Chapter 6
Initial Phase Results

What's Covered in Chapter 6:

♦　　　Neighborhood-Specific Results

♦　　　Considerations Regarding Use of Results

♦　　　Uncertainty and Limitations

This chapter presents the results of the initial phase of the RAIMI pilot for the Port Neches Assessment Area in Jefferson County, Texas. Consistent with RAIMI Pilot Study objectives, the results presented within this chapter provide the detailed contaminant-specific, source-specific, and receptor-specific information to support the identification and prioritization of risk management opportunities. The results presented represent exposure via inhalation of contaminants in air (i.e., inhalation exposure pathway) based on impacts from emission sources with available contaminant-specific emissions data. However, regardless of whether modeling a single source or multiple sources, a single exposure pathway or multiple exposure pathways, or whether contaminant specific emissions data is not available for all sources; if a potential risk level of concern is indicated by these results, then the responsible source or sources should still be prioritized for further scrutiny and risk management considerations. As discussed in Section 6.2, a more complete characterization of emissions within the Port Neches Assessment Area would be expected with increased regulatory and facility focus on prioritized sources identified by the RAIMI Pilot Study.

While presentation of results in this report provides information necessary to achieve the very basic design objectives of the RAIMI Pilot Study, the multi-facility, multi-source, multi-receptor risk assessment built around a dynamic project platform provides significant additional opportunities for the identification and implementation of risk management solutions. Several possible scenarios can be quickly conceived, including:

- Evaluating the change in risk impacts to a neighborhood due to reductions in actual or allowable emissions from select emission sources;

- Evaluating the change in risk impacts by implementing a new emission control technology on a particular source, or on all similar emission sources of a particular process at multiple facilities;

- Addressing cross-program emissions permitting issues for sources and facilities regulated by multiple statutes; and

- Evaluating the changes in estimated potential risks due to changes to emissions reporting requirements.

The prioritization objective is to identify, at a minimum, all emission sources that may potentially contribute to a risk level of concern when also considering the combined impacts from surrounding sources. The risk levels of concern adopted in the RAIMI Pilot Study for the Port Neches Assessment Area are based on historical regulatory concern levels, of which 10^{-5} for risk and 0.25 for hazard are consistent with the range of central values (Travis et al. 1987). Other studies, given other objectives, might identify different levels for prioritization or indication of risk concern. These risk and hazard levels are adopted as a basis to identify exposure concerns, and to facilitate presentation and discussion of results. As such, use of these risk and hazard levels in the RAIMI Pilot Study should be viewed as a quantitative threshold for scope of analysis (i.e., which sources and associated mass of emitted contaminants potentially result in significant impacts based on available data) and presentation of results. Section 6.1 presents neighborhood-specific results of impacts from emissions evaluated in the initial phase of the RAIMI Pilot Study on the Port Neches Assessment Area. Section 6.2 discusses identified data limitations that may effect interpreting results.

6.1   NEIGHBORHOOD-SPECIFIC RESULTS

As discussed in Chapter 5, for each source and contaminant modeled, output from the execution of the single-pass air modeling approach and risk modeling allows for the generation of risk and hazard values at one or all of the air modeling receptor grid nodes of interest within the assessment area. However, focus for the RAIMI Pilot Study, as stated in the objectives and presented in this chapter, is prioritization of potential risk concerns for specific neighborhoods within the Port Neches Assessment Area subject to impacts from any combination of sources and/or contaminants. Estimated risk and hazard values at additional locations, other than highly impacted neighborhood areas, have also been presented in this report to illustrate that source attribution and impacts can vary with geographic location and distance from sources. It is important to note, that although this approach and presentation focuses on selection of locations of concern to view results in comparison of a certain risk-based floor, the RAIMI method allows for determination and viewing of results for all locations and contaminants for the entire assessment area, providing an "estimated risk surface" for the whole area, whether or not it rises at any given point to levels anyone would consider of interest.

To identify exposure locations within a residential land use or neighborhood, all air parameter values within ISCST3 output plot files for each modeled source and within the boundaries of the residential land use areas or neighborhoods were identified following the procedures described in the HHRAP and as discussed in Section 5.3. For the emission sources modeled in the Port Neches Assessment Area, this analysis identifies two distinct maximum impacted neighborhood areas. These two residential exposure areas are labeled as the Port Neches/Nederland and Groves neighborhoods, and are identified on Figure 6-1.

The Port Neches/Nederland neighborhood is located in the central part of the Port Neches assessment area. The Groves neighborhood is located in the southeastern part of the assessment area. The neighborhoods themselves are separated from one another by a large complex of industrial facilities. Presentation and discussion of results in the RAIMI Pilot Study focuses on the location of predicted maximum impact for each of the two neighborhoods. For each neighborhood, the text includes a discussion of (1) modeled risk levels, (2) source attribution, (3) applicable monitoring data, and (4) risk management considerations. Discussion of results is complemented, as appropriate, with figures and supporting data.

Contaminant specific results at the neighborhood exposure locations are summarized in Table 6-1. As discussed in the introduction to this chapter, results of the Pilot Study that are presented and discussed in this chapter include those results that exceed risk or hazard levels of 10^{-5} and 0.25, respectively. These levels are adopted as a basis to identify exposure concerns, and to facilitate presentation and discussion of results, and do not represent, for the purpose of this study, any regulatory threshold. The information in Table 6-1 indicates that modeled emissions of contaminants resulted in resident adult and resident child cancer risk and non-cancer hazard levels greater than the levels established for prioritization. Table 6-2 presents the contaminant-specific toxicity benchmarks used to calculate risk and hazard impacts for those contaminants identified in Table 6-2. The hierarchy used for toxicity benchmarks in

TABLE 6-1

RISK SUMMARY

Contaminant	Port Neches / Nederland Neighborhood				Groves Neighborhood			
	Adult		Child		Adult		Child	
	Risk	Hazard	Risk	Hazard	Risk	Hazard	Risk	Hazard
Benzene	$9x10^{-6}$	NC	$4x10^{-6}$	NC	**$3x10^{-5}$**	NC	**$1x10^{-5}$**	NC
1,3-Butadiene[a]	**$5x10^{-4}$**	NA	**$2x10^{-4}$**	NA	**$1x10^{-4}$**	NA	**$5x10^{-5}$**	NA
1,3-Butadiene (proposed)[b]	$7x10^{-6}$	**1**	$3x10^{-6}$	**2**	$2x10^{-6}$	**0.3**	$8x10^{-7}$	**0.6**
Ethylene Oxide	**$2x10^{-5}$**	NC	$9x10^{-6}$	NC	**$2x10^{-5}$**	NC	**$1x10^{-5}$**	NC
Formaldehyde	$5x10^{-6}$	0.0	$2x10^{-6}$	0.0	**$2x10^{-5}$**	0.0	$7x10^{-6}$	0.0
Benzo(a)anthracene	$9x10^{-6}$	NC	$4x10^{-6}$	NC	**$2x10^{-5}$**	NC	**$1x10^{-5}$**	NC
Benzo(a)pyrene	**$3x10^{-5}$**	NC	**$1x10^{-5}$**	NC	**$7x10^{-5}$**	NC	**$3x10^{-5}$**	NC
Benzo(b)fluoranthene	$9x10^{-6}$	NC	$4x10^{-6}$	NC	**$2x10^{-5}$**	NC	$9x10^{-6}$	NC
Acrolein	NC	**2.6**	NC	**5.8**	NC	**9.1**	NC	**20.2**

Notes:

[a]   Risk values calculated using the current unit risk factor contained in EPA's Integrated Risk Information System (IRIS) (see Table 6-2)

[b]   Risk and hazard values calculated using proposed toxicity benchmarks as recommended by EPA's National Center for Environmental Assessment (see Table 6-2)(U.S. EPA 2001).

NA   Not applicable

NC   Not calculated due to toxicity benchmarks not being available.

Bold type indicates risk greater than $1x10^{-5}$ or hazard greater than 0.25.

Values determined based on modeled air concentrations of reported actual emission rates for 1997 (see Chapter 3).

TABLE 6-2

TOXICITY FACTORS FOR PRIORITIZED CONTAMINANTS

Contaminant	Inhalation URF (per µg/m^3)	Source	Notes	RfD	Source	Notes
1,3-Butadiene	0.00028	IRIS URF (U.S. EPA 2000e)	See note below.	0.00126 mg/kg-d	See note below.	Consistent with NCEA recommendation.
1,3-Butadiene (proposed)	0.00001	Proposed NCEA URF (U.S. EPA 2001)	See note below.	--	--	--

BUTADIENE NOTES REGARDING URF: Integrated Risk Information System (IRIS) currently (as of April 2001) provides a unit risk factor (URF) of 0.00028 per µg/m^3, based on EPA (1985) [corrected in Cote and Bayard (1990), as cited in IRIS], which was based on National Toxicology Program (1984) findings (cited in IRIS) and based on mouse data. More recently, EPA's National Center for Environmental Assessment (NCEA) released an external review draft, dated February 1998, that recommended a URF of 9E-03 per ppm, or 4.07E-06 per µg/m^3, based on human data (U.S. EPA 1998f). Follow up recommendation based on input resulting from review by the EPA Science Advisory Board has led to the most current use of 1.0E-05 per µg/m^3 in the NATA National-Scale Assessment, as cited in Appendix G, page G-5 (U.S. EPA 2001). However, this value has not yet been finalized and does not appear in IRIS.

BUTADIENE NOTES REGARDING RfD: Per e-mail from the 1,3-butadiene chemical manager, Aparna Koppikar, to Jeff Yurk on March 1, 2000, the chronic draft RfC is 2 ppb (U.S. EPA 2000f). This would equate to a chronic RfC of 4.42 µg/m^3 and an RfD (assuming route-to-route extrapolation) of 0.00126 mg/kg-d following conversions (U.S. EPA 1998b; 1997c) where an RfC may be back-calculated to an RfD by the equation RfD = (RfC x 20 m^3/day)/(70 kg).

Contaminant	Inhalation URF (per µg/m^3)	Source	Notes	RfD	Source	Notes
Acrolein	--	--	--	Inhalation RfD 5.71429E-06	Calculated from IRIS Inhalation RfC (U.S. EPA 2000e)	See note below

TABLE 6-2

TOXICITY FACTORS FOR PRIORITIZED CONTAMINANTS

Contaminant	Inhalation URF (per µg/m³)	Source	Notes	RfD	Source	Notes
ACROLEIN NOTES REGARDING Inhalation RfD: .Integrated Risk Information System (IRIS) currently (as of August 2002) provides a Inhalation RfCof 2E-5 mg/cu.m. The inhalation RfD of 5.71429E-06was back-calculated using the RfC to RfD conversion equation $RfD = (RfC \times 20 \ m^3/day)/(70 \ kg)$, as provided in Appendix A-3 of the Human Health Risk Assessment Protocol for Hazardous Waste Combustion Facilities (HHRAP) (U.S. EPA 1998b).						
Benzene	0.0000083	Previous IRIS URF (U.S. EPA 1998g)	URF of 7.8E-6 reflects upper end of IRIS range (U.S. EPA 2000e)	--	--	--
BENZENE NOTES REGARDING URF: As per the IRIS file for benzene (U.S. EPA 2000e): "The numerical difference between the 1985 [previous IRIS file] risk estimate (8.1E-6 at 1 µg/m³) compared to the new high-end risk (7.8E-6 at 1 µg/m³) is insignificant and no scientific inference about one value versus the other should be made." Therefore, although the current IRIS URF is slightly different from the value used, the difference is insignificant.						
Benzo(a)anthracene	0.000208571	Calculated per U.S. EPA 1993	See note below.	NA	--	--
BENZO(A)ANTHRACENE NOTES: The benzo(a)anthracene URF was calculated from BAP URF assuming a relative potency factor of 0.1. Carcinogenic potential of benzo(a)anthracene has not been individually quantitated in IRIS. Rather, a relative potency factor of 0.1 was established by EPA (1993) for PAH compounds in relation to BAP. Therefore, benzo(a)anthracene is projected to be tenfold less carcinogenic than BAP, and its URF is reduced from that of BAP by multiplying the BAP URF by 0.1. (TNRCC 1999e) uses 8.8E-5 per µg/m³ as a benzo(a)anthracene URF, citing a Region 4 value (U.S. EPA 1995b), which was attributed to NCEA.						

TABLE 6-2

TOXICITY FACTORS FOR PRIORITIZED CONTAMINANTS

Contaminant	Inhalation URF (per µg/m^3)	Source	Notes	RfD	Source	Notes
Benzo(a)pyrene	0.0020857142	Calculated from IRIS oral CSF (U.S. EPA 2000e)	See note below.	NA	--	--
BAP NOTES: A URF may be derived from an inhalation slope factor (SFi) using the expression URF = (SFi x 20 m^3/day) / (1000 µg/mg x 70 kg) as per HEAST (U.S. EPA 1997c). Direct route-to-route extrapolation was used, as the SFi was assumed equal to the CSF given in IRIS (U.S. EPA 2000e). (TNRCC 1999e) uses 8.8E-4 per µg/m^3 as a BAP URF, citing a Region 4 value (EPA 1995b), which was attributed to NCEA.						
Benzo(b)fluoranthene	0.000208571	Calculated per EPA 1993	See note below.	NA	--	--
BENZO(B)FLUORANTHENE NOTES: The benzo(b)fluoranthene URF was calculated from BAP URF assuming a relative potency factor of 0.1. Carcinogenic potential of benzo(b)fluoranthene has not been individually quantitated in IRIS. Rather, a relative potency factor of 0.1 was established by EPA (1993) for PAH compounds in relation to BAP. Therefore, benzo(b)fluoranthene is projected to be tenfold less carcinogenic than BAP, and its URF is reduced from that of BAP by multiplying the BAP URF by 0.1. (TNRCC 1999e) uses 8.8E-5 per µg/m^3 as a benzo(b)fluoranthene URF, citing a Region 4 value (EPA 1995b), which was attributed to NCEA.						

Notes: As indicated in the table above, both current and proposed toxicity benchmarks are presented for 1,3-butadiene. To prevent confusion, risk values for 1,3-butadiene are presented throughout this chapter based on the current IRIS URF, unless otherwise stated.

BAP	Benzo(a)pyrene
CSF	Oral cancer slope factor
HEAST	Health Effects Assessment Summary Tables
IRIS	Integrated Risk Information System
kg	Kilogram
m^3	Cubic meter
mg	Milligram
NA	Not available
NCEA	National Center for Environmental Assessment.
PAH	Polycyclic aromatic hydrocarbon

RfD   Oral reference dose, expressed in terms of milligrams contaminant per kilogram body weight per day (mg/kg-d).

RfC   Inhalation reference concentration, expressed in terms of milligrams of the contaminant per cubic meter of air (mg/m^3).

Sfi   Inhalation slope factor

TNRCC   Texas Natural Resource Conservation Commission

µg   Microgram

URF   Inhalation unit risk factor, expressed in terms of lifetime risk of exposure to one microgram of the contaminant per cubic meter of air ($µg/m^3$).

the Port Neches Pilot was basically, in order of preference, values from IRIS and HEAST. In addition to IRIS and HEAST and at the request of TNRCC, both the current and proposed (NCEA Provisional) toxicity benchmarks are presented for 1,3-butadiene (see also Table 6-2) (to prevent confusion, risk values for 1,3-butadiene are presented throughout this chapter based on the current IRIS URF, unless otherwise stated). However, it should be noted that this hierarchy of toxicity benchmarks is specific to the Port Neches Pilot Study, and that the hierarchy of toxicity benchmarks to be used in a localized assessment is a consideration to be determined prior to each assessment based, at a minimum, on (1) data quality objectives of the assessment, and (2) up front site-specific knowledge of contaminants that may be highly suspect (e.g., high monitoring detections, heavy production or use in the area, etc.), but do not have values in IRIS or HEAST. Complete results of risk modeling for all evaluated contaminants can be found in Appendix IRAP.

Available air monitoring data for the prioritized contaminants is discussed specific to each neighborhood. It is important to note that the use of this data in this report is intended to provide available supporting information associated with the identification of potential risk concerns. As discussed in Section 6.2.6, it is not included as a comparison to modeled values or intended as a verification of modeling methods. Instead, the intent is to include all relevant and available information for consideration in the identification of potential risk concerns and prioritizations.

6.1.1   Port Neches/Nederland Neighborhood

As noted in Table 6-1, four contaminants have modeled concentrations that correspond to a potential risk or hazard level of 10^{-5} or 0.25, respectively. The highest modeled risk, based on available emissions characterization data, is 5×10^{-4}, a result of 1,3-butadiene emissions. The highest modeled hazard, based on available emissions characterization data, is 5.8, a result of acrolein emissions. Source attribution is contaminant specific with both grouped and individual emission sources contributing significantly. Ambient air monitoring data for the Port Neches/Nederland neighborhood is available at station T136 for two of the four contaminants discussed in this section. Risk management considerations center on the need for additional emissions characterization data to assert confidence in modeled impacts for contaminants currently identified as not resulting in significant impacts, and to more accurately define source attribution. The following subsections further discuss results for the initial phase of the RAIMI Pilot Study specific to the Port Neches/Nederland neighborhood.

