Appendix B: Derivation of chemical- and instrument-specific baselines for investigation level derivation

The purpose of setting an instantaneous baseline-derived investigation level (iBDIL) is to identify the presence of an abnormally high concentration of any monitored chemical in the ambient air. This allows for identification of non-spurious concentrations that warrant a follow-up source investigation, with further actions carried out if needed. To set the iBDIL, the maximum non-signal baseline noise (baseline level) must be determined for each chemical and for each monitoring instrument. This appendix addresses chemical measurements made using the Selected Ion Flow Tube-Mass Spectrometer (SIFT), Differential Ultra-Violet Absorption Spectrometer (DUVAS), Picarro, and nephelometer instruments. The iBDIL is set 10-times higher than the chemical- and instrument- specific baseline. The baseline and iBDIL for a number of chemicals measured by the SIFT and the DUVAS are provided in Table B - 1. The following sections describe the specific baseline determinations for each chemical and instrument.

Table B - 1. Baseline and iBDIL values of chemicals monitored by SIFT and DUVAS instruments.

Chemical(s)	Applicable Instrument(s)	SIFT Baseline (ppb)	DUVAS Baseline (ppb)	iBDIL (ppb)
Acetylene	SIFT	8	N/A	80
Ammonia	DUVAS	N/A	ND	ND
Benzene	SIFT, DUVAS	8	14	80 [a]
1,3-Butadiene	SIFT, DUVAS	4	6	40 [a]
Butane	SIFT	ND	N/A	ND
1-Butene (1-Butylene)	SIFT	11	N/A	110
C3 - C4 Saturated	SIFT	96	N/A	960
Cyclohexane	SIFT	12	N/A	120
Ethane + Ethylene	SIFT	ND	N/A	ND
Ethylbenzene	DUVAS	N/A	35	350
Ethylbenzene + Xylenes	SIFT	6	N/A	60
Formaldehyde	DUVAS	N/A	ND	ND
Hexane	SIFT	34	N/A	340
Isobutane	SIFT	28	N/A	280
Octane	SIFT	16	N/A	160
Propane	SIFT	54	N/A	540

Chemical(s)	Applicable Instrument(s)	SIFT Baseline (ppb)	DUVAS Baseline (ppb)	iBDIL (ppb)
Propylene	SIFT	ND	N/A	ND
Styrene	SIFT, DUVAS	6	8	60 [a]
Sulfur Dioxide	DUVAS	N/A	7	70
Toluene	SIFT, DUVAS	7	40	70 [a]
***m*-Xylene**	DUVAS	N/A	ND	ND
***o*-Xylene**	DUVAS	N/A	ND	ND
***p*-Xylene**	DUVAS	N/A	ND	ND

[a] iBDIL derived using baseline from the SIFT instrument.; iBDIL – instantaneous baseline derived investigation level; N/A – not applicable; ND – not derived; ppb – parts per billion; SIFT – Selected Ion Flow Tube-Mass Spectrometer; and DUVAS – Differential Ultra-Violet Absorption Spectrometer.

SIFT Instrument Chemical Baseline Derivations

The SIFT instrument was utilized to conduct more than 300 mobile monitoring surveys between September 10, 2020, and November 10, 2021, in the Beaumont, Houston, and Corpus Christi areas of Texas (TCEQ regions 10, 12, and 14, respectively). Some or all these surveys measured the following chemicals: acetylene, benzene, 1,3-butadiene, butane, 1-butene (1-butylene), C3-C4 saturated, cyclohexane, ethane + ethylene, ethylbenzene + xylenes, hexane, isobutane, isobutene, octane, propane, propylene, styrene, and toluene. Not all surveys were evaluated to determine the baseline for each chemical, but rather a subset of surveys were chosen based on criteria discussed in Section 3.2. A summary of the monitoring surveys identified as having the maximum non-signal baseline noise, and therefore used for the derivation of chemical-specific baseline levels, is provided in Table B - 2.

Table B - 2. SIFT monitoring surveys used to derive chemical-specific baseline levels.

Chemical(s)	Event	Date	Location	Survey Number	Baseline (ppb)
Acetylene	Hurricane Laura	9/16/2020	Orange, TX	A	8
Benzene	Hurricane Laura	9/10/2020	Port Arthur, TX	E (Stat)	8
1,3-Butadiene	Winter Storm Uri	2/23/2021	Houston, TX	A (Stat)	4
Butane					ND
1-Butene (1-Butylene)	Hurricane Delta	10/11/2020	Port Arthur, TX	A	11
C3 – C4 Saturated	Hurricane Laura	9/10/2020	Port Neches, TX	B	96

Chemical(s)	Event	Date	Location	Survey Number	Baseline (ppb)
Cyclohexane	Hurricane Laura	9/10/2020	Port Arthur, TX	C (Stat)	12
Ethane + Ethylene					ND
Ethylbenzene + Xylenes	N/A	6/16/2021	Port Neches, TX	9-L	6
Hexane	Hurricane Laura	9/10/2020	Port Arthur, TX	C (Stat)	34
Isobutane	Winter Storm Uri	2/23/2021	Houston, TX	A	28
Octane	Winter Storm Uri	3/7/2021	Corpus Christi, TX	BG	16
Propane	Winter Storm Uri	3/9/2021	Port Neches, TX	AM	54
Propylene					ND
Styrene	N/A	10/25/2021	Channelview, TX	B	6
Toluene	Winter Storm Uri	3/30/2021	Channelview, TX	BJ	7

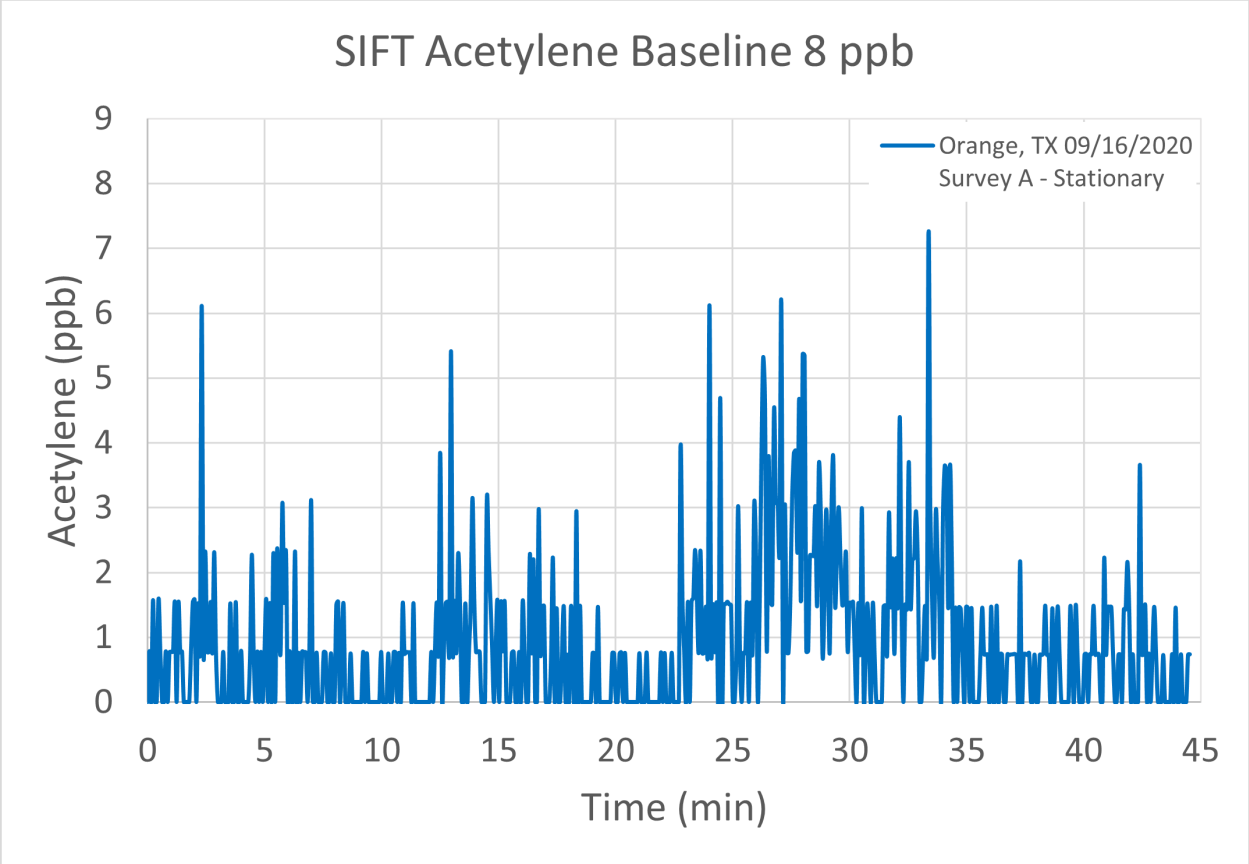
Stat – Stationary survey; ND – not derived; N/A – not applicable; and ppb – parts per billion.

Acetylene

Of the 145 SIFT surveys that measured acetylene, a total of 20 surveys were selected and evaluated to determine the acetylene baseline level. The survey with the maximum non-signal baseline noise was survey A from September 16, 2020, in Orange, TX (Region 10), shown below (Figure B - 1). The maximum noise from the survey was 7.24 ppb, which was rounded[1] to 8 ppb to generate the baseline level for acetylene. The iBDIL for acetylene was calculated as 10-times the baseline level and therefore the acetylene iBDIL was set at 80 ppb.

[1] Because the baseline value represents the top of the range of instrument noise and background ambient concentrations, we rounded the highest non-signal concentrations observed for that chemical and instrument up to the nearest part per billion. Exceptions to this rounding convention are noted for specific chemicals/instruments.

