



SunCoke Energy

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August 19, 2021

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**RE: Consent Decree, *United States, et al. v. Indiana Harbor Coke Company, et al.*
Draft SOF Report**

To Whom It May Concern,

The United States, the State of Indiana, Indiana Harbor Coke Company (IHCC), SunCoke Energy, Inc. (SunCoke), and Cokenergy, LLC (Cokenergy) are parties to a Consent Decree (CD) lodged in federal court on January 25, 2018 with an Effective Date of October 25, 2018.

Pursuant to Paragraph 30.b of the CD, IHCC is submitting a draft report of Solar Occultation Flux testing conducted at the facility within 90 days of test completion. If you have any questions regarding this report, please contact me at 740-370-8710 or email me at kmbatten@suncoke.com.

Sincerely,

Katie Batten
Director of Health, Safety and Environmental
SunCoke Energy, Inc.

Solar Occultation Flux Testing at Indiana Harbor Coke Company

*Developed in accordance with Paragraph 30.a of Consent Decree, Case No.
2:18-cv-00035 (Oct. 25, 2018)*

Draft REPORT
19 August 2021



Date: 19 August 2021

Title: Solar Occultation Flux Testing at Indiana Harbor Coke Company

Developed in accordance with Paragraph 30.a of Consent Decree, Case No. 2:18-cv-00035 (Oct. 25, 2018).

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PO SC311104579, "Solar Occultation Flux Testing at Indiana Harbor Coke Company"
Prepared for SunCoke Energy

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EXECUTIVE SUMMARY

A VOC (volatile organic compounds) and sulfur dioxide (SO₂) emissions test was conducted at the Indiana Harbor Coke Company in May 2021. The test was done to satisfy the requirements of paragraph 30 of the Consent Decree among the United States, the State of Indiana, SunCoke Energy Inc., IHCC, and Cokenergy LLC entered in the U.S. District Court for the Northern District of Indiana on October 25, 2018 (Case No. 2:18-cv-00035).

The main objectives of the test were to measure overall emissions of VOCs (volatile organic compounds) and SO₂ (sulfur dioxide) from the plant and identify primary sources of the emissions.

Measurements were conducted over the period 10-21 May 2021 for a total of 11 days. Weather was favorable for successful measurements and site operations ran smoothly during the survey period, with few upsets or other reported anomalies. On average 128 ovens were charged daily, with 5122 tons coal/day charged in total.

A total VOC emission rate of 5.5 kg/h was measured, of which 85% or 4.7 kg/h corresponded to alkanes (95% Confidence Interval (CI): 4.1 - 5.2 kg/h), and 15% of BTEX and alkenes, *Table ES 1*. The total site emissions of SO₂ were measured at 701 kg/h (95% CI: 663 - 738 kg/h).

Table ES 1. Summary of test results for emissions of SO₂, alkanes and total VOC measured at Indiana Harbor Coke Company, May 2021.

Area	SO ₂ kg/h	Alkanes kg/h	Total VOC kg/h
Process plant	701	4.7	5.5

The test involved measurements of fenceline emissions and characterization of emissions closer to potential sources (such as coke ovens, HRSGs, and flue gas treatment systems). It should be noted that the coking process is a batch process with operational variability and does not operate at steady state. Emissions measurements taken over a specific period are not necessarily representative of the levels of potential emissions over a longer period.

SOF (Solar Occultation Flux) was used to measure emissions of VOCs, combining measured slant vertical columns with wind speed and wind direction measurements. SkyDOAS (zenith-sky Differential Optical Absorption Spectroscopy) was used to measure vertical columns of SO₂. Wind speed and wind direction were obtained on a continuous basis by means of wind masts and a vertical wind profiler (LIDAR, light detection and ranging) with range 10-300 m (32 - 984') above ground.

Plume concentration ratios of benzene, BTEX (benzene, toluene, ethylbenzene and xylene) and ethene to alkanes were characterized both at the fenceline and closer to sources, for indirect emission assessment. Extractive (mobile) Fourier Transform InfraRed spectroscopy and ultraviolet DOAS were used for the concentration measurements of VOCs and SO₂, with supporting canister sample data.

Overlapping data sets between different instrumentations were compared as a consistency check. The Cokenergy plant was measured to have an average SO₂ emission of 670±177 kg/h, based on 64 observations over 9 days. This compares very well with the CEMS stack data, showing an average of 677 kg/h for the corresponding time window. SOF and SkyDOAS showed comparable results for total site SO₂ emissions, 676±137 kg/h and 701±161 kg/h, respectively.

MeDOAS and MeFTIR fenceline integrations showed a benzene to alkane average mass fraction of 4.1% ± 1.8%, whereas canister samples averaged a benzene to alkane mass fraction of 4.3%.

TABLE OF CONTENTS

EXECUTIVE SUMMARY	3
1 INTRODUCTION	5
1.1 Summary of test program	5
1.2 Key personnel	6
2 Source and sampling location descriptions	7
2.1 Process description	7
2.1.1 General Overview	7
2.1.2 Plant Description	7
2.1.3 Production Activity Description	9
2.2 Sampling locations	11
3 Summary and discussion of results	12
3.1 Test Matrix	12
3.2 Summary of results	14
3.2.1 VOC emissions measured by SOF	19
3.2.2 SO ₂ emissions measured by SkyDOAS and SOF	21
3.2.3 Plume characterization by extractive FTIR, DOAS and canister sampling	26
3.3 Process data	32
4 Sampling and analytical procedures	33
4.1 Emission test methods	33
4.2 Sample identification and custody	34
5 QA/QC activities	35
5.1 SOF	35
5.2 SkyDOAS	35
5.3 MeFTIR	36
5.4 MEDOAS	36
5.5 Wind LIDAR	37
5.6 Wind tower	37
5.7 Canisters	37
Appendices	38
A - Methods	38
B - Wind data	51
C - Canister data	68
D - Coal terminal measurements	73

1 INTRODUCTION

1.1 Summary of test program

This test program relates to an emissions test at Indiana Harbor Coke Company (IHCC) located at 3210 Watling Street, East Chicago, Indiana. Measurements were conducted by FluxSense Inc. (113 W G St #757, San Diego, CA 92101). Testing was conducted to satisfy the requirements of paragraph 30 of the Consent Decree among the United States, the State of Indiana, SunCoke Energy, Inc., IHCC, and Cokenergy LLC entered in the U.S. District Court for the Northern District of Indiana on October 25, 2018 (Case No. 2:18-cv-00035).

The main objectives of the test were to measure overall emissions of VOCs (volatile organic compounds) and SO₂ (sulfur dioxide) from the plant and identify primary sources of the emissions.

The IHCC plant produces coke from metallurgical coal in heat-recovery coke ovens. In the heat recovery process, VOCs evolved from the pyrolyzed coal are combusted to completion within a negative pressure system. Residual heat in the combusted flue gas is extracted by heat recovery steam generators (HRSGs). Flue gas sulfur dioxide is treated by a flue gas desulfurization (FGD) system.

The test involved measurements of fenceline emissions and characterization of emissions closer to potential sources (such as coke ovens, HRSGs, and flue gas treatment systems).

SOF (Solar Occultation Flux) was used to measure emissions of VOCs, combining measured slant vertical columns with wind speed and wind direction measurements.

SkyDOAS (zenith-sky Differential Optical Absorption Spectroscopy) was used to measure vertical columns of SO₂ combined with wind speed and wind direction measurements.

Concentration ratios of benzene and BTEX (benzene, toluene, ethylbenzene and xylene) to alkanes and SO₂ were characterized both at the fenceline and closer to sources, for indirect emission assessment. Mobile and stationary extractive Fourier Transform InfraRed spectroscopy (MeFTIR) and ultraviolet DOAS (Mobile Whitecell DOAS) were used for the concentration measurements of VOCs and SO₂, with supporting canister sample data in particular locations.

Wind speed and wind direction were measured at multiple locations by means of wind masts and a moveable vertical wind profiler (LIDAR, light detection and ranging) on a continuous basis.

The test was conducted during the period 10 May – 21 May 2021.

1.2 Key personnel

SunCoke project coordinator and manager:

Dr. Jonathan Perkins, M: (610) 858-7706, jhperkins@suncoke.com

IHCC site coordinator:

Nancy Estrada, M: (219) 895-5976, nestrada@suncoke.com

IHCC site safety coordinators:

Elizabeth Moore, M: (270) 556-5268, ewmoore@suncoke.com

Anthony Rivera, M: (219) 378-3924, arivera@suncoke.com

FluxSense Inc. project coordinator:

Marianne Ericsson, M: (775) 830-5272, marianne.ericsson@fluxsense.com

FluxSense Inc. test director:

Jerker Samuelsson, M: +46-70-3099669, jerker.samuelsson@fluxsense.com

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FluxSense Inc. test crew:

Brian Offerle (as above)

Anthony Babore, M: (619) 806-4644, anthony.babore@fluxsense.com

2 Source and sampling location descriptions

2.1 Process description

2.1.1 General Overview

IHCC operates an advanced heat-recovery process to transform metallurgical coal into coke. In the process, coal is charged into a high temperature oven. A portion of the coal pyrolyzes and produces volatile matter (VM). The remaining fixed carbon polymerizes into coke. The VM is combusted within the oven to provide the heat to continue the coking process. The combusted flue gas is directed through heat recovery steam generators (HRSGs) where the residual heat is extracted and steam is produced. The steam can be used to generate electricity supplied to the steel plant. The cooled flue gas is scrubbed in a flue gas desulfurization (FGD) system and exhausted. The finished coke is pushed from the oven, quenched with water, screened to remove fine material and delivered to the customer.

2.1.2 Plant Description

As shown in Figure 1, the IHCC plant is arranged in four batteries (A, B, C, & D) of 67 ovens each. There are two quench towers (one shared by batteries A&B and one shared by batteries C&D). Each battery has four HRSGs and emergency vent stacks. The HRSGs are owned and operated by Cokenergy. The combusted and cooled flue gas is directed to the FGD system in the Cokenergy facility comprised of a spray dry absorber (SDA), baghouse and main stack. There are two parallel induced draft fans at the base of the main stack that draw the flue gas through the entire system.

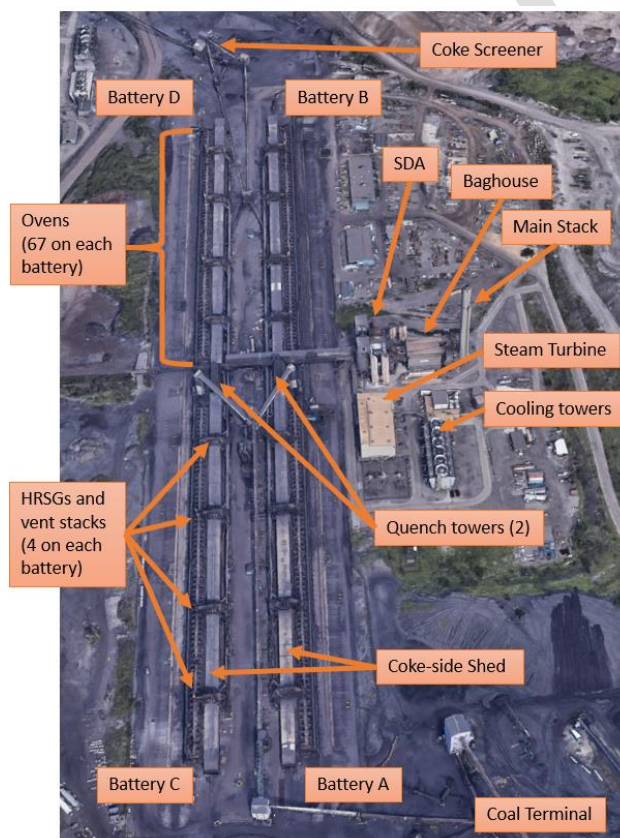


Figure 1. Plant overview.

For the purposes of an atmospheric plume detection trial, it is important to determine the approximate heights of various structures and potential sources. These heights and locations are described in Table 1 and Figure 2.

Table 1. Approximate height of main plant installations.

Site part	Approximate height above ground (feet)
Main stack	300'
Top of the SDA penthouse	150'
Bypass vent stacks	81'
Top of the common flue gas tunnel	29'
Top of the ovens	15'
Top of HRSG	55'
Quench tower	60'
Shed	42'
STG building and cooling towers	60'
Coal surge bin	118'

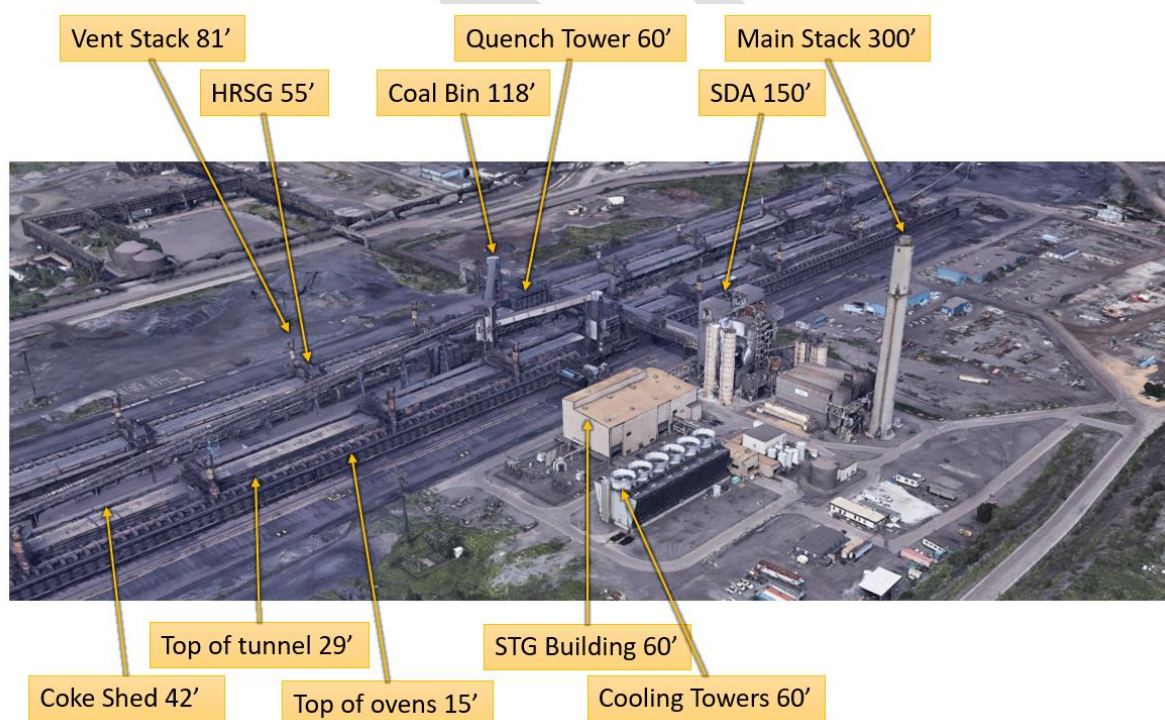


Figure 2. Approximate heights of main buildings and installations.