Important Notes Regarding the Figures Used to Present RAIMI Pilot Study Results

Figures are used to graphically present the results of the RAIMI Pilot Study. Most of these figures were designed to communicate the neighborhood-specific and contaminant-specific results for each contaminant and the attribution of neighborhood-specific impacts to specific sources.

Contaminant and receptor-specific results for each compound are graphically depicted using shaded islopleths to represent the level of impacts across the assessment area. The shaded isopleths are drawn across the assessment area for continuity and visual comprehension of the risk and hazard impacts. Thus some industrial areas, where residential exposure is unlikely to occur, were included in the shading. The illustration of shaded isopleths over non-residential land use areas is not intended to portray risk information for non-residential exposure conditions. Also, it is important to note that all depicted results are based on available emissions characterization data as described in Chapter 3; with potential limits discussed in Section 6.2.

It should also be noted that unshaded areas on the results maps is an indication that the risk or hazard level in those areas is less than 1×10^{-5} or 0.25, respectively; unshaded areas should not be interpreted to have no risk or hazard.

Locations to facilitate the discussion of attribution of neighborhood-specific impacts to specific sources is graphically depicted on the results maps. Attribution data tables are included to describe the apportionment of risk and hazard impacts to the individual sources.

The following information is also included on the results maps:

- Aerial photography of the assessment area showing residential and industrial development
- Location of predicted maximum impact at an actual residential location
- Air monitoring stations
- Facility boundaries
- Individual source locations to identify the points of emissions attribution

---

6.1.1.1 Cancer Risk Values

Contaminants 1,3-butadiene, ethylene oxide, and benzo(a)pyrene are identified at receptor grid nodes in and around the Port Neches/Nederland neighborhood as having concentrations that would correspond to a potential risk or hazard level exceeding 10^{-5} or 0.25, respectively, given the basic exposure scenario used. Corresponding risk values for ethylene oxide and benzo(a)pyrene are an order of magnitude less than 1,3-butadiene. Based on evaluation of the air inhalation pathway for adult and child residents, using currently available emissions data, the adult resident air inhalation pathway is more significant. Pilot Study results for these contaminants are discussed below. Risk values for all contaminants evaluated are available for review in Appendix IRAP.

1,3-Butadiene: As noted in Table 6-1, the contaminant with a modeled concentration that corresponds to the highest carcinogenic risk value is 1,3-butadiene, which results in a risk estimate of 5×10^{-4}. The

location of predicted maximum impact from 1,3-butadiene in the Port Neches/Nederland neighborhood is in a residential area northwest of several impoundments at the Huntsman facility. Figure 6-2 illustrates the spatial distribution of risk impacts from 1,3-butadiene across the Port Neches/Nederland neighborhood.

As indicated in Table 6-2, the primary risk modeling for 1,3-butadiene, as presented throughout this chapter, is based on the current IRIS unit risk factor (URF). However, as a result of interest expressed by permitting programs, the risk modeling for 1,3-butadiene was also conducted with the most current proposed URF as cited in Table 6-2. The proposed URF value for 1,3-butadiene results in estimates of adult and child inhalation risk values in the Port Neches/Nederland neighborhood of 1×10^{-5} and 4×10^{-6}, respectively.

Ethylene Oxide: Table 6-1 indicates that emissions of ethylene oxide resulted in concentrations which would correspond to adult resident inhalation risk values of 2×10^{-5}. The spatial distribution of modeled risk values for ethylene oxide is shown on Figure 6-3. The location of predicted maximum impact from ethylene oxide in the Port Neches/Nederland neighborhood is in a residential area in the east part of the neighborhood, adjacent to the Huntsman and Motiva facilities.

Benzo(a)pyrene: Table 6-1 indicates that emissions of benzo(a)pyrene resulted in concentrations which would correspond to adult resident inhalation risk values of 3×10^{-5}. The spatial distribution of modeled risk values for benzo(a)pyrene is shown on Figure 6.4. The location of predicted maximum impact from benzo(a)pyrene in the Port Neches/Nederland neighborhood is along the northern edge of a residential area in the north-central part of the neighborhood.

6.1.1.2 Non-Cancer Hazard Values

As noted in Table 6-1, emissions of two contaminants, 1,3-butadiene and acrolein, resulted in estimated hazard levels exceeding 0.25 in the Port Neches/Nederland neighborhood. These results are discussed below. Hazard values for some contaminants, including ethylene oxide and benzo(a)pyrene, could not be calculated because toxicity benchmarks are not available (see Table 6-2). Hazard values for all contaminants evaluated are available for review in Appendix IRAP.

1,3-Butadiene: As illustrated in Figure 6-5, 1,3-butadiene emissions resulted in a modeled concentration that corresponds to a non-carcinogenic hazard value of 2.0. The location of predicted maximum impact from 1,3-butadiene in the Port Neches/Nederland neighborhood is in a residential area northwest of

several impoundments at the Huntsman facility, and is the same location identified for the maximum risk value identified in Section 6.1.1.1. The maximum hazard value is obtained from the child resident air inhalation pathway.

Acrolein: As illustrated in Figure 6-6, the contaminant with a modeled concentration that corresponds to the highest non-carcinogenic hazard value is acrolein, which results in a hazard estimate of 5.8. The location of predicted maximum impact from acrolein in the Port Neches/Nederland neighborhood is in a residential area in the northern part of Nederland, south of several tank farms and terminal facilities.   The maximum hazard value is obtained from the child resident air inhalation pathway.

6.1.1.3 Source Attribution

Attribution of impacts in the Port Neches/Nederland neighborhood area to specific emission sources is contaminant dependent, with significant contributions identified from both grouped and individual emission sources. It is important to note that presented findings are based on modeling available emissions characterization data, the limits of which are further discussed in Section 6.2.

1,3-Butadiene: Table 6-3 summarizes the attribution profile for the most significant 1,3-butadiene emissions sources contributing to impacts at the modeled location of maximum impact in the Port Neches/Nederland neighborhood. This table also includes a prioritization of the most significant 1,3-butadiene emissions sources for risk management, based on modeling available emissions data as described in Chapter 3. The locations of the prioritized individual sources are illustrated on Figure 6-2 for cancer risk and Figure 6-5 for non-cancer hazard. At the location of predicted maximum impact, individual 1,3-butadiene emissions sources, mostly at the Huntsman facilities, account for most of the predicted impacts.

Review of risk results across the assessment area indicate, however, that a substantially different attribution profile is exhibited for other locations in the Port Neches/Nederland neighborhood with distance from industrial sources. To illustrate this point, Figure 6-2 identifies an additional location that was selected for presentation and discussion. The attribution profile and risk-based prioritization specific to this additional receptor location are presented in Table 6-4. The random location is somewhat

TABLE 6-3

ATTRIBUTION PROFILE AND RISK-BASED PRIORITIZATION
AT THE LOCATION OF PREDICTED MAXIMUM IMPACT IN THE PORT NECHES/NEDERLAND NEIGHBORHOOD
FROM 1,3-BUTADIENE EMISSIONS

	Source Description[a,b]	Permit Status	Source-Specific Percentage of Pathway Risk	Cancer Risk		Non-Cancer Hazard	
				Resident Adult	Resident Child	Resident Adult	Resident Child
1	*Huntsman Corporation, Wastewater JWWTP Blending Station #B-14* FIN: JWB14 EPN: JWB14	G	23.5%	1×10^{-4}	5×10^{-5}	0.1	0.3
2	*Huntsman Corporation, Wastewater JWWTP Neutralization Basin #B-16* FIN: JWB16 EPN: JWB16	G	14.9%	7×10^{-5}	3×10^{-5}	0.07	0.2
3	*Huntsman Corporation,* South B.D.E. Equipment Fugitives FIN: BDFUGS EPN: BDFUGS	P	12.4%	6×10^{-5}	3×10^{-5}	0.06	0.1
4	*Huntsman Corporation,* TNRCC Name: Fugitives EPN: C4FU	UN	6.9%	4×10^{-5}	2×10^{-5}	0.04	0.08
5	*Huntsman Corporation, Wastewater JWWTP Primary Clarifier #C-6* FIN: JWC6 EPN: JWC6	G	6.8%	3×10^{-5}	2×10^{-5}	0.04	0.08
	All Other Modeled Sources - 22 Individual and 14 Grouped Sources - 7 of these individual sources resulted in risk exceeding 1×10^{-5}	NA	35.4%	2×10^{-4}	8×10^{-5}	0.2	0.4
	Total[c]		**100.0%**	**5.0×10^{-4}**	**2.2×10^{-4}**	**0.5**	**1**

TABLE 6-3

**ATTRIBUTION PROFILE AND RISK-BASED PRIORITIZATION
AT THE LOCATION OF PREDICTED MAXIMUM IMPACT IN THE PORT NECHES/NEDERLAND NEIGHBORHOOD
FROM 1,3-BUTADIENE EMISSIONS**

Notes: As indicated in the Table 6-2, both current and proposed toxicity benchmarks are presented for 1,3-butadiene. To prevent confusion, risk values for 1,3-butadiene are presented throughout this chapter based on the current IRIS URF, unless otherwise stated.

[a]   The locations of prioritized individual sources are shown on Figure 6-2 for cancer risk impacts, and Figure 6-5 for non-cancer hazard impacts.

[b]   Complete source descriptions can be found in Appendix ESC, and complete modeled risk results are in Appendix IRAP

[c]   Totals may vary due to rounding

EPN   Emissions point number

FIN   Facility identification number

G   Grandfathered Source

P   Permitted Source

NA   Not Applicable–grouped source category

UN   Unknown

TABLE 6-4

ATTRIBUTION PROFILE AND RISK-BASED PRIORITIZATION
AT A RANDOM RECEPTOR LOCATION
IN THE PORT NECHES/NEDERLAND NEIGHBORHOOD
FROM 1,3-BUTADIENE EMISSIONS

	Source Description[a,b]	Permit Status	Source-Specific Percentage of Pathway Risk	Cancer Risk	
				Resident Adult	Resident Child
1	*Light Duty Gasoline Vehicles (LDGV)* Surrogate: On-Road Mobile	NA	27.7%	1×10^{-5}	6×10^{-6}
2	*Light Duty Gasoline Trucks 1&2 (LDGT)* Surrogate: On-Road Mobile	NA	22.0%	1×10^{-5}	5×10^{-6}
3	*Huntsman Corporation, Wastewater JWWTP Blending Station #B-14* FIN: JWB14 EPN: JWB14	G	6.9%	3×10^{-6}	2×10^{-6}
4	*Huntsman Corporation, Wastewater JWWTP Neutralization Basin #B-16* FIN: JWB16 EPN: JWB16	G	5.1%	3×10^{-6}	1×10^{-6}
5	*Huntsman Corporation,* South B.D.E. Equipment Fugitives FIN: BDFUGS EPN: BDFUGS	P	4.8%	2×10^{-6}	1×10^{-6}
	All Other Modeled Sources (24 Individual and 12 Grouped Sources)	NA	33.5%	2×10^{-6}	7×10^{-6}
	Total[c]		**100.0%**	**5×10^{-5}**	**2×10^{-5}**

Notes: As indicated in the Table 6-2, both current and proposed toxicity benchmarks are presented for 1,3-butadiene. To prevent confusion, risk values for 1,3-butadiene are presented throughout this chapter based on the current IRIS URF, unless otherwise stated.

[a]   The locations of prioritized individual sources are shown on Figure 6-2
[b]   Complete source descriptions can be found in Appendix ESC, and complete modeled risk results are in Appendix IRAP
[c]   Totals may vary due to rounding
EPN   Emissions point number
FIN   Facility identification number
G   Grandfathered Source
P   Permitted Source
NA   Not Applicable–grouped source category

removed from large industrial facilities, although several tank farms and bulk terminal facilities are located to the north. At this location, the predicted risk value from 1,3-butadiene emissions is $5x10^{-5}$, one order of magnitude smaller than at the location of predicted maximum impact located closer to the industrial sources. As noted in Table 6-4, approximately half of the potential risk impacts at this location are attributable to two grouped emissions source subcategories-light duty gasoline vehicles and light duty gasoline trucks.

The attribution of potential risk impacts to individual and grouped sources across the Port Neches/Nederland neighborhood is also represented in the shaded isopleth pattern illustrated on Figure 6-2. Three features on this map, in particular, illustrate how attribution of modeled impacts across the neighborhood are discernable between individual and grouped emission sources. First, there is a north-south trend that is centered on the significant individual sources at the Huntsman facility and includes the areas of highest modeled impacts for the neighborhood. This orientation correlates with the prevailing northerly/southerly winds in the assessment area.

Second, the shaded area indicated on Figure 6-2 (representing modeled risk levels greater than 10^{-5}) extends west of the heavily industrialized areas, into the residential and commercial center of the Port Neches/Nederland neighborhood. Modeled risk in these areas include significant contributions from mobile grouped source subcategories (light duty gasoline vehicles and light duty gasoline trucks). The emissions inventory for these subcategories was developed based on a census tract population surrogate. Therefore, maximum modeled impacts from these subcategories could be expected where population density is highest, as is the case in the central neighborhood areas of Nederland and Port Neches.

Third, on the western part of Figure 6-2 there is a shaded area, west of the main isopleth coverage area, indicating a relative increase in modeled risk estimates. This isopleth area is anticipated to be somewhat influenced by the grouped source modeling methodology as described in Section 4.1.3, and would require further refinement before defining as local "hot spots" of risk impacts.

Ethylene Oxide: Table 6-5 summarizes the attribution profile for the significant ethylene oxide emissions sources contributing to impacts at the predicted location of maximum impact in the Port Neches/Nederland neighborhood. The locations of the prioritized individual sources are illustrated on Figure 6-3. At the location illustrated, individual emissions sources of ethylene oxide at the Huntsman facilities account for most of the modeled impacts.

TABLE 6-5

**ATTRIBUTION PROFILE AND RISK-BASED PRIORITIZATION
AT THE LOCATION OF PREDICTED MAXIMUM IMPACT
IN THE PORT NECHES/NEDERLAND NEIGHBORHOOD
FROM ETHYLENE OXIDE EMISSIONS**

	Source Description[a,b]	Permit Status	Source-Specific Percentage of Pathway Risk	Cancer Risk	
				Resident Adult	Resident Child
1	*Huntsman Corporation*, R. & S. with Scrubber R-0-62" FIN: RSER062 EPN: RSELRBMTW	G	19.6%	4×10^{-6}	2×10^{-6}
2	*Huntsman Corporation*, R. & S.E. Process Fugitives FIN: RSEFUG EPN: RSEFUG	P	16.2%	3×10^{-6}	2×10^{-6}
3	*Huntsman Corporation*, F4 Unit Process Fugitives FIN: F4FUG EPN: F4FUG	P	14.7%	3×10^{-6}	1×10^{-6}
4	*Huntsman Corporation*, F6 Unit Process Fugitives FIN: F6FUG EPN: F6FUG	P	13.8%	3×10^{-6}	1×10^{-6}
5	*Huntsman Corporation*, Utilities East Cooling Towers FIN: UEUL22 EPN: UEUL22	P	12.5%	3×10^{-6}	1×10^{-6}
	All Other Modeled Sources (10 Individual and 4 Grouped Sources)	NA	23.3%	5×10^{-6}	2×10^{-6}
	Total[c]		**100.0%**	**2×10^{-5}**	**9×10^{-6}**

Notes:

[a] The locations of prioritized individual sources are shown on Figure 6-3

[b] Complete source descriptions can be found in Appendix ESC, and complete modeled risk results are in Appendix IRAP

[c] Totals may vary due to rounding

EPN Emissions point number
FIN Facility identification number
G Grandfathered Source
P Permitted Source
NA Not Applicable–Grouped source category

Similar to 1,3-butadiene, review of risk results across the assessment area indicate that a substantially different attribution profile is exhibited for other locations in the Port Neches/Nederland neighborhood with distance from industrial sources. To illustrate this point, Figure 6-3 identifies an additional location, which is located along the northern edge of a residential area in the north-central part of the Port Neches/Nederland neighborhood, that was selected for presentation and discussion. The attribution profile specific to this location is presented in Table 6-6. At this location, grouped source subcategories account for a risk value of about 1×10^{-5}. Significant grouped source subcategories contributing to this risk include industrial organic chemicals manufacturing and hospital sterilizers.

TABLE 6-6

**ATTRIBUTION PROFILE AND RISK-BASED PRIORITIZATION
AT A RANDOM RECEPTOR LOCATION IN THE PORT NECHES/NEDERLAND
NEIGHBORHOOD
FROM ETHYLENE OXIDE EMISSIONS**

Source Description[a]		Permit Status	Source-Specific Percentage of Pathway Risk	Cancer Risk	
				Resident Adult	Resident Child
1	*Industrial Organic Chemicals Manufacturing* Surrogate: Industrial Land Use	NA	69.2%	8×10^{-6}	4×10^{-6}
2	*Hospital Sterilizers* Surrogate: Commercial Land Use	NA	16.5%	2×10^{-6}	9×10^{-7}
	All Other Modeled Sources (15 Individual and 2 Grouped Sources)	NA	14.4%	2×10^{-6}	8×10^{-7}
		Total[b]	**100.0%**	**1×10^{-5}**	**5×10^{-6}**

Notes: [a] Complete source descriptions can be found in Appendix ESC, and complete modeled risk results are in Appendix IRAP
  [b] Totals may vary due to rounding
NA Not Applicable–Grouped emissions source

Consideration of the risk isopleths and attribution information on Figure 6-3 yields further understanding of the neighborhood emissions characterization. For example, the shaded areas indicating the highest risk impacts illustrated on Figure 6-3 coincide with the areas adjacent to the Huntsman facility–which contains the only individual sources of ethylene oxide in the assessment area based on available emissions characterization data. Additionally, several small isolated isopleth areas evident on Figure 6-3 are anticipated to be somewhat influenced by the grouped source modeling methodology as described in Section 4.1.3, and would require further refinement before defining as local "hot spots" of risk impacts.