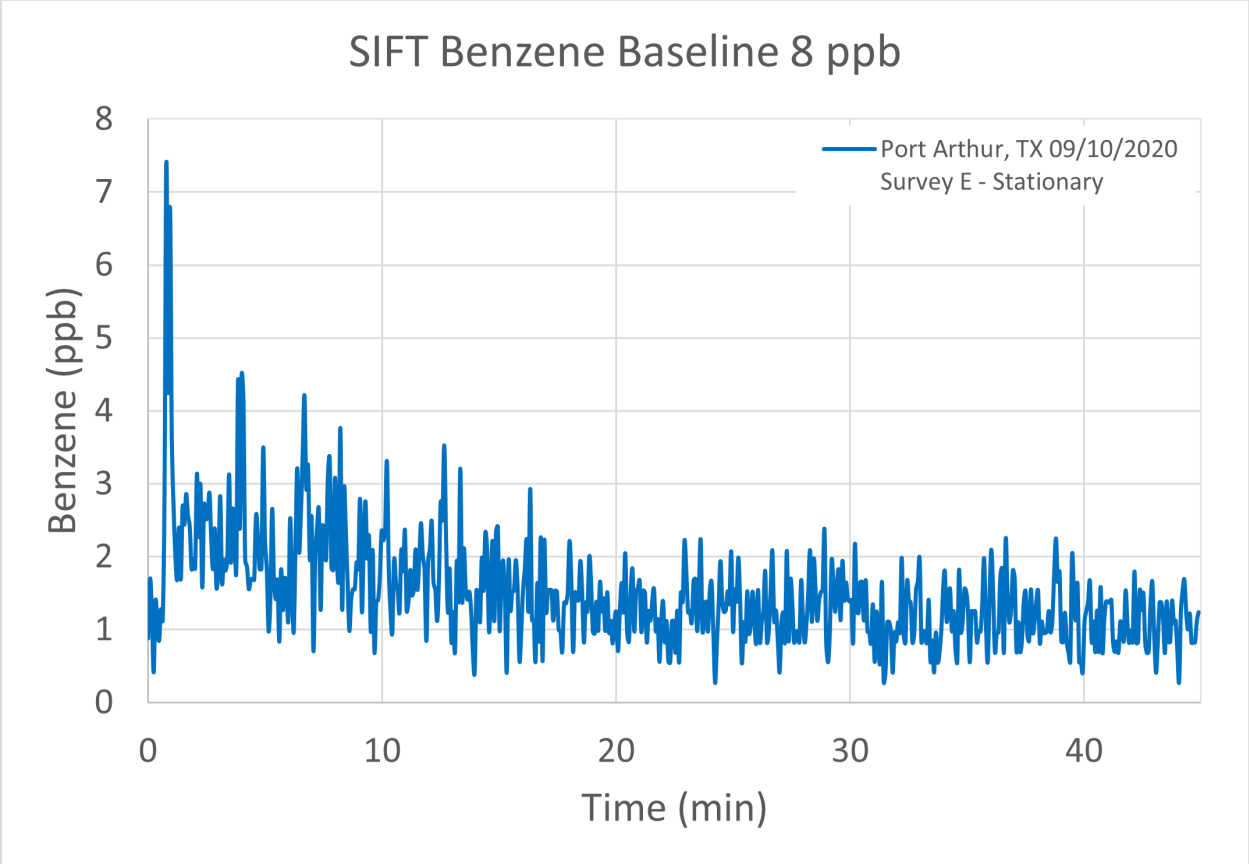
Figure B - 1. Time-concentration graph of acetylene collected during a SIFT instrument survey that was selected as the acetylene maximum non-signal baseline level.



Benzene

Of the 304 SIFT surveys that measured benzene, a total of 18 surveys were selected and evaluated to determine the benzene baseline level. The survey with the maximum non-signal baseline noise was Survey E -Stationary from September 10, 2021, in Port Arthur, TX (Region 10), shown below (Figure B - 2). The maximum noise from the survey was 7.40 ppb, which was rounded to 8 ppb to generate the baseline level for benzene. The iBDIL for benzene was calculated as 10-times the baseline level and therefore the benzene iBDIL was set at 80 ppb.

Figure B - 2. Time-concentration graph of benzene collected during a SIFT instrument survey that was selected as the benzene maximum non-signal baseline level.

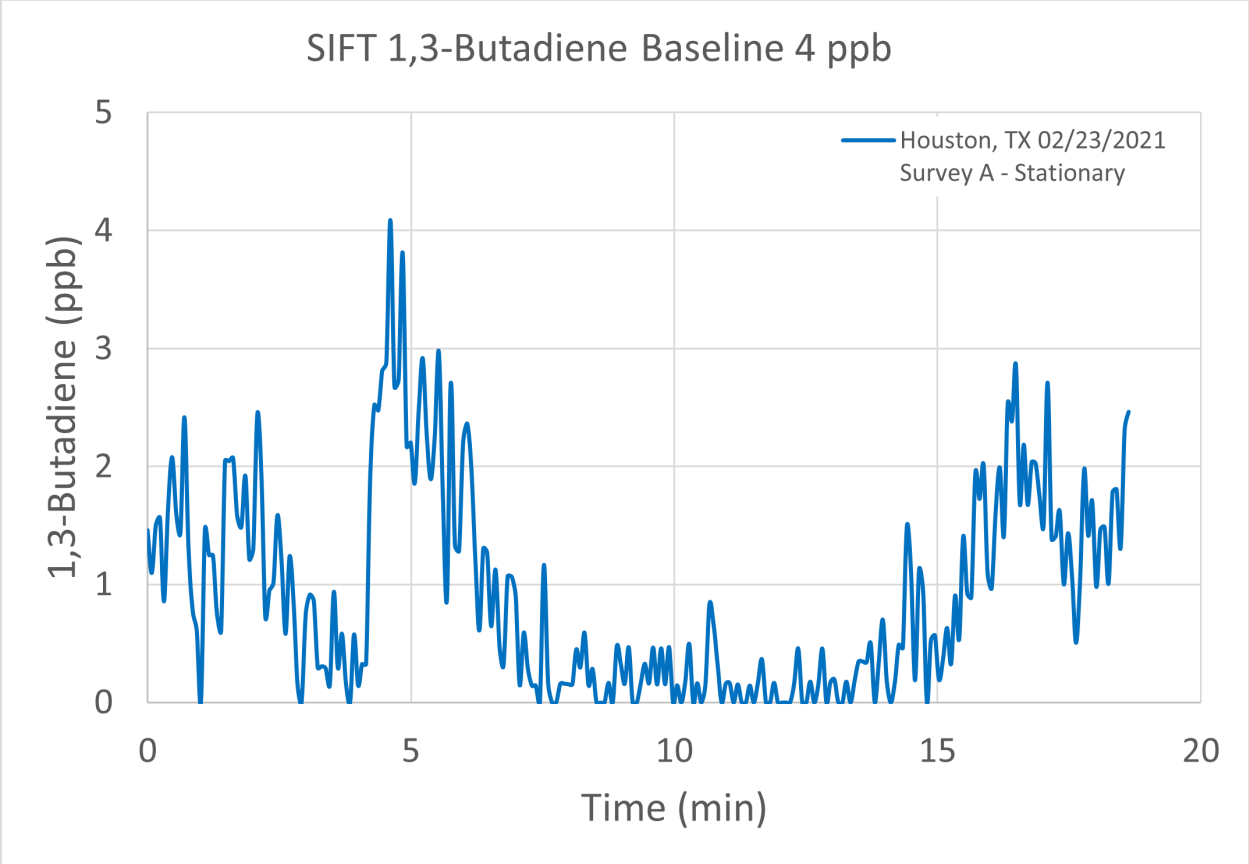


1,3-Butadiene

Of the 304 SIFT surveys that measured 1,3-butadiene, a total of 12 surveys were selected and evaluated to determine the 1,3-butadiene baseline level. The survey with the maximum non-signal baseline noise was Survey A-Stationary from February 23, 2021, in Houston, TX (Region 12), shown below (Figure B - 3). The maximum noise from the survey was 4.09 ppb, which was rounded down to 4 ppb to generate the baseline level for 1,3-butadiene.[2] The iBDIL for 1,3-butadiene was calculated as 10-times the baseline level and therefore the 1,3-butadiene iBDIL was set at 40 ppb.

[2] Because the maximum non-signal baseline for 1,3-butadiene was < 0.1 ppb higher than 4 ppb, the decision was made to round the baseline level down to 4 ppb.

Figure B - 3. Time-concentration graph of 1,3-butadiene collected during a SIFT instrument survey that was selected as the 1,3-butadiene maximum non-signal baseline level.



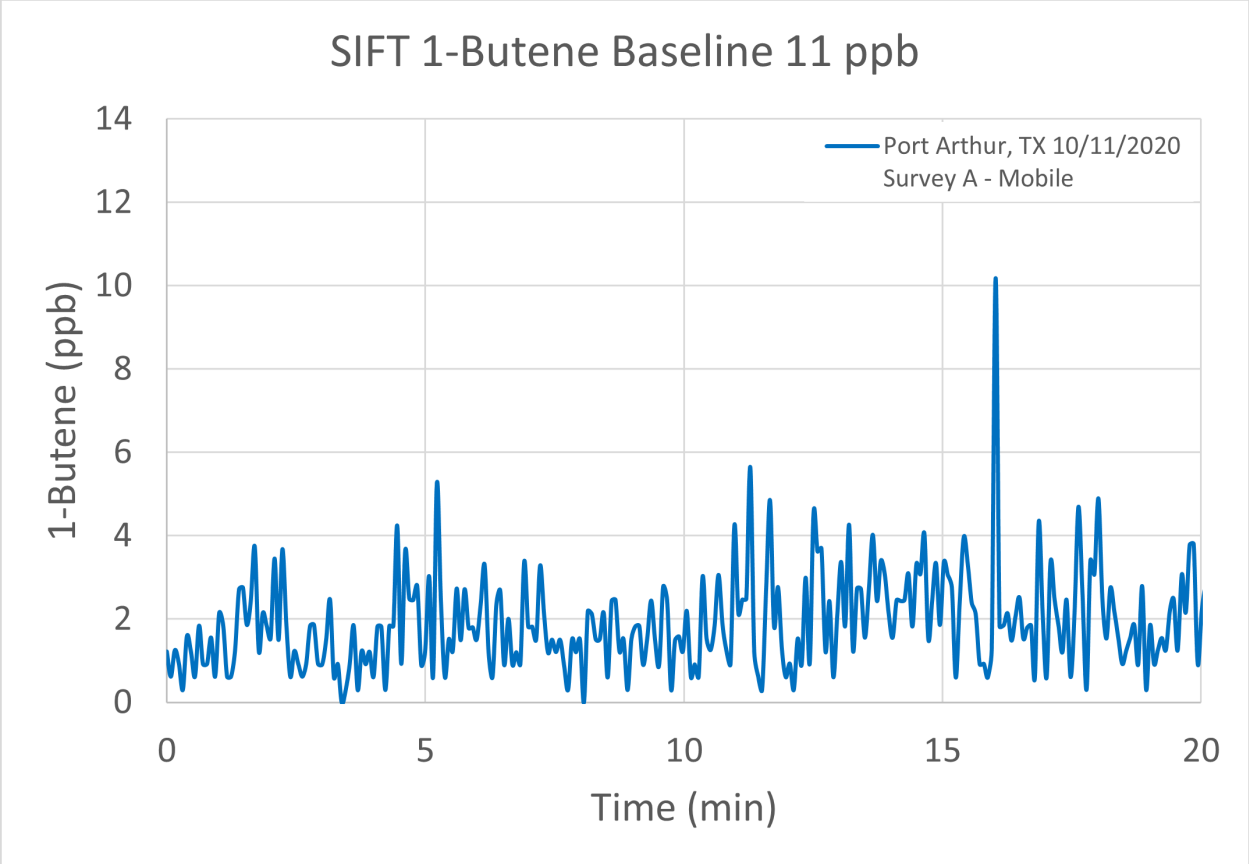
Butane

The baseline was not determined for butane due to the variation observed in the baseline noise among surveys.

1-Butene

Of the 151 SIFT surveys that measured 1-butene, a total of 26 surveys were selected and evaluated to determine the 1-butene baseline level. The survey with the maximum non-signal baseline noise was survey A from October 11, 2020, in Port Arthur, TX (Region 10), shown below (Figure B - 4). The maximum noise from the survey was 10.18 ppb, which was rounded to 11 ppb to generate the baseline level for 1-butene. The iBDIL for 1-butene was calculated as 10-times the baseline level and therefore the 1-butene iBDIL was set at 110 ppb.