2.1.3 Production Activity Description

Figure 3 illustrates the generic process for heat-recovery coke making.

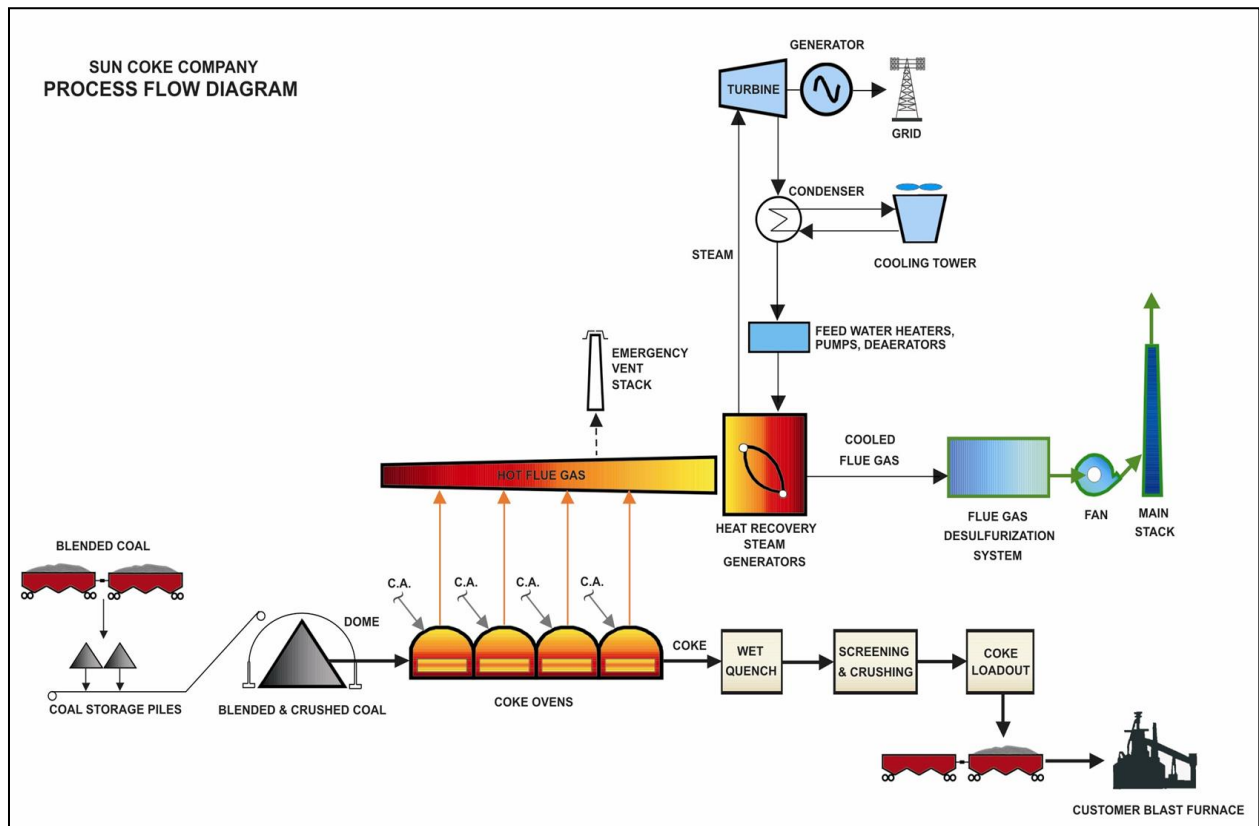


Figure 3. Heat Recovery Coke Making Process Flow Diagram.

In the normal production process at IHCC, crushed and blended coal is brought into the plant from the terminal via conveyor belt and temporarily stored in two coal bins. During the typical daily production cycle (typically 2:30PM to 6:00AM), 134 ovens (half of the plant) are pushed and charged. The timing of the pushing of individual ovens is determined by when they are deemed fully coked (ready to push) in accordance with regulatory requirements.

To push an oven, the Pusher-Charger-Machine (PCM) removes the oven door on the push side of the battery and aligns the pusher ram with the oven. On the coke side, the door machine removes the oven door and aligns the coke chute. The hot car is positioned under the coke chute. The PCM then rams the coke through the oven into the hot car. The hot car then trams to the quench tower. The distance from the quench tower to the furthest oven is 1,100 ft. The hot car tramping to the quench tower is done within a coke shed enclosure that has a dust removal system. In the quench tower, the coke is drenched in water to cool the coke down to a safe level. The quench process takes about 90 seconds. The hot car then dumps the coke onto the wharf. The coke is then metered onto the coke conveyor belt. The belt transports the coke to the screening deck where the small coke (breeze) is removed. The final product coke (known as furnace coke) is then transported by conveyor belt to the adjacent customer facility.

After the coke is pushed out, fresh coal is charged into the empty oven. On the coke side, the door machine replaces the door. On the push side, the PCM removes the ram and then aligns the leveling conveyor. A specific amount (typically 35-42 tons) of coal is then transferred by conveyor belt from the coal bins to the PCM. The PCM then loads the coal charge into the oven via the leveling conveyor through the push side opening. The PCM then replaces the door. The pushing/charging process takes approximately 10 minutes to complete.

The coal in the oven carbonizes to coke over a period of approximately 48 hours. Each day, half the ovens in the plant are pushed and charged. To even out the mass flow in the flue gas system, the oven pushes are spread out over the time of the production shift, spread out over the batteries and spread out over the ovens under individual HRSGs. Both sides of the plant (A&B batteries and C&D batteries) operate at the same time. Thus, potential fugitive emission sources from the pushing/charging process are typically distributed over approximately 17 hours and the length of the plant (2,300 ft).

In the oven, the pyrolyzing coal releases volatile matter (VM). Air is drawn into the oven which then combusts the VM in the crown space above the bed and in the flue below the bed, as illustrated in Figure 4.

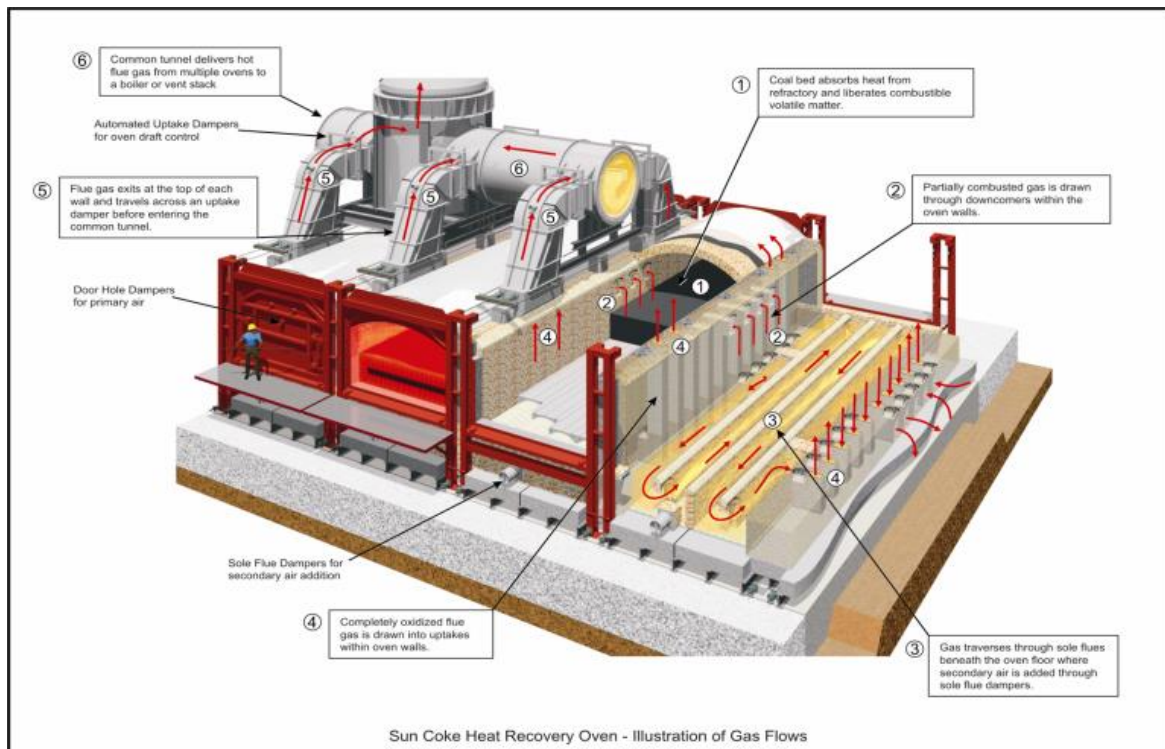


Figure 4. Heat Recovery Coke Oven Detail.

Heat recovery ovens are designed to operate under negative pressure during the coking cycle to minimize fugitive emissions compared with ovens at byproduct coke plants that operate under positive pressure. The VM is combusted completely, resulting in comparatively low VOCs. The flue gas generated by the coking process is ducted into a common tunnel which is designed to act as an afterburner. The common tunnel carries the flue gas to the heat recovery steam generators (HRSGs), which produce steam for use in the process or generating electricity.

After passing through the HRSGs, the flue gases are cleaned and filtered by a flue gas desulfurization (FGD) unit before being exhausted through the main stack by an induced draft fan. The induced draft fan creates the negative pressure throughout the system all the way back to the ovens. The FGD consists of a spray dry absorber (SDA) that contacts lime slurry ($\text{Ca}(\text{OH})_2$) with the flue gas and a baghouse for collection of particulate matter (CaSO_4 particles).

Each HRSG is matched with an emergency vent stack. During normal facility operations, the vent stack lids remain closed. In the event of a process upset or HRSG outage that inhibits oven exhaust transport to the FGD and the main stack, the vent stack lid will open to allow the combusted flue gas from the associated ovens to exhaust to the atmosphere through the vent stack while maintaining negative pressure in the system.

2.2 Sampling locations

Measurements were conducted both in mobile mode, where the mobile lab was driven alongside near the facility installations and further away at the fenceline, and in a stationary mode where detailed concentration screening was conducted near the potential sources.

Figure 3 displays main routes for the mobile measurements. The mobile measurements were conducted both upwind and downwind of the facility in order to observe if there were any incoming emissions from neighboring sites to be considered.

The close-by measurement route no. 1 was driven slowly in order to obtain good spatial resolution in the continuous measurements, and hence gain knowledge of specific areas of emissions. This also applies for the intermediate route no. 3 in between the oven batteries.

The fenceline route no. 2 was used to screen the overall site emissions as well as to attempt to identify any interfering emissions from neighboring sites.

As expected, the prevailing wind direction was from the lakeside (N-SE) sector. During periods of northwest-southwest winds, background emissions from nearby steelworks or refineries were screened for.

The wind was monitored by a moveable vertical wind profiler (LIDAR) that was placed near the location of the measurements. The wind LIDAR monitored the wind in the 10 m – 300 m vertical range. The LIDAR was complemented by a stationary wind mast (10 m height). The mobile lab was also equipped with a wind meter mounted on the roof, although only for plume interpretation purposes in real-time.

Sampling was also conducted by the main stack at the Cokenergy facility, both by vertical column measurements using SOF and SkyDOAS, and by concentration sampling utilizing the CEMS line at the main stack.

Concentration measurements for screening and concentration ratios were done both from the mobile lab platform on routes 1-4, and for stationary extractive sampling assisted by having the inlet tubing attached to a sky-lift. An operator controlled the sky-lift to position the extractive tubing at specific sampling positions. This sampling procedure was used to obtain concentration ratios of BTEX and benzene versus other VOCs as measured by DOAS and FTIR in the cross section of different plumes.



Figure 3. Overview of the site and approximate measurement routes.

3 Summary and discussion of results

The test matrix is described in section 3.1. The field test results are given in section 3.2.

3.1 Test Matrix

Table 2. Test matrix of main measurement targets. (Planned) / Actual

Sampling location	No. of days	No. of runs	Pollutant / entity	Sample type	Sampling Method	Analytical method
Fenceline, overall site, route 1&2 ^{a)}	(5+) / 8	(25+) / 43	VOCs	Vertical columns	SOF	FTIR
Fenceline, overall site, route 1&2 ^{a)}	(5+) / 10	(25+) / 74	SO ₂	Vertical columns	SkyDOAS	DOAS
Fenceline, overall site, route 1&2 ^{a)}	(5+) / 8	(25+) / 41	VOCs, SO ₂ , BTEX, Benzene	Concentration	MeFTIR, MeDOAS	FTIR, DOAS
Fenceline, overall site, route 1&2 ^{a)}	(2) / 2	(10) / 11	VOCs ^{b)}	Concentration	Canisters	GC-FID, external lab
Main stack	(2+) / 6	(10+) / 18	VOCs	Vertical columns	SOF	FTIR
Main stack	(2+) / 9	(10+) / 64	SO ₂	Vertical columns	SkyDOAS	DOAS
Main stack, CEMS line	(2) / 2	(2+) / 2	VOCs, SO ₂ , BTEX, Benzene	Concentration	MeFTIR, MeDOAS	FTIR, DOAS
Main stack, CEMS line	(1) / 1	(4) / 4	VOCs ^{b)}	Concentration	Canister samples	GC-FID, external lab
Coke ovens, close-by screening along route 1&3 ^{a)} . Detailed screening min. 4 ovens per battery.	(2) / 2	(16) / 16	VOCs, SO ₂ , BTEX, Benzene	Concentration	MeFTIR, MeDOAS	FTIR, DOAS
Coke conveyance, close-by screening along route 1&3 ^{a)}	(1) / 1	(2) / 2	VOCs, SO ₂ , BTEX, Benzene	Concentration	MeFTIR, MeDOAS	FTIR, DOAS
Vent stacks, Detailed screening min. 1 vents per battery.	(1) / 1	(4) / 4	VOCs, SO ₂ , BTEX, Benzene	Concentration	MeFTIR, MeDOAS	FTIR, DOAS
Quench towers, Detailed screening	(1) / 2	(2) / 2	VOCs, SO ₂ , BTEX, Benzene	Concentration	MeFTIR, MeDOAS	FTIR, DOAS
HRSBs, min. 1 per battery, Detailed screening	(1) / 2	(4) / 4	VOCs, SO ₂ , BTEX, Benzene	Concentration	MeFTIR, MeDOAS	FTIR, DOAS
Charging/Pushing unit, detailed screening	(2) / 2	(5+) / 8	VOCs, SO ₂ , BTEX, Benzene	Concentration	MeFTIR, MeDOAS	FTIR, DOAS

Charging/Pushing unit, detailed screening	(1) / 1	(4) / 4	VOCs ^{b)}	Concentration	Canister samples	GC-FID, external lab
All site	All days	All runs	Wind field	Wind speed and wind direction	Wind LIDAR and tower monitor	Wind induced doppler shift, rotational RPM and direction

a) See Figure 3.

b) Canister samples were collected in parallel to the extractive FTIR and DOAS instruments (at the inlet of the optical cells) for QA-QC purposes. Sampling was done using Silonite-coated evacuated canisters. The samples were analyzed for C₂-C₉ alkanes and C₆-C₉ aromatic compounds and C₂-C₄ olefins.