Benzo(a)pyrene: Table 6-7 summarizes the attribution profile for the significant benzo(a)pyrene
emissions sources contributing to impacts at the predicted location of maximum impact in the Port
Neches/Nederland neighborhood. This table also includes a prioritization of significant benzo(a)pyrene
emissions sources for risk management. The emissions characterization for the Port Neches assessment
area did not identify any individual sources of benzo(a)pyrene emissions; only grouped emissions source
categories were identified, as indicated on Table 6-7.

TABLE 6-7

ATTRIBUTION PROFILE AND RISK-BASED PRIORITIZATION
AT THE LOCATION OF PREDICTED MAXIMUM IMPACT
IN THE PORT NECHES/NEDERLAND NEIGHBORHOOD
FROM BENZO(A)PYRENE EMISSIONS

Source Description[a]		Permit Status	Source-Specific Percentage of Pathway Risk	Cancer Risk	
				Resident Adult	Resident Child
1	*Gasoline Distribution Stage 1* Surrogate: Commercial Land Use and Industrial Land Use	NA	67.0%	2×10^{-5}	9×10^{-6}
2	*Consumer Products Usage* Surrogate: Population	NA	20.5%	6×10^{-6}	3×10^{-6}
3	*Open Burning: Scrap Tires* Surrogate: Industrial Land Use	NA	5.4%	2×10^{-6}	7×10^{-7}
4	*Surface Coatings: Industrial Maintenance* Surrogate: Industrial Land Use	NA	3.4%	1×10^{-6}	5×10^{-7}
	All Other Modeled Sources (17 Grouped Sources)	NA	3.7%	1×10^{-6}	5×10^{-7}
	Total[b]		**100.0%**	**3×10^{-5}**	**1×10^{-5}**

Notes: [a]   Complete source descriptions can be found in Appendix ESC, and complete modeled risk
                     results are in Appendix IRAP
         [b]   Totals may vary due to rounding
         NA   Not Applicable–grouped source category

Attribution of benzo(a)pyrene to grouped sources is indicated by the spatial distribution of modeled risk
impacts on Figure 6-4. This figure identifies several non-contiguous isopleth areas of relatively increased
modeled risk estimates, and the position of these isopleth areas correspond to grouped source modeling
pseudo-source locations illustrated on Figure 4-1 as described in Section 4.1.3. This indicates

that the risk values indicated by the shaded areas may be influenced to some degree by the emissions allocation scheme and modeling procedure for grouped emissions sources. As described in Section 3.3.2, this method of characterizing grouped source emissions is intended to identify areas for further evaluation based on potential risk impacts. Therefore, assessment of benzo(a)pyrene emissions impacts could be further evaluated by modeling benzo(a)pyrene emissions sources based on the frequency of actual occurrence in the assessment area, as described in Section 3.3.2.

Acrolein: Table 6-8 summarizes the attribution profile for the significant acrolein emissions sources contributing to impacts at the predicted location of maximum impact in the Port Neches/Nederland neighborhood. This table also includes a prioritization of significant acrolein emissions sources for risk management. The emissions characterization for the Port Neches assessment area did not identify any individual sources of acrolein emissions; only grouped emissions source categories were identified, as indicated on Table 6-8.

Attribution of acrolein to grouped sources is indicated by the spatial distribution of modeled risk impacts on Figure 6-6. This figure identifies several non-contiguous isopleth areas of relatively increased modeled risk estimates, and the position of these isopleth areas correspond to grouped source modeling pseudo-source locations illustrated on Figure 4-1 as described in Section 4.1.3. This indicates that the risk values indicated by the shaded areas may be influenced to some degree by the emissions allocation scheme and modeling procedure for grouped emissions sources. As described in Section 3.3.2, this method of characterizing grouped source emissions is intended to identify areas for further evaluation based on potential risk impacts. Therefore, assessment of acrolein emissions impacts could be further evaluated by modeling acrolein emissions sources based on the frequency of actual occurrence in the assessment area, as described in Section 3.3.2.

6.1.1.4 Applicable Air Monitoring Data

As discussed in Chapter 2, ambient air monitoring data is available at station T136 for the Port Neches/Nederland neighborhood (see Figure 6-7). However, of the contaminants prioritized in the Pilot Study as being of potential concern in the Port Neches/Nederland neighborhood based on modeled air concentrations, only measured data for 1,3-butadiene and acrolein are available at T136 (TNRCC 1997a; U.S. EPA 1998h). Review of the Community Air Toxics Monitoring Network Report (January–December 1994-1997) and the Aerometric Information Retrieval System (AIRS) database

TABLE 6-8

**ATTRIBUTION PROFILE AND RISK-BASED PRIORITIZATION
AT THE PREDICTED LOCATION OF MAXIMUM IMPACT
IN THE PORT NECHES/NEDERLAND NEIGHBORHOOD FROM ACROLEIN EMISSIONS**

	Source Description[a]	Permit Status	Source-Specific Percentage of Pathway Risk	Non-Cancer Hazard	
				Resident Adult	Resident Child
1	Light Duty Gasoline Vehicles (LDGV) Surrogate: On-Road Mobile	NA	29.7 %	0.78	1.73
2	Light Duty Gasoline Trucks 1 & 2 (LDGT) Surrogate: On-Road Mobile	NA	13.2 %	0.35	0.77
3	Marine Vessels, Commercial Surrogate: Water-Based Land Use	NA	12.2 %	0.32	0.71
4	All Off-highway Vehicle Diesel Surrogate: Off-Road Mobile	NA	12.2 %	0.32	0.71
5	Heavy Duty Gasoline Vehicles (HDGV) Surrogate: On-Road Mobile	NA	10.5 %	0.27	0.61
6	Heavy Duty Diesel Vehicles (HDDV) Surrogate: On-Road Mobile	NA	8.4 %	0.22	0.49
7	Structure Fires Surrogate: Population	NA	5.8 %	0.15	0.34
	All Other Modeled Sources (11 Grouped Sources)	NA	8.0 %	0.21	0.47
		Total[b]	**100.0 %**	**2.62**	**5.83**

Notes: [a]   Complete source descriptions can be found in Appendix ESC, and complete modeled risk
results are in Appendix IRAP
[b]   Totals may vary due to rounding
NA   Not Applicable–Grouped source category

indicates that measured air concentration data are not available at this station for ethylene oxide or benzo(a)pyrene (TNRCC 1997a; U.S. EPA 1998h).

Average annual measured air concentrations of 1,3-butadiene are available at T136 for the years 1994 through 2000 (TNRCC 1997a; U.S. EPA 1998h). To illustrate measured concentrations on a risk basis, tables in Figure 6-7 present modeled risk and hazard levels based on extrapolating the average air concentrations, for the available average yearly monitoring data summarized in the table, into the future for the length of applicable exposure duration (e.g., 30 years for the adult). A simplified exposure scenario, as described in Chapter 5, was utilized consisting of breathing outdoor air 24 hours a day for 350 days a year. Resulting adult risk values range from 10^{-4} to 10^{-3}; calculated using the toxicity factor value reported in IRIS (see Table 6-2). Child hazard values range from about 2.0 to 6.0.

For acrolein, average annual measured air concentrations are available at T136 for the years 1995 through 1997 (TNRCC 1997a; U.S. EPA 1998h). Similarly, the tables in Figure 6-7 illustrate measured concentrations on a non-cancer hazard basis based on extrapolation and a simplified exposure scenario. The resulting child hazard value was 14.6, and the adult hazard value was about 6.6.

Although measured air concentration data are not available at station T136 for ethylene oxide or benzo(a)pyrene, inputting average annual air concentration data available for formaldehyde does result in risk and/or hazard levels of concern. Even though formaldehyde was not modeled as a contaminant of concern in the Port Neches/Nederland neighborhood, its risk based measured concentrations are presented due to potential for secondary formation (see Section 6.2.5). Air monitoring data for formaldehyde is available at this location only for the years 1995 through 1997 (U.S. EPA 1998h). Also, monitoring data for formaldehyde at Station T136 is very limited (four samples in 1995 and 1996, and 2 samples in 1997). In contrast, data for the other contaminants discussed above are based on about 50 samples for each reported year. Risk modeling results for formaldehyde are included in Figure 6-7.

With regard to available ambient air monitoring data, it is important to note that the use of this data in this report is intended to provide available supporting information associated with the identification of potential risk concerns. As discussed in Section 6.2.6, it is not included as a comparison to modeled values or intended as a verification of modeling methods. Instead, the intent is to include all relevant and available information for consideration in the identification of potential risk concerns and prioritizations.

6.1.1.5 Risk Management Considerations

Risk management considerations in this section focus on information identified during Pilot Study implementation that relates to the confidence in presented results [i.e., results that exceed criteria (see introduction to Chapter 6) for presentation and discussion], and is included such that it can be considered by risk managers when assessing risk priorities and important data gaps in the Port Neches/Nederland neighborhood. It should be noted that these discussions are limited since they primarily focus on information that affects prioritized results that are presented in this chapter and do not equally consider information that may affect the confidence in low priority results that are not as scrutinized (i.e., results that are considered a lower priority since they do not exceed a $1x10^{-5}$ risk level or a 0.25 hazard level). Additional risk management considerations not necessarily specific to the profiling of this neighborhood location are presented in Section 6.2. The primary risk management consideration for results on the Port Neches/Nederland neighborhood is the need for additional emissions characterization data to assert confidence in modeled impacts for contaminants currently identified as not resulting in significant impacts and for emissions of contaminants that are identified as resulting in impacts of potential concern, to more accurately define source attribution.

Speciation of Emissions

In some cases reported emissions may be in the form of a grouping of constituents that are not adequately speciated into individual contaminants for air dispersion and risk modeling. Unspeciated emissions are therefore mixtures of multiple contaminants (e.g., non-methane VOCs, VOC gas mixtures, gasoline, crude oil, and jet fuel). Specific to the speciation of emissions from permitted and non-permitted sources at facilities contributing to impacts in the Port Neches/Nederland neighborhood, the emissions characterization data indicate the following:

- For the Huntsman facilities:

  - Speciated emissions of 1,3-butadiene (238 tons) and ethylene oxide (44 tons) are recorded in the 1997 PSDB (TNRCC 1999d).
  - 722 tons of unspeciated emissions that may contain 1,3-butadiene, ethylene oxide, and other contaminants, were also reported in the 1997 PSDB (TNRCC 1999d).
  - 2,409 tons of unspeciated non-methane VOC emissions, which may include 1,3-butadiene, ethylene oxide, and other contaminants, were reported in the 1997 Source Status Survey (described in Section 6.2.1; TNRCC 1999c).

- For the Ameripol Synpol facility:

  – Speciated emissions of 1,3-butadiene (5.8 tons) are recorded in the 1997 PSDB (TNRCC 1999d).
  – 72 tons of unspeciated emissions, which may include 1,3-butadiene and other contaminants, were also reported in the 1997 PSDB (TNRCC 1999d).
  – 228 tons of unspeciated non-methane VOC emissions, which may include 1,3-butadiene and other contaminants, were reported in the 1997 Source Status Survey (TNRCC 1999c).

Unspeciated emissions of 1,3-butadiene, ethylene oxide, or other contaminants from facilities in the assessment area may also contribute to impacts that can not be evaluated at this time because sufficient information for air and risk modeling was not available based on emissions characterization. A total of 3,429 tons of unspeciated emissions were reported for facilities in the Port Neches assessment area (TNRCC 1999d).

As with permitted emission sources, emissions from grandfathered and exempt sources may result in impacts that cannot be modeled without detailed speciated emissions information. Specific to the sources and facilities contributing to impacts in the Port Neches/Nederland neighborhood, the 1997 PSDB and the 1997 TNRCC Source Status Survey indicate the following emissions based on source permit status:

- Documented grandfathered and exempt emissions from the Huntsman facilities include:

  – Grandfathered emissions of 1,3-butadiene (137.7 tons), and ethylene oxide (21.7 tons) are recorded in the 1997 PSDB (TNRCC 1999d).
  – Emissions of non-methane VOCs from grandfathered sources (6.6 tons) and exempt sources (0.3 tons) are recorded in the 1997 PSDB (TNRCC 1999d).
  – Emissions of non-methane VOCs from grandfathered (1,014 tons) and exempt (220 tons) sources were reported during the 1997 TNRCC Source Status Survey (TNRCC 1999c).

- Documented grandfathered and exempt emissions from the Ameripol Synpol facility include:

  – Emissions of 1,3-butadiene from grandfathered (5.3 tons) and exempt (0.5 tons) sources are recorded in the 1997 PSDB (TNRCC 1999d).
  – Emissions of non-methane VOCs from grandfathered sources (4.9 tons) and VOC gas mixtures from grandfathered (7.3 tons) and exempt (5.6 tons) sources are recorded in the 1997 PSDB (TNRCC 1999d).
  – Emissions of non-methane VOCs from grandfathered (48.7 tons) and exempt (6.2 tons) sources were reported during the 1997 TNRCC Source Status Survey (TNRCC 1999c).

Grandfathered and exempt emissions from other facilities in the assessment area may also contribute to impacts that cannot be evaluated at this time due to insufficient information for air and risk modeling. A

total of 3,251 tons of grandfathered and exempt emissions of non-methane VOCs were voluntarily reported to TNRCC for the 1997 Source Status Survey by facilities in the Port Neches assessment area (TNRCC 1999c). Risk managers should be aware that unspeciated emissions from grandfathered and exempt sources may be present in the study area.

Characterization of Grouped Emissions Source

Risk levels greater than 10^{-5} were modeled for emissions from grouped sources of ethylene oxide, benzo(a)pyrene, and acrolein in the Port Neches/Nederland neighborhood. Grouped emissions sources were characterized to provide emissions estimates based on a census-tract surrogate, as described in Chapter 3.   However, further refinement may be required to support risk management decisions. These emissions estimates could be further refined by evaluating the actual frequency or occurrence of specific sources within a census tract. For example, emissions estimates for Stage I gasoline distribution–emissions from petroleum product storage facilities– was based on county and census tract employment within SIC 5171 (petroleum bulk stations and terminals). Since similar facilities exist within the assessment area, these facilities could be modeled based on actual location, which would provide a more realistic picture of resulting risk impacts.

Toxic Release Inventory Data

The 1997 PSDB indicates that Huntsman emitted more than 238 tons of 1,3-butadiene to the airshed (TNRCC 1999d). This value is significantly greater than the 120 tons of 1,3-butadiene reported in the TRI (U.S. EPA 2000g). The 1997 TRI also indicates that Ameripol Synpol emitted more than 9 tons of 1,3-butadiene, but the 1997 PSDB reports only 5.8 tons of this contaminant (TNRCC 1999d; U.S. EPA 2000g). As discussed in Section 2.2.5, it is important to note that major differences in data resolution exist between the TRI and PSDB due to these databases representing different regulatory programs with different objectives and emissions reporting requirements. Also, while TRI represents a generalized database that only report emissions on a facility wide basis, TNRCC's PSDB reports emissions data at a resolution specific to individual sources (see Sections 2.2.5, 3.2, and 4.3.2).

Secondary Formation

No individual sources of acrolein emissions were identified in the Port Neches assessment area. However, 1,3-butadiene, an important precursor compounds to atmospheric formation of acrolein is emitted in very large quantities. The PSDB indicates that approximately 249 tons of 1,3-butadiene were

emitted from sources within the Port Neches/Nederland Assessment area, and about 272 tons were emitted from sources in Jefferson County. Reported emissions of acrolein precursor compounds are subject to the same emissions characterization limitations as other contaminants. Risk management considerations regarding the secondary formation of formaldehyde are discussed in greater detail in Section 6.2.

6.1.2   Groves Neighborhood

As noted in Table 6-1, eight contaminants have modeled concentrations which correspond to a potential risk or hazard level at or above 10^{-5} or 0.25, respectively. These prioritized results are presented in this section. The highest modeled risk value based on available emissions characterization data is $1x10^{-4}$ as a result of 1,3-butadiene emissions. The highest modeled hazard value is 20.2, as a result of acrolein emissions. Source attribution is contaminant specific. Ambient air monitoring data for the Groves neighborhood is available at station T119 for two of the seven contaminants discussed in this section. Risk management considerations center on the need for additional emissions characterization data to assert confidence in modeled impacts for contaminants currently identified as not resulting in significant impacts, and to more accurately define source attribution. The following subsections further discuss results for the initial phase of the RAIMI Pilot Study specific to the Groves neighborhood.

