard Index: COPC HI = 0.0995

2. Maximum Exposed Individual (MEI) Cancer Risk

   Excess Lifetime Cancer Risk: COPC ELCR = 9.42E-06

The acute scenario is:

1. Maximum Exposed Individual (MEI) Acute Non-Cancer Risk

   Hazard Quotient: All COPC HQ's are less than 1.0

The MEI is the individual who is exposed to the modeled maximum ground-level concentrations. The risks for the two scenarios are not unacceptable.

[4] *NIOSH Pocket Guide to Chemical Hazards* http://www.cdc.gov/niosh/npg/default.html

Table 1 Addendum – Summary of DEP's Air Quality Analysis Results for Chronic Risk Scenario for Maximum Exposed Individual

Compounds of Potential Concern	**Chronic Cancer Risk**	**Concentration (µg/m³)**	**Chronic Non Cancer HQ**	**Concentration (µg/m³)**
1,3-Butadiene	**8.01E-07**	2.67E-02	**0.01334226**	2.67E-02
2-Methylnaphthalene	-	7.78E-07	-	7.78E-07
3-Methylchloranthrene	6.70E-11	1.06E-08	-	1.06E-08
7,12-Dimethylbenz(a)anthracene	6.71E-09	9.45E-08	-	9.45E-08
Acenaphthene	-	2.23E-08	-	2.23E-08
Acenaphthylene	-	3.18E-08	-	3.18E-08
Acetaldehyde	3.82E-10	1.74E-04	0.00001929	1.74E-04
Acrolein	-	1.01E-04	**0.00502669**	1.01E-04
Ammonia	-	6.64E-02	0.00013274	6.64E-02
Anthracene	-	2.30E-08	-	2.30E-08
Arsenic	5.09E-09	1.18E-06	0.00007874	1.18E-06
Barium	-	2.60E-05	0.00005197	2.60E-05
Benz(a)anthracene	1.98E-12	1.80E-08	-	1.80E-08
Benzene	**3.86E-06**	4.95E-01	**0.01650183**	4.95E-01
Benzo(a)pyrene	8.97E-12	8.15E-09	-	8.15E-09
Benzo(b)fluoranthene	1.37E-12	1.25E-08	-	1.25E-08
Benzo(g,h,i)perylene	-	7.09E-09	-	7.09E-09
Benzo(k)fluoranthene	1.27E-12	1.15E-08	-	1.15E-08
Beryllium	1.70E-10	7.08E-08	0.00000354	7.08E-08
Biphenyl	-	6.50E-06	0.00001626	6.50E-06
Cadmium	1.17E-08	6.50E-06	0.00064960	6.50E-06
Chromium VI	**1.53E-06**	1.82E-05	**0.00228033**	1.82E-05
Chrysene	1.54E-13	1.40E-08	-	1.40E-08
Cobalt	4.46E-09	4.96E-07	0.00008268	4.96E-07
Copper	-	4.42E-06	-	4.42E-06
Dibenz(a,h)anthracene	1.18E-11	9.83E-09	-	9.83E-09
Dichlorobenzene	7.80E-11	7.09E-06	0.00000001	7.09E-06
Ethylbenzene	1.40E-08	5.60E-03	0.00000558	5.60E-03
Ethylene Oxide	-	0.00E+00	-	0.00E+00
Fluoranthene	-	5.25E-08	-	5.25E-08
Fluorene	-	1.47E-07	-	1.47E-07
Formaldehyde	2.14E-08	1.65E-03	0.00016769	1.64E-03
n-Hexane	-	2.04E+01	**0.02912909**	2.04E+01
Indeno(1,2,3-cd)pyrene	1.39E-12	1.26E-08	-	1.26E-08
Lead	3.48E-11	2.90E-06	0.00001935	2.90E-06
Manganese	-	2.24E-06	0.00004488	2.24E-06
Mercury	-	1.54E-06	0.00000512	1.54E-06
Methanol	-	2.56E-02	0.00000128	2.56E-02
Molybdenum	-	6.50E-06	-	6.50E-06
Naphthalene	**3.16E-06**	9.29E-02	**0.03093346**	9.29E-02
Nickel	5.95E-09	1.24E-05	0.00088582	1.24E-05
PAH (as benzo(a)pyrene)	1.91E-09	1.74E-06	-	1.74E-06
n-Pentane	-	1.54E-02	0.00001535	1.54E-02
Phenanthrene	-	2.68E-07	-	2.68E-07
Phenol	-	2.86E-05	0.00000014	2.86E-05
Propane	-	9.45E-03	-	9.45E-03
Propylene Oxide	2.78E-11	7.51E-06	0.00000025	7.51E-06
Pyrene	-	7.90E-08	-	7.90E-08
Selenium	-	1.42E-07	0.00000001	1.42E-07
Styrene	-	3.16E-02	0.00003152	3.16E-02
Toluene	-	6.57E-02	0.00001315	6.57E-02
Vanadium	-	1.24E-05	-	1.24E-05
Xylenes	-	2.12E-03	0.00002121	2.12E-03
ELCR	**9.42E-06**	**HI**	**0.09945984**	