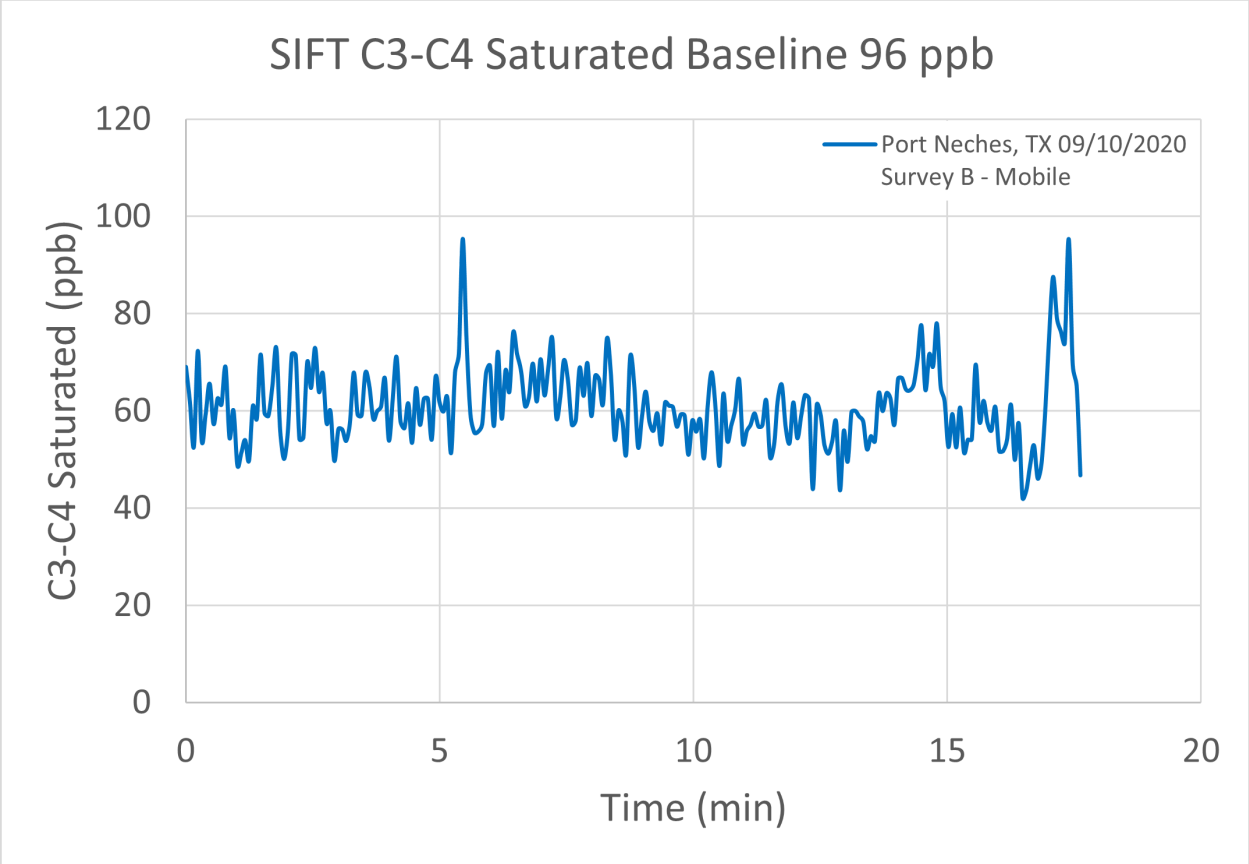
Figure B - 4. Time-concentration graph of 1-butene collected during a SIFT instrument survey that was selected as the 1-butene maximum non-signal baseline level.



C3-C4 Saturated

Of the 77 SIFT surveys that measured C3-C4 saturated, a total of 28 surveys were selected and evaluated to determine the C3-C4 saturated baseline level. The survey with the maximum non-signal baseline noise was Survey B from September 10, 2020, in Port Neches, TX (Region 10), shown below (Figure B - 5). The maximum noise from the survey was 95.40 ppb, which was rounded to 96 ppb to generate the baseline level for C3-C4 saturated. The iBDIL for C3-C4 saturated was calculated as 10-times the baseline level and therefore the C3-C4 iBDIL was set at 960 ppb.

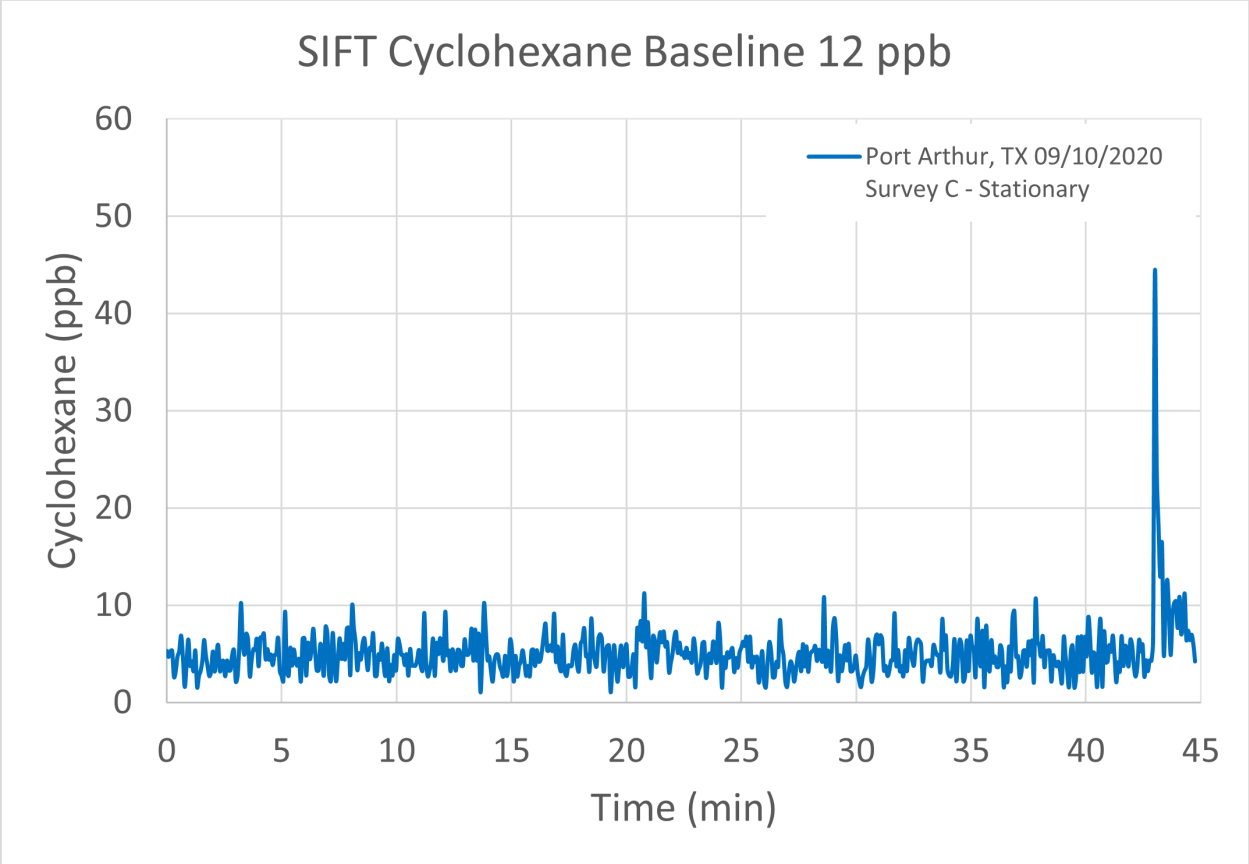
Figure B - 5. Time-concentration graph of C3-C4 saturated collected during a SIFT instrument survey that was selected as the C3-C4 saturated maximum non-signal baseline level.



Cyclohexane

Of the 100 SIFT surveys that measured cyclohexane, a total of 28 surveys were selected and evaluated to determine the cyclohexane baseline level. The survey with the maximum non-signal baseline noise was survey C (stationary) from September 10, 2020, in Port Arthur, TX (Region 10), shown below (Figure B - 6). The maximum noise from the survey was 11.30 ppb, which was rounded to 12 ppb to generate the baseline level for cyclohexane. The iBDIL for cyclohexane was calculated as 10-times the baseline level and therefore the iBDIL was set at 120 ppb.

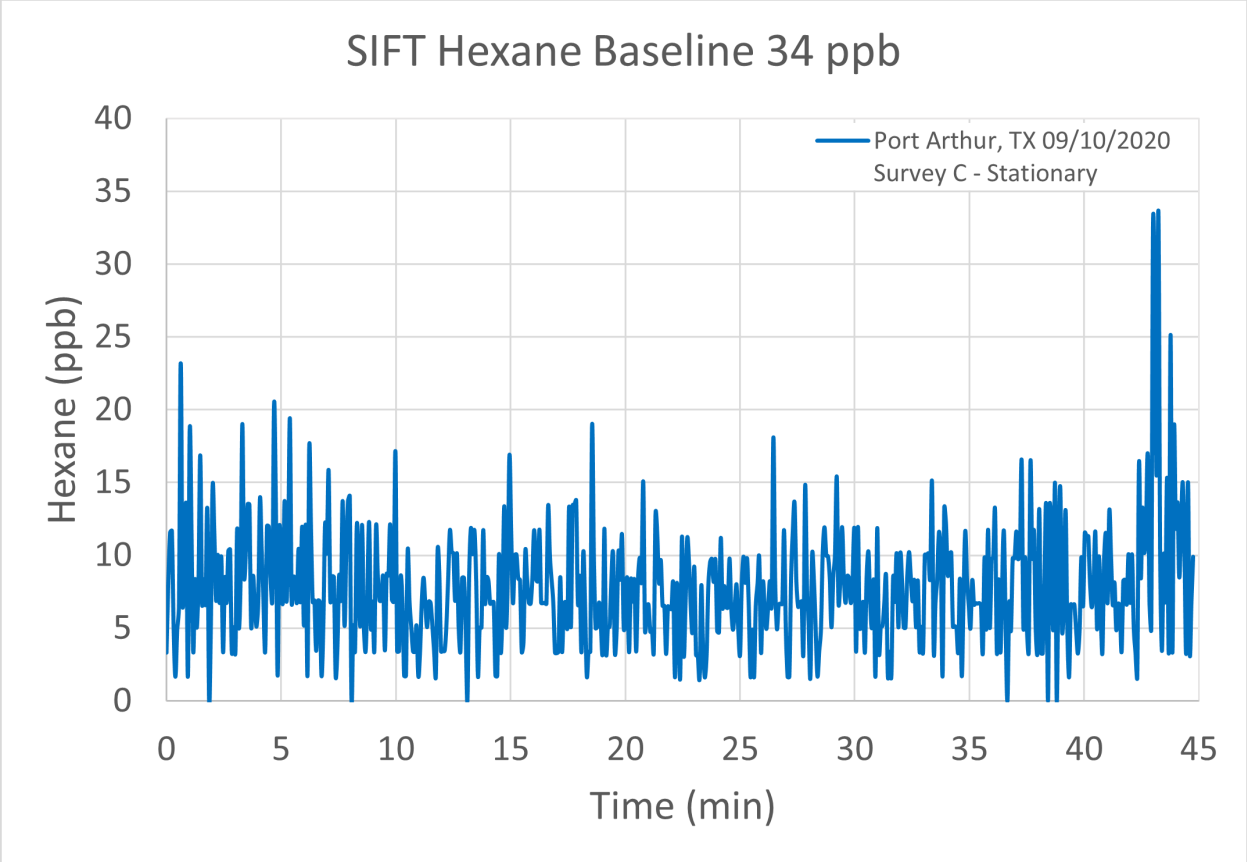
Figure B - 6. Time-concentration graph of cyclohexane collected during a SIFT instrument survey that was selected as the cyclohexane maximum non-signal baseline level.



n-Hexane

Of the 104 SIFT surveys that measured n-hexane, a total of 23 surveys were selected and evaluated to determine the n-hexane baseline level. The survey with the maximum non-signal baseline noise was survey C (stationary) from September 10, 2021, in Port Arthur, TX (Region 10), shown below (Figure B - 7). The maximum noise from the survey was 33.65 ppb, which was rounded to 34 ppb to generate the baseline level for n-hexane. The iBDIL for n-hexane was calculated as 10x the baseline level and therefore the n-hexane iBDIL was set at 340 ppb.