6.1.2.1 Cancer Risk Values

Eight contaminants–benzene, 1,3-butadiene, ethylene oxide, formaldehyde, benzo(a)anthracene, benzo(a)pyrene, benzo(b)fluoranthene, and acrolein–are identified in Table 6-1 as having modeled concentrations that would correspond to risk levels exceeding 10^{-5} in the Groves neighborhood. RAIMI Pilot Study results for these contaminants are discussed below. Based on evaluation of the air inhalation pathway for adult and child residents, using currently available emissions data, the adult resident air inhalation pathway is more significant. Risk and hazard values for all contaminants modeled are available for review in Appendix IRAP.

Benzene: Table 6-1 indicates that benzene emissions result in modeled concentrations that would correspond to an adult resident inhalation risk value of $3x10^{-5}$ in the Groves neighborhood. The location of predicted maximum impact from benzene emissions is in a residential area in the eastern part of Groves, as shown on Figure 6-8, which illustrates the spatial distribution of potential risk values across the Groves neighborhood.

1,3-Butadiene: As noted in Table 6-1 and illustrated in Figure 6-9, the highest modeled carcinogenic risk value of $1x10^{-4}$ is attributable to emissions of 1,3-butadiene when evaluating exposure using current benchmarks indicated on Table 6-2.   The location of predicted maximum impact in the Groves neighborhood from 1,3-butadiene emissions is in a residential area in the eastern part of Groves, as shown on Figure 6-9. It should be noted that on Figure 6-9, the shaded risk level isopleth terminates along the southern edge of the Port Neches Assessment Area, south of the Groves neighborhood. This is a result of the air modeling receptor grid array not extending beyond the assessment area.

As indicated in Table 6-2, the primary risk modeling for 1,3-butadiene, as presented throughout this chapter, is based on the current IRIS URF. However, as a result of interest expressed by permitting programs, the risk modeling for 1,3-butadiene was also conducted with the most current proposed URF as cited in Table 6-2. The proposed URF value for 1,3-butadiene results in estimated adult and child inhalation risk values in the Groves neighborhood of $3x10^{-6}$ and $1x10^{-6}$, respectively.

Ethylene Oxide: Table 6-1 indicates that emissions of ethylene oxide result in modeled concentrations corresponding to an adult resident inhalation risk value of $2x10^{-5}$. The spatial distribution of modeled risk values for ethylene oxide is shown on Figure 6-10. The location of predicted maximum impact from ethylene oxide in the Groves neighborhood is in a residential area in the eastern part of the neighborhood.

Formaldehyde: Table 6-1 indicates that emissions of formaldehyde result in modeled concentrations corresponding to an adult resident inhalation risk value of $2x10^{-5}$. The spatial distribution of modeled risk values for formaldehyde is shown on Figure 6-11. The location of predicted maximum impact from formaldehyde in the Groves neighborhood is in a residential area in the eastern part of the neighborhood.

Benzo(a)anthracene: Table 6-1 indicates that emissions of benzo(a)anthracene result in modeled concentrations corresponding to an adult resident inhalation risk value of $2x10^{-5}$. The spatial distribution of modeled risk values for benzo(a)anthracene is shown on Figure 6-12. The location of predicted maximum impact from benzo(a)anthracene in the Groves neighborhood is in a residential area in the eastern part of the neighborhood.

Benzo(a)pyrene: Table 6-1 indicates that emissions of benzo(a)pyrene result in modeled concentrations corresponding to an adult resident inhalation risk value of $7x10^{-5}$. The spatial distribution of modeled risk values for benzo(a)pyrene is shown on Figure 6-13. The location of predicted maximum impact from

benzo(a)pyrene in the Groves neighborhood is along the northern edge of a residential area in the eastern part of the neighborhood.

Benzo(b)fluoranthene: Table 6-1 indicates that emissions of benzo(b)fluoranthene result in modeled concentrations corresponding to an adult resident inhalation risk value of $2x10^{-5}$. The spatial distribution of modeled risk values for benzo(b)fluoranthene is shown on Figure 6-14. The location of predicted maximum impact from benzo(a)fluoranthene in the Groves neighborhood is in a residential area in the eastern part of the neighborhood.

6.1.2.2 Non-Cancer Hazard Values

Predicted hazard values for 1,3-butadiene and acrolein exceed 0.25 in the Groves. Hazard values for ethylene oxide, benzo(a)anthracene, benzo(a)pyrene, and benzo(b)fluoranthene could not be calculated because toxicity benchmarks are not available for these contaminants (see Table 6-2). The highest hazard value is obtained from the child resident air inhalation pathway. Hazard values for all contaminants evaluated are available for review in Appendix IRAP.

1,3-Butadiene: Emissions of 1,3-butadiene resulted in a modeled hazard value of 0.6 (see Table 6-1). The location of predicted maximum impact from 1,3-butadiene emissions is in the eastern part of the Groves neighborhood (see Figure 6-15).

Acrolein: Emissions of acrolein resulted in a modeled hazard value of 20.2 (see Table 6-1). The location of predicted maximum impact from acrolein emissions is in the eastern part of the Groves neighborhood (see Figure 6-16).

6.1.2.3 Source Attribution

Attribution of impacts in the Groves neighborhood to specific emissions sources is contaminant specific, with significant contributions identified from both grouped and individual emissions sources, as discussed below. It is important to note that presented findings are based on modeling available emissions characterization data, the limits of which are further discussed in Section 6.2.

Benzene: Table 6-9 summarizes the attribution profile for significant benzene emission sources contributing to impacts at the predicted location of maximum impact in the Groves neighborhood (see

Figure 6-8). This table also includes a prioritization of the significant emissions sources. The emissions characterization of Port Neches identified individual sources and grouped source categories for benzene emissions, but only the grouped source categories resulted in significant impacts.

The shaded risk isopleths illustrated on Figure 6-8 indicate areas of relatively higher modeled risk estimates, which are non-contiguous and small in areal extent. As described in Section 6.1.1.3, in the attribution discussion for benzo(a)pyrene, the spatial distribution of benzene impacts depicted on Figure 6-8 is anticipated to be influenced by the emissions allocation scheme and air dispersion modeling procedure for grouped sources. However, as described in Section 3.3.2, further assessment based on the frequency and actual occurrence of sources within the assessment area would provide a more refined prediction of impacts from benzene emissions in the neighborhood.

TABLE 6-9

ATTRIBUTION PROFILE AND RISK-BASED PRIORITIZATION
AT THE PREDICTED LOCATION OF MAXIMUM IMPACT
IN THE GROVES NEIGHBORHOOD FROM BENZENE EMISSIONS

	Source Description[a]	Permit Status	Source-Specific Percentage of Pathway Risk	Cancer Risk	
				Resident Adult	Resident Child
1	*Light Duty Gasoline Vehicles (LDGV)* Surrogate: On-Road Mobile	NA	34.5%	1×10^{-5}	5×10^{-6}
2	*Gasoline Distribution Stage 1* Surrogate: Commercial Land Use and Industrial Land Use	NA	30.8%	1×10^{-5}	4×10^{-6}
3	*Light Duty Gasoline Trucks 1&2 (LDGT)* Surrogate: On-Road Mobile	NA	25.2%	8×10^{-6}	4×10^{-6}
	All Other Modeled Sources (36 Individual and 25 Grouped Sources)	NA	9.6%	3×10^{-6}	1×10^{-6}
		Total[b]	**100.0%**	**3×10^{-5}**	**1×10^{-5}**

Notes: [a]   Complete source descriptions can be found in Appendix ESC, and complete modeled risk results are in Appendix IRAP
   [b]   Totals may vary due to rounding
   NA   Not Applicable–Grouped source category

1,3-Butadiene: Table 6-10 summarizes the attribution profile for the significant 1,3-butadiene emissions sources contributing to impacts–cancer risk and non-cancer hazard–at the location of predicted maximum impact in the Groves neighborhood (see Figure 6-9). This table also includes a prioritization of the most significant 1,3-butadiene emissions sources for risk management. At the location of predicted maximum impact, grouped 1,3-butadiene emissions sources account for most of the predicted impacts.

The risk results indicate, however, that other locations in the Groves neighborhood may exhibit a substantially different attribution profile. For example, Figure 6-9 also identifies a random receptor location for results presentation and discussion. The attribution profile and risk-based prioritization specific to this receptor location are presented on Table 6-11. This location is in a residential alcove surrounded on three sides by the Huntsman facility. At this location, the modeled risk value from 1,3-butadiene emissions is 6×10^{-5}. However, the most significant sources contributing to impacts at this location are individual sources at the Huntsman facility, as indicated on Table 6-11.

Ethylene Oxide: Table 6-12 summarizes the attribution profile for the significant ethylene oxide emissions source contributing to impacts at the predicted location of maximum impact in the Groves neighborhood (see Figure 6-10). This table also includes a prioritization of the most significant ethylene oxide emissions sources for risk management. At the location of predicted maximum impact, grouped emissions sources account for most of the predicted impacts. Additionally, this location coincides with a single, isolated local maxima on Figure 6-10, the characteristics of which are consistent with those identified for benzo(a)pyrene in the Port Neches/Nederland neighborhood (see Section 6.1.1.3) and for benzene in the Groves neighborhood (see above). Therefore, as described in Section 3.3.2, further assessment based on the frequency and actual occurrence of sources within the assessment area would provide a more refined prediction of impacts from grouped source ethylene oxide emissions in the neighborhood.

However, other locations in the Groves neighborhood may exhibit a substantially different attribution profile, as indicated on Table 6-13 and illustrated on Figure 6-10. A random receptor location, identified on Figure 6-9, was also selected to demonstrate the variation in attribution profile between two receptor locations in the neighborhood. At this location, in the northwest part of the Groves neighborhood, significant risk levels are attributable to individual ethylene oxide emissions sources at Huntsman, and modeled grouped source categories are not independently significant. The Huntsman facility is the only facility in the Port Neches Assessment Area for which individual sources of ethylene oxide emissions were identified during emissions characterization.

TABLE 6-10

ATTRIBUTION PROFILE AND RISK-BASED PRIORITIZATION
AT THE LOCATION OF PREDICTED MAXIMUM IMPACT
IN THE GROVES NEIGHBORHOOD FROM 1,3-BUTADIENE EMISSIONS

Source Description[a]	Permit Status	Source-Specific Percentage of Pathway Risk	Cancer Risk		Non-Cancer Hazard	
			Resident Adult	Resident Child	Resident Adult	Resident Child
1 *Light Duty Gasoline Vehicles (LDGV)* Surrogate: On-Road Mobile	NA	42.2%	5×10^{-5}	2×10^{-5}	0.05	0.1
2 *Light Duty Gasoline Trucks 1&2 (LDGT)* Surrogate: On-Road Mobile	NA	33.6%	4×10^{-5}	2×10^{-5}	0.04	0.09
3 *Heavy Duty Gasoline Vehicles (HDGV)* Surrogate: On-Road Mobile	NA	5.5%	7×10^{-6}	3×10^{-6}	0.007	0.02
4 *Heavy Duty Diesel Vehicles (HDDV)* Surrogate: On-Road Mobile	NA	3.1%	4×10^{-6}	2×10^{-6}	0.004	0.008
5 *All Off-highway Vehicle: Gasoline, 4-Stroke* Surrogate: Off-Road Mobile	NA	2.5%	3×10^{-6}	1×10^{-6}	0.003	0.007
All Other Modeled Sources (27 Individual and 9 Grouped Sources)	NA	13.2%	2×10^{-5}	7×10^{-6}	0.02	0.04
Total[b]		**100.0%**	**1×10^{-4}**	**5×10^{-5}**	**0.1**	**0.3**

Notes: As indicated in the Table 6-2, both current and proposed toxicity benchmarks are presented for 1,3-butadiene. To prevent confusion, risk values for 1,3-butadiene are presented throughout this chapter based on the current IRIS URF, unless otherwise stated.

[a]   Complete source descriptions can be found in Appendix ESC, and complete modeled risk results are in Appendix IRAP
[b]   Totals may vary due to rounding
NA   Not Applicable–grouped source category

TABLE 6-11

**ATTRIBUTION PROFILE AND RISK-BASED PRIORITIZATION
AT A RANDOM RECEPTOR LOCATION IN THE GROVES NEIGHBORHOOD
FROM 1,3-BUTADIENE EMISSIONS**

	Source Description[a,b]	Permit Status	Source-Specific Percentage of Pathway Risk	Cancer Risk	
				Resident Adult	Resident Child
1	*Huntsman Corporation,* Wastewater JWWTP Blending Station #B-14 FIN: JWB14 EPN: JWB14	G	20.4%	1×10^{-5}	6×10^{-6}
2	*Huntsman Corporation,* Wastewater JWWTP Neutralization Basin #B-16 FIN: JWB16 EPN: JWB16	G	16.0%	1×10^{-5}	5×10^{-6}
3	*Huntsman Corporation*, South B.D.E. Equipment Fugitives FIN: BDFUGS EPN: BDFUGS	P	10.1%	7×10^{-6}	3×10^{-6}
4	*Huntsman Corporation,* Fugitives EPN: C4FUG	UN	7.3%	5×10^{-6}	2×10^{-6}
5	*Huntsman Corporation*, Cooling Tower EPN: C4CT	UN	6.6%	4×10^{-6}	2×10^{-6}
	All Other Modeled Sources (22 Individual and 14 Grouped Sources)	NA	39.6%	3×10^{-5}	1×10^{-6}
	Total[c]		**100.0%**	**6×10^{-5}**	**3×10^{-5}**

Notes: As indicated in the Table 6-2, both current and proposed toxicity benchmarks are presented for 1,3-butadiene. To prevent confusion, risk values for 1,3-butadiene are presented throughout this chapter based on the current IRIS URF, unless otherwise stated.

[a]   The locations of prioritized sources are shown on Figure 6-9
[b]   Complete source descriptions can be found in Appendix ESC, and complete modeled risk results are in Appendix IRAP
[c]   Totals may vary due to rounding
EPN   Emissions point number
FIN   Facility identification number
G   Grandfathered Source
P   Permitted Source
NA   Not Applicable
UN   Unknown

TABLE 6-12

**ATTRIBUTION PROFILE AND RISK-BASED PRIORITIZATION
AT THE LOCATION OF PREDICTED MAXIMUM IMPACT IN THE GROVES
NEIGHBORHOOD FROM ETHYLENE OXIDE EMISSIONS**

	Source Description[a]	**Permit Status**	**Source-Specific Percentage of Pathway Risk**	**Cancer Risk**	
				Resident Adult	**Resident Child**
1	*Industrial Organic Chemicals Manufacturing* Surrogate: Industrial Land Use	NA	76.2%	2×10^{-5}	8×10^{-6}
2	*Hospital Sterilizers* Surrogate: Commercial Land Use	NA	19.4%	4×10^{-6}	2×10^{-6}
	All Other Modeled Sources (15 Individual and 2 Grouped Sources)	NA	4.4%	1×10^{-6}	4×10^{-6}
	Total[b]		**100.0%**	$\mathbf{2 \times 10^{-5}}$	$\mathbf{1 \times 10^{-5}}$

Notes: [a]   Complete source descriptions can be found in Appendix ESC, and complete modeled risk results are in Appendix IRAP
        [b]   Totals may vary due to rounding
        NA   Not Applicable

TABLE 6-13

**ATTRIBUTION PROFILE AND RISK-BASED PRIORITIZATION
AT A RANDOM RECEPTOR LOCATION IN THE GROVES NEIGHBORHOOD
FROM ETHYLENE OXIDE EMISSIONS**

	Source Description[a,b]	Permit Status	Source-Specific Percentage of Pathway Risk	Cancer Risk	
				Resident Adult	Resident Child
1	*Huntsman Corporation,* F6 Unit Process Fugitives FIN: F6FUG EPN: F6FUG	P	24.2%	3×10^{-6}	1×10^{-6}
2	*Huntsman Corporation,* Utilities East Cooling Towers FIN: UEUL22 EPN: UEUL22	P	16.6%	2×10^{-6}	8×10^{-7}
3	*Huntsman Corporation,* F4 Unit Process Fugitives FIN: F4FUG EPN: F4FUG	P	15.5%	2×10^{-6}	8×10^{-7}
4	*Huntsman Corporation,* F2 Unit Process Fugitives FIN: F2FUG EPN: F2FUG	P	12.8%	1×10^{-6}	6×10^{-7}
5	*Huntsman Corporation,* Utilities East Cooling Towers FIN: UEUL31 EPN: UEUL31	P	12.0%	1×10^{-6}	6×10^{-7}
	All Other Modeled Sources (10 Individual and 4 Grouped Sources)	NA	19.0%	2×10^{-6}	9×10^{-7}
	Total[c]		**100.0%**	**1×10^{-5}**	**5×10^{-6}**

Notes: [a]   The locations of prioritized individual sources are shown on Figure 6-10
          [b]   Complete source descriptions can be found in Appendix ESC, and complete modeled risk
                results are in Appendix IRAP
          [c]   Totals may vary due to rounding
          EPN   Emissions point number
          FIN   Facility identification number
          G   Grandfathered Source
          P   Permitted Source
          NA   Not Applicable

Formaldehyde: Table 6-14 summarizes the attribution profile for the significant formaldehyde emissions sources contributing to impacts at the predicted location of maximum impact in the Groves neighborhood (see Figure 6-11). At the location of predicted maximum impact, grouped emissions sources account for all of the predicted impacts, as no individual sources of formaldehyde emissions in the Port Neches Assessment Area were identified during the emissions characterization.