3.2 Summary of results

Measurements were conducted for 11 days during the period of 10-21 May. Weather was generally favorable for SOF and SkyDOAS measurements, especially during the first week of testing, with clear skies and northeasterly winds bringing in cleaner homogenous background air to the site from the lakeside.

A total VOC emission rate of 5.5 kg/h was measured, of which 85% or 4.7 kg/h corresponded to alkanes (95% Confidence Interval (CI): 4.1 - 5.2 kg/h), and 15% of BTEX and alkenes, Table 3. The total site emissions of SO₂ were 701 kg/h (95% CI: 663 - 738 kg/h).

Table 3. Summary of test results for emissions of SO₂, alkanes and total VOC measured at Indiana Harbor Coke Company, May 2021.

Area	SO ₂ kg/h	Alkanes kg/h	Total VOC kg/h
Process plant	701	4.7	5.5

On average 128 ovens were charged daily, with 5122 tons coal/day charged in total, corresponding to 39.8 tons per oven. The sulfur content of the charged coal was on average 0.91% with a coal moisture of 8.1%. Production mode (charging/pushing) in general took place in the 2:30 PM - 6:00 AM window, with a few occasions stretching into the maintenance window outside of this time period.

It should be noted that the coking process is a batch process with operational variability and does not operate at steady state. Emissions measurements taken over a specific period are not necessarily representative of the levels of potential emissions over a longer period.

VOCs

Solar Occultation Flux (SOF) was used to directly measure the emissions of alkanes from the overall site. Plume characterization by mobile extractive FTIR and DOAS (MeFTIR, MeDOAS) and canister sampling was then combined with the SOF alkane emission results to derive a total VOC emission estimate including alkane, alkene and BTEX compounds.

A total VOC emission rate of 5.5 kg/h was measured, of which 85% or 4.7 kg/h corresponded to alkanes (95% Confidence Interval (CI): 4.1 - 5.2 kg/h), and 15% of BTEX and alkenes. The alkane emission rate is based on an average of the 43 individual SOF measurements that passed the QA/QC steps.

Alkene and BTEX to alkane mass fractions were established by MeFTIR, MeDOAS and canister samples, showing the core of the plume corresponding to alkanes, with smaller contributions from BTEX and olefins. Fenceline route samples showed an average mass composition of 85% alkanes, 9.3% BTEX and 5.7% alkenes from the process.

Figure 4 shows a typical SOF transect for alkane emissions on 12 May, 10:18-10:25 AM. Note that the column scale is very low compared to measured SO₂ columns here. For comparison, the SO₂ max column in a corresponding measurement of SO₂ in Figure 9 is 500 mg/m². When comparing column values, as well as concentrations, between different measurements one should also consider the impact of wind speed.

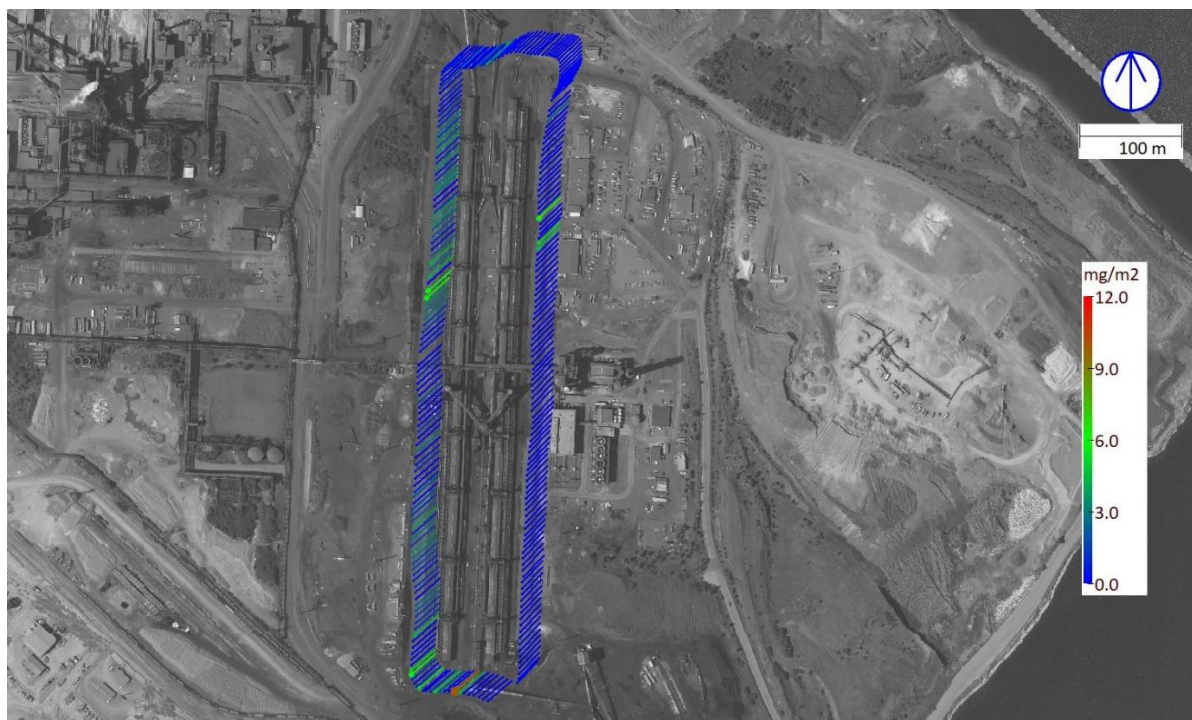


Figure 4. SOF measurement of alkanes from the process plant on 12 May, 2021, 10:15-10:25 AM. Wind was blowing from northeast at 4 m/s as indicated by the coloured lines (pointing up in wind). The alkane column is colour coded from background (blue) to 12 mg/m² shown on a linear scale. Map from Google Earth™, 2021.

Example ground level concentrations of benzene, toluene, p-xylene and alkanes are shown in Figure 5 through Figure 8. The corresponding plot for SO₂ is given in Figure 12.

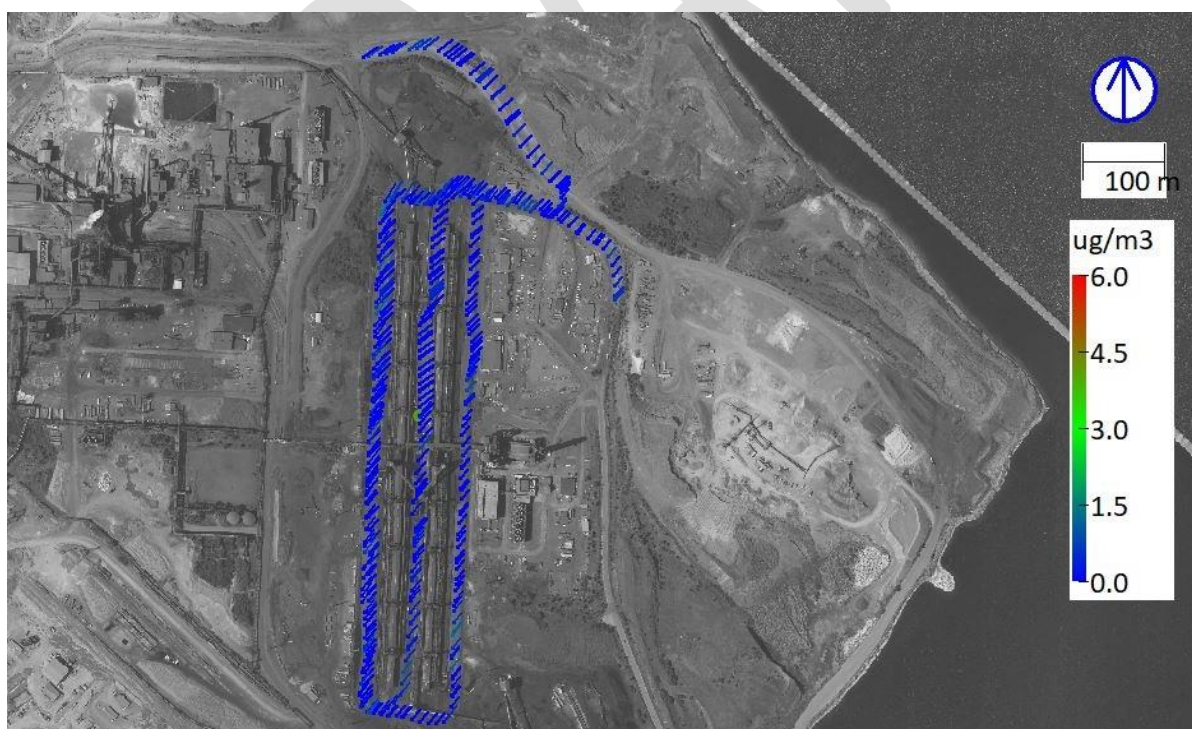


Figure 5. Example concentration mapping of benzene at ground level by mobile extractive DOAS (MeDOAS), 16 May 2021, 2:20-3:00 PM. Winds were 4.7 m/s from northeast as indicated by the coloured lines (pointing up in wind). The benzene concentration is colour-coded from background (blue) to 6 µg/m³. Map from Google Earth™, 2021.

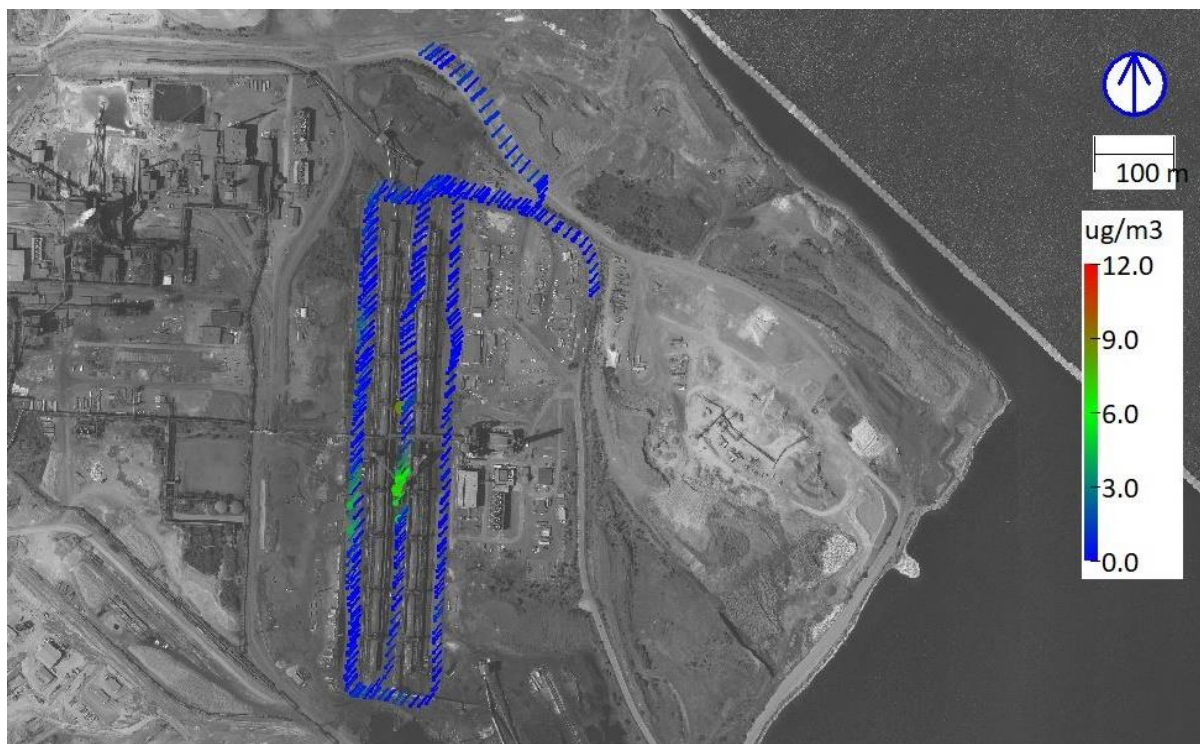


Figure 6. Example concentration mapping of toluene at ground level by mobile extractive DOAS (MeDOAS), 16 May 2021, 2:20-3:00 PM. Winds were 4.7 m/s from northeast as indicated by the coloured lines (pointing up in wind). The concentration is colour-coded from background (blue) to 12 $\mu\text{g}/\text{m}^3$. Map from Google Earth™, 2021.

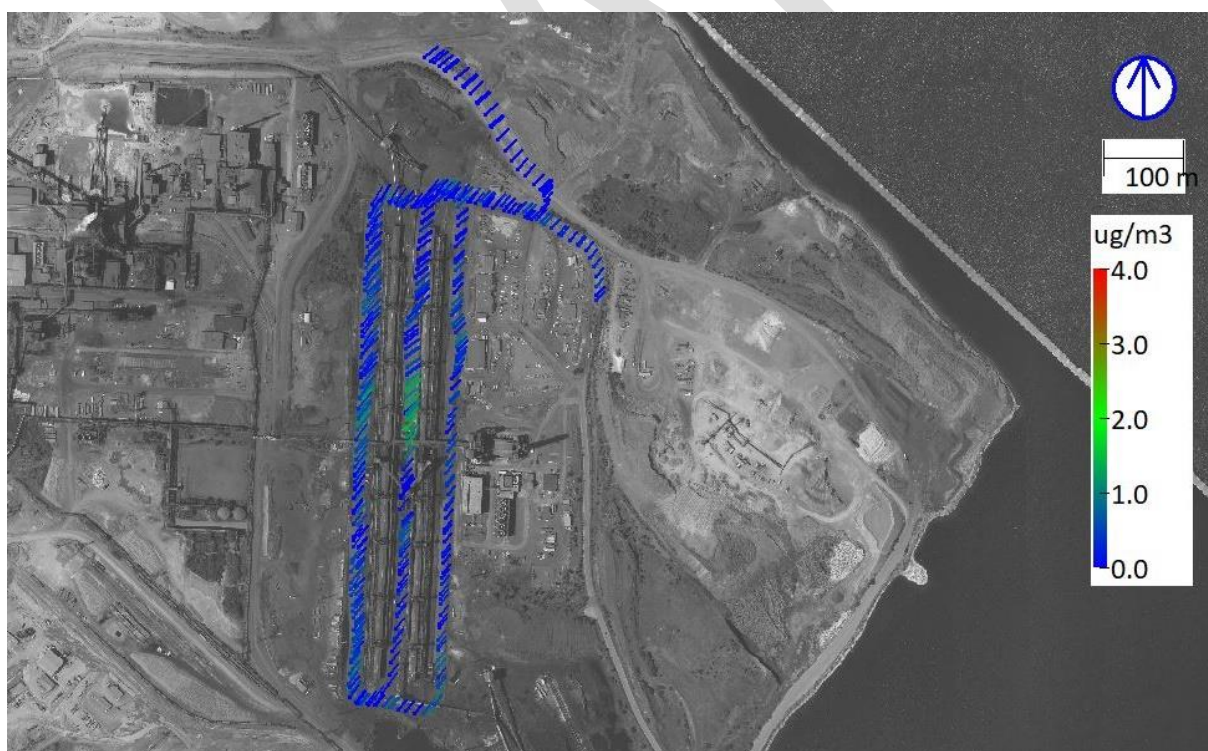


Figure 7. Example concentration mapping of p-xylene at ground level by mobile extractive DOAS (MeDOAS), 16 May 2021, 2:20-3:00 PM. Winds were 4.7 m/s from northeast as indicated by the coloured lines (pointing up in wind). The concentration is color-coded from background (blue) to 4 $\mu\text{g}/\text{m}^3$. Map from Google Earth™, 2021.