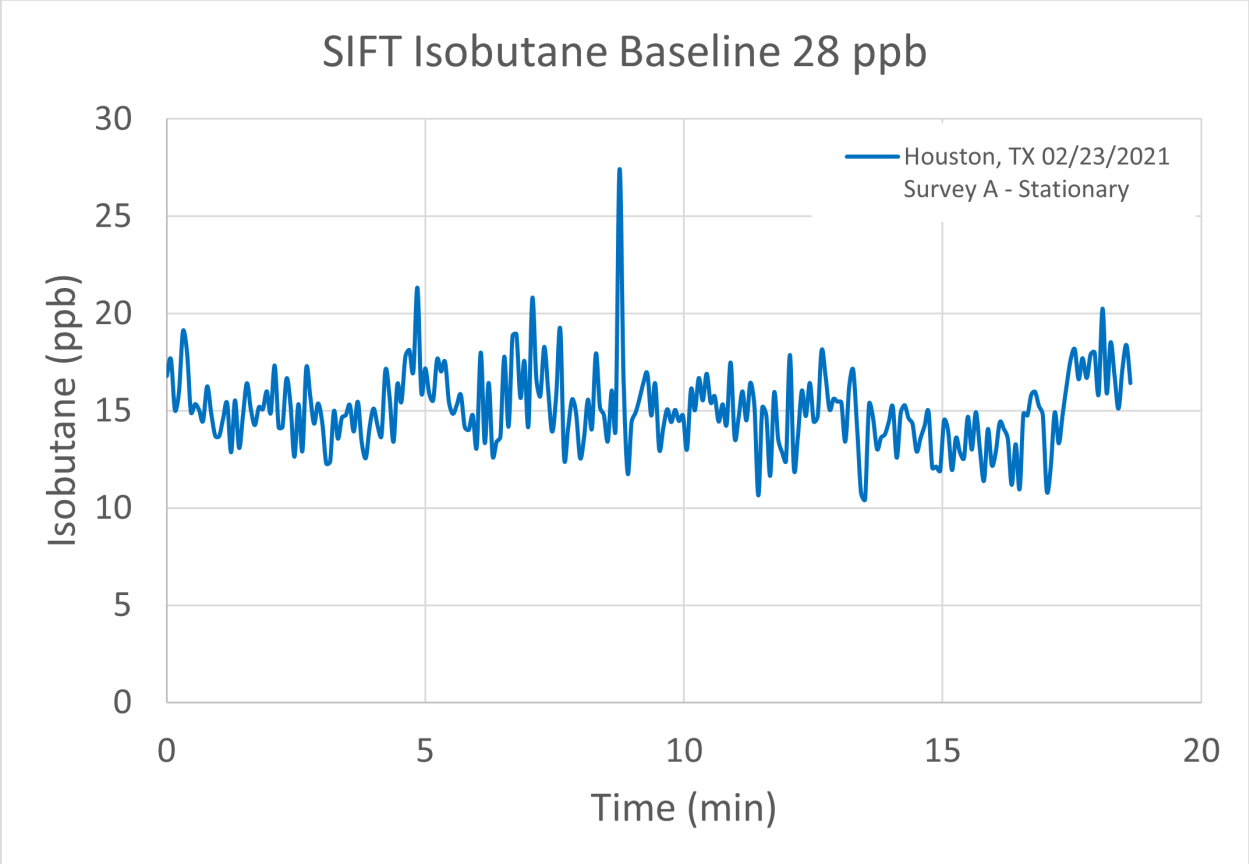
Figure B - 7. Time-concentration graph of n-hexane collected during a SIFT instrument survey that was selected as the n-hexane maximum non-signal baseline level.



Isobutane

Of the 145 SIFT surveys that measured isobutane, a total of 27 surveys were selected and evaluated to determine the isobutane baseline level. The survey with the maximum non-signal baseline noise was survey A (stationary) from February 23, 2021, in Houston, TX (Region 12), shown below (Figure B - 8). The maximum noise from the survey was 27.42 ppb, which was rounded to 28 ppb to generate the baseline level for isobutane. The iBDIL for isobutane was calculated as 10-times the baseline level and therefore the isobutane iBDIL was set at 280 ppb.

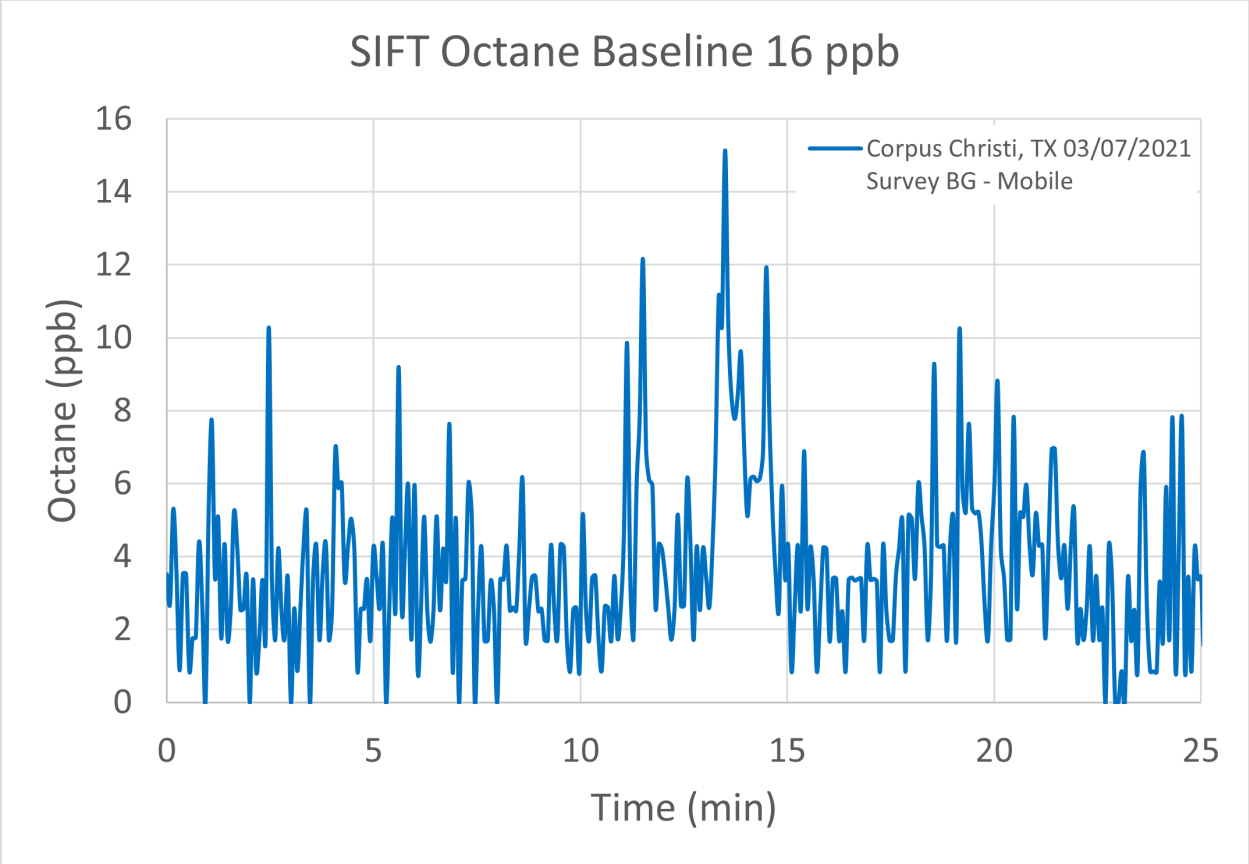
Figure B - 8. Time-concentration graph of isobutane collected during a SIFT instrument survey that was selected as the isobutane maximum non-signal baseline level.



n-Octane

Of the 100 SIFT surveys that measured n-octane, a total of 45 surveys were selected and evaluated to determine the n-octane baseline level. The survey with the maximum non-signal baseline noise was survey BG from March 7, 2021, in Corpus Christi, TX (Region 14), shown below (Figure B - 9). The maximum noise from the survey was 15.14 ppb, which was rounded to 16 ppb to generate the baseline level for n-octane. The iBDIL for n-octane was calculated as 10-times the baseline level and therefore the n-octane iBDIL was set at 160 ppb.

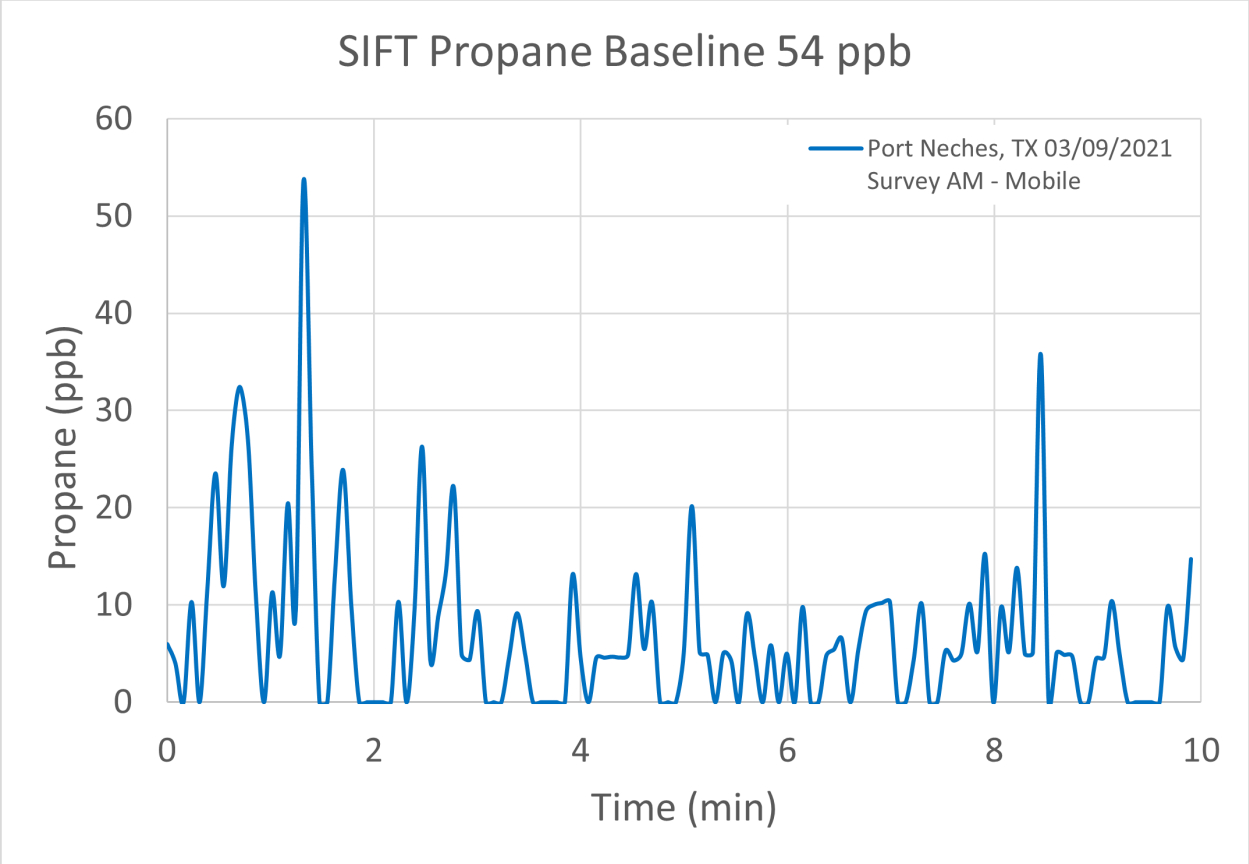
Figure B - 9. Time-concentration graph of n-octane collected during a SIFT instrument survey that was selected as the n-octane maximum non-signal baseline level.