Additionally, this predicted maximum impact location coincides with one of two isolated local maxima on Figure 6-11, the characteristics of which are consistent with those identified for benzo(a)pyrene in the Port Neches/Nederland neighborhood (see Section 6.1.1.3) and for benzene in the Groves neighborhood (see above). Therefore, as described in Section 3.3.2, further assessment based on the frequency and actual occurrence of sources within the assessment area would provide a more refined prediction of impacts from grouped source formaldehyde emissions in the neighborhood.

Benzo(a)anthracene: Table 6-15 summarizes the attribution profile for the significant benzo(a)anthracene emissions sources contributing to impacts at the predicted location of maximum impact in the Groves neighborhood (see Figure 6-12). This table also includes a prioritization of the most significant benzo(a)anthracene emissions sources for risk management. At the location of predicted maximum impact, grouped emissions sources account for all of the predicted impacts, as no individual sources of benzo(a)anthracene emissions in the Port Neches Assessment Area were identified during the emissions characterization. It should also be noted that values presented are based only on modeled vapor concentrations.

Additionally, this predicted maximum impact location coincides with a single isolated local maxima on Figure 6-12, the characteristics of which are consistent with those identified for benzo(a)pyrene in the Port Neches/Nederland neighborhood (see Section 6.1.1.3) and for benzene in the Groves neighborhood (see above). Therefore, as described in Section 3.3.2, further assessment based on the frequency and actual occurrence of sources within the assessment area would provide a more refined prediction of impacts from grouped source benzo(a)anthracene emissions in the neighborhood.

Benzo(a)pyrene: Table 6-16 summarizes the attribution profile for the significant benzo(a)pyrene emissions sources contributing to impacts at the predicted location of maximum impact in the Groves neighborhood (see Figure 6-13). This table also includes a prioritization of the most significant benzo(a)pyrene emissions sources for risk management. At the location of predicted maximum impact,

TABLE 6-14

**ATTRIBUTION PROFILE AND RISK-BASED PRIORITIZATION
AT THE LOCATION OF PREDICTED MAXIMUM IMPACT IN THE GROVES
NEIGHBORHOOD FROM FORMALDEHYDE EMISSIONS**

Source Description[a]		Permit Status	Source-Specific Percentage of Pathway Risk	Cancer Risk	
				Resident Adult	Resident Child
1	*Light Duty Gasoline Vehicles (LDGV)* Surrogate: On-Road Mobile	NA	27.4%	5×10^{-6}	2×10^{-6}
2	*Light Duty Gasoline Trucks 1&2 (LDGT)* Surrogate: On-Road Mobile	NA	25.7%	4×10^{-6}	2×10^{-6}
3	*Heavy Duty Diesel Vehicles (HDDV)* Surrogate: On-Road Mobile	NA	13.3%	2×10^{-6}	1×10^{-6}
4	*Industrial Organic Chemicals Manufacturing* Surrogate: Industrial Land Use	NA	11.7%	2×10^{-6}	9×10^{-7}
5	*All Off-highway Vehicle: Diesel* Surrogate: Off-Road Mobile	NA	9.2%	2×10^{-6}	7×10^{-7}
	All Other Modeled Sources (19 Grouped Sources)	NA	12.7%	2×10^{-6}	9×10^{-7}
	Total[b]		**100.0%**	**2×10^{-5}**	**8×10^{-6}**

Notes: [a]   Complete source descriptions can be found in Appendix ESC, and complete modeled risk results are in Appendix IRAP
           [b]   Totals may vary due to rounding
        NA   Not Applicable

TABLE 6-15

**ATTRIBUTION PROFILE AND RISK BASED PRIORITIZATION
AT THE LOCATION OF PREDICTED MAXIMUM IMPACT IN THE GROVES
NEIGHBORHOOD FROM BENZO(A)ANTHRACENE EMISSIONS**

	Source Description[a]	Permit Status	Source-Specific Percentage of Pathway Risk	Cancer Risk	
				Resident Adult	Resident Child
1	*Gasoline Distribution Stage 1* Surrogate: Commercial Land Use and Industrial Land Use	NA	63.9%	1×10^{-5}	6×10^{-6}
2	*Consumer Product Usage* Surrogate: Population	NA	23.8%	5×10^{-6}	2×10^{-6}
3	*Open Burning: Scrap Tires* Surrogate: Industrial Land Use	NA	5.0%	1×10^{-6}	5×10^{-7}
	All Other Modeled Sources (18 Grouped Sources)	NA	7.4%	2×10^{-6}	7×10^{-7}
		Total[b]	**100.0%**	**2×10^{-5}**	**1×10^{-5}**

Notes: [a] Complete source descriptions can be found in Appendix ESC, and complete modeled risk results are in Appendix IRAP
        [b] Totals may vary due to rounding
        NA   Not Applicable

TABLE 6-16

**ATTRIBUTION PROFILE AND RISK-BASED PRIORITIZATION
AT THE LOCATION OF PREDICTED MAXIMUM IMPACT
IN THE GROVES NEIGHBORHOOD
FROM BENZO(A)PYRENE EMISSIONS**

Source Description[a]		Permit Status	Source-Specific Percentage of Pathway Risk	Cancer Risk	
				Resident Adult	Resident Child
1	*Gasoline Distribution Stage 1* Surrogate: Commercial Land Use and Industrial Land Use	NA	63.9%	4×10^{-5}	2×10^{-5}
2	*Consumer Product Usage* Surrogate: Population	NA	23.8%	2×10^{-5}	7×10^{-6}
3	*Open Burning: Scrap Tires* Surrogate: Industrial Land Use	NA	5.0%	3×10^{-6}	2×10^{-6}
	All Other Modeled Sources (18 Grouped Sources)	NA	7.4%	5×10^{-6}	2×10^{-6}
		Total[b]	**100.0%**	**7×10^{-5}**	**3×10^{-5}**

Notes: [a]   Complete source descriptions can be found in Appendix ESC, and complete modeled risk
                results are in Appendix IRAP
         [b]   Totals may vary due to rounding
       NA   Not Applicable

grouped emissions sources account for all of the predicted impacts, as no individual sources of
benzo(a)pyrene emissions in the Port Neches Assessment Area were identified during the emissions
characterization. It should also be noted that values presented are based only on modeled vapor
concentrations.

Additionally, this predicted maximum impact location coincides with a one of several isolated and non-
contiguous local maxima on Figure 6-13, the characteristics of which are consistent with those identified
for benzo(a)pyrene in the Port Neches/Nederland neighborhood (see Section 6.1.1.3) and for benzene in
the Groves neighborhood (see above). Therefore, as described in Section 3.3.2, further assessment based
on the frequency and actual occurrence of sources within the assessment area would provide a more
refined prediction of impacts from grouped source benzo(a)pyrene emissions in the neighborhood.

Benzo(b)fluoranthene: Table 6-17 summarizes the attribution profile for the significant benzo(b)fluoranthene emissions sources contributing to impacts at the predicted location of maximum impact in the Groves neighborhood (see Figure 6-14). This table also includes a prioritization of the most significant benzo(b)fluoranthene emissions sources for risk management. At the location of predicted maximum impact, grouped emissions sources account for all of the predicted impacts, as no individual sources of benzo(b)fluoranthene emissions in the Port Neches Assessment Area were identified during the emissions characterization. It should also be noted that values presented are based only on modeled vapor concentrations.

Additionally, this predicted maximum impact location coincides with a one of several isolated and non-contiguous local maxima on Figure 6-14, the characteristics of which are consistent with those identified for benzo(a)pyrene in the Port Neches/Nederland neighborhood (see Section 6.1.1.3) and for benzene in the Groves neighborhood (see above). Therefore, as described in Section 3.3.2, further assessment based on the frequency and actual occurrence of sources within the assessment area would provide a more refined prediction of impacts from grouped source benzo(a)fluoranthene emissions in the neighborhood.

Acrolein: Table 6-18 summarizes the attribution profile for the significant acrolein emissions sources contributing to impacts at the predicted location of maximum impact in the Groves neighborhood (see Figure 6-16). This table also includes a prioritization of the most significant acrolein emissions sources for risk management. At the location of predicted maximum impact, grouped emissions sources account for all of the predicted impacts, as no individual sources of acrolein emissions in the Port Neches Assessment Area were identified during the emissions characterization.

Additionally, this predicted maximum impact location coincides with a one of several isolated and non-contiguous local maxima on Figure 6-16, the characteristics of which are consistent with those identified for benzo(a)pyrene in the Port Neches/Nederland neighborhood (see Section 6.1.1.3) and for benzene in the Groves neighborhood (see above). Therefore, as described in Section 3.3.2, further assessment based on the frequency and actual occurrence of sources within the assessment area would provide a more refined prediction of impacts from grouped source acrolein emissions in the neighborhood.

TABLE 6-17

**ATTRIBUTION PROFILE AND RISK-BASED PRIORITIZATION
AT THE LOCATION OF PREDICTED MAXIMUM IMPACT
IN THE GROVES NEIGHBORHOOD
FROM BENZO(B)FLUORANTHENE EMISSIONS**

	Source Description[a]	Permit Status	Source-Specific Percentage of Pathway Risk	Cancer Risk	
				Resident Adult	Resident Child
1	*Gasoline Distribution Stage 1* Surrogate: Commercial Land Use and Industrial Land Use	NA	63.9%	1×10^{-5}	6×10^{-6}
2	*Consumer Product Usage* Surrogate: Population	NA	23.8%	5×10^{-6}	2×10^{-7}
3	*Open Burning: Scrap Tires* Surrogate: Industrial Land Use	NA	5.0%	1×10^{-6}	5×10^{-7}
	All Other Modeled Sources (18 Grouped Sources)	NA	7.4%	2×10^{-6}	7×10^{-7}
		Total[b]	**100.0%**	**2×10^{-5}**	**9×10^{-6}**

Notes: [a]   Complete source descriptions can be found in Appendix ESC, and complete modeled risk
              results are in Appendix IRAP
        [b]   Totals may vary due to rounding
        NA   Not Applicable

TABLE 6-18

**ATTRIBUTION PROFILE AND RISK-BASED PRIORITIZATION
AT THE PREDICTED LOCATION OF MAXIMUM IMPACT
IN THE GROVES NEIGHBORHOOD FROM ACROLEIN EMISSIONS**

	Source Description[a]	Permit Status	Source-Specific Percentage of Pathway Risk	Non-Cancer Hazard	
				Resident Adult	Resident Child
1	*Light Duty Gasoline Vehicles (LDGV)* Surrogate: On-Road Mobile	NA	31.4 %	2.86	6.36
2	*Light Duty Gasoline Trucks 1 & 2 (LDGT)* Surrogate: On-Road Mobile	NA	14.0 %	1.27	2.82
3	*Heavy Duty Gasoline Vehicles (HDGV)* Surrogate: On-Road Mobile	NA	11.1 %	1.01	2.24
4	*Marine Vessels, Commercial* Surrogate: Water-Based Land Use	NA	9.9 %	0.90	1.99
5	*Structure Fires* Surrogate: Population	NA	9.0 %	0.82	1.82
6	*Heavy Duty Diesel Vehicles (HDDV)* Surrogate: On-Road Mobile	NA	8.9 %	0.81	1.80
7	*All Off-highway Vehicle Diesel* Surrogate: Off-Road Mobile	NA	8.7 %	0.79	1.76
8	*Railroads-Diesel* Surrogate: Railroad Miles	NA	3.8 %	0.35	0.77
	All Other Modeled Sources (10 Grouped Sources)	NA	3.2 %	0.29	0.66
	Total[b]		**100 %**	**9.10**	**20.22**

Notes: [a]   Complete source descriptions can be found in Appendix ESC, and complete modeled risk
               results are in Appendix IRAP
        [b]   Totals may vary due to rounding
        NA   Not Applicable–Grouped source category

6.1.2.4 Applicable Air Monitoring Data

As discussed in Chapter 2, ambient air monitoring data is available at station T119 for the Groves neighborhood (see Figure 6-6). However, of the contaminants prioritized in the Pilot Study as being a risk concern based on modeled air concentrations, only measured data for benzene and 1,3-butadiene are available at station T119 (TNRCC 1997a; U.S. EPA 1998h). Review of the Community Air Toxics Monitoring Network Report (January–December 1997) and the Aerometric Information Retrieval System (AIRS) database indicates that measured air concentration data are not available at this station for ethylene oxide, formaldehyde, benzo(a)anthracene, benzo(a)pyrene, benzo(b)fluoranthene, or acrolein (TNRCC 1997a; U.S. EPA 1998h).

Average annual measured air concentrations of benzene and 1,3-butadiene are available at T119 for the years 1993 through 2000 (TNRCC 1997a; U.S. EPA 1998h). To illustrate measured concentrations on a risk basis, tables in Figure 6-6 present modeled risk and hazard levels based on extrapolating the average air concentrations, for the available average yearly monitoring data summarized in the table, into the future for the length of applicable exposure duration (e.g., 30 years for the adult). A simplified exposure scenario, as described in Chapter 5, was utilized consisting of breathing outdoor air 24 hours a day for 350 days a year. For benzene data, resulting adult risk values range from 10^{-6} to 10^{-5}, and child hazard values range from 0.058 to 0.18. For ambient air 1,3-butadiene data, resulting risk values range from the 10^{-5} to 10^{-4} level; calculated using the toxicity factor value reported in IRIS (see Table 6-2). Hazard values for 1,3-butadiene range from 0.33 to 1.27.

With regard to available ambient air monitoring data, it is important to note that the use of this data in this report is intended to provide available supporting information associated with the identification of potential risk concerns. As discussed in Section 6.2.6, it is not included as a comparison to modeled values or intended as a verification of modeling methods. Instead, the intent is to include all relevant and available information for consideration in the identification of potential risk concerns and prioritizations.

6.1.2.5 Risk Management Considerations

Risk management considerations in this section focus on information identified during Pilot Study project implementation that relates to the confidence in presented results [i.e., results that exceed criteria (see introduction to Chapter 6) for presentation and discussion], and is included such that it can be considered

by risk managers when assessing risk priorities and important data gaps in the Groves neighborhood. It should be noted that these discussions are limited since they primarily focus on information that affects prioritized results that are presented in this chapter and do not equally consider information that may affect the confidence in low priority results that are not as scrutinized (i.e., results that are considered a lower priority since they do not exceed a $1x10^{-5}$ risk level or a 0.25 hazard level).   Additional risk management considerations not necessarily specific to the profiling of this neighborhood location are presented in Section 6.2. The primary risk management consideration for results on the Groves neighborhood is the need for additional emissions characterization data to assert confidence in modeled impacts for contaminants currently identified as not resulting in significant impacts and for emissions of contaminants that are identified as resulting in impacts of potential concern, to more accurately define source attribution.

Speciation of Emissions

In some cases reported emissions may be in the form of a grouping of constituents that are not adequately speciated into individual contaminants for air dispersion and risk modeling. Unspeciated emissions are therefore mixtures of multiple contaminants (e.g., non-methane VOCs, VOC gas mixtures, gasoline, crude oil, and jet fuel). Specific to the speciation of emissions from permitted and non-permitted sources at facilities contributing to impacts in the Groves neighborhood, the emissions characterization data indicate the following:

- For the Huntsman facilities:

    – Speciated emissions of benzene (22 tons), 1,3-butadiene (238 tons) and ethylene oxide (44 tons) are recorded in the 1997 PSDB (TNRCC 1999d).
    – 722 tons of unspeciated emissions that may contain benzene, 1,3-butadiene, ethylene oxide, and other contaminants, were also reported in the 1997 PSDB (TNRCC 1999d).
    – 2,409 tons of unspeciated non-methane VOC emissions, which may include benzene, 1,3-butadiene, ethylene oxide, and other contaminants, were reported in the 1997 Source Status Survey (further described in Section 6.2.1; TNRCC 1999c).

- For the Ameripol Synpol facility:

    – Speciated emissions of 1,3-butadiene (5.8 tons) are recorded in the 1997 PSDB (TNRCC 1999d).
    – 72 tons of unspeciated emissions, which may include 1,3-butadiene and other contaminants, were also reported in the 1997 PSDB (TNRCC 1999d).

    – 228 tons of unspeciated non-methane VOC emissions, which may include 1,3-butadiene and other contaminants, were reported in the 1997 Source Status Survey (TNRCC 1999c).

Unspeciated emissions of these and other contaminants from other facilities in the assessment area may also contribute to impacts to the Groves neighborhood that can not be evaluated at this time because sufficient information for air and/or risk modeling is not available based on emissions characterization. A total of 3,429 tons of unspeciated emissions were reported for facilities in the Port Neches assessment area (TNRCC 1999d). Risk managers should be aware that unspeciated emissions from sources within the assessment area may contain contaminants that could effect the risk modeling results.

As with permitted emission sources, emissions from grandfathered and exempt sources may result in impacts that cannot be modeled without detailed emissions information. Specific to the sources and facilities contributing to impacts in the Groves neighborhood, the 1997 PSDB and the TNRCC Source Status Survey indicate the following information based on source permit status:

- Documented grandfathered and exempt emissions from the Fina Port Arthur Refinery include:

  – Emissions of benzene from grandfathered sources (32.7 tons) and exempt sources (0.5 tons) are recorded in the 1997 PSDB (TNRCC 1999d).
  – Emissions of non-methane VOCs from grandfathered (86.7 tons) and exempt sources (5.5 tons), and VOC gas mixtures emissions from grandfathered (114.9 tons) and exempt sources (27.1 tons) are recorded in the 1997 PSDB (TNRCC 1999d).
  – Emissions of non-methane VOCs from grandfathered (530 tons) and exempt (53 tons) sources were reported during the 1997 TNRCC Source Status Survey (TNRCC 1999c).