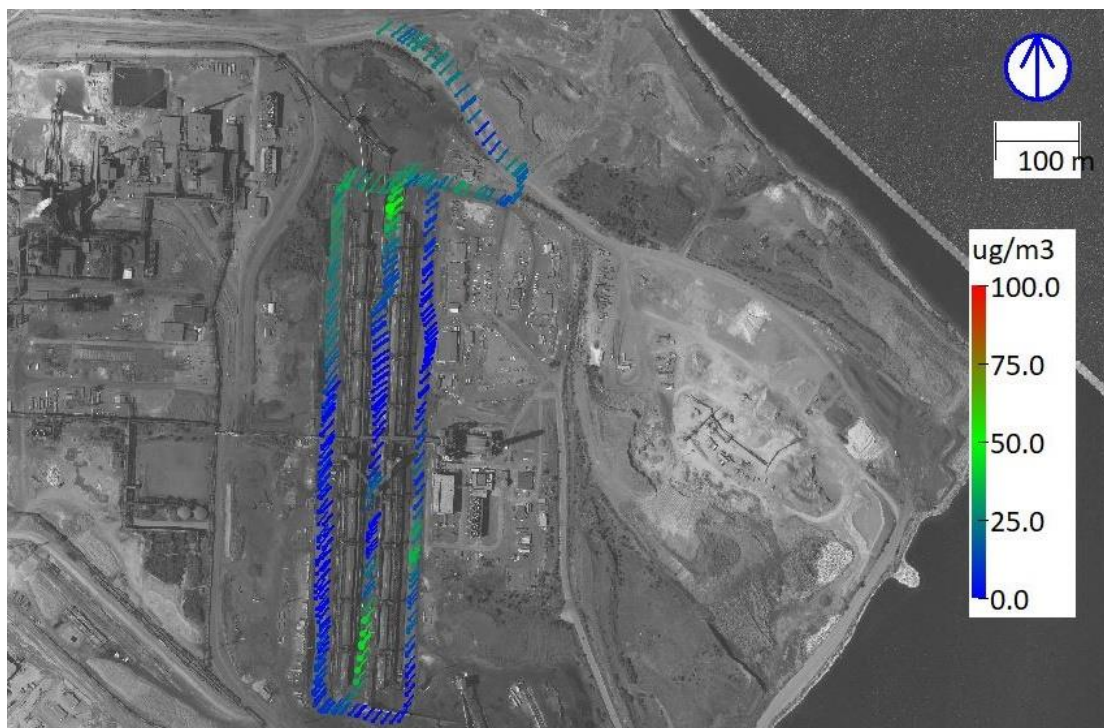


Figure 8. Example concentration mapping of alkanes at ground level by mobile extractive FTIR (MeFTIR), 16 May 2021, 2:20-3:00 PM. Winds were 4.7 m/s from northeast as indicated by the coloured lines (pointing up in wind). The concentration is color-coded from background (blue) to 100 $\mu\text{g}/\text{m}^3$. Map from Google Earth™, 2021.

SO₂

The overall process plant emission (IHCC + Cokenergy) of SO₂ was measured by SkyDOAS over 8 days, showing an average emission of 701 kg/h (95% CI: 663 - 738 kg/h). Figure 9 shows an example SO₂ measurement at the site from the 12 May, 2021.

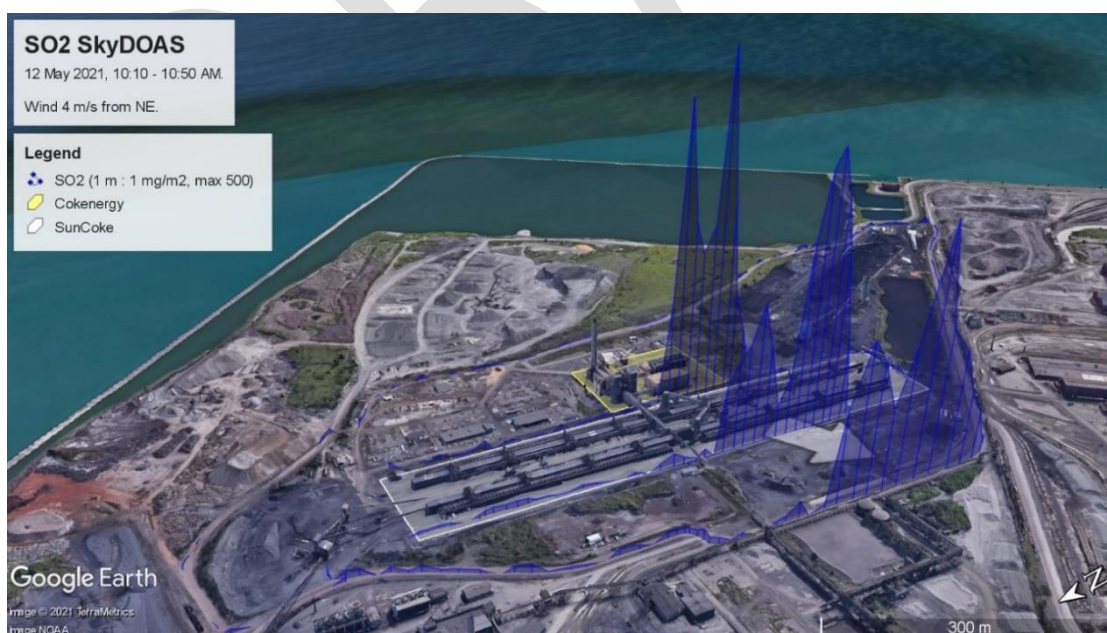


Figure 9. Example SkyDOAS measurement of SO₂ on 12 May, 10:10 - 10:50 AM, including a clean upwind transect, one run in between Cokenergy and IHCC and two downwind transects at different distances to the plant. Winds were 4 m/s from northeast. Map from Google Earth™, 2021.

As can be seen, there was no SO₂ flux from the upwind side, and the Cokenergy plant emission is the dominant source. The nearby Cokenergy plant transect has the highest columns, and the plume is then measured at two downwind distances, with subsequently lower column values as the plume is dispersed and broadened. Figure 10 shows another SO₂ measurement by SkyDOAS in colour-coded 2D-representation of the SO₂ columns (12 May 2021, 09:36-09:48 AM).



Figure 10. Example SkyDOAS SO₂ measurement 12 May 2021, 09:36-09:48 AM. Wind was blowing from northeast at 4.4 m/s as indicated by the coloured lines (pointing up in wind). The sulfur dioxide column is colour coded from background (blue) to 680 mg/m². Map from Google Earth™, 2021.

In order to better visualize the emissions contribution from oven batteries, Figure 11 focuses on the north half of the plant and shows the aggregate emissions from B and D batteries, including ovens, vent stacks and HRSGs.



Figure 11. Example SkyDOAS measurement of SO₂ on 12 May, 10:00 AM. Winds were 4 m/s from northeast. The picture view focuses on emissions from B and D batteries, reaching a maximum column of 58 mg/m², whereas the main stack plume (going through the roof of the view) reaches 748 mg/m². Map from Google Earth™, 2021.

Figure 12 shows an example ground level concentration mapping of SO₂ by MeDOAS measurements on 16 May 2021, 2:20-3:00 PM. The concentration pattern typically changes with production activities. Note concentrations close to background on the upwind side, and then the highest concentrations downwind the batteries. Concentrations get dispersed both by vertical plume lift and horizontal dispersion, as seen by lower concentrations on the furthestmost downwind transect.

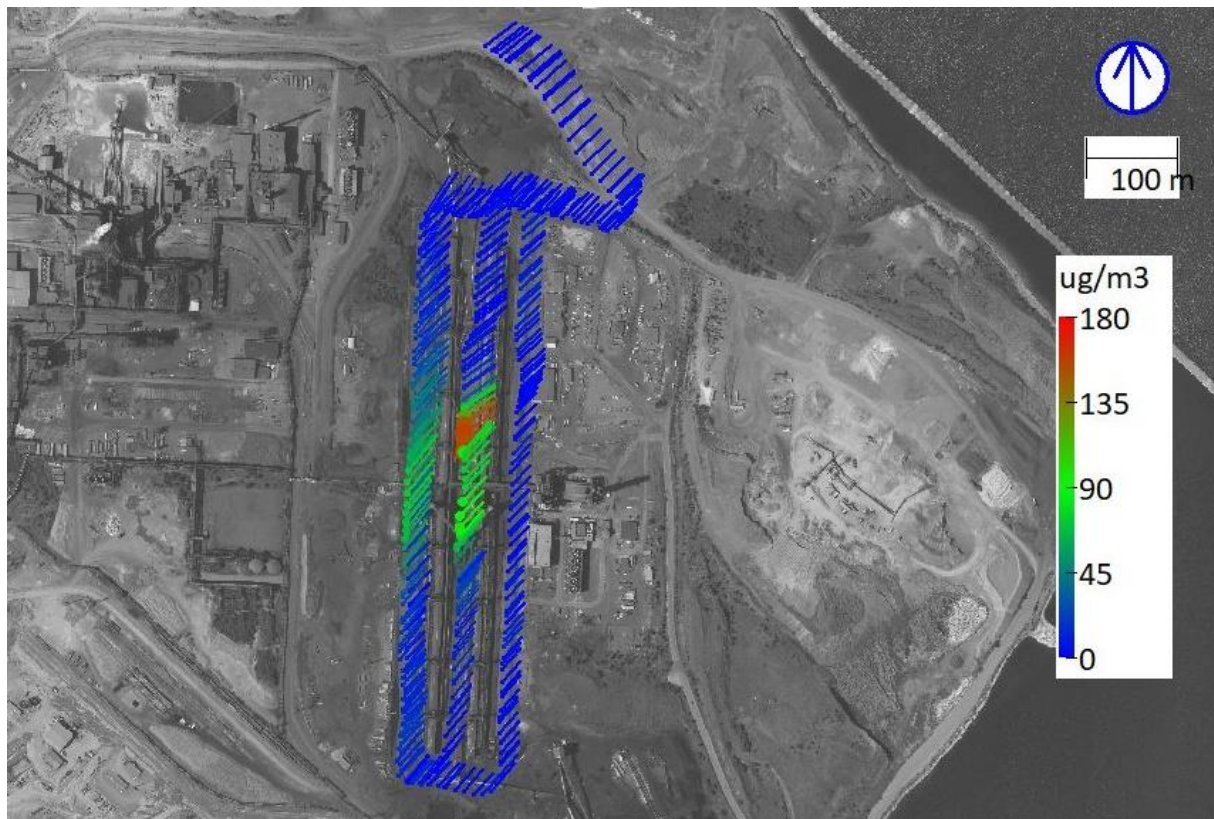


Figure 12. Example concentration mapping of SO₂ at ground level by mobile extractive DOAS (MeDOAS), 16 May 2021, 2:20-3:00 PM. Winds were 4.7 m/s from northeast as indicated by the coloured lines (pointing up in wind). The concentration is colour-coded from background (blue) to 180 µg/m³. Map from Google Earth™, 2021.

3.2.1 VOC emissions measured by SOF

Key findings by SOF VOC emission measurements are summarized in Table 4.

The overall process plant emission (IHCC + Cokenergy) was measured on six days and a total of 43 plume transects, spanning from 9:36 AM - 5:13 PM over the day. SOF measured a VOC (alkane) emission of 4.7 kg/h (95% CI: 4.1 - 5.2 kg/h).

Table 4. Overall process (IHCC + Cokenergy) VOC emissions (alkane) measured by SOF. (N.B. Method protocol requires averaging of multiple measurements).

Date	Start time	Stop time	Emission (kg/h)	Wind Speed (m/s)	Wind Dir (deg)
210510	131024	131458	1.37	7.2	38
210510	132913	133305	3.51	7.4	51
210510	142237	142601	3.66	8.4	20
210510	151116	151351	3.53	8.3	22
210510	162912	163147	5.64	7.6	11
210511	103241	103959	1.99	3.3	25
210511	111057	111555	6.99	3.7	18
210511	132515	132958	7.14	6.5	23
210511	134807	135215	5.43	6.1	31
210511	135335	135807	3.16	6	31
210511	140218	140816	5.53	6.8	30
210511	141106	141343	8.09	7.3	30
210511	141941	142256	3.17	8.1	27
210511	145549	150052	7.14	6.8	38
210511	154554	154914	8.61	7.5	29
210511	161011	161430	6.31	7.8	23
210511	162528	162904	7.8	7.9	21
210512	93635	94131	4.84	4.4	53
210512	94753	95139	4.48	4.3	48
210512	100929	101421	5.33	3.8	48
210512	102013	102434	3.42	3.9	50
210512	103511	103937	3.39	4.2	46
210512	105136	105322	5.39	3.8	51
210512	111010	111353	5.05	4.2	43
210512	112853	113334	3.37	4	42
210512	113833	114250	3.8	3.8	46
210512	135705	140316	4.36	3.5	21
210512	140439	140923	2.87	3.6	19
210512	141317	141821	4.46	3.5	18
210512	142947	143325	1.76	4.1	17
210512	154323	154723	6.2	4.4	25
210512	171520	172023	6.04	5	34
210513	124940	125259	3.65	2.7	90
210513	125847	130314	3.04	2.6	80
210513	130628	131001	2.18	2.7	85
210513	162608	163104	7.59	3.7	78
210513	164759	165158	5.04	3.5	81
210513	170859	171320	5.62	3.8	68
210514	113944	114418	3.64	3.1	33
210514	115002	115430	4.21	3.7	51
210514	135300	135659	3.51	4.7	58
210514	141152	141515	4.64	5.2	49
210516	114628	115146	4.2	2.8	42
Emission average 95% CI: 4.1-5.2 kg/h					

3.2.2 SO₂ emissions measured by SkyDOAS and SOF

SO₂ emissions measured by SkyDOAS

Key findings of SO₂ emissions measured by SkyDOAS are summarized in Table 5 and Table 6.