Propane

Of the 304 SIFT surveys that measured propane, a total of 18 surveys were selected and evaluated to determine the propane baseline level. The survey with the maximum non-signal baseline noise was survey AM from March 9, 2021, in Port Neches, TX (Region 10), shown below (Figure B - 10). The maximum noise from the survey was 53.63 ppb, which was rounded to 54 ppb to generate the baseline level for propane. The iBDIL for propane was calculated as 10-times the baseline level and therefore the propane iBDIL was set at 540 ppb.

Figure B - 10. Time-concentration graph of propane collected during a SIFT instrument survey that was selected as the propane maximum non-signal baseline level.



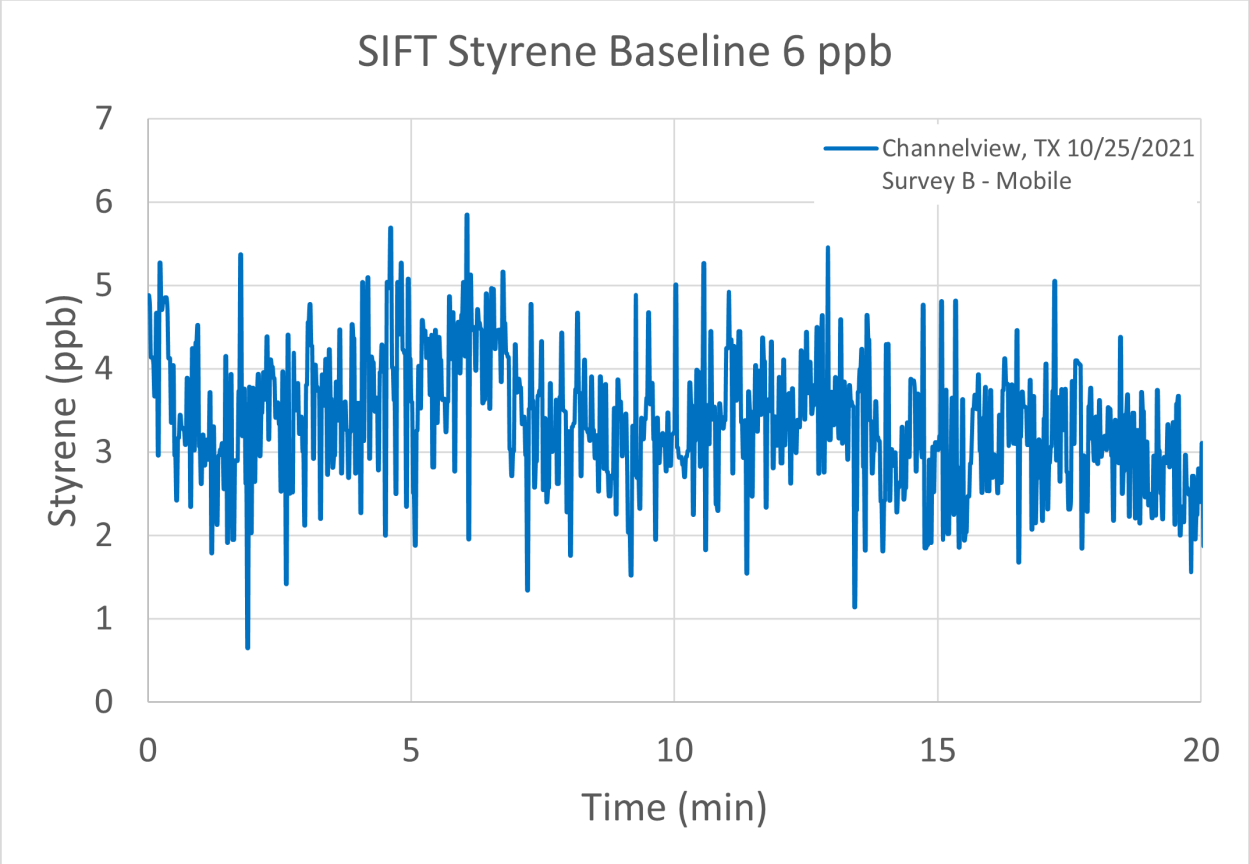
Propylene

The baseline was not determined for propylene due to the large variability observed in the baseline between regions and events.

Styrene

Of the 304 SIFT surveys that measured styrene, a total of 27 surveys were selected and evaluated to determine the styrene baseline level. The survey with the maximum non-signal baseline noise was survey B from October 25, 2021, in Channelview, TX (Region 12), shown below (Figure B - 11). The maximum noise from the survey was 5.8 ppb, which was rounded to 6 ppb to generate the baseline level for styrene. The iBDIL for styrene was calculated as 10-times the baseline level and therefore the styrene iBDIL was set at 60 ppb.

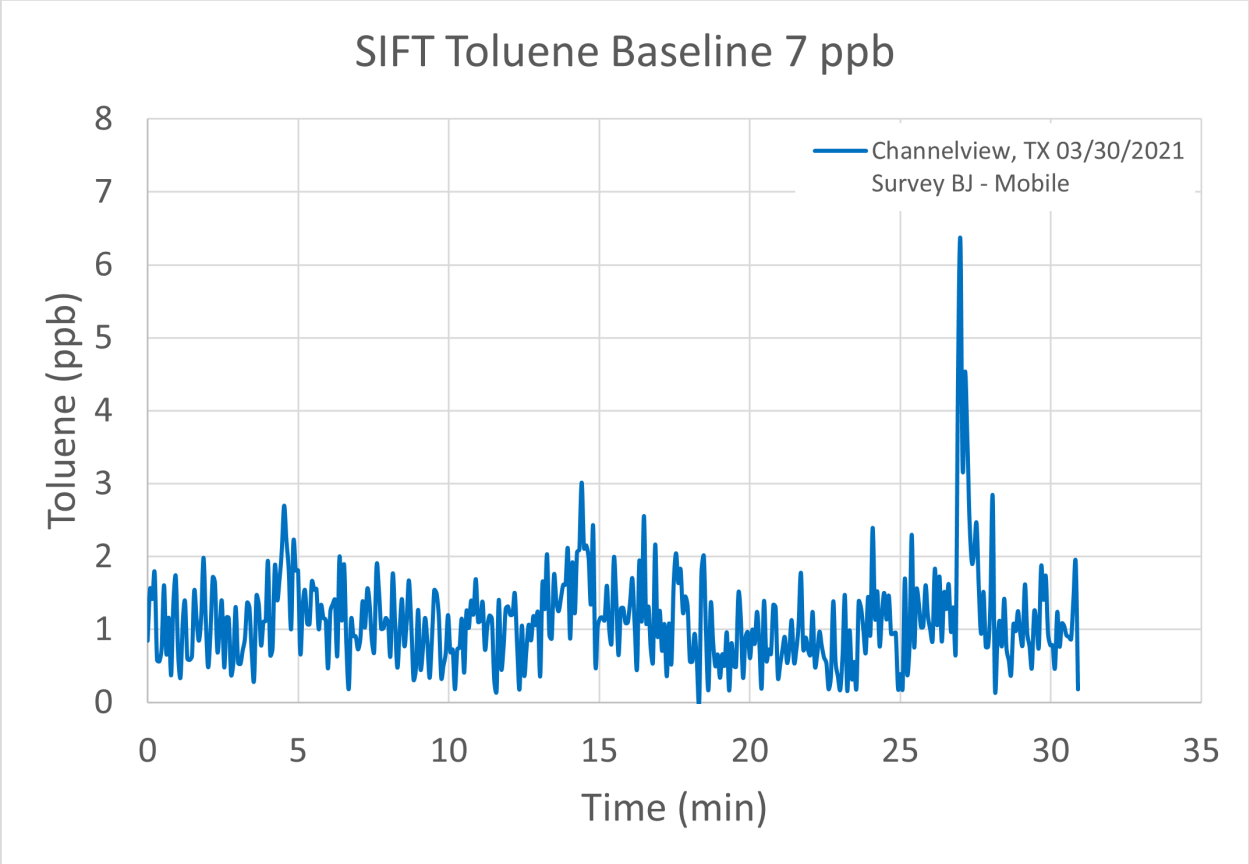
Figure B - 11. Time-concentration graph of styrene collected during a SIFT instrument survey that was selected as the styrene maximum non-signal baseline level.



Toluene

Of the 304 SIFT surveys that measured toluene, a total of 29 surveys were selected and evaluated to determine the toluene baseline level. The survey with the maximum non-signal baseline noise was Survey BJ from March 30, 2021, in Channelview, TX (Region 12), shown below (Figure B - 12). The maximum noise from the survey was 6.35 ppb, which was rounded to 7 ppb to generate the baseline level for toluene. The iBDIL for toluene was calculated as 10-times the baseline level and therefore the toluene iBDIL was set at 70 ppb.