- Documented grandfathered and exempt emissions from the Huntsman facilities include:

  – Grandfathered emissions of benzene (22 tons), 1,3-butadiene (137.7 tons), and ethylene oxide (21.7 tons) are recorded in the 1997 PSDB (TNRCC 1999d).
  – Emissions of non-methane VOCs from grandfathered sources (6.6 tons) and exempt sources (0.3 tons) are recorded in the 1997 PSDB (TNRCC 1999d).
  – Emissions of non-methane VOCs from grandfathered (1,014 tons) and exempt (220 tons) sources were reported during the 1997 TNRCC Source Status Survey (TNRCC 1999c).

- Documented grandfathered and exempt emissions from the Ameripol Synpol facility include:

  – Emissions of 1,3-butadiene from grandfathered (5.3 tons) and exempt (0.5 tons) sources are recorded in the 1997 PSDB (TNRCC 1999d).

       –   Emissions of non-methane VOCs from grandfathered sources (4.9 tons) and VOC gas mixtures from grandfathered (7.3 tons) and exempt (5.6 tons) sources are recorded in the 1997 PSDB (TNRCC 1999d).

       –   Emissions of non-methane VOCs from grandfathered (48.7 tons) and exempt (6.2 tons) sources were reported during the 1997 TNRCC Source Status Survey (TNRCC 1999c).

Grandfathered and exempt emissions from other facilities in the assessment area may also contribute to impacts that cannot be evaluated at this time due to insufficient information for air and risk modeling. A total of 3,251 tons of grandfathered and exempt emissions of non-methane VOCs were voluntarily reported to TNRCC for 1997 by facilities in the Port Neches assessment area (TNRCC 1999c). Risk managers should be aware that unspeciated emissions from grandfathered and exempt sources in the assessment area may contain contaminants that could effect the risk modeling results.

Characterization of Grouped Emissions Source

Risk and hazard levels greater than 10^{-5} and 0.25, respectively, were modeled for emissions from grouped sources of benzene, 1,3-butadiene, ethylene oxide, formaldehyde, benzo(a)anthracene, benzo(a)pyrene, benzo(b)fluoranthene, and acrolein in the Groves neighborhood. Grouped emissions sources were characterized to provide emissions estimates based on a census-tract surrogate, as described in Chapter 3. However, further refinement may be required to support risk management decisions. These emissions estimates could be further refined by evaluating the actual frequency or occurrence of specific sources within a census tract. For example, emissions estimates for Stage I gasoline distribution–emissions from petroleum product storage facilities– was based on county and census tract employment within SIC 5171 (petroleum bulk stations and terminals). Since similar facilities exist within the assessment area, these facilities could be modeled based on actual location, which would provide a more realistic picture of resulting risk impacts.

Secondary Formation

No individual sources of formaldehyde or acrolein emissions were identified in the Port Neches assessment area. However, several important precursor compounds to atmospheric formation of formaldehyde (1,3-butadiene, propylene, and ethylene) and acrolein (1,3-butadiene) are emitted in very large quantities (see Table 6-19). Reported emissions of formaldehyde and acrolein precursor compounds are subject to the same emissions characterization limitations as other contaminants. Risk

TABLE 6-19

FORMALDEHYDE AND ACROLEIN PRECURSOR EMISSIONS

Precursor	1997 Emissions Facilities in the Port Neches Assessment Area (tons)	1997 Emissions Facilities in Jefferson County (tons)
1,3-Butadiene (Formaldehyde and Acrolein)	248.6978	271.8328
Propylene (Formaldehyde only)	108.3100	487.8798
Ethylene (Formaldehyde only)	146.8202	769.5876

Source: TNRCC 1999d

management considerations regarding the secondary formation of formaldehyde are discussed in greater detail in Section 6.2.

The CEP results indicate that formaldehyde concentrations in Jefferson County may be significant on a county-wide basis (see Table 2-8)(U.S. EPA 1999a). However, the RAIMI Pilot Study results for formaldehyde (see Figure 6-11 and Table 6-14) identify formaldehyde impacts nominally exceeding the 10^{-5} risk level only in very localized areas within the Groves neighborhood. One significant difference between the CEP and RAIMI methodologies is that the CEP considered the atmospheric formation of formaldehyde from precursor compounds; the RAIMI Pilot Study did not consider atmospheric formation in the initial phase.

Although no individual sources of formaldehyde emissions in the Port Neches assessment area were identified in the PSDB, modeling of emissions inventoried for the group source subcategory of industrial organic chemicals manufacturing indicates formaldehyde emissions of potential concern to the Groves neighborhood. This suggests that individual industrial sources of formaldehyde may exist in the assessment area.

6.2   CONSIDERATIONS REGARDING USE OF RESULTS

This section notes important considerations with regard to how the results of RAIMI Pilot Study may be used to identify and prioritize risk management opportunities, evaluate permit conditions, or otherwise be

used by regulatory agencies and facilities. As noted in Chapter 3, the most significant limit to the usability of results is the lack of complete emissions characterization in the form of unidentified and unspeciated emissions data. Therefore, most of the considerations described in this section pertain to emissions characterization. Other considerations in addition to emissions characterization includes use of actual versus allowable emission rates, adjusting for process upsets, secondary formation of contaminants, and aspects of monitoring versus modeling. This section also discussed some of the major uncertainties in the Pilot Study analysis, which will be discussed further in Section 6.3.

The RAIMI Pilot Study is designed to use readily available databases containing speciated emissions data, but an unknown, yet suspected significant portion of the assessment area emissions are not included in the inventories maintained by federal and state agencies. In addition, a significant portion of the reported data are not speciated to adequate contaminant-specific detail or in an appropriate format that allows for evaluation of risk impacts. Because of the incomplete nature of available emissions characterization data, it is possible that the RAIMI Pilot Study initial phase results underestimate risk and hazard impacts. Users of these results are cautioned to recognize these data gaps when risk management opportunities are identified and implemented.

6.2.1   Limits of Regulatory Reported Data

With regard to emissions of individual contaminants and the information necessary to assess risk impacts to individual receptors at the neighborhood level, the existing requirements for reporting emissions to state and federal emissions databases are not adequate to ensure that all significant emissions sources are being reported. Generally, the regulatory reporting requirements were not developed with the specific focus of obtaining sufficient data to evaluate exposure to neighborhood receptors. However, comparing emissions records across regulatory reporting databases can provide insight into the nature of the inadequacies of emissions databases. Table 6-20 compares the emissions data from the 1997 TRI and the 1997 Texas PSDB. The information presented in Table 6-20 is limited to those contaminates profiled in Section 6.1 for which emissions are also reported in the TRI or PSDB databases. Although the TRI was not designed to be a data repository for air dispersion and/or risk modeling data, the information in Table 6-20 does indicate a wide variance in the actual reported emissions across regulatory databases. The TNRCC emissions inventory program is acting to minimize these discrepancies–whether they are due to misinterpretation of the reporting requirements, typographical errors, or other factors–by sending a request to the reporting facilities, asking that they correct their reported emissions.

TABLE 6-20

COMPARISON OF 1997 TRI AND PSDB DATA

Facility	Contaminant	TRI Air Emissions (Pounds)	PSDB Air Emissions (Pounds)
Ameripol Synpol Corp.	1,3-Butadiene	18,500	11,660
Carotex, Inc.	Benzene	0	9,106
Clark Port Arthur Pipeline Company	Benzene	0	4,984
DuPont Dow Elastomers	1,3-Butadiene	8,599	7,508
DuPont Beaumont Plant	Benzene	15,265	15,285
Fina Oil & Chemical Co.	Benzene	54,666	97,611
Huntsman Corp. - C4/O&O Plant	Benzene	1,570	45,436
	1,3-Butadiene	214,000	476,456
	Ethylene Oxide	52,000	89,002

Source: U.S. EPA 2000g; TNRCC 1999d

The following subsections describe specific aspects of regulatory reported data that effect the content and completeness of emissions characterization for the purpose of generating and using RAIMI Pilot Study results.

CAA Operating Permits

Under the CAA, an operating permit is required only for the construction of a new major sources or for the major modification of an existing source. As described in Chapter 3, a major source is one that emits more than 100 tons per year of a criteria pollutant, greater than 10 tons per year of a single HAP, or greater than 25 tons per year of a combination of HAPs.   The CAA operating permit, also known as a Title V permit, documents actual and projected emissions and includes the required stack parameters for air and risk modeling. However, a complete inventory of emissions, even for major sources, is not required and, therefore, not available for inclusion into the RAIMI Pilot Study.

Sources emitting up to 100 tons per year of criteria pollutants, and up to 10 tons per year of HAPs, are not classified as major sources and are not required to get operating permits under the CAA. Therefore, some CAA sources (i.e. those with emissions of contaminants less than 10 tons per year, but in quantities that could contribute to risk) do not have regulatory requirements to provide emissions data for inclusion into the emissions databases, and thus are not available for evaluation in the RAIMI Pilot Study.

The collection of additional required data on source emissions is anticipated under the Title V operating permit program, which is in progress. Many source categories of interest to the RAIMI Pilot Study, such as refineries and chemical plants which may have hazardous air pollutant emissions, were required to submit Title V applications to the State of Texas in the year 2000. However, subsequent review and approval may delay data availability. Permit application dates have been established based on emissions source category.   In the Port Neches Assessment Area, Title V applications have been received from Fina, Huntsman, and Ameripol Synpol. Most process description, process flow diagram, and plot plans were provided for these three facilities. However, detailed speciation of emissions were not included in the Title V applications.

Risk managers should be aware that upcoming Title V permit applications for other source categories of interest may contain important and relevant information for emissions characterization and risk modeling, although the availability of the data is dependent on the submittal date and regulatory review.

Grandfathered and Exempt Sources

Depending on state reporting requirements, emission sources that meet certain regulatory exemptions, including grandfathered status, are not always required to report emissions or to apply for an operating permit. For the state of Texas and consistent with TNRCC Emissions Inventory requirements, all major sources are required to report emissions, regardless of permit status. However, prior to 1997, sufficient data did not exist to differentiate these emissions by the operating authority of the unit: grandfathered, exempt, or permitted. To correct this deficiency in the data, House Bill 3019 of the 75th Texas Legislature gave TNRCC the authority to request that all companies submitting an emissions inventory also update a survey form (Source Status Survey) with the operating status and permitting authority of all equipment on site (TNRCC 1999c).   Although the emissions apportioning exercise is voluntary, the TNRCC reports excellent participation from the regulated community.

TNRCC annually requests the voluntary participation in the emissions inventory survey of sources not requiring permits. These sources include CAA major sources that have not been modified (and do not require an operating permit) and grandfathered facilities (operating prior to 1972). Non-major sources, including sources exempt from regulation under the CAA, are also requested to participate. The completeness of the Table 1(a) forms as part of the emissions inventory survey is dependent on the voluntary submittal of accurate data by these sources.

Emissions from these grandfathered or exempt sources may be significant from a risk perspective. For example, at the location of maximum risk at an actual residential location in the Port Neches/Nederland neighborhood, three grandfathered sources account for 45 percent of the adult cancer risk from 1,3-butadiene (see Table 6.3). Table 6-21 contains a summary of 1997 non-methane VOC emissions for grandfathered, exempt, and permitted sources in the Port Neches Assessment Area. This information indicates that the grandfathered and exempt sources account for about 49 percent of the total reported non-methane VOC emissions in the Texas PSDB. A summary of 1997 PSDB emissions with respect to permit status for benzene, 1,3-butadiene, and ethylene oxide is presented on Table 6-22. Grandfathered emissions of benzene and 1,3-butadiene account for a significant portion of the total emissions for these contaminants. Users of the RAIMI Pilot Study results are cautioned about the limitations presented by the absence of adequate emissions characterization data for grandfathered and exempt sources.

Regulated Contaminants

The CAA regulates a list of 188 HAPs. However, many contaminants that may pose significant risks are not included in the list of HAPs under the CAA, but are identified under other regulatory programs. For example, the HHRAP identifies over 200 contaminants of potential concern, and the State of Texas publishes a list of over 1800 contaminants that may have adverse effects on the exposed public. These additional contaminants not regulated under the CAA may contribute to aggregate risk. However, emissions data required to evaluate the impacts of these contaminants are not available due to a lack of regulatory requirements to provide these data under the CAA.

TABLE 6-21

PERMIT STATUS-SPECIFIC EMISSIONS OF NON-METHANE VOCS

Facility	Permit Status			
	Grandfathered Emissions (tpy)	Exempt Emissions (tpy)	Permitted Emissions (tpy)	Total Emissions (tpy)
Air Liquide America Corporation	0.0	0.0	6.5	6.5
Ameripol. Synpol. Corporation	48.7	6.2	173.2	228.0
BASF Corporation	0.1	1.8	112.7	114.6
Beaumont Methanol, Ltd.	0.0	0.0	41.7	41.7
Carotex Incorporated	0.0	0.0	51.7	51.7
Clark Port Arthur Pipeline Company	192.7	0.2	59.4	252.3
Duke Energy Field Services, Inc.	0.0	8.5	0.0	8.5
Dupont Dow Elastomers L.L.C.	0.0	24.1	453.1	477.2
E.I. du Pont De Nemours & Company	2.7	4.3	203.1	210.2
Fina Oil and Chemical Company	529.6	53.2	801.7	1384.5
Huntsman Corporation	862.8	0.0	916.7	1779.5
Huntsman Corporation	150.9	220.2	259.0	630.1
I.C.I. Acrylics, Incorporated	0.0	0.0	13.2	13.2
Mobil Oil Corporation	10.6	0.0	1.7	12.2
Mobil Pipe Line Company	54.5	0.0	0.0	54.5
Motiva Enterprises, L.L.C.	3.2	17.7	1.0	21.8
Southern Manufacturing Company	0.0	0.0	41.7	41.7
Sun Marine Terminal	164.0	0.0	87.7	251.6
Te Products Pipeline Company, L.P.	169.6	123.3	0.0	292.8
Tejas Gas Pipeline Company	0.0	0.9	0.0	0.9
UCAR Pipeline Inc	0.0	20.3	0.0	20.3
Union Oil Company of California	519.6	61.9	124.3	705.7
Total	**2708.8**	**542.6**	**3348.3**	**6599.7**
Percent of Total	**41%**	**8%**	**51%**	**100%**

Source: TNRCC 1999c

Note: Data was obtained for 1997 from the TNRCC Source Status Survey.
         tpy = tons per year

TABLE 6-22

CONTAMINANT EMISSIONS AND PERMIT STATUS

Contaminant	Grandfathered Emissions (tons)	Exempt Emissions (tons)	Permitted Emissions (tons)	Total Emissions (tons)
Benzene	67.7	2.7	28.9	99.3
1,3-Butadiene	143.5	0.7	104.5	248.7
Ethylene Oxide	21.7	0.0	22.8	44.5
Total	**233.0**	**3.4**	**156.2**	**392.5**

Source: 1999c
Note: Three facilities (General Atlantic Resources, Sun Marine Terminal, and U.S. Intec) did not report permit
         status for their benzene emissions. The total annual benzene emissions for those three facilities was 0.83
         tons.

6.2.2   Lack of Emissions Speciation

A significant portion of the reported data are not speciated adequately to facilitate evaluation in the

RAIMI Pilot Study. The lack of adequately speciated emissions data imposes a significant limit to

emissions characterization, and subsequent inclusion in risk modeling. A review of the 1997 PSDB

emissions for the Port Neches Assessment Area (see Table 2-7), indicates that emissions are reported to

varying degrees of speciation, as follows:

- Speciated to specific contaminant, which enables risk modeling because contaminant-specific toxicity factors can be obtained (e.g., benzene, 1,3-butadiene)

- Unspeciated as a product or process mixture that may be manually speciated with an appropriate apportionment scheme (e.g., gasoline, crude oil)

- Unspeciated as a categorical mixture that cannot be further speciated, except, possibly, by the facility (e.g., non-methane VOCs, particulates)

Table 6-23 summarizes the speciated and unspeciated facility specific data from the 1997 PSDB.

Unspeciated data accounts for 42 percent of the PSDB emissions, not including certain criteria pollutants

(nitrogen oxides, carbon oxides, and sulfur dioxide). The RAIMI Pilot Study did not undertake an effort

to speciate emissions that were not adequately speciated in the emissions databases used for the study.