$$Modeled\ Maximum\ Exposure\ Concentration * Unit\ Risk\ Factor\ (URF) = Chronic\ Cancer\ risk$$

$$\frac{Modeled\ Maximum\ \ Exposure\ Concentration}{Reference\ Concentration\ (RfC)} = \ HQ$$

Table 2 Addendum– Summary of DEP's Air Quality Analysis Results for Acute Risk Scenario

Compounds of Potential Concern	**DEP Max 1-Hr Conc (µg/m³)**	**DEP Acute HQ**
1,3-Butadiene	1.87E+00	0.006803345
2-Methylnaphthalene	1.58E-02	0.000005250
3-Methylchloranthrene	1.00E-05	0.000000135
7,12-Dimethylbenz(a)anthracene	7.00E-05	-
Acenaphthene	1.62E-03	0.000000450
Acenaphthylene	3.19E-03	0.000000319
Acetaldehyde	3.96E+00	0.000878969
Acrolein	2.44E+00	**0.121938000**
Ammonia	4.84E+01	**0.080624533**
Anthracene	5.00E-04	0.000001852
Arsenic	9.20E-04	0.004600000
Barium	2.03E-02	0.000270400
Benz(a)anthracene	3.20E-04	0.000010667
Benzene	1.59E+01	**0.079474200**
Benzo(a)pyrene	9.00E-05	0.000003000
Benzo(b)fluoranthene	3.80E-04	-
Benzo(g,h,i)perylene	1.00E-05	0.000000000
Benzo(k)fluoranthene	8.00E-05	0.000004211
Beryllium	6.00E-05	0.000240000
Biphenyl	1.01E-01	0.000670133
Cadmium	5.09E-03	**0.016966667**
Chromium VI	1.08E-02	0.001081000
Chrysene	5.30E-04	0.000017667
Cobalt	3.90E-04	0.000130000
Copper	3.92E-03	0.001568000
Dibenz(a,h)anthracene	1.50E-04	-
Dichlorobenzene	5.56E-03	0.000000741
Ethylbenzene	1.30E-01	0.000009555
Ethylene Oxide	0.00E+00	-
Fluoranthene	6.06E-03	-
Fluorene	1.78E-03	-
Formaldehyde	2.50E+01	**0.408839347**
n-Hexane	2.41E+01	0.000892257
Indeno(1,2,3-cd)pyrene	1.50E-04	-
Lead	2.31E-03	0.000308000
Manganese	1.75E-03	0.000023333
Mercury	1.20E-03	0.000120000
Methanol	2.23E+00	0.000273889
Molybdenum	5.09E-03	0.000011311
Naphthalene	2.84E+00	0.001516037
Nickel	9.68E-03	0.004302222
PAH (benz(a)pyrene RfC)	6.20E-02	0.002065333
n-Pentane	1.20E+01	0.003996483
Phenanthrene	1.41E-02	-
Phenol	1.14E-02	0.000001898
Propane	7.36E+00	0.000027261
Propylene Oxide	7.01E-03	0.000009736
Pyrene	1.48E-03	-
Selenium	1.10E-04	0.000003667
Styrene	7.40E-01	0.000174078
Toluene	1.53E+00	0.000109574
Vanadium	1.06E-02	0.000006057
Xylenes	8.72E-02	0.000005357

$$\frac{Modeled\ Maximum\ Exposure\ Concentration}{Reference\ Concentration\ (RfC)} = Hazard\ Quotient$$

Table 3 – Summary of DEP's Risk Factors

Chemical Name	CAS No.	RfC ($\mu g/m^3$)	Chronic RfC reference	URF ($m^3/\mu g$)	URF Reference	Acute RfC (mg/m3)	STEL (mg/m3)	Ceiling (mg/m3)	TLV (mg/m3)	IDLH (mg/m3)	Reference
1,3-Butadiene	106-99-0	2.00	EPA IRIS	0.00003	EPA IRIS	0.275	11		2.2		OSHA
1,4-Dichlorobenzene	106-46-7	801.5	Cal EPA	0.000011	Shell	7.5	301				ACGIH
2-Methylnaphthalene	91-57-6	NR		NR		3					Shell
3-Methylchloranthrene	56-49-5	NR		0.0063	CalEPA	0.074					Shell
7,12-Dimethylbenz[a]anthracene	57-97-6	NR		0.071	CalEPA						
Acenaphthene	83-32-9	NR		NR		3.6					Shell
Acenaphthylene	208-96-8	NR		NR		10					Shell
Acetaldehyde	75-07-0	9.00	EPA IRIS	0.0000022	EPA IRIS	4.5		45			ACGIH
Acrolein	107-02-8	0.02	EPA IRIS	NR		0.02	0.8				NIOSH
Ammonia	7664-41-7	500	EPA IRIS	NR		0.6	35		25		ACGIH
Anthracene	120-12-7	NR		NR		0.27					Shell
Arsenic	7440-38-2	0.015	Cal EPA	0.00431	EPA IRIS	0.0002		0.002			NIOSH
Barium	7440-39-3	0.5	HEAST	NR		0.075			0.5		ACGIH
Benz[a]anthracene	56-55-3	NR		0.00011	CalEPA	0.03			0.2		Shell
Benzene	71-43-2	30.00	EPA IRIS	0.0000078	EPA IRIS	0.2	8				ACGIH
Benzo[a]pyrene (PAH)	50-32-8	NR		0.0011	CalEPA	0.03			0.2		OSHA
Benzo[b]fluoranthene	205-99-2	NR		0.00011	CalEPA						
Benzo[g,h,i]perylene	191-24-2	NR		NR		30					Shell
Benzo[k]fluoranthene	207-08-9	NR		0.00011	CalEPA	0.019					Shell
Beryllium	7440-41-7	0.02	EPA IRIS	0.0024	EPA IRIS	0.00025	0.01				ACGIH
Biphenyl	92-52-4	0.4	PPRTV	NR		0.15			1		NIOSH
Cadmium	7440-43-9	0.01	ATSDR	0.0018	EPA IRIS	0.0003			0.002		ACGIH
Chromium III	16065-83-1	NR		NR		0.075			0.5		ACGIH
Chromium VI	18540-29-9	0.008	EPA IRIS	0.084	EPA IRIS	0.01		0.1			OSHA
Chrysene	218-01-9	NR		0.000011	CalEPA	0.03			0.2		OSHA
Cobalt	7440-48-4	0.006	PPRTV	0.009	PPRTV	0.003			0.02		ACGIH
Copper	7440-50-8	NR		NR		0.0025	0.1				ACGIH
Dibenz[a,h]anthracene	53-70-3	NR		0.0012	CalEPA						
Ethylbenzene	100-41-4	1000	EPA IRIS	0.0000025	CalEPA	13.6	543				ACGIH
Ethylene Oxide	75-21-8	30	Cal EPA	0.003	EPA IRIS	0.225	9				OSHA
Fluoranthene	206-44-0	NR		NR							
Fluorene	86-73-7	NR		NR							

Formaldehyde	50-00-0	9.8	ATSDR	0.000013	EPA IRIS	0.0615	2.5				OSHA
Indeno[1,2,3-cd]pyrene	193-39-5	NR		0.00011	CalEPA						
Lead	7439-92-1	0.15	NAAQS	0.000012	CalEPA	0.0075			0.05		ACGIH
Manganese	7439-96-5	0.05	EPA IRIS	NR		0.075	3				NIOSH
Mercury	7439-97-6	0.30	EPA IRIS	NR		0.01		0.1			OSHA
Methanol	67-56-1	20000	EPA IRIS	NR		8.125	325				NIOSH
Molybdenum		NR		NR		0.45			3		
Naphthalene	91-20-3	3.00	EPA IRIS	0.000034	CalEPA	1.875	75				NIOSH
n-Hexane	110-54-3	700	EPA IRIS	NR		27			180		ACGIH
Nickel	7440-02-0	0.014	Cal EPA	0.00048	EPA IRIS	0.00225			0.015		NIOSH
n-Pentane	109-66-0	1000	PPRTV	NR		180		1800			NIOSH
Phenanthrene	85-01-8	NR		NR							
Phenol	108-95-2	200	Cal EPA	NR		6		60			NIOSH
Propane	74-98-6	NR		NR		270			1800		OSHA
Propylene Oxide	75-56-9	30	EPA IRIS	0.0000037	EPA IRIS	0.7125			4.8		ACGIH
p-Xylene	106-42-3	100	EPA IRIS	NR		16.275	651				ACGIH
Pyrene	129-00-0	NR		NR							
Selenium	7782-49-2	19.99	Cal EPA	NR		0.03			0.2		ACGIH
Styrene	100-42-5	1001	EPA IRIS	NR		4.25	170				ACGIH
Toluene	108-88-3	5000	EPA IRIS	NR		14	560				NIOSH
Vanadium	7440-62-2	NR		NR		1.75				35	NIOSH