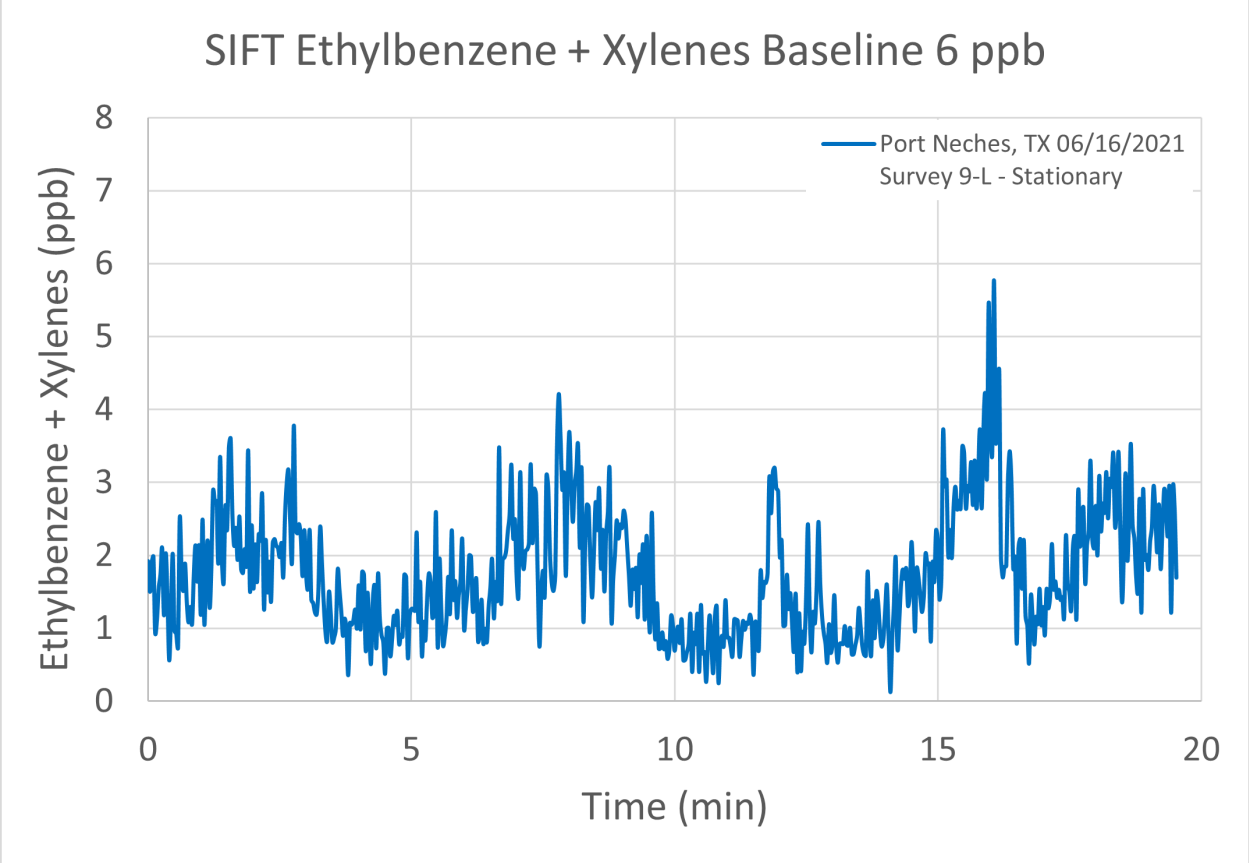
Figure B - 12. Time-concentration graph of toluene collected during a SIFT instrument survey that was selected as the toluene maximum non-signal baseline level.



Xylenes + Ethylbenzene

Of the 304 SIFT surveys that measured xylenes + ethylbenzene, a total of 54 surveys were selected and evaluated to determine the xylenes + ethylbenzene baseline level. The survey with the maximum non-signal baseline noise was survey 9-L (stationary) from June 16, 2021, in Port Neches, TX (Region 10), shown below (Figure B - 13). The maximum noise from the survey was 5.77 ppb, which was rounded to 6 ppb to generate the baseline level for xylenes + ethylbenzene. The iBDIL for xylenes + ethylbenzene was calculated as 10-times the baseline level and therefore the xylenes + ethylbenzene iBDIL was set at 60 ppb.

Figure B - 13. Time-concentration graph of xylenes + ethylbenzene collected during a SIFT instrument survey that was selected as the xylenes + ethylbenzene maximum on-signal baseline level.



DUVAS Instrument Chemical Baseline Derivations

The DUVAS instrument was utilized to conduct more than 500 mobile monitoring surveys between August 28, 2020, and March 4, 2022, in the Beaumont, Houston, and Corpus Christi, areas of Texas (TCEQ Regions 10, 12, and 14 respectively). Of those, 198 surveys conducted in Beaumont and Houston beginning in September 2021 had one-second data available for analysis and so those surveys were used for the DUVAS baseline derivations. Some or all these surveys measured the following chemicals: ammonia, benzene, 1,3-butadiene, ethylbenzene, formaldehyde, styrene, sulfur dioxide, toluene, and xylenes. Not all surveys were evaluated to determine the baseline for each chemical, but rather a subset of surveys were chosen based on criteria discussed in Section 3.2. A summary of the monitoring surveys identified as having the maximum non-signal baseline noise, and therefore used for the derivation of chemical-specific baseline levels is provided in Table B - 3. For consistency, the TCEQ chose to designate a single iBDIL for chemicals measured by both the SIFT and DUVAS (benzene, 1,3-butadiene, styrene, and toluene).

Table B - 3. DUVAS monitoring surveys used to derive chemical-specific baselines.

Chemical(s)	Date	Location	Survey Number	Baseline (ppb)
Ammonia				ND
Benzene	10/12/2021	Port Neches, TX	Datalog 4-3	14
1,3-Butadiene	10/13/2021	Port Neches, TX	Datalog 6-3	6
Ethylbenzene	9/16/2021	Texas City, TX	H	35
Formaldehyde				ND
Styrene	10/13/2021	Beaumont, TX	Datalog 1-3	8
Sulfur Dioxide	10/28/2021	Pasadena, TX	10	7
Toluene	11/12/2021	Channelview, TX	4	40
***m*-Xylene**				ND
***o*-Xylene**				ND
***p*-Xylene**				ND

ND – not derived and ppb – parts per billion.

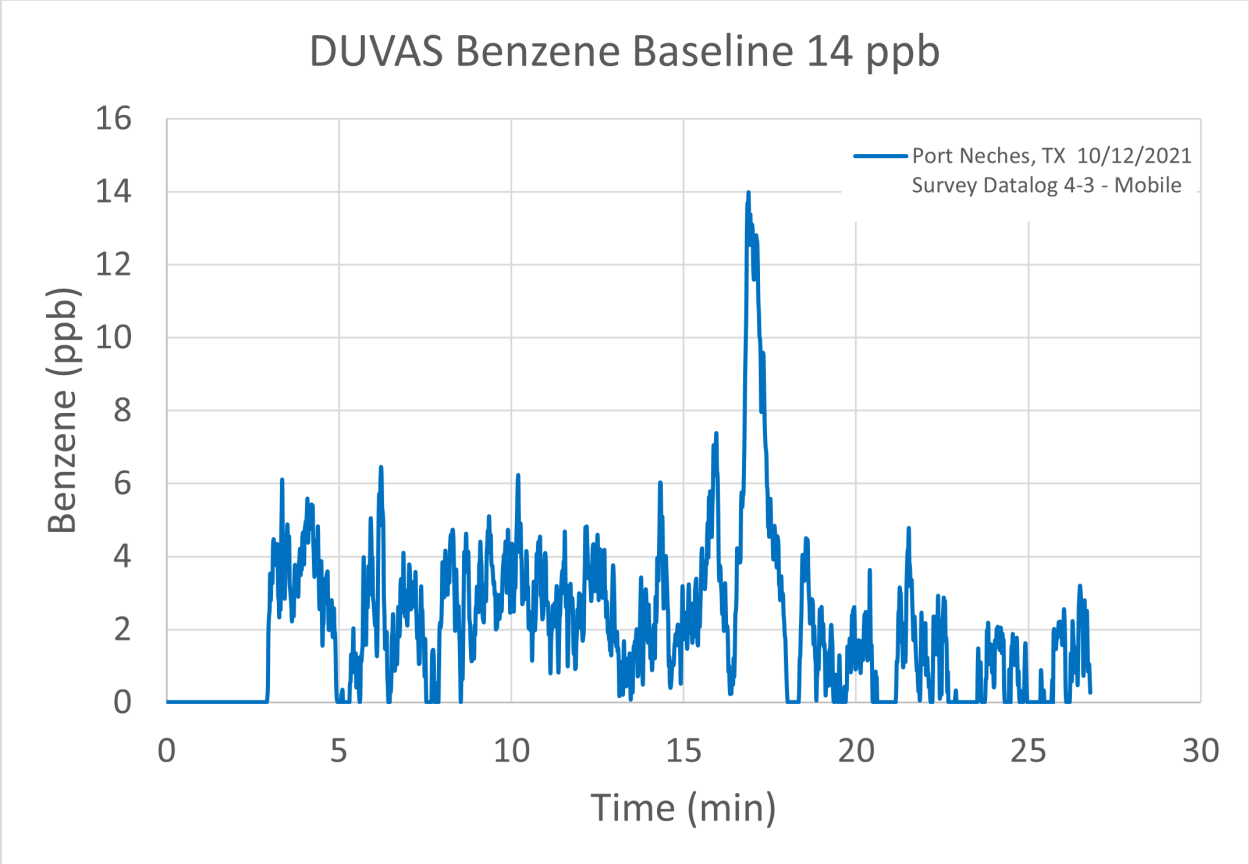
Ammonia

The baseline was not determined for ammonia due to the large variation observed among the baseline surveys, with many surveys reporting a concentration of zero for most if not all of the survey.

Benzene

Of the 198 DUVAS surveys that measured benzene and reported one-second data, a total of 23 surveys were selected and evaluated to determine the benzene baseline level. The survey with the maximum non-signal baseline noise was survey Datalog 4-3 from October 12, 2021, in Port Neches, TX (Region 10), shown below (Figure B - 14). The maximum noise from the survey was 13.98 ppb, which was rounded to 14 ppb to generate the baseline level for benzene. The baseline level for benzene is similar between the SIFT and the DUVAS. Because using the SIFT baseline level for benzene generates a lower iBDIL and so triggers a source investigation at a lower chemical concentration, the SIFT baseline was used to set the benzene iBDIL at 80 ppb.