The overall process plant emission (IHCC + Cokenergy) was measured on 8 different days and a total of 74 plume transects, spanning from 9:20 AM - 6:00 PM in the day. SkyDOAS measured an average SO₂ emission of 701 kg/h (95% CI: 663 - 738 kg/h), Table 5.

The Cokenergy plant (main stack + baghouse and other operations) was measured to have an average SO₂ emission of 669 kg/h (95% CI: 625 - 714 kg/h), based on 64 observations on 9 days, Table 6. This compares very well with the CEMS data, averaging 677 kg/h for the corresponding time window.

Table 5. Process (IHCC + Cokenergy) SO₂ emissions measured by SkyDOAS. (N.B. Method protocol requires averaging of multiple measurements).

Date	Start time	Stop time	Emission (kg/h)	Wind Speed (m/s)	Wind Dir (deg)
210510	142233	142618	787.1	8.4	20
210510	145022	145552	589.1	8.9	20
210510	151059	151547	785.1	8.3	23
210510	163302	163608	1217.8	8	15
210510	162855	163150	731.1	8.3	16
210510	164051	164357	888.9	7.7	14
210510	164427	164733	918.0	8.1	17
210510	172926	173718	753.0	7.4	21
210510	175444	180004	941.8	7.6	14
210511	111150	111832	619.5	3.7	18
210511	112338	112814	614.6	3.6	17
210511	134609	135139	716.2	6.1	30
210511	141834	142209	763.6	8	27
210511	135251	140031	756.1	6.1	31
210511	140316	140826	685.4	6.8	30
210511	141106	141634	728.6	7.4	30
210511	145718	150150	879.9	6.7	38
210511	150410	150903	647.7	6.4	38
210511	151131	151746	665.2	6	34
210511	151948	152505	718.4	6.5	37
210511	153514	153910	311.2	7.8	28
210511	154534	154858	611.8	7.5	28
210511	155722	160218	473.1	7.5	23
210511	160951	161431	459.4	7.8	23
210511	162459	163027	798.8	8.3	22
210511	164514	165030	1197.1	6.7	18
210511	171444	172138	514.9	6.7	22
210512	91958	92427	640.9	4.6	52
210512	93626	94130	505.6	4.4	53
210512	94744	95136	522.2	4.3	48
210512	95630	100138	562.6	3.8	51
210512	102011	102454	498.6	3.9	50

210512	100933	101419	525.0	3.8	48
210512	103509	103956	571.4	4.2	46
210512	110902	111411	857.4	4.2	43
210512	112945	113410	460.8	4	42
210512	141125	141725	676.3	3.5	18
210512	142905	143349	610.3	4.6	15
210512	134744	135307	761.6	2.9	40
210512	135423	135956	669.6	3.4	15
210512	140626	141055	701.2	3.5	18
210512	154149	154654	501.7	5.1	26
210512	163730	164655	850.4	5.5	34
210512	170137	170720	784.8	5.2	33
210512	171505	172048	725.9	5	34
210513	162624	163406	849.1	3.7	79
210513	164716	165240	794.3	3.5	81
210513	170849	171319	436.6	3.8	68
210513	173536	174006	637.1	3.9	77
210513	125948	130221	836.3	2	80
210513	130721	131300	860.6	2.2	89
210513	145408	150008	699.1	3	43
210513	162542	163142	893.9	3.7	78
210514	111214	112114	768.3	3.4	24
210514	114935	115441	690.1	3.7	51
210514	133437	134101	592.8	4.5	48
210514	134155	135058	586.5	4.3	56
210514	135149	135725	750.1	4.7	58
210514	135800	140036	822.7	4.8	58
210514	140209	140615	492.3	4.8	51
210514	140557	140957	693.8	5.1	49
210514	141031	141510	603.8	5.2	49
210514	141516	141852	544.8	5	51
210516	134049	134755	661.2	5.3	25
210516	135813	140425	961.1	5.8	54
210516	142005	142717	609.0	4.8	47
210516	150231	150737	583.6	5.1	55
210516	162916	163946	807.0	4.4	68
210518	105910	110514	981.7	7.8	135
210518	111013	112937	779.5	7.9	143
210518	124456	125856	732.1	8.9	138
210518	130104	131004	753.6	9.8	145
210518	133655	134451	571.4	8.9	157
210520	164020	164756	662.5	9.5	194

Emission average 95% CI: 663-738 kg/h

Table 6. SO₂ emissions from Cokenergy plant measured by SkyDOAS. (N.B. Method protocol requires averaging of multiple measurements).

Date	Start time	Stop time	Emission (kg/h)	Wind Speed (m/s)	Wind Dir (deg)
210510	143043	143328	1032.98	9	25
210510	151847	152629	761	8.6	13
210510	160942	161312	574.27	7.4	16
210511	115209	115609	550.08	4.5	19
210511	124828	125353	502.03	5.8	38
210511	132042	132510	564.37	6.8	32
210511	154114	154522	679.73	8.4	28
210511	155146	155730	634.18	8.2	26
210511	160523	160955	669.06	7.6	27
210511	161623	162459	518.12	8.6	22
210511	162459	162651	772.94	8.1	23
210512	92534	92731	614.14	5	54
210512	94139	94515	576.94	4.8	52
210512	95226	95348	432.32	4.6	51
210512	100133	100634	556.52	4.1	52
210512	101421	101819	438.87	4.1	50
210512	102507	102745	727.97	4.4	55
210512	142517	142905	574.03	4.5	15
210512	151157	151733	652.8	4.9	21
210512	151913	152119	778.18	4.9	22
210512	152625	152929	794.8	4.8	26
210512	153102	153246	486.5	5	26
210512	164648	164910	635.73	5.4	36
210512	170714	170949	571.32	6.2	31
210512	172035	172920	654.63	6.3	30
210513	125439	125700	813.26	2	86
210513	172006	172712	504.77	3.9	67
210514	115450	115729	932.55	4.1	59
210514	121009	121233	701.73	3.7	53
210514	121753	122223	541.92	3.9	58
210514	123914	124150	586.19	3.9	57
210514	132655	133204	546.11	4.5	46
210516	92602	93122	724.85	2.5	103
210516	93934	94306	730.78	3.7	105
210516	134807	135155	717.39	5.7	46
210516	142723	143159	569.51	4.4	56
210516	170517	170741	532.04	4	79
210518	102409	102649	884.06	8.2	139
210518	114245	114809	963.06	8.3	152
210518	120544	120744	742.86	9.3	141
210518	152057	152233	675.45	8.9	157
210518	153501	153641	1135.35	8.1	153
210518	153933	154049	516.39	9.5	152
210518	155925	160301	709.92	8.6	155

210518	160512	160747	595.09	8.5	157
210518	170440	170635	967.24	8.5	165
210518	170700	170805	552.03	8	168
210519	154905	155113	1067.1	9.3	182
210520	104553	104725	403.25	7.8	173
210520	104816	105352	620.93	8.2	174
210520	115948	120412	668.86	8.6	181
210520	134159	134347	1064.72	9	172
210520	134402	134549	849.14	9	185
210520	134820	134956	602.5	8.8	165
210520	135020	135511	830.46	9.2	168
210520	135743	141035	640.3	9.1	171
210520	141102	141737	566.33	9.9	179
210520	142837	143131	645.28	10.1	182
210520	143316	143610	670.06	9.7	179
210520	150747	151047	828.56	9.1	176
210520	152619	152739	825.79	10.1	172
210520	160140	160248	317.34	10.4	179
210520	164336	164756	663.62	10.5	191
210520	170631	170951	187.5	9.9	182

Emission average 95% CI: 625-714 kg/h

SO₂ emissions measured by SOF

SO₂ emissions from the overall site were also measured with SOF, as a complementary quality assurance to the main SkyDOAS measurements. Table 7 summarizes the results, showing an average SO₂ emission of 676 kg/h (95% CI: 622-731 kg/h), based on 28 observations on 6 days. The SOF data set is a subset of the SkyDOAS data, with 28 measurement transects compared to 74 for SkyDOAS (701 kg/h, 95% CI: 663-738 kg/h), but results are well in line for the two different methods utilizing infrared and ultraviolet light absorption respectively.

Table 7. Process (SunCoke + Cokenergy) SO₂ emissions measured by SOF. (N.B. Method protocol requires averaging of multiple measurements).

Date	Start time	Stop time	Emission (kg/h)	Wind Speed (m/s)	Wind Dir (deg)
210510	131024	131533	855.1	7.2	38
210510	132913	133309	604.2	7.4	51
210510	142237	142639	608.4	8.4	20
210511	103233	104023	628.3	3.3	25
210511	140218	140816	608.8	6.8	30
210511	141941	142256	985.2	8.1	27
210511	145549	150141	563.0	6.8	38
210511	152052	152444	691.8	6.5	36
210512	100924	101421	417.6	3.8	48
210512	102004	102441	542.3	3.9	50
210512	103447	104030	515.0	4.2	46
210512	111010	111433	513.3	4.1	43
210512	112948	113502	511.4	4	41
210512	113802	114303	790.0	3.8	46
210512	135532	140225	673.3	3.5	16
210512	140629	140938	722.3	3.6	18
210512	141251	141836	621.8	3.5	18
210512	154223	154723	699.1	4.4	25
210513	124940	125259	1015.7	2.7	90
210513	125847	130314	747.1	2.6	80
210513	162636	163104	692.7	3.7	78
210513	164828	165209	825.8	3.6	81
210514	113851	114426	609.6	3.1	33
210514	114944	115430	647.1	3.7	51
210514	135300	135708	630.6	4.7	58
210514	141152	141515	867.3	5.2	49
210514	141524	141812	660.5	5	51
210520	115841	120517	692.7	8.1	184
Emission average 95% CI: 622-731 kg/h					

3.2.3 Plume characterization by extractive FTIR, DOAS and canister sampling

Plume characterization was conducted by MeFTIR, MeDOAS and canister samples both as integrated fenceline samples and at a few specific locations, as described in the test matrix (Table 2).

Fenceline concentration ratios

MeFTIR and MeDOAS were used to characterize concentrations alongside the same fenceline routes used for the SOF and SkyDOAS measurements. Canister samples were collected in key areas for improved speciation and quality assurance.

Table 8 shows benzene to alkane mass fractions as integrated by MeDOAS and MeFTIR respectively. 41 integrations were done across the tested fenceline areas, with a benzene to alkane average mass fraction of 4.1% (95% CI: 3.5-4.7%). In all, 9 integrated canister samples were collected for the fenceline routes (subsample). These averaged a benzene to alkane mass fraction of 4.3%, comparing well to the extractive methods.

For BTEX compounds the extractive instrumentation (excluding o-xylene) showed an average mass fraction versus alkanes of 9.9% (95% CI: 8.1-11.7%), based on 27 measurements over 7 days, see Table 9. This compares well to the canister mass fraction estimate of 12.1%.

Table 8. Benzene versus alkane mass fraction integrated across the tested fenceline areas.

Date	Time	N
210512	103531 -172009	5
210513	125737 -174012	4
210514	84558 -161518	9
210516	91956 -172129	9
210517	161333 -162249	1
210518	100505 -154608	7
210520	170951 -171627	1
210521	90509 -113920	5
Mass fraction average 95% CI: 3.5-4.7%		

Table 9. BTEX versus alkane mass fraction integrated across the tested fenceline areas.

Date	Time	N
210512	103531 -172009	5
210513	125737 -174012	4
210514	104356 -161518	6
210516	91956 -154506	7
210517	161333 -162249	1
210518	100505 -154608	3
210521	113355 -113920	1
Mass fraction average 95% CI: 8.1-11.7%		

Table 10 summarizes mass fraction of ethene versus alkane mass for 42 fenceline integrations. An average ethene to alkane mass fraction of 3.5% (95% CI: 3.1-3.9%) was found. The corresponding (subsample) canister mass fraction was 2.9%.

Table 10. Ethene versus alkane mass fraction integrated across the tested fenceline areas.

Date	Time	N
210512	103427 -172009	5
210513	125737 -174012	4
210514	84558 -161518	9
210516	91956 -172129	10
210517	161333 -162249	1
210518	100505 -154608	7
210520	170951 -171627	1
210521	90509 -113920	5

Mass fraction average 95% CI: 3.1-3.9%

Table 11 shows a summary of 9 canister samples integrated along the fenceline route for the SOF and SkyDOAS emission transects. Of the overall VOC content (alkanes+alkenes+BTEX) analyzed by gas chromatograph in those samples, alkanes were dominant with about 85% of the overall VOC mass, followed by almost 9% BTEX and remaining 5% alkenes (olefins). This suggests SOF alkane emissions of 4.7 kg/h should be expanded by 17.6% ($1/0.85$) to resemble the overall VOC emissions, e.g. 5.5 kg/h, from the process area.

Table 11. Canister sample summary for fenceline samples.

Canister ID	Location	Sample date	Sample ID	Concentration ($\mu\text{g}/\text{m}^3$)			Mass fraction (%) of sum of all		
				BTEX	Alkanes	Alkenes	BTEX	Alkanes	Alkenes
1036	Fenceline	2021-05-16	230939	1.33	9.82	0.86	11.1	81.7	7.2
3156	Fenceline	2021-05-16	230940	1.90	10.98	0.66	14.0	81.1	4.9
1043	Fenceline	2021-05-16	230941	1.41	13.82	0.87	8.8	85.8	5.4
3152	Fenceline	2021-05-16	230942	1.43	14.28	0.73	8.7	86.9	4.4
3153	Fenceline	2021-05-18	230943	0.65	15.48	1.23	3.8	89.1	7.1
3157	Fenceline	2021-05-18	230944	1.95	18.34	1.13	9.1	85.6	5.3
3165	Fenceline	2021-05-18	230945	1.69	17.45	0.82	8.5	87.4	4.1
3162	Fenceline	2021-05-18	230946	2.53	11.76	1.08	16.4	76.5	7.1
3160	Fenceline	2021-05-18	230947	1.22	34.25	2.20	3.2	90.9	5.8
Average:				1.6	16.2	1.1	9.3	85.0	5.7

CEMS line concentration ratios, Main stack

Three canister samples were collected at the CEMS line on the Main Stack, one during production and two during non-production mode. Weighing the production canister sample in by 2/3 and the non-production mode sample by 1/3 in order to resemble the temporal mode distribution, resulted in a mass composition of 76% alkanes, 16.5% BTEX and 7% alkenes in the stack flow.