For example, emissions reported as a mixture, such as gasoline, are not apportioned into the speciated

TABLE 6-23

SPECIATED AND UNSPECIATED EMISSIONS

Facility	Speciated Emissions (pounds)	Unspeciated Emissions (pounds)
Air Liquide Port Neches Plant	0	63,366
Ameripol Synpol Corp.	1,046,134	142,832
BASF Corp.	117,888	126,120
Beaumont Methanol L.P.	342,077	57,348
Carotex, Inc.	44,432	50,978
Clark Port Arthur Pipeline Company	53,793	442,260
Duke Energy Field Services, Inc.	0	59,880
Dupont Dow Elastomers L.L.C	914,103	47,508
E.I. Du Pont De Nemours & Company	4,019,511	100,496
Fina Oil and Chemical Company	364,530	2,977,700
General Atlantic Resources	0	3,320
Huntsman Corporation	2,762,771	1,486,186
Huntsman Petrochemical Corporation	176,507	0
I.C.I. Acrylics, Inc.	18,371	16,288
Mobil Oil Corporation	183,945	1,023,042
Mobil Pipe Line Company	0	0
Motiva Enterprises, LLC	0	0
Oiltanking Beaumont Partners, L.P.	0	0
Southern Manufacturing Company	0	0
Sun Marine Terminal	0	0
Te Products Pipeline Company, L.P.	0	0
Tejas Gas Pipeline Company	0	0
U S Intec Incorporated	0	0
UCAR Pipeline, Inc.	0	0
Union Oil Company of California	1,037,700	334,720
Port Neches Assessment Area Total	**11,081,762**	**6,932,044**
Percent of Total	**62%**	**38%**

Source: TNRCC 1999d

Notes: Tabulated data includes particulates and vapors, but does not include emissions of carbon oxides, nitrogen oxides, or sulfur dioxide.

Values reported in Table 6-23 do not include emissions for sources that reported less than 2,000 pounds of emissions for 1997.

constituents that make up that mixture. For this example, the reported mixture emissions would not be included in the RAIMI Pilot Study. As a result, risk managers should be aware that the RAIMI Pilot Study results are generated based on using the available facility reported speciated emissions data. Therefore, the results of the RAIMI Pilot Study are derived from a fraction of the total emissions reported in the Texas PSDB.   TNRCC has recognized the heightened regulatory focus on individual HAPs in recent years, and that data on grouped classes of contaminants (e.g., non-methane VOCs) does not always provide adequate information to accurately assess health risks. Therefore, TNRCC emissions inventory program instructs facilities to provide speciation data for 90 percent of HAP emissions for those sources with emissions rates greater than 1 tpy, or 0.1 tpy for any individual HAP. Adherence to these instructions by facilities reporting emissions to the PSDB would significantly improve the speciation–and thus usability–of the PSDB for risk management purposes.

6.2.3   Use of Actual or Allowable Emissions Data

As discussed in Section 3.2.2, reported actual emission rates constitute the primary source of emissions characterization information for individual sources modeled in the RAIMI Pilot Study. The modeling of only actual emission rates may underestimate potential risk in some cases by not including emissions from any permitted sources identified in the PSDB known to be operating, but with no reported actual emissions. The RAIMI emissions characterization also contains allowable emission rates for some permitted sources, in which the allowable emission rate is established by the permit. Evaluating allowable emission rates, or substituting allowable emission rates for data gaps in reported actual emission rates, may be beneficial in considering risk management opportunities, and also support a better understanding the magnitude of uncertainty associated with underestimating potential risk by evaluating only actual, facility-reported emissions data. Modeling of allowable emissions for permitted sources within the assessment area may provide risk managers with important information to better support or assess regional permitting and cross-program permitting. Modeling allowable emissions could also provide a metric by which permitting programs–RCRA, CAA, or State programs–measure reductions in localized impacts through implementation of emissions reduction efforts.

However, there are several notable limitations to the use of allowable emissions rates as well. These limitations are best described by specific examples from the Port Neches Assessment Area. Consider emissions of 1,3-butadiene from permitted sources in the Port Neches Assessment Area (the following data was compiled from references TNRCC 1999c and 1999d). Emissions characterization identifies 45 permitted sources of 1,3-butadiene. Reported actual emissions from these permitted sources total about 105 tons per year (tpy), and reported allowable emissions of 129 tpy. Although the reported

allowable emissions exceed the actual emissions as a whole, significant source-specific inconsistencies

are noted as follows:

- Allowable emission rates are reported for 20 of the 45 permitted emission sources;

- Nine of these sources reported actual emissions in excess of reported allowable emission
  rates
  - average ratio of actuals to allowables is 3.1
  - average difference between actuals and allowables is 4.9 tpy

- Seven of the 20 sources reported allowable emissions in excess of actual emissions
  - average ratio allowables to actuals is 6.6
  - average difference between allowables and actuals is 12.9 tpy

- Four of the 20 sources reported zero actual emissions of 1,3-butadiene
  - these four sources report a total of 15 tpy of allowable emissions

- An allowable emission rate of zero is reported for 25 permitted emission sources (note
  that it is not certain whether a zero allowable emission rate indicates that the allowable
  emission rate is in fact "zero", or that the data field was not reported and interpreted as
  zero)
  - 12 of these sources report zero actual and zero allowable emissions
  - 13 of these sources report actual emissions ranging from 0.0009 to about 18 tpy,
    with an average emission rate of about 2.8 tpy

Based on this information there is not a consistent and reliable relationship between reported actual and

allowable emission rates that would facilitate evaluation of impacts from allowable emissions as a "worst

case" assessment, nor is there adequate information to use allowable data to estimate actual emission

rates. To do so would require source-specific allocation of an emission rate for modeling, which would

introduce further uncertainties that may not be consistent among the many sources.

Additionally, allowable emission rates are only available for permitted sources; a permitted allowable

emission rate is not applicable to a grandfathered or exempt source. As shown in Tables 6-19 and 6-20,

grandfathered sources in the Port Neches Assessment Area contribute significant actual emissions for

which allowable emissions rates are not available. Impacts from grandfathered or exempt sources would

not be evaluated under a strategy that exclusively considers allowable emission rates.

6.2.4   Accounting for Process Upsets

The PSDB does not specifically account for process upset conditions, or other special conditions, in

which emissions are elevated above the usual operating conditions. These upsets may contribute

additional emissions into the atmosphere for certain processes and facilities with poor maintenance

histories. Examples of process upsets can include maintenance, startup, or shutdown emissions, which are not reported in emissions inventory.

Although the PSDB does not specifically include emissions during U&M conditions, TNRCC requires industry to report upset and maintenance (U&M) conditions with an estimate of air emissions during the U&M activity. These requirements are described in 30 TAC 101.6 Notification Requirements for Major Upset, and 101.7 Notification Requirements for Maintenance, under General Rules [see TNRCC website, or TAG document "CSR TAG Upset Emissions" (WP, 6/21/00)]. Additionally, facilities are subject to 101.4 Nuisance rules during U&M conditions. As a mechanism to monitor and track U&M emissions, TNRCC incorporates reported emissions estimates into a U&M inventory database (TNRCC 2000). A review of this database for the RAIMI Pilot Study indicated the following:

- Statewide, 307 of the 1836 facilities tracked in the database report non-zero emissions, and only 229 facilities report more than 1 ton released. The facility reporting the largest U&M emissions for 1997 is Clark Refining in Jefferson County with 32,780 tons total U&M releases, of which all were from upset events (32,690 tons of CO and 90 tons of SO_2). Two facilities in the database indicated releases of greater than 10,000 tons, 18 facilities released more than 1,000 tons, 63 facilities released more than 100 tons, and 131 released more than 10 tons. Total reported statewide 1997 U&M emissions of NMOC were 14,459 tons. Total reported statewide U&M emissions of PM10 were 600 tons.

- In Jefferson County, there were 38,605 tons of pollutants reported by industry in 1997 as released into the air during U&M events that are not listed as emissions in the PSDB

- In Jefferson county, 18 facilities accounted for all of the reported 1997 emissions,

- In Jefferson County, 98% of 1997 emissions were from Upset events, and 2% from Maintenance.

- In Jefferson County, 6% of total U&M emissions (or 2,327 tons, 2,280 tons as Upsets and 47 tons as Maintenance) were reported as NMOC and are therefore not suitable for air dispersion or risk modeling without further speciation.

- In Jefferson County, there were no reported U&M emissions of PM10.

Of particular concern with regard to the reporting and tracking of U&M emissions is the possibility that significant U&M data reported to TNRCC regional offices are not being inventoried in the statewide U&M database maintained by TNRCC offices in Austin.   The facility may, for some of these reports, request that this information be classified in Regional "confidential" files, and thus the data may not be reported to the U&M inventory in Austin. An effort to develop higher confidence that the available

inventories–PSDB and the U&M database–are adequately comprehensive and complete would require extensive effort and site-specific file review at the TNRCC Regional offices.

6.2.5   Secondary Formation of Contaminants

Many industrial areas have emissions of reactive toxic contaminants and other non-toxic precursors which transform into derivative toxic contaminants in the atmosphere. The secondary formation of certain contaminants, such as formaldehyde or acrolein, may account for higher ambient concentrations than are attributable to the primary emissions of these contaminants. Similarly, the National Air Toxic Assessment (NATA) results of the National Scale Assessment suggest the contribution of secondary formation to ambient formaldehyde concentrations may be underestimated (U.S. EPA 2001). For example, relatively small quantities of formaldehyde emissions that have been documented by the TNRCC in the Port Neches Assessment Area, do not account for the high formaldehyde concentrations at the monitoring stations. However, the area has high documented emissions of formaldehyde precursors, such as 1,3-butadiene, ethylene, and propylene, and an acrolein precursor (1,3-butadiene). Formaldehyde is known to form from reactions of 1,3-butadiene with two radicals prevalent in the study area, the hydroxyl (OH) radical, which photolysizes during daylight hours, and NO_3 which reacts during nighttime. Therefore, source-specific contribution to the secondary formation of contaminants, such as formaldehyde and acrolein, should be considered.

Direct simulation of the atmospheric transformation processes which relate the precursors to the secondary formations is complex and requires additional research to better understand the interactions. Current representations of secondary contaminant formation derive from ozone formation models as implemented in regional scale air models, with simplified reactions and long residence times (several hours to several days) for reactive precursors to transform into the derivative contaminants. These regional models typically are not designed for evaluating individual sources (U.S. EPA 1999d).

Two recently published studies have attempted to model secondary formation of formaldehyde (U.S. EPA 1999a; 1999h). The Science Advisory Board review of the Cumulative Exposure Project commended consideration of secondary formation using the simple approach in that project. For the CEP modeling effort, numerical calculations were performed by categorizing precursor reactivity and executing the air model using time-variable decay rates derived from the ambient concentration of the hydroxyl radical at the different times of the day during differing atmospheric mixing conditions. In the Air Dispersion Modeling of Toxic Pollutants in Urban Areas study, the ozone formation model, OZIPR, is modified with inputs to simulate formaldehyde formation (U.S. EPA 1999j). Both methods require extensive resources

to evaluate the various air modeling scenarios that account for the precursor reactivity rates, ambient
concentrations of radicals, residence times, and atmospheric conditions throughout the year. In addition
to being resource intensive, both of these modeling approaches are limited in their ability to adequately
address the design objectives of the RAIMI Pilot Study. The continued development and implementation
of secondary simulation methods will be assessed by the RAIMI Pilot Study for potential future
consideration.

Where representative monitoring data has identified ambient concentration levels of concern for
contaminants in the study area, such as formaldehyde, the RAIMI Pilot Study method evaluates the
source-specific impacts based on the relative impacts of the formaldehyde precursor emissions. Where
existing monitoring data is not available, the same method may be used to identify monitor sites at the
points of highest cumulative impacts of known contaminant precursors. For both circumstances, the
evaluation of ambient impacts based on precursor emissions provides significant information for source-
specific decision-making based on relative contribution of precursors to known contaminants of concern.

For the potential future consideration of secondary formation impacts, one approach the RAIMI Pilot
Study project may evaluate is to:

- Identify the potential for secondary formation as a contributing factor to risk in a study area. The risk potential may be identified based on existing monitored data showing high concentrations of chemicals known to result from secondary formation, existence of emissions of known precursor chemicals, or similarity of industry type in study area to other areas with known secondary formation concerns.

- Air model all identified precursors with emissions in the study area using ISCST3 for an inert (non-reactive) chemical with unit emission rate (1.0 grams per second). Unit concentration at each grid node is called 'Unit-Conc'.

- Determine each precursor concentration at each grid node by multiplying the unit concentration by the precursor emission rate, 'PER'.

- Apply the molecular conversation ratios from each precursor to the secondary chemical using the mole factor, called 'MF'.

- Develop a residence time nomogram, or table, of conversion ratios from precursor to the secondary chemical based on the distance from the precursor release location to the grid node to be evaluated. These 'residence time factors' (RTF) will have a different value at each downwind distance for each precursor reactivity category (e.g., very high, high, medium-high). To estimate the highest potential for conversion to the secondary chemical, the RTF nomogram will be developed assuming the longest residence time with a wind speed of 1 meter per second in ISCST3.

–   Calculate the potential for secondary formation for each precursor at each grid node of interest using the following equation:

$$C_{secondary} = C_{unit} \ \text{x} \ PER_i \ \text{x} \ MF_i \ \text{x} \ RTF_i$$

where:

$C_{secondary}$	=	Concentration of compound derived through secondary formation
C_{unit}	=	Unit concentration
PER	=	Precursor emission rate
MF	=	Mole factor
RTF	=	Residence time factor

–   Sum all the secondary concentration estimates [Conc-Secondary(i)] from each precursor at the grid node to be evaluated to identify a high estimate of the potential for secondary formation at the grid node:

$$\sum C_{secondary, \ i}$$

for i =1 through n
where n = number of precursor compounds

Should this procedure identify potential for secondary formation to contribute significantly to the risk in the area, a more refined method could be used to improve the estimate. However, with this method, the amounts and sources for precursor emissions that indicate potential for highest contributions to secondary formation could be identified for setting potential permit limits or identifying an overall reduction strategy for the area. Also, potential locations for siting monitors may be identified for locations with the highest impact potential. The results will assist in identifying contaminants that should be included in a monitoring study that otherwise may be excluded because of difficulties associated with sampling or analysis.

6.2.6   Monitoring Versus Modeling

The RAIMI Pilot Study tests the development and implementation of risk-based methods for identifying the relationships between specific sources and representative receptors on a localized scale, more refined than the county or census tract level typical of national studies. The comparison of air concentrations estimated by air modeling to monitored concentrations from an existing network operated by the State of Texas was not an objective. However, available ambient air monitoring data relevant to results in Chapter 6 is presented in corresponding sections with the intent to provide available supporting information associated with the identification of potential risk concerns and prioritizations. As discussed in this section, these available data can be viewed as a weight of evidence or a relative trending comparison on a risk-basis applicable to the context of the RAIMI Pilot Study. However, as with

conducting a complex measured to modeled comparison, various technical aspects (e.g., scope, technical feasibility, and data gaps) require consideration.

The RAIMI provides a risk-based application for prioritizing risk concerns. Specific to the RAIMI Pilot Study, the scope of comparison should be appropriate to make available to decision-makers the overall capabilities, limitations and reliability of estimated results for consideration in subsequent risk-based determinations. As illustrated in Table 6-24, modeled results from the Pilot Study provide the same relative risk-based prioritization of contaminants as for the measured results, when measured data are available. Although numerical closure within this comparison would be ideal, it is anticipated that a more controlled exercise (e.g., designed correlation of air modeling parameterization with air monitoring siting and operations) and resolution of critical data gaps (e.g., limits in emissions characterization), as feasible, would provide an improved numerical correlation.

6.2.6.1 Controlled Study Considerations

While the relative comparison illustrated in Table 6-24 provides confidence in the overall capabilities of the RAIMI approach to conduct risk-based prioritizations, it does not preclude conducting a more complex comparison, if warranted, and if technically feasible. As noted in the previous paragraph, numerical closure in compared values would be expected with design of a more controlled exercise and resolution of critical data gaps. To support comparison of modeled and monitored values, emissions characterization requires control of, or detailed information on, the speciated emission rate, source location, stack height and diameter, stack gas exit velocity and temperature, start-up and shutdown conditions, and control device operations to evaluate consistency with the assumption of steady-state emissions. Average or typical operations reported in annual summaries or inventories are insufficient for emissions characterization, which must occur contemporaneous to the air monitoring operations for identification of data outliers prior to the statistical analysis of the data sets. Similarly, the siting and

TABLE 6-24

**COMPARISON OF ADULT CANCER RISK RESULTS
FROM MONITORED AND AIR MODELED CONCENTRATIONS**

Contaminant	Groves Neighborhood Monitoring Location T119		Port Neches/Nederland Neighborhood Monitoring Location T136	
	Risk Based on 1997 Monitoring Data	**Risk Based on Air Modeling of Actual 1997 Emissions**	**Risk Based on 1997 Monitoring Data**	**Risk Based on Air Modeling of Actual 1997 Emissions**
Benzene	7×10^{-6}	2×10^{-6}	4×10^{-6}	1×10^{-6}
1,3-Butadiene	4×10^{-5}	1×10^{-5}	1×10^{-3}	2×10^{-4}
Ethylene Oxide	Not Monitored	8×10^{-7}	Not Monitored	5×10^{-6}
Formaldehyde	Not Monitored	2×10^{-7}	2×10^{-5}	3×10^{-7}
Benzo(a)anthracene	Not Monitored	2×10^{-7}	Not Monitored	5×10^{-7}
Benzo(b)fluoranthene	Not Monitored	3×10^{-7}	Not Monitored	6×10^{-7}
Benzo(a)pyrene	Not Monitored	7×10^{-7}	Not Monitored	1×10^{-6}

Notes: Risk levels presented in this table are based on extrapolating the average air concentrations, from 1997 monitoring data or air dispersion modeling of 1997 emissions, into the future for the length of applicable exposure duration (e.g., 30 years for the adult). A simplified exposure scenario, as described in Chapter 5, was utilized consisting of breathing outdoor air 24 hours a day for 365 days a year.