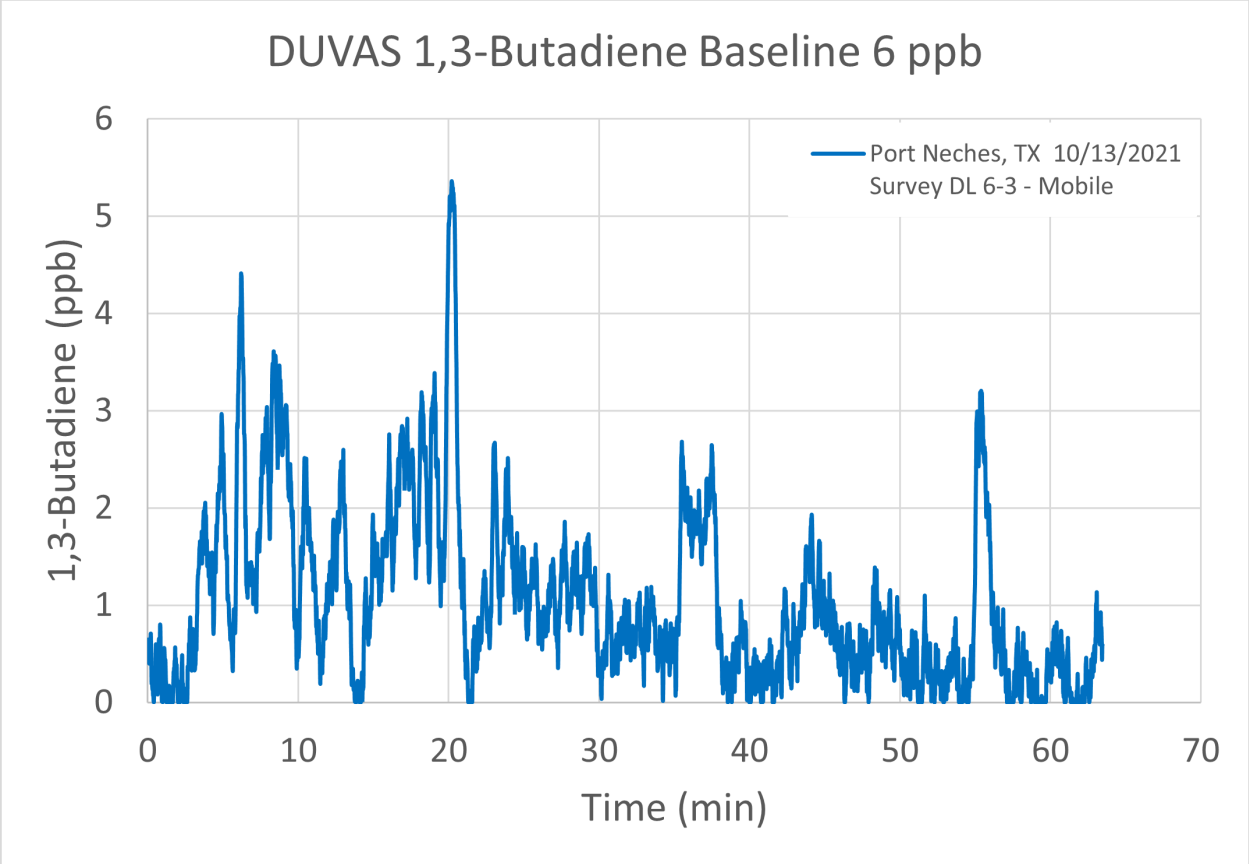
Figure B - 14. Time-concentration graph of benzene collected during a DUVAS instrument survey that was selected as the benzene maximum non-signal baseline level.



1,3-Butadiene

Of the 190 DUVAS surveys that measured 1,3-butadiene and reported one-second data, a total of 24 surveys were selected and evaluated to determine the 1,3-butadiene baseline level. The survey with the maximum non-signal baseline noise was survey Datalog 6-3 from October 13, 2021, in Port Neches, TX (Region 10), shown below (Figure B - 15). The maximum noise from the survey was 5.36 ppb, which was rounded to 6 ppb to generate the baseline level for 1,3-butadiene. The baseline level for 1,3-butadiene is similar between the SIFT and the DUVAS. Because using the SIFT baseline level for 1,3-butadiene generates a lower iBDIL and so triggers a source investigation at a lower chemical concentration, the SIFT baseline was used to set the 1,3-butadiene iBDIL at 40 ppb.

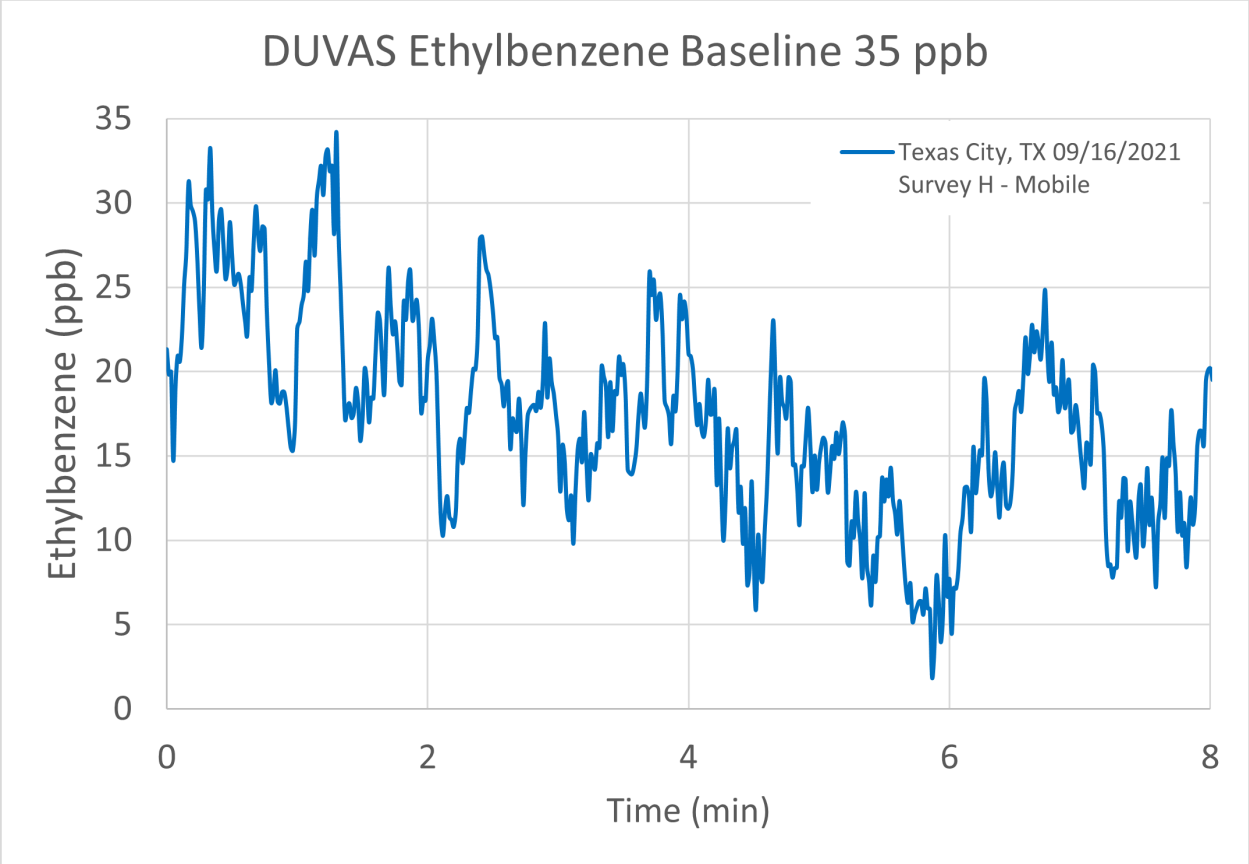
Figure B - 15. Time-concentration graph of 1,3-butadiene collected during a DUVAS instrument survey that was selected as the 1,3-butadiene maximum non-signal baseline level.



Ethylbenzene

Of the 198 DUVAS surveys that measured ethylbenzene and reported one-second data, a total of 42 surveys were selected and evaluated to determine the ethylbenzene baseline level. The survey with the maximum non-signal baseline noise was survey H from September 16, 2021, in Texas City, TX (Region 12), shown below (Figure B - 16). The maximum noise from the survey was 34.21 ppb, which was rounded to 35 ppb to generate the baseline level for ethylbenzene. The iBDIL for ethylbenzene was calculated as 10-times the baseline level and therefore the ethylbenzene iBDIL was set at 350 ppb.

Figure B - 16. Time-concentration graph of ethylbenzene collected during a DUVAS instrument survey that was selected as the ethylbenzene maximum non-signal baseline level.



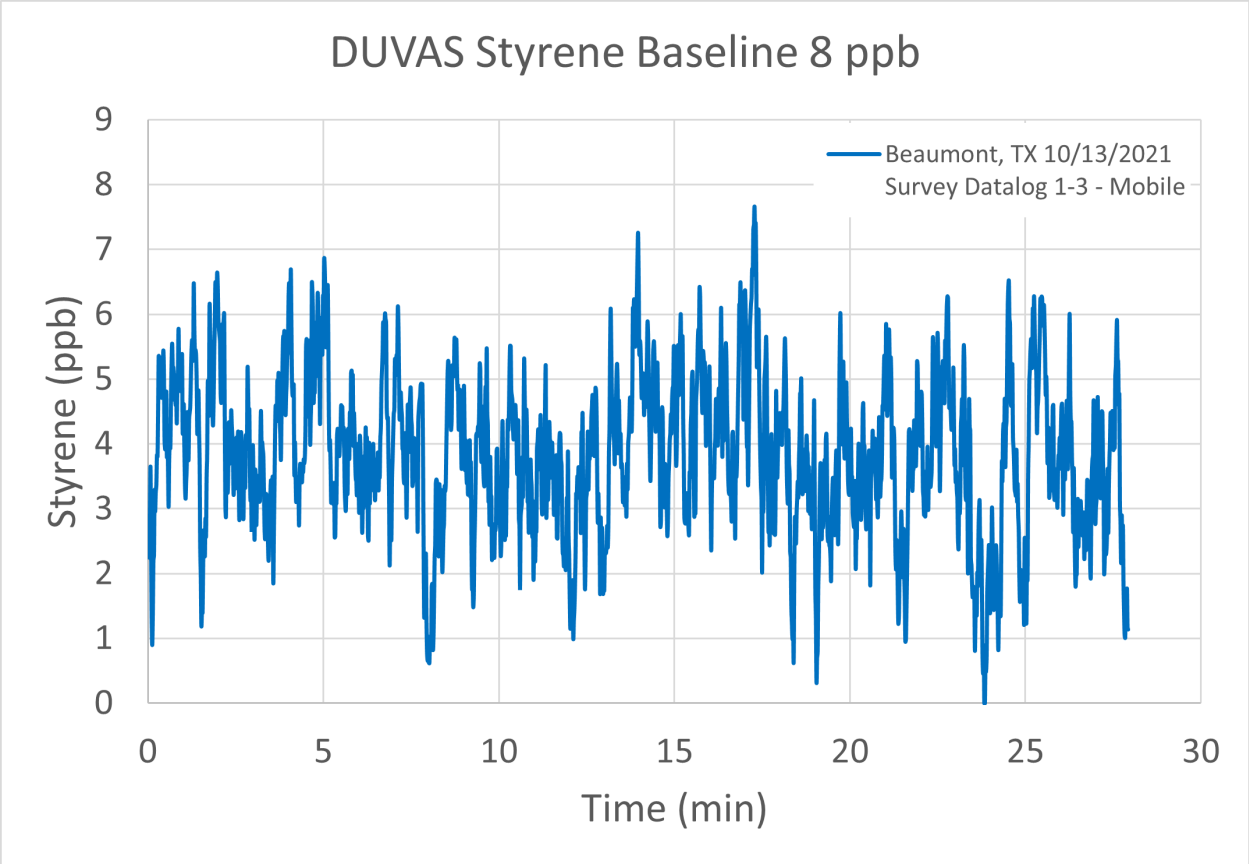
Formaldehyde

The baseline was not determined for formaldehyde due to the large variation observed among the baseline surveys, with many surveys reporting a concentration of zero for most if not all of the survey.