Table 12. CEMS line canister samples. p = production mode, np = non-production mode.

Canister ID	Location	Sample date	Sample ID	Concentration ($\mu\text{g}/\text{m}^3$)			Mass fraction (%) of sum of all		
				BTEX	Alkanes	Alkenes	BTEX	Alkanes	Alkenes
1044	CEMS ^{np}	2021-05-17	230952	2.7	13.6	0.8	15.7	79.7	4.6
1046	CEMS ^p	2021-05-17	230953	2.2	10.2	1.2	16.2	75.3	8.5
1153	CEMS ^{np}	2021-05-17	230954	2.6	10.5	0.5	19.3	77.3	3.3
Production mode weighted average:				2.4	10.9	1.0	16.6	76.5	6.9

Detailed process source characterization

This section describes results from near field screening of selected sources/operations by means of extractive FTIR and DOAS, connected with Teflon tubing to reach and pump sample air from near sources. Note that sampling includes periods of time both in and out of the moving plume (if present), so higher concentrations were seen intermittently, and comparisons should only be made on a relative scale between compounds and similar targets rather than in absolute terms between all source types. Observed concentrations and concentration fractions can be used to verify operational performance and indicate potential impact of a source on observed emissions.

Ovens

Four ovens per battery were screened in the near field with extractive FTIR and DOAS and attached Teflon tubing to reach to the sample point. Ovens A40, A41, A42 and A43 were screened in the A battery. B23-B26 were sampled in the B battery, C44-C47 in the C battery and D23-D26 in the D battery. The ovens were first sampled on top of the oven and then by the oven door. Average concentrations for the complete screening period, including both the top and door screening, is given in Table 13.

Table 13. Average concentration at ovens during near source screening.

Source	SO ₂ (µg/m ³)	Alkanes (µg/m ³)	Ethylene (µg/m ³)	Benzene (µg/m ³)	Toluene (µg/m ³)
Oven A40	5.4	0.1	0.6	0.6	0.8
Oven A41	5.2	3.0	6.7	1.8	1.5
Oven A42	7.4	8.0	0.0	0.5	0.4
Oven A43	27.5	6.5	0.0	0.5	0.5
Oven B23	3.8	2.4	1.2	0.3	0.2
Oven B24	1.5	3.0	0.8	0.4	0.1
Oven B25	5.2	3.7	0.5	0.0	0.6
Oven B26	1.8	1.4	1.4	0.2	0.1
Oven C44	1.2	8.1	1.8	0.0	0.0
Oven C45	12.4	16.6	4.7	0.2	0.8
Oven C46	6.2	7.3	4.8	0.5	0.4
Oven C47	8.9	7.9	3.8	1.4	0.7
Oven D23	644.7	36.7	5.6	1.9	NA
Oven D24	211.8	57.5	9.4	4.9	NA
Oven D25	24.6	15.6	1.7	0.4	0.2
Oven D26	16.0	3.3	1.0	0.4	0.3

PCM

Eight different push operations and eight charge operations were screened with the extractive instrumentation in the near field on 14 May 2021. Table 14 shows average concentrations for all the push and charge samples, respectively.

Table 14. Average concentration at ovens at oven push and charge operations during near source screening.

Source	SO ₂ (µg/m ³)	Alkanes (µg/m ³)	Ethylene (µg/m ³)	Benzene (µg/m ³)	Toluene (µg/m ³)
PCM Push	216.7	132.0	16.1	10.8	23.0
PCM Charge	196.4	18.2	4.7	4.9	5.9

Vent stacks

Oven battery vent stacks A3, B2, C3 and D2 were screened with extractive FTIR and DOAS nearby the top of the vent stack. Figure 13 shows the procedure at vent stack A3 on the 14 May 2021, 08:40 AM. A Sky-lift was used to reach with a long 1"-diameter Teflon-tubing extending from the FTIR and DOAS instruments in the mobile lab to the elevated plume location.

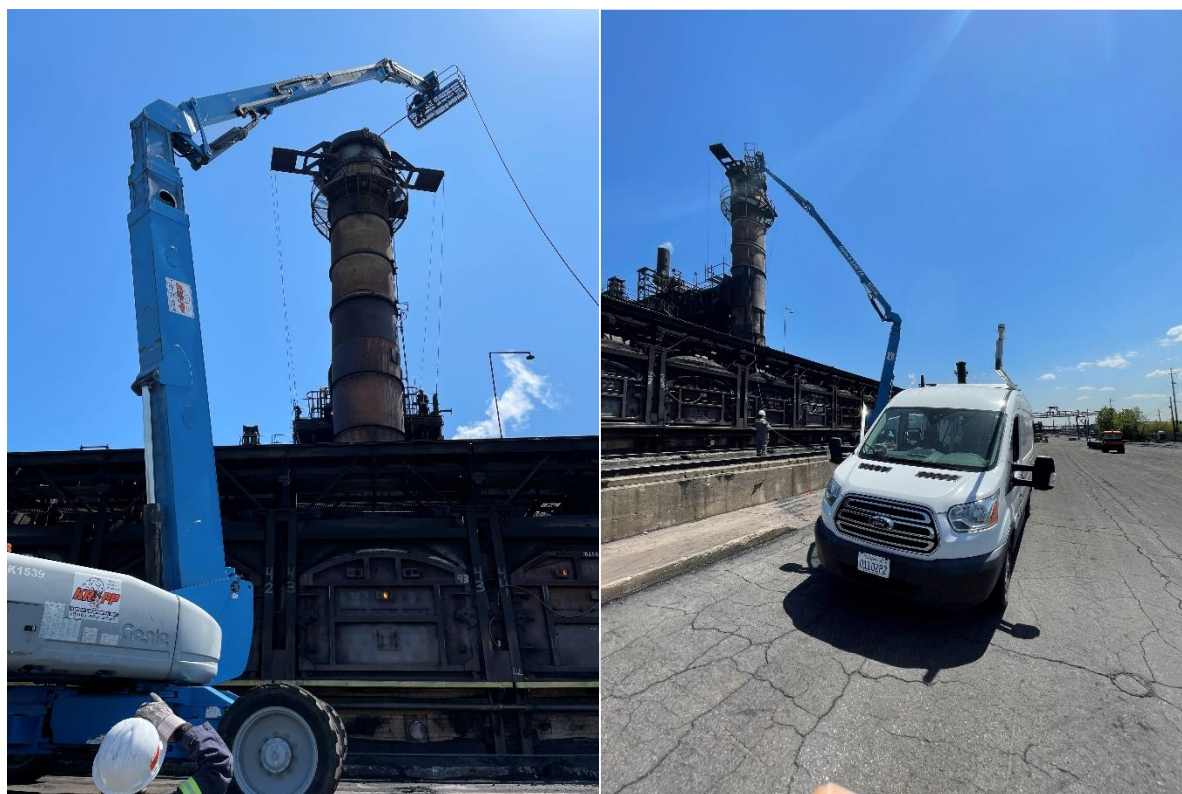


Figure 13. Near source concentration screening with extractive FTIR and DOAS at vent stack A3, 14 May 2021, 08:40 AM.

Table 15 shows the average concentrations measured near the vent stack top for vent stack A3, B2, C3, and D2.

Table 15. Average concentration at vent stacks during near source screening.

Source	SO ₂ (µg/m ³)	Alkanes (µg/m ³)	Ethylene (µg/m ³)	Benzene (µg/m ³)	Toluene (µg/m ³)
Vent A3	3273.2	11.2	2.0	NA	NA
Vent B2	19.6	1.7	2.3	0.0	0.6
Vent C3	81.2	2.1	1.0	0.3	0.0
Vent D2	47.0	7.5	0.0	0.0	1.8

HRSGs

HRSGs A3, B2, C3 and D2 were screened in near field with extractive FTIR and DOAS with attached Teflon tubing on the same occasion as the vent stack. Two positions were tested on each HRSG, Table 16.

Table 16. Average concentration at HRSGs during near source screening.

Source	SO ₂ (µg/m ³)	Alkanes (µg/m ³)	Ethylene (µg/m ³)	Benzene (µg/m ³)	Toluene (µg/m ³)
HRSG A3	2.9	3.0	1.1	0.2	0.3
HRSG B2	0.3	2.4	1.1	0.2	0.7
HRSG C3	38.1	6.1	0.0	0.9	0.0
HRSG D2	18.4	3.8	0.0	0.9	0.8

Wharf

The wharf was screened during production both at the A-B-battery side and the C-D-battery side on 14 May, 4:20-5:20 PM. The near source plume was sampled with extractive FTIR and DOAS, as summarized in Table 17.

Table 17. Average concentration during near source screening at Wharf production.

Source	SO ₂ (µg/m ³)	Alkanes (µg/m ³)	Ethylene (µg/m ³)	Benzene (µg/m ³)	Toluene (µg/m ³)
Wharf CD	517.2	46.3	8.5	0.0	0.0
Wharf AB	353.2	17.1	1.1	0.0	0.0

Quench

The CD battery quench plume was sampled in near field with extractive FTIR and DOAS on 17 May 3:25 PM. Table 18 summarizes the average concentrations detected during the near field quench screening.

Table 18. Average concentrations during quench screening.

Source	SO ₂ (µg/m ³)	Alkanes (µg/m ³)	Ethylene (µg/m ³)	Benzene (µg/m ³)	Toluene (µg/m ³)
Quench (near field)	5.2	12.7	2.6	0.1	0.2

3.3 Process data

In order to cross-correlate observed emission plumes with plant operation activities, during the test period IHCC obtained pertinent process data and maintain detailed logs including:

- production rates and times for pushing and charging of the different ovens.
- time log for the quenching episodes.
- coal usage rates and % sulfur content in the used coal.

Logs were kept to documenting any upsets from normal production, specifically any events that might affect observed emissions such as bypass venting. Logs were kept both for the production (~ 2:30 PM – 6 AM) and the service/maintenance-window (~ 6 AM – 2:30 PM).

Table 19 summarizes the coal charge going to the ovens daily during the survey period, along with sulfur and moisture content.

Table 19. Oven coal charge data.

Date	Charged ovens	Tons coal	Tons/oven	Coal sulfur % (db)	Coal moisture (%)
2021-05-09	133	5305.8	39.89	-	-
2021-05-10	120	4794.8	39.96	0.910	8.13
2021-05-11	133	5304.1	39.88	0.910	8.13
2021-05-12	128	5104.7	39.88	0.910	8.13
2021-05-13	132	5245.1	39.74	0.910	8.16
2021-05-14	126	5028.6	39.91	0.910	8.14
2021-05-15	130	5168.1	39.75	0.910	8.12
2021-05-16	128	5101.7	39.86	0.910	8.14
2021-05-17	118	4676.5	39.63	0.910	8.14
2021-05-18	139	5535.7	39.83	0.900	8.11
2021-05-19	124	4915.0	39.64	0.900	8.18
2021-05-20	123	4881.8	39.69	0.900	8.15
2021-05-21	139	5518.2	39.70	0.915	8.09
Average	128.7	5121.5	39.8	0.908	8.13
SD	6.5	262.7	0.1	0.005	0.02

4 Sampling and analytical procedures

4.1 Emission test methods

The FluxSense measurement vehicle or “mobile lab” was equipped with four optical instruments for gas monitoring during the survey: SOF (Solar Occultation Flux), SkyDOAS (Differential Optical Absorption Spectroscopy), MeFTIR (Mobile extractive Fourier Transformed Infrared spectrometer) and MeDOAS (Mobile extractive White cell DOAS). The individual measurement methods are described in Appendix A.

SOF and SkyDOAS both measure gas columns through the atmosphere by means of light absorption. SOF utilizes infrared light from the direct sun whereas SkyDOAS measures scattered ultraviolet light from the sky. MeFTIR and MeDOAS both measure ground level concentrations of alkanes and BTEX respectively. Both instruments are used in extractive mode where ambient air is pumped from attached inlet tubing through the optical cell while being analyzed in real time.

Accurate wind data is necessary in order to compute emission fluxes. Wind information is derived from several different sources. A moveable wind LIDAR was used to measure vertical profiles of wind speed and wind direction from 10-300 m height. The LIDAR data is combined with data from wind mast(s). Figure 14 gives a general overview of the measurement setup and the data flow.

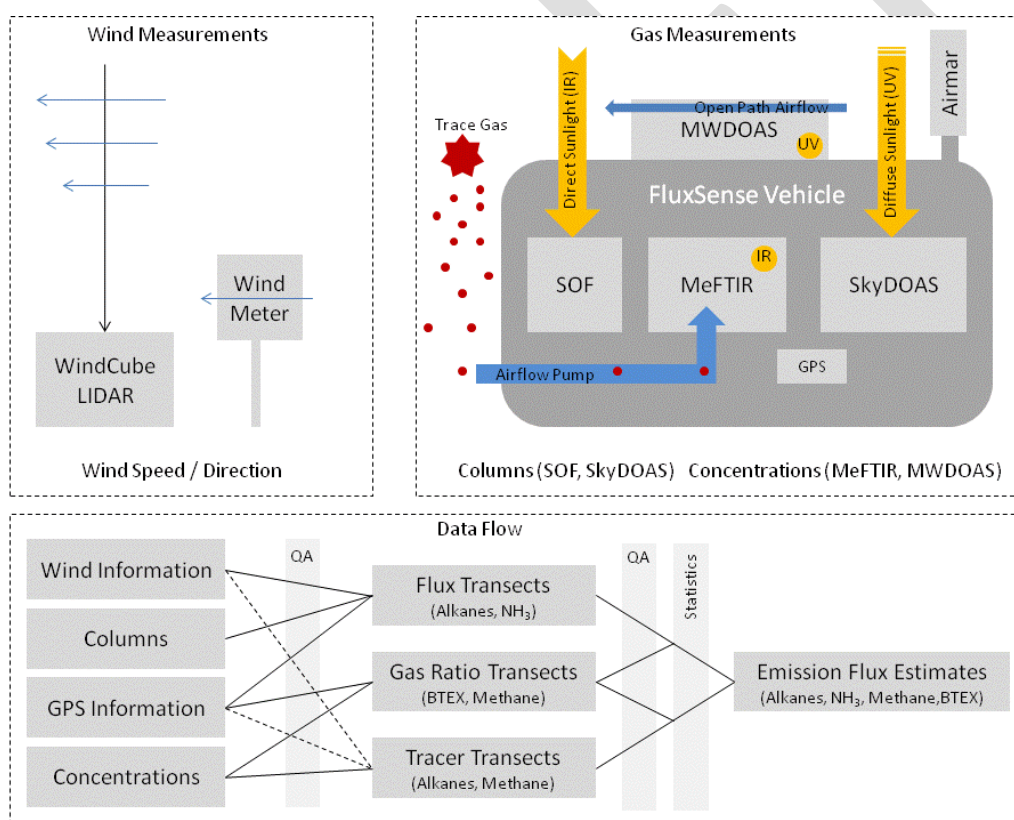


Figure 14. Overview of the FluxSense mobile lab main instruments; SOF, MeFTIR, MWDOAS and SkyDOAS (upper right panel) and wind measurements (upper left panel) and simplified data flow diagram (lower panel). SOF and SkyDOAS are column integrating passive techniques using the Sun as the light source while MeFTIR and MWDOAS sample local air concentrations using active internal light sources. The data flow describes what information that goes into the flux emission estimates. Direct flux emissions are given from measured columns (SOF and SkyDOAS) of alkanes and SO₂ while indirect fluxes are calculated via gas concentration ratios (MeFTIR and MWDOAS) of BTEX and benzene. See appendix 1 for principal equations. All emission flux estimates are based on statistical analysis of measured data. Q.C. = Quality Control, S.A.= Statistical Analysis (see Appendix A for details).

In order to derive final emission flux estimates, the GPS-tagged gas column measurements by SOF and SkyDOAS are combined with wind data and integrated across plume transects at the various source locations. Gas mass ratio measurements by MeFTIR and MeDOAS are then used to indirectly estimate the emissions for BTEX.

The overall uncertainty for emission estimates based on optical remote sensing methods, such as SOF and SkyDOAS for this survey, is dominated by uncertainties in the wind field. In the flux calculation, the measured (vertical or slant) concentration columns are associated with an average plume transportation speed. In this process the wind speed and direction are first measured, and in the next stage the concentration profile, e.g. the plume allocation by height, is addressed in order to attribute a plume transportation speed.

Silonite-coated and evacuated canisters were sampled in key plumes for supporting speciation and quality assurance. Canisters were analyzed at the Swedish Environmental Research Institute (IVL) (external accredited laboratory) by GC FID-MS. C₂-C₉ alkanes, C₂-C₄ alkenes and C₆-C₉ aromatic hydrocarbons were on the analyte list.

4.2 Sample identification and custody

All SOF, SkyDOAS, MeFTIR and MeDOAS measurements of columns and concentrations were uniquely geo-tagged with latitude and longitude position and time according to GPS receivers connected to the instruments. All FTIR and DOAS spectra have been stored on back-up discs.

Wind data (wind speed, wind direction, height) from wind mast and the wind LIDAR were geo-tagged with position and time according to GPS connected to the wind instruments. All wind data has been stored on back-up discs.

Chain of custody was kept for the canister samples all the way from preparation until analyzed at the laboratory. Each canister was uniquely tagged and a log was kept for the sampling time, position and circumstances.

5 QA/QC activities

The following procedures/quality checks were undertaken on a recurrent basis to ensure appropriate operations during the survey. Paragraph 5.1 through 5.7 cover the different instrumentations used.

5.1 SOF

- Verify that detector is cooled
- Verify that FTIR spectrometer is operational, (e.g. that all internal operational check flags are in order, such as laser amplitude, interferometer block etc.)
- Verify that GPS is operational and has sufficient amount of satellites (3+)
- Check that data storage disc has sufficient space
- Check that amplification for the solar tracker is properly set so that the tracker can lock properly on the sun without oscillating
- Check that vibration mounts are sufficiently filled with air
- Check light intensity so that the ADC (analog-digital converter) receives more than 1500 for the InSb (indium antimonide) detector
- Check interferogram for any abnormal oscillations
- Check that an RMS of <0.15% can be achieved in stationary mode
- Check retrieved concentration columns in different vehicle orientations to verify that the tracker is properly aligned (alkane column offsets <2.5 mg/m²)
- Check stationary stability in retrieved concentration columns to verify operation and stable background
- Check for consistent background columns at the plume edges before and after the plume scan and note significant deviations
- Check spectral fit to observe any interfering absorption not handled by the evaluation retrieval

5.2 SkyDOAS

- Verify that detector is cooled
- Verify that DOAS spectrometer is operational, (e.g. that all internal operational check flags are in order, such as shutter, slit width, grating etc.)
- Verify that GPS is operational and has sufficient amount of satellites (3+)
- Check that data storage disc has sufficient space
- Check that telescope is open and pointed vertically to the sky without obstruction
- Check that vibration mounts are operational
- Check light intensity and adjust exposure so that the detector does not get saturated at any wavelength (e.g. less than 65000 counts for a single spectrum at all columns of the CCD)
- Check that an RMS of <0.01% can be achieved in stationary mode
- Check stationary stability in retrieved concentration columns to verify operation and stable background
- Check for consistent background columns at the plume edges before and after the plume scan and note significant deviations
- Check spectral fit to observe any interfering absorption not handled by the evaluation retrieval

5.3 MeFTIR

- Verify that detector is cooled
- Verify that FTIR spectrometer is operational, (e.g. that all internal operational check flags are in order, such as laser amplitude, interferometer block etc.)
- Verify that GPS is operational and has sufficient amount of satellites (3+)
- Check that data storage disc has sufficient space
- Check that amplification for the sandwich detector is properly set so that both channels are operational without saturation
- Check that vibration mounts are sufficiently filled with air
- Check that light intensity is sufficient
- Check interferogram for any abnormal oscillations
- Verify pump operation and pressure in the gas cell (a few mbars below ambient in normal operation)
- Check that an RMS of $<0.2\%$ can be achieved in stationary mode
- Check stationary stability in retrieved concentration to verify operation and stable background
- Check for consistent background concentrations at the plume edges before and after the plume scan and note significant deviations. Consistent concentrations at the plume edges along with upwind measurements will indicate if significant interfering inflow of the target species is taking place.
- Check spectral fit to observe any interfering absorption not handled by the evaluation retrieval
- Check background concentrations for consistency (CH_4 , N_2O)
- Verify pathlength with laser/halogen lamp
- Conduct spike tests with methane gas ($\sim 5\text{-}15$ ppmv concentration)

5.4 MEDOAS

- Verify that detector is cooled
- Verify that DOAS spectrometer is operational, (e.g. that all internal operational check flags are in order, such as shutter, slit width, grating etc.)
- Verify that GPS is operational and has sufficient amount of satellites (3+)
- Check that data storage disc has sufficient space
- Check that vibration mounts are operational
- Verify pump operation and pressure in the gas cell (a few mbars below ambient in normal operation)
- Check light intensity and adjust exposure so that the detector does not get saturated at any wavelength (e.g. less than 65000 counts for a single spectrum at all columns of the CCD)
- Check that an RMS of $<0.01\%$ can be achieved in stationary mode
- Check stationary stability in retrieved concentrations to verify operation and stable background
- Check for consistent background concentrations at the plume edges before and after the plume scan and note significant deviations. Consistent concentrations at the plume edges along with upwind measurements will indicate if significant interfering inflow of the target species is taking place.
- Check spectral fit to observe any interfering absorption not handled by the evaluation retrieval
- Verify pathlength with laser/halogen lamp

- Conduct spike tests with p-xylene (or corresponding BTEX compound) (~ 100 ppbv range)

5.5 Wind LIDAR

- Verify that the LIDAR is aligned towards true north (e.g. compensate for the magnetic declination at the site)
- Verify that the instrument has a free field of view within a ± 17 degrees cone from zenith
- Verify that power supply is operational and battery capacity sufficient
- Check that backscatter signal is sufficient for wind data retrieval in the 10-300 m range
- Check that data storage disc has sufficient space
- Observe wind LIDAR data output at start-up
- Backup wind data on a daily basis

5.6 Wind tower

- Verify that the wind tower is aligned towards true north (e.g. compensate for the magnetic declination at the site)
- Verify that the wind meter is not obstructed
- Verify that power supply is operational and battery capacity sufficient
- Check that wind speed and direction data are reasonable
- Check that data logger has sufficient space
- Observe wind logger data at start-up
- Backup wind data on a daily basis

5.7 Canisters

- Maintain chain of custody
- Check canister for vacuum prior to sampling
- Flush any sample restrictors/nozzles prior to sampling
- Record time from vacuum to full canister for consistency check
- Note initial and final canister pressure
- Label canister with location, time (start and stop), date and operator

Appendices

A - Methods

The SOF method

The SOF method [Mellqvist 1999, 2008a, 2008b, 2009, 2010; Kihlman 2005a; Johansson 2014] is based on the recording of broadband infrared spectra of the sun with a Fourier transform infrared spectrometer (FTIR) that is connected to a solar tracker. The latter is a telescope that tracks the sun and reflects the light into the spectrometer independent of the orientation of the vehicle. Using multivariate optimization, it is possible from these solar spectra to retrieve the path-integrated concentrations (referred to as column concentrations), in the unit mg/m^2 , of various species between the sun and the spectrometer. The system used in this project consists of a custom-built solar tracker, transfer optics and a Bruker IRCube FTIR spectrometer with a spectral resolution of 0.5 cm^{-1} , equipped with a dual InSb (Indium Antimonide) / MCT (Mercury Cadmium Telluride) detector. A reference spectrum is taken outside the plume so that atmospheric background concentrations are removed. This means that all measured SOF columns are analyzed relative to the background column concentrations.

The system is installed in a measurement vehicle which allows consecutive column concentration measurements to be performed while driving. The flux of a species in a plume from an industry is measured by collecting spectra while driving the vehicle so that the light path from the sun to the instrument gradually cuts through the whole plume, preferably as orthogonally as possible to the wind direction, see Figure A 1 and Figure A 2.

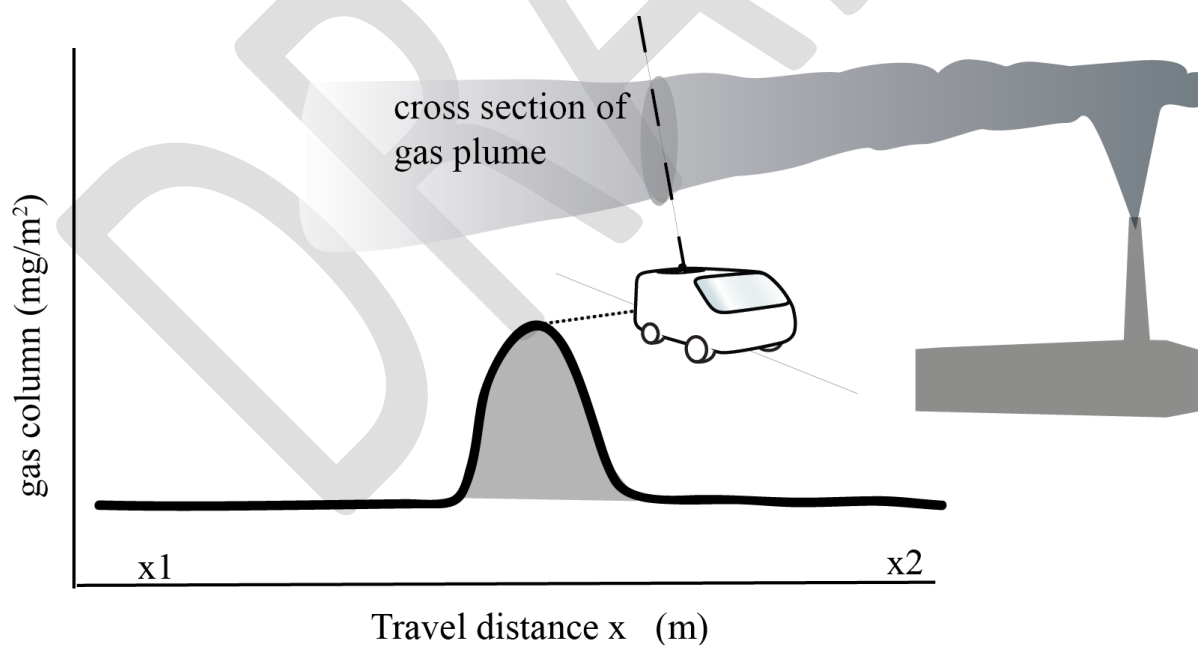


Figure A 1. Schematic of the SOF measurement where the vehicle is driven across the prevailing wind so that the solar beam cuts through the emission plume while the sun is locked into the FTIR spectrometer by the solar tracking device on the roof. The VOC mass (or other compound of interest) is integrated through the plume cross section.

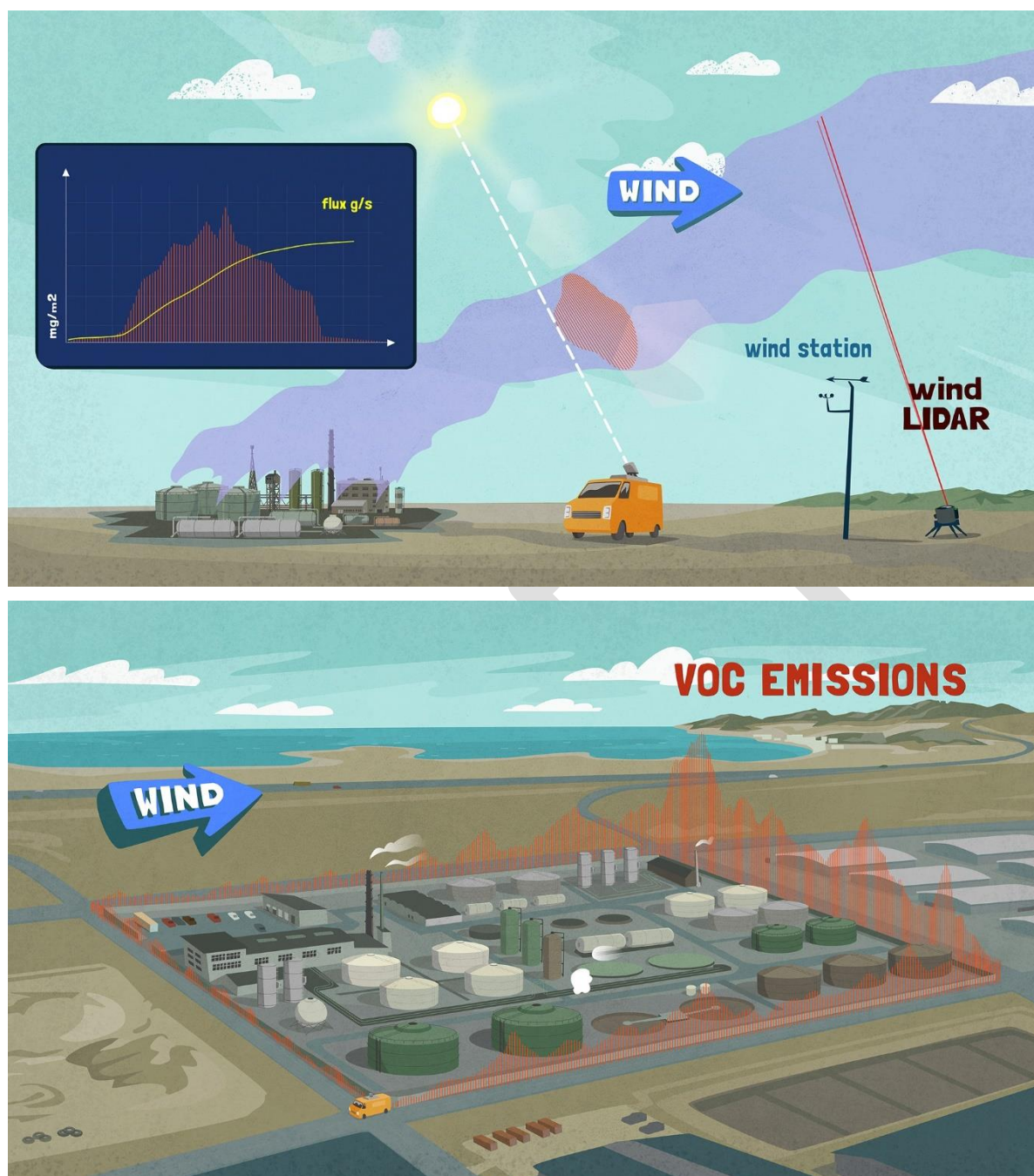


Figure A 2 Schematic of SOF and SkyDOAS measurement where the vehicle is driven across the prevailing wind so that the solar beam or zenith sky light beam cuts through the emission plume while the sun is locked into the FTIR spectrometer by the solar tracking device on the roof. The VOC mass (or other compound of interest) is integrated through the plume cross section. Usually, the measurements are carried by encircling the individual sources, in order to remove the influence of the upwind (background) emissions.

For each spectrum a column concentration of the species is retrieved using custom software (QESOF, i.e. *Quantitative evaluation of SOF*) [Kihlman 2005b]. These column concentrations, together with positions recorded with a GPS (Global Positioning System) receiver and the solar angle calculated from the time of the measurements, are used to calculate the area integrated column of the species in the intersection area between the plume and the light path. The flux of the species is then obtained by multiplying this area integrated concentration with the orthogonal wind speed vector component.

The IR spectra recorded by the SOF instrument are analyzed in QESOF by fitting a set of spectra from the HITRAN infrared database [Rothman 2003] and the PNNL (Pacific Northwest National Laboratory) database [Sharpe 2004] in a least-squares fitting procedure. Calibration data from the HITRAN database is used to simulate absorption spectra for atmospheric background compounds present in the atmosphere with high enough abundance to have detectable absorption peaks in the wavelength region used by SOF. Spectra, including water vapor, carbon dioxide and methane, are calibrated at the actual pressure and temperature and degraded to the instrumental resolution of the measurements. The same approach is applied for several retrieval codes for high resolution solar spectroscopy developed within Network for the Detection of Atmospheric Composition Change (NDACC) [Rinsland 1991; Griffith 1996] and QESOF has been tested against these with good agreement, better than 3%. For the retrievals, high resolution spectra of ethylene, propene, propane, n-butane and n-octane were obtained from the PNNL database and these are degraded to the spectral resolution of the instrument by convolution with the instrument line shape. The uncertainty in the absorption strength of the calibration spectra is about 3.5% for all five species.

In this project, the SOF method is used to measure VOCs in two different modes. Most VOCs with C-H bonds absorb strongly in the 3.3-3.7 μm (2700-3005 cm^{-1}) spectral region. This region is mainly used for alkane measurements using a spectral resolution of 8 cm^{-1} . Alkenes (including ethylene and propylene) and ammonia are instead measured in the spectral region between 910 and 1000 cm^{-1} using a spectral resolution of 0.5 cm^{-1} . In the alkane mode – the IR light absorption is essentially sensitive to the total alkane mass (number of alkane C-H bonds) present in the plume. The absorption structures (cross sections) for the various alkane compounds are rather similar, with the absorption strength scaling to the mass of the alkane species. Hence, the actual mix of alkanes in the plume does not affect the retrieved total alkane mass flux much, although only cross sections from a subset of all alkanes (propane, n-butane and octane) are fitted in the spectral analysis. Typically, the rare event of significant absorption from other species in the plume shows up as elevated residuals and is further investigated in the re-analysis. For the alkene mode the specificity of the measurements is good, since the absorption of different species is rather unique in this so called “fingerprint region” and absorption features are often sharp and well separable from each other at 0.5 cm^{-1} resolution.

SOF is a technique employed by FluxSense in over 100 fugitive emission studies around the world. In Europe the SOF technique is considered one of the Best Available Technology [European Commission 2015] for measurements of fugitive emission of VOCs from refineries; and in Sweden it is used together with tracer correlation and optical gas imaging for annual screening of all larger refineries and petrochemical plants. The estimated uncertainty for the SOF emissions measurements is typically 30 % for the total site emissions. This uncertainty has been calculated from several controlled release experiments (blind and non-blind) and side-by-side measurements with other measurement techniques.

Mobile SkyDOAS

The principle for Mobile SkyDOAS (Mobile Differential Optical Absorption Spectroscopy) measurements is very similar to that of SOF. Instead of measuring direct sun light in the infrared region, scattered light in the UV and visible region is measured in zenith angle with a telescope connected with an optical fiber to a Czerny-Turner spectrometer with a CCD camera. Column concentrations are retrieved from spectra in a similar way as with the SOF, although absorption is generally weaker. The system consists of a quartz telescope (20 mrad field of view, diameter 7.5 cm) connected with an optical fiber (liquid guide, diameter 3 mm) to a 303 mm focal length Czerny-Turner spectrometer with a 1024 by 255 pixels, thermoelectrically cooled CCD camera, see Figure A 3.



Figure A 3. The mobile SkyDOAS system: Zenith looking telescope, optical fiber and spectrometer. The SOF system is seen in the center of the sun roof.

The system was installed in the same measurement vehicle as the SOF system. Plumes were transected in the same way as with the SOF system and the retrieved column concentrations used to calculate fluxes exactly the same way, except that the SkyDOAS measurement direction is always zenith.

In this project, mobile SkyDOAS is used to measure SO_2 , NO_2 and H_2CO . NO_2 is retrieved in the wavelength region between 324 and 350 nm and SO_2 in the region 310-325 nm. H_2CO is measured in the region 322-350 nm. Apart from SO_2 , NO_2 and H_2CO the spectral analysis also includes other atmospheric compounds such as O_3 and O_4 . The rare event of significant absorption from other species in the plume than those included in the spectral fit shows up as elevated residuals and is further investigated in the re-analysis. The absorption line parameters of the retrieved compounds are well established in published databases, stating an uncertainty of 4% (Vandaele *et al.* 1998) for the UV cross section of NO_2 and less than 2% for the SO_2 cross sections (Bogumil *et al.* 2003).

The DOAS technique was introduced in the 1970's (Platt *et al.* 1979) and has since then become an increasingly important tool in atmospheric research and monitoring both with artificial light sources and in passive mode utilizing the scattered solar light. In recent time the multi axis DOAS technique (scanning passive DOAS) has been applied in tropospheric research for instance measuring formaldehyde (Heckel *et al.* 2005; Pikelnaya *et al.* 2007).

Passive DOAS spectroscopy from mobile platforms has also been quite extensively applied in volcanic gas monitoring (Galle *et al.* 2003) for SO_2 flux measurements and for mapping of formaldehyde flux measurements in megacities (Johansson *et al.* 2009). Mobile SkyDOAS has been used in several studies for measurements of industries i.e. SO_2 , NO_2 and H_2CO for several campaigns in Texas including NO_2 measurements at Longview in 2012 (Johansson *et al.* 2014a; Johansson & Mellqvist 2013). (Rivera 2009) did SO_2 measurements on a power plant in Spain for validation purposes. They also made measurements at an industrial conglomerate in Tula in Mexico (Rivera *et al.* 2009a) and measurements of SO_2 , NO_2 and H_2CO during the TexAQs 2006 campaign (Rivera *et al.* 2009b; Rivera *et al.* 2010).

Mobile extractive FTIR (MeFTIR)

Mobile Extractive FTIR (MeFTIR) [Galle 2001, Börjesson 2009] in combination with tracers has been used to quantify VOC emissions from refinery and petrochemical sources in Europe and in the U.S. Alkanes and alkenes are typically measured, but also methane and other climate gases can be retrieved. In the present project MeFTIR will measure both concentrations of total VOCs (as observed by C-H-stretch absorption in the 2700-3100 cm^{-1} wavenumber region) and methane.

MeFTIR is an optical technique capable of monitoring gas concentrations at ppb-sensitivity in mobile field operations. It is used both independently for concentration mapping and flux measurements, but often combined together with simultaneous SOF flux measurements to provide more detailed VOC speciation of plumes and for plume height assessments [Johansson et. al. 2013a]. The plume height can be estimated by dividing measured columns (mg/m^2) with ground concentrations (mg/m^3), assuming that the plume is evenly distributed up to the plume height (and zero above).

The MeFTIR system contains a mid-infrared spectrometer with medium resolution (0.5 cm^{-1}). It utilizes an internal glow bar as an infrared radiation source, and by customized optics this light is transmitted through an optical multi-pass measurement cell with path-length of typically 107 meters. The system is mounted on a vibration dampening platform to allow for real time plume mapping from a mobile platform, such as a vehicle or boat, see Figure A 4.



Figure A 4. The MeFTIR instrumentation consisting of a Bruker FTIR spectrometer connected to an optical multi-pass cell.

The transmitted light is detected simultaneously with an InSb-detector in the 2.5–5.5 μm (1800–4000 cm^{-1}) region and an MCT detector in the 8.3–14.3 μm (700–1200 cm^{-1}) region. Temperature and pressure in the cell are averaged over the duration of each measurement. Atmospheric air is continuously pumped at high flow rate through the optical cell from the outside, taking in plume air from the roof of the vehicle (2.5 m height) through a Teflon tube. A high flow pump is used to ensure that the gas volume in the cell is fully replaced within a few seconds. Spectra are typically recorded with an integration time of 10-15 seconds. A GPS-receiver is used to register the position of the vehicle every second. Extended Teflon tubing can be attached to the system for elevated sampling or leak search purposes.

The concentration in the spectra is analyzed in real time by fitting a set of calibrated spectra from the HITRAN infrared database [Rothman 2003] and the PNNL database [Sharpe 2004] in a least-squares fitting procedure. Compounds being analyzed include ethylene, propylene, total alkane mass (based on fitting cross sections of ethane, propane, n-butane, i-pentane, n-octane), water, methane, CO, CO₂ and N₂O. The analysis routines are very similar to the ones for SOF, but less complex because strong

absorption by atmospheric trace gases (water, methane, CO₂) has less consequence at the shorter path length in the MeFTIR measurement cell.

The MeFTIR tracer approach has been tested in a so-called gas release “blind test” together with other techniques in U.S. [ERF 2011]. In that test, methane was released from an area-distributed source in four different configurations and flow rates ranging from 1.1-3.3 g/s. At a downwind distance of 400 meters MeFTIR retrieved the fluxes within 6% in 3 cases and 19% in the fourth. This is consistent with other validation experiments, showing a flux estimate accuracy of better than 20%. Concentration measurement by FTIR is a widely used procedure, and the main uncertainties are associated with the absorption cross sections (typically < 3.5%) and spectral retrieval, with an aggregate uncertainty better than 10% in the analysis.

Concentrations are monitored in real time in order to detect emission plumes and to judge whether any interfering sources are being sampled. Unwanted signals from local traffic exhaust or from the measurement vehicle itself could be filtered out by looking at exhaust compound signatures like carbon monoxide concentrations. Measurements of ambient concentrations of methane and carbon dioxide (with known atmospheric concentrations) are used for consistency check.

Mobile White Cell DOAS (MWDOAS or MeDOAS)

The mass concentrations of benzene, toluene, ethylbenzene, m- and p-xylene (BTEX) are measured using a mobile real-time system: Mobile White cell DOAS (MWDOAS or MeDOAS). The MWDOAS system consists of a long optical White cell that is mounted on the measurement vehicle (see Figure A 5). By multiple reflections in the White cell mirror system an overall path length of up to 118 m is obtained depending on configuration, resulting in low detection limits (ppb). The light from the internal lamp is transmitted through the White cell and then analyzed in a DOAS spectrometer, using the UV wavelength region 255 - 285 nm. The system comes in two versions – one open path model and one extractive gas cell model (similar to the MeFTIR system), dependent on application.



Figure A 5. The MeDOAS instrument having an overall optical path-length of up to 118 m.

A measurement begins by acquiring a reference spectrum outside the plume, usually upwind of the facility. Spectra are then sampled and averaged continuously while driving through emission plumes. The averaging time is set to around 6 seconds in order to achieve acceptable SNR (see below). The spatial sampling is also dependent on the vehicle's velocity. A typical driving speed for MWDOAS measurements is 10-20 km/h for sufficient plume sampling. The spectra are geo-tagged and evaluated online using the standard DOAS technique, giving information of plume locations and constituents. Published absorption cross-sections included in the DOAS evaluation routine are tabulated in Table A. 1.

The MWDOAS data is later merged with the corresponding MeFTIR data to produce a plume specific BTEX/Alkane mass ratio. The mass ratio of BTEX/Alkanes is then used to calculate the aromatic flux from individual sub areas where alkane fluxes have been measured by SOF, assuming they have the same source. Specific area plumes are ideally probed at several times, and an overall average of all plume transect BTEX/Alkane ratios is made. The method requires in situ access to the plume of the studied source.

Table A. 1. The UV-cross-sections used in the evaluation of the MWDOAS spectra.

Chemical compound	Origin of reference cross section
O ₃	[Burrows 1999]
SO ₂	[Bogumil 2003]
O ₂	[Bogumil 2003]
Toluene	[Fally 2009]
Benzene	[Etzkorn 1999]
1,3,5-Trimethylbenzene	[Etzkorn 1999]
1,2,4-Trimethylbenzene	[Etzkorn 1999]
Styrene	[Etzkorn 1999]
Phenol	[Etzkorn 1999]
p-Xylene	[Etzkorn 1999]
m-Xylene	[Etzkorn 1999]
Ethylbenzene	[Etzkorn 1999]

The MWDOAS technique has been validated in various surveys by comparison with canister samples acquired at several different locations and which were subsequently analyzed by gas chromatography (GC-FID). The validation shows that the result from MWDOAS lies well within 10% of the result of the certified canister results for BTEX. Due to an absorption cross-section too weak to be used with reliability in the MWDOAS analysis, the ortho isomer of the xylene has been omitted in this