Formaldehyde monitoring data at Station T136 is very limited (two samples in 1997). In contrast, data for the other listed contaminants for which monitoring data are available are based on about 50 samples.

Source of monitoring data: U.S. EPA 1998h. "Aerometric Information Retrieval System (AIRS)". Office of Air Quality Planning and Standards (OAQPS), Information Transfer and Program Integration Division (ITPID). Research Triangle Park, North Carolina.

operation of the air monitoring network must be designed for targeted contaminants, sampling methods, averaging periods, quality controls and laboratory analysis that supports subsequent point-by-point comparison. As these ideal conditions rarely occur unless incorporated in the initial study scope, most published comparisons identify limitations on data representativeness prior to reporting comparison results. Additionally, air model reliability should be considered in context of the conditions used.

6.2.6.2 Air Model Reliability

As federal, state and local authorities by consensus have adopted air models for estimating air concentrations to support regulatory decisions, the prescribed conditions and limitations for use should be incorporated into the study. In the Guideline on Air Quality Models, the national regulatory recommendations for model applications are summarized (U.S. EPA 1999d). Air models were developed to support quantitative regulatory decisions under the Clean Air Act for permitting and compliance with specified limits on ambient air concentration, or permissible increases in concentrations above previous levels. Atmospheric scientists have confirmed through a number of studies on model accuracy that (1) models are more reliable for estimating long-term (annual) averages than short-term (24 hours or less), and (2) models are reasonably reliable in estimating the magnitude of highest concentrations occurring sometime and somewhere within an area. For example, highest concentrations are found to be within 10 to 40 percent of highest measured values in an area, but comparison to specific values at specific locations at specific times are not well-correlated. These values are typically within the long-recognized 'factor-of-two' accuracy. Therefore, the Guideline recommends that air dispersion models be used as a "best estimate" of measured values. These accuracies are acceptable for risk-based decisions within an order of magnitude.

Uncertainties associated with these accuracies are classified as 'inherent' or 'reducible'. Inherent uncertainty is unavoidable when representing mathematically complex atmospheric processes, such as turbulence, using theory that is incomplete and the knowledge of the parameter values is indiscernible. For example, variability in wind direction during a measurement period is observable and may be bounded within ranges of variations. However, for practicality of representation in an air dispersion model, a mean or average value must be used to represent wind direction, ignoring the range of variability during the measurement period. Inherent uncertainty has been reported as responsible for variations in concentration from measured values by as much as 50 percent. Reducible uncertainty, such as emissions characteristics, measurement errors, and formula simplification in an imperfect model, accounts for the remaining observed differences between measured and predicted model values. Even a perfect model,

with removal of all reducible uncertainty, will retain the inherent uncertainty that limits air modeling to the factor-of-two accuracy.

6.2.6.3 Review of Other Studies

A brief review of modeled to monitored concentrations reported by other studies indicates the range of variability for these types of air models. The most significant observation noted by each study is a systematic under-prediction of the monitored concentrations by the Gaussian steady-state plume models. The CEP modeled 1990 emissions inventory data and compared the estimated concentrations to the monitoring data for 1990 at 259 carbon monoxide monitoring across the United States (U.S. EPA 1999a). The results of the estimated model concentration to observed concentration was an under-prediction (arithmetic mean 0.52) for the annual average concentration value, with a range of 0.12 to 1.81. This indicates 60 percent of all values were within a factor of 1, 74 percent within a factor of 2, and 79 percent within a factor of 3.

Similarly, the National Air Toxic Assessment (NATA) used 1996 emissions and monitoring data which noted a general underestimation of monitored values by the air dispersion modeling for annual average HAP concentrations at exact locations of monitors (U.S. EPA 2001). For the seven reported HAPs, the percentage of estimated modeled concentrations lower than the monitored value at the exact monitor location ranged from 59 percent for benzene to 91 percent for acetaldehyde and lead. For locations 10 kilometers from the exact monitor location, the model estimated lower concentrations in 25 percent to 65 percent of the comparisons. For locations 50 kilometers from the exact monitor location, the estimated modeled concentrations ranged from 6 percent to 34 percent of monitored value. This example, testing the source location relative to monitor, identifies that there is an improvement in the accuracy of models when exact location of estimate is not required. Potential reasons are identified as incomplete emission inventory, underestimation of emission rates, monitor siting for peak impacts near sources and not long-term average high values, and monitor accuracy. NATA found 90 percent of long-term estimates within a factor of two of monitored values. Three key recommendations of the NATA analysis based on the results of the monitored and modeled concentration comparison are that (1) better data must be obtained on the source locations and releases for pollutants dominated by point sources, (2) improved area source spatial allocation methods are needed below the county level, and (3) better estimates of background concentrations are required on a regional rather than national basis.

One last comparison provides ISCST3 results for long-term averages as compared to long-term air monitoring data sets. In the evaluation of the proposed AERMOD model, U.S. EPA contracted for a

model evaluation of ISCST3 and AERMOD to monitoring data (U.S. EPA 1998i). Five comparisons with data sets are in flat terrain, as in the RAIMI Pilot Study. Four areas are rural and one is urban. For all data sets, the emission sources are tall stacks (taller than 84 meters) with buoyant plumes. However, only two data sets compared long-term annual averages of modeled to monitored concentrations, Kincaid and Baldwin in rural Illinois. As noted by the AERMIC peer review, these conditions are not representative of most industrial sources with medium to low level stacks, and area or volume sources of fugitive emissions or surface impoundments. ISCST3 had a ratio of modeled to monitored of 0.14 for Kincaid and 0.63 for Baldwin for annual average peak concentrations. These results are consistent with other published findings of under-estimating concentrations using the ISCST3 air model. Unfortunately, the impacts of more typical shorter stacks and fugitive sources within the Port Neches Assessment Area are not addressed by these findings. It should be noted that the more refined proposed AERMOD model also under-estimated monitored concentrations with ratios of 0.30 and 0.97 for the two data sets.

6.2.6.4 Consideration of Critical Data Gaps

Numerical closure in compared values would be expected with resolution of critical data gaps. As described in Section 6.2, critical data gaps have been identified specific to emissions characterization. Consideration of emissions characterization data gaps can be critical since they effect both the accuracy of the air modeling (e.g., lack or accuracy of source parameter values) and risk modeling (e.g., lack of speciated emissions) components, and because their numerical effect at a given receptor location can be significant. To further illustrate this point, the following example specific to the Pilot Study is provided relative to achieving numerical closure at monitoring station T136 located in the Port Neches/Nederland neighborhood.

Inventory Completeness - Case Study

An important aspect is to evaluate the completeness of the emissions databases. That is, to determine whether the available emissions data is accurate with respect to the universe of emissions sources and emitted contaminants in the assessment area. The Pilot Study assumes that the integrity of these emissions databases sufficiently provide adequate information to develop a prioritization of risk concerns from emissions sources in the assessment area. These results are therefore constrained by the completeness of these emissions inventories. To achieve an acceptable level of confidence in the completeness of emissions inventories–and thus results–requires reported emissions to be validated by cross-checking with other databases and emissions estimating resources. The EPA Office of Air Quality Planning and Standards (OAQPS) maintains several resources that can assist with estimating an

anticipated emission level of specific contaminants from specific processes. These algorithms can be used to calculate potential emissions levels by factoring production rates, process types and equipment, and emissions control equipment. It should be noted that the identification of additional emissions may take the form of non-reporting actual emissions, under-reporting of actual emissions, or reporting actual emissions of specific contaminants as part of an unspeciated class of emissions (e.g., non-methane VOCs, jet fuel, crude oil, etc.). The following discussion carries this example through for the case study of Ameripol Synpol. This exercise focuses on determining if there exists ample reason to suspect the presence of additional 1,3-butadiene sources in the Port Neches Assessment Area–beyond those reported to and documented in the emissions databases.

For this example, the potential for other sources of 1,3-butadiene emissions from the Ameripol Synpol facility was evaluated by reviewing emissions estimating literature for similar facilities and by comparing the emissions inventories with data reported to TRI. OAQPS developed a "Locating and Estimating" document to identify sources and estimate emissions of 1,3-Butadiene. (U.S. EPA 1996b).   Butadiene may be released directly into the air as a primary pollutant from industrial sources, and through secondary formation from other sources, particularly mobile sources.   In addition, emissions of styrene may also provide an important check on reported emissions of 1,3-butadiene, as it is released directly as a primary pollutant from an industrial source and not formed as a secondary chemical in the air. A comparison of styrene emissions with 1,3-butadiene emissions from processes that are expected to emit both may be a good indicator of emissions potential for 1,3-butadiene as a primary contaminant from unreported sources. A Locating and Estimating document for Styrene is also available (U.S. EPA 1993b).

The U.S. EPA Locating and Estimating document for 1,3-butadiene states that the Ameripol Synpol Port Neches facility had a 1993 production capacity of styrene-butadiene vinylpyridine (SBV) latex of 372,200 tpy, which is very similar with the 1990 production rate of 370,500 tpy reported in the Locating and Estimating Document for styrene. The following emissions potential and reported emissions data are summarized for styrene:

- The Locating and Estimating document emissions estimating factors for styrene indicate the total uncontrolled potential for styrene emissions at a plant with a similar capacity to that of the Ameripol Synpol Port Neches facility would be 377 tpy, with 222 tpy emitted from the drying units and 155 tpy from storage tanks;

- The 1997 PSDB reports 165 tpy of actual (148 tpy from stack sources and 17 tpy from fugitive sources) and 494 tpy of allowable styrene emissions from Ameripol Synpol; and

- The 1997 TRI reports styrene releases to air totaling 173 tons (145 tpy from stack sources and 28 from fugitive sources).

Similarly, the following emissions potential and reported and emissions data are summarized for

1,3-butadiene:

- • The Locating and Estimating document emissions estimating factors for 1,3-butadiene indicate the total uncontrolled potential for 1,3-butadiene emissions at a plant with a similar capacity to that of the Ameripol Synpol Port Neches facility would be 1,381tpy, with 1,321 tpy emitted from process vents, 56 tpy from wastewater, and 4 tpy from other fugitive sources;

- • The 1997 PSDB reports 5.83 of actual (3 tpy from a single wastewater source and 2.83 tpy from 28 other sources) and zero tpy of allowable 1,3-butadiene emissions from Ameripol Synpol; and

- • The 1997 TRI reports 1,3-butadiene releases to air totaling 9 tons (1 tpy from stack sources and 8 tpy from fugitive sources).

The PSDB and TRI emissions of styrene, although not in complete agreement, generally appear to be

consistent with the estimate for the same size facility using the Locating and Estimating document,

allowing for variations in operations and emissions controls. However, unlike styrene, the reported

emissions data for 1,3-butadiene are grossly inconsistent with the emissions potential calculated using the

Locating and Estimating document. Both 1,3-butadiene and styrene are raw materials for the production

of SBV latex. This indicates potential discrepancies between potential and reported emissions of these

contaminants.

Acknowledging that many additional considerations must be addressed to determine a representative

emission rate of 1,3-butadiene from a facility other than total production capacity and emission factors

from similar facilities, there appears to be potential for significant unreported 1,3-butadiene emissions at

the Ameripol Synpol facility. Due to its close proximity to the ambient monitoring station T136 location,

even a moderate increase in estimated emissions will have a dramatic impact on the butadiene air

concentrations computed by the air model. The 1998 TRI reports 22 tpy of 1,3-butadiene emissions from

Ameripol Synpol. This represents a nearly 4-fold increase from the 1997 PSDB reported value of

5.83 tpy, which would correspond to a similar increase in modeled risk impacts. The potential for

unreported emissions of 1,3-butadiene from the Ameripol Synpol facility alone would account for most of

the observed differences in the measured and modeled air concentrations of butadiene in the RAIMI Pilot

Study.

6.3   UNCERTAINTY AND LIMITATIONS

This section notes important considerations with regard to how the results of RAIMI Pilot Study may be used to identify and prioritize risk management opportunities, evaluate permit conditions, or otherwise be used by regulatory agencies and facilities. As noted in Chapter 3, the most significant limit to the usability of results is the lack of complete emissions characterization in the form of unidentified and unspeciated emissions data. Therefore, most of the considerations described in this section pertain to emissions characterization. Other considerations in addition to emissions characterization includes use of actual versus allowable emission rates, adjusting for process upsets, secondary formation of contaminants, and aspects of monitoring versus modeling.

The RAIMI Pilot Study was designed to test a risk-based tool for prioritizing concerns (e.g., facilitating air toxics reduction strategies) at a local level. Limitations and uncertainties associated with the tool are directly related to the scope and objectives of the study to be performed. For example, the tool is designed on a dynamic platform such that multiple air model types (i.e., ISCST3, CALPUFF, AERMOD, etc.) could be utilized in the implementation of the tool. Each of these air models would have uncertainties and limitations associated with their use and site-specific application. The purpose of this section is to highlight the major limitations and uncertainties generally encountered at the local level of assessment and provide examples illustrated in the RAIMI Pilot Study utilized to demonstrate this tool.

In general, uncertainties and limitations fall into two categories, those associated with the scope of the assessment and those associated with major technical components of the assessment such as emissions characterization, air modeling and risk modeling. For example, the scope of the initial phase of the RAIMI Pilot Study inherently limited the evaluation to (1) outdoor emission sources, (2) 188 air pollutants, and (3) only the inhalation exposure pathway. Also, since results represent what was occurring in 1997, they may not accurately reflect conditions in this area today. Uncertainties associated with scope include those resulting from; modeling mobile and area emission sources as groups, allocating emissions to grouped sources based on surrogates such as population or land use, and utilizing a simple exposure scenario which assumes a person breathes outdoor air 24 hours a day, 350 days per year, and for 6 (child) or 30 (adult) years.

General uncertainties and limitations associated with emissions characterization include variability and quality and accuracy of emission estimation methods and data gaps, respectively. For example, specific to the RAIMI Pilot Study, there were uncertainties associated with source definition (e.g., point versus fugitive) and location. There were also limitations associated with gaps in speciated emissions

(e.g., emissions reported as non-methane VOCs, gasoline mixtures, etc.). See Chapter 3 for discussion of these uncertainties and limitations as they pertain to the RAIMI Pilot Study.

General uncertainties and limitations associated with air modeling include variability and representativeness of air model input parameters (see Appendix SEN for sensitivity analysis of input parameters of ISCST3), as well as limitations of the air model implemented in the Pilot Study. For example, specific to the RAIMI Pilot Study, there were uncertainties associated with meteorological data and surface roughness calculations. There were also limitations with the range of the ISCST3 model (i.e., 50 kilometers), and the inability to accurately account for secondary formation, decay, and building downwash. Decay and building downwash limitations are based on scope of the project, whereas range of the air model and its ability to address secondary formation are limitations of the model utilized in the Pilot Study. See Chapter 4 for discussion of these uncertainties and limitations as they pertain to the RAIMI Pilot Study.

General uncertainties and limitations associated with risk modeling include those associated with toxicity, terrestrial fate and transport of deposited emissions, and those associated with exposure. Uncertainties associated with toxicity data (i.e., RfDs and CSFs) are inherent to the risk assessment process in general (U.S. EPA 1998a; 1998b) and are mitigated through application of uncertainty factors (i.e., for RfDs) or utilization of the upper 95 percent bound for the slope factors (i.e., CSFs). There is also a limitation imposed by the lack of toxicity data for many contaminants. For the RAIMI Pilot Study, oral RfDs and CSFs were utilized for contaminants lacking inhalation RfDs and CSFs to reduce the effects of this limitation. Also, for the RAIMI Pilot Study, terrestrial fate and transport of deposited emissions is not within the scope of the initial phase. Limitations and uncertainties associated with the simple exposure scenario utilized in the RAIMI Pilot Study are specific to the scope of the assessment and limitations in available emissions data. For example, to prioritize sources on a risk basis it was not deemed practical to develop the data necessary to accurately portray exposure. Also, emissions data is presented in State and Federal databases on an annual basis. Measured data collected at the facility fenceline for one contaminant (1,3 butadiene) on a 15 minute basis continually for a year indicated that measured air concentrations varied by several orders of magnitude over time and it would be extremely difficult to match activity pattern with emissions. See Chapter 5 for discussion of these uncertainties and limitations as they pertain to the RAIMI Pilot Study.

Acceptable levels of accuracy and precision to assessment results are directly tied to the scope and objectives of a study. There are several ways to quantitatively or qualitatively assess the effect uncertainties and limitations have on the results. For example, in the RAIMI Pilot Study, two methods

were applied to ensure the accuracy and precision of assessment results commensurate with study design objectives. First, modeled concentrations of the most significantly emitted contaminants were compared to measured concentrations. Although there are uncertainties and limitations associated with comparison of monitoring and modeling (see Section 6.2.6), it serves as a way to focus and add confidence to interpretation of results. Secondly, a sensitivity analysis of the air model input parameters was conducted to bound the effects of selection of model inputs. Results and discussion of the comparison of measured to modeled results and the air model input sensitivity analysis are presented in Section 6.2.6 and Appendix SEN, respectively.