Styrene

Of the 190 DUVAS surveys that measured styrene and reported one-second data, a total of 22 surveys were selected and evaluated to determine the styrene baseline level. The survey with the maximum non-signal baseline noise was survey Datalog 1-3 from October 13, 2021, in Beaumont, TX (Region 10), shown below (Figure B - 17). The maximum noise from the survey was 7.66 ppb, which was rounded to 8 ppb to generate the baseline level for styrene. The baseline level for styrene is similar between the SIFT and the DUVAS. Because using the SIFT baseline level for styrene generates a lower iBDIL and so triggers a source investigation at a lower chemical concentration, the SIFT baseline was used to set the styrene iBDIL at 60 ppb.

Figure B - 17. Time-concentration graph of styrene collected during a DUVAS instrument survey that was selected as the styrene maximum non-signal baseline level.

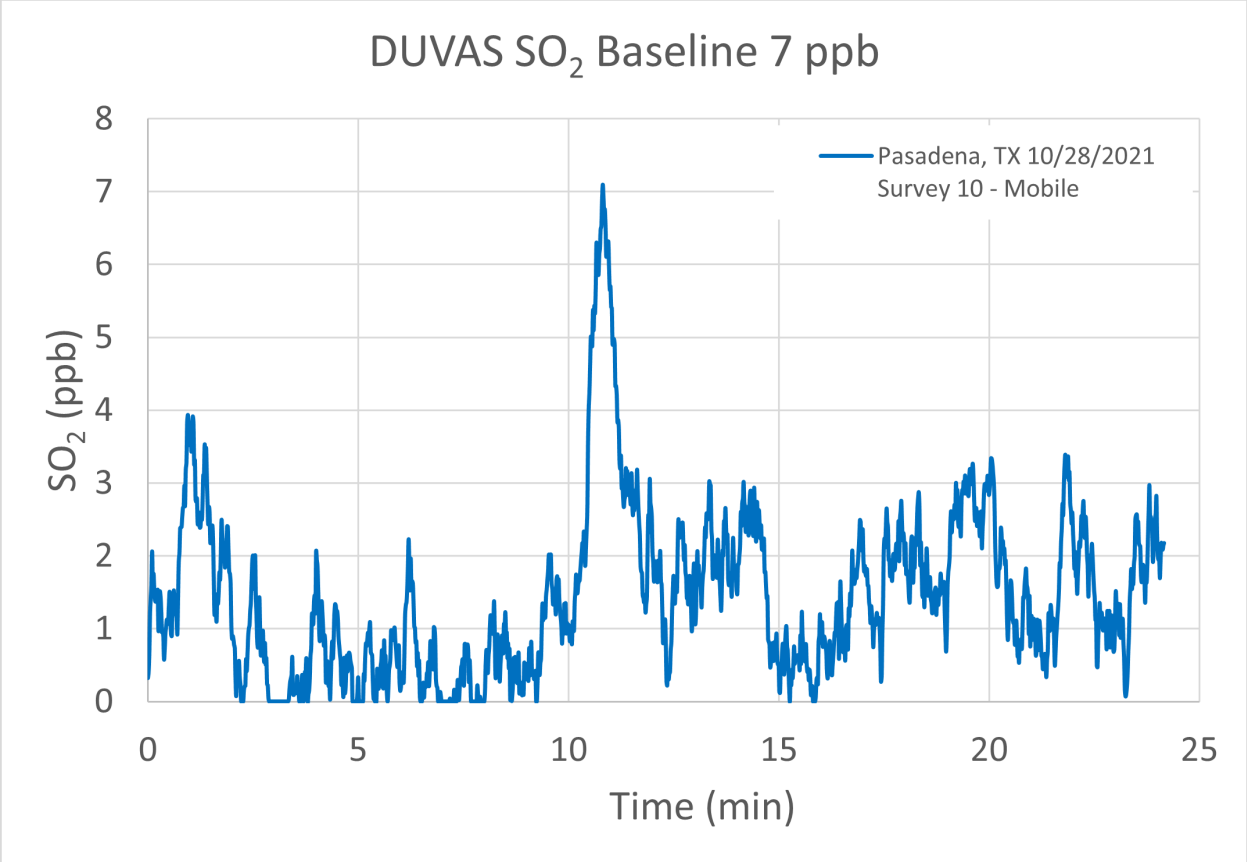


Sulfur dioxide

Of the 167 DUVAS surveys that measured sulfur dioxide (SO_2) and reported one-second data, a total of 23 surveys were selected and evaluated to determine the sulfur dioxide baseline level. The survey with the maximum non-signal baseline noise was survey 10 from October 28, 2021, in Pasadena, TX (Region 12), shown below (Figure B - 18). The maximum noise from the survey was 7.09 ppb, which was rounded down to 7 ppb to generate the baseline level for sulfur dioxide. The iBDIL for sulfur dioxide[3] was calculated as 10-times the baseline level and therefore the sulfur dioxide iBDIL was set at 70 ppb.

[3] Because the maximum non-signal baseline for sulfur dioxide was < 0.1 ppb higher than 7 ppb, the decision was made to round the baseline level down to 7 ppb.

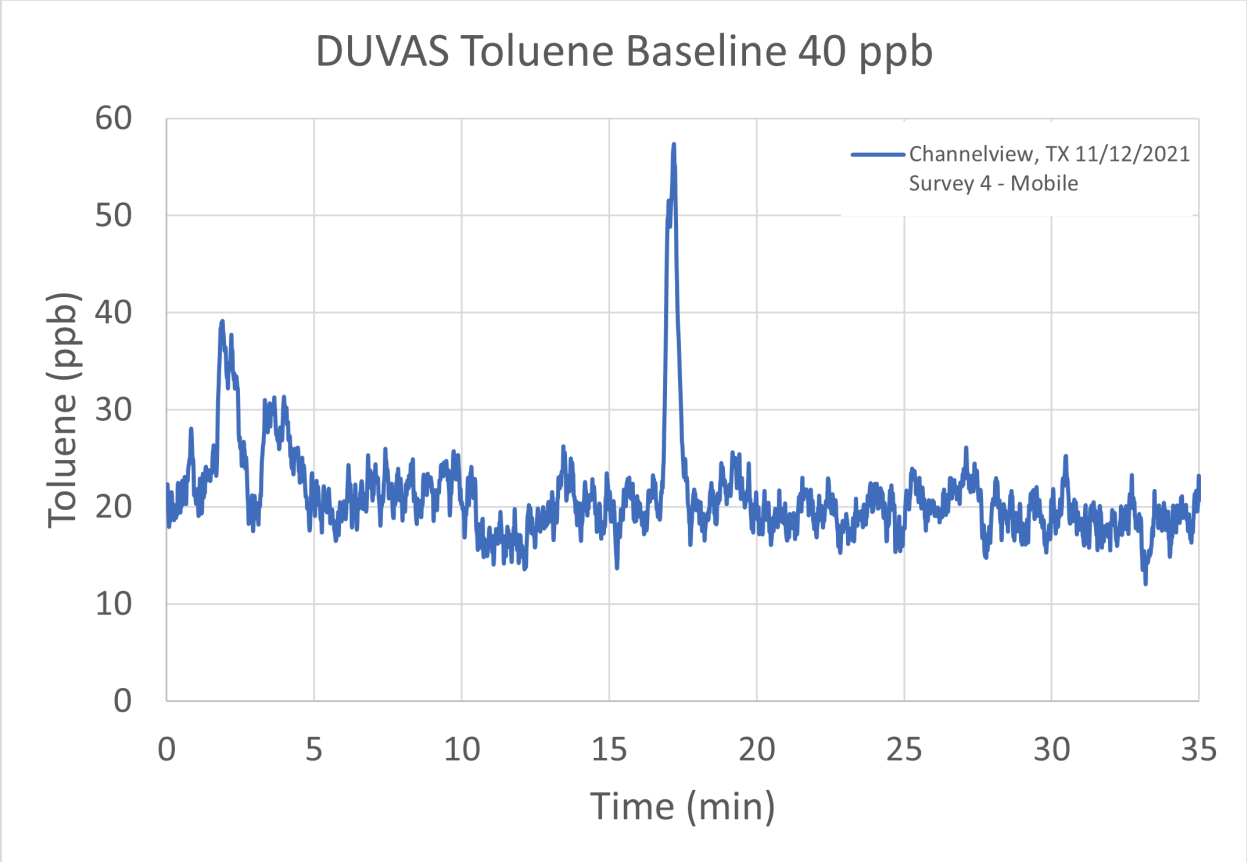
Figure B - 18. Time-concentration graph of sulfur dioxide collected during a DUVAS instrument survey that was selected as the sulfur dioxide maximum non-signal baseline level.



Toluene

Of the 190 DUVAS surveys that measured toluene and reported one-second data, a total of 54 surveys were selected and evaluated to determine the toluene baseline level. The survey with the maximum non-signal baseline noise was survey 4 from November 12, 2021, in Channelview, TX (Region 12), shown below (Figure B - 19). The maximum noise from the survey was 39.15 ppb, which was rounded to 40 ppb to generate the baseline level for toluene. Because using the SIFT baseline level for toluene generates a lower iBDIL and so triggers a source investigation at a lower chemical concentration, the SIFT baseline was used to set the toluene iBDIL at 70 ppb.

Figure B - 19. Time-concentration graph of toluene collected during a DUVAS instrument survey that was selected as the toluene maximum non-signal baseline level.



Xylenes

The baseline was not determined for any of the three xylenes due to the large variation observed among the baseline surveys, with many surveys reporting a concentration of zero for most if not all of the survey.

Picarro Instrument Chemical Baseline Derivation

Hydrogen Sulfide

The Picarro instrument was utilized to conduct 97 mobile monitoring surveys (31 stationary, 66 mobile) between October 12, 2021, and October 13, 2022, in El Paso, West Odessa, Port Neches, and Nederland, Texas (TCEQ Regions 6, 7, 10, and 10, respectively). Twenty-seven surveys (6 stationary, 21 mobile) were analyzed for evaluation of baseline concentrations. The baseline concentrations were inconsistent and highly variable and ranged from 3.3 to 64 ppb; therefore, a straight-forward iBDIL (10-times the baseline concentration) cannot be determined. The selected AHBCV/iHPIL for hydrogen sulfide is 70 ppb, and this can be used as the value to trigger source investigation/characterization.

Nephelometer Instrument Baseline Derivation

Particular Matter 2.5 and 10 ($PM_{2.5}$ and PM_{10})

The Nephelometer instrument was utilized to conduct 40 surveys between November 2, 2022, and February 22, 2023, in the Houston area (TCEQ Region 12). $PM_{2.5}$ and PM_{10} data from 19 surveys were analyzed for evaluation of baseline concentrations. The baseline noise from the instruments was extremely low at an approximately 20 ng/m^3 level, while the concentrations of PM detected during the surveys were in the µg/m^3 range. Together, the baseline concentrations (noise plus background ambient concentrations) of PM varied greatly, from 5 to 40 µg/m^3 for $PM_{2.5}$ and from 10 to 100 µg/m^3 for PM_{10} over the course of a day, reflecting known ambient variability in PM concentrations within a day and from day to day. Because of this variability in daily PM concentrations, we concluded that the method for setting an iBDIL using constant chemical baseline cannot be applied to the nephelometer PM data; therefore, no iBDIL for $PM_{2.5}$ or PM_{10} was derived. Instead, the initial investigation level for $PM_{2.5}$ and PM_{10} will be set at the iHPIL as discussed in Section 3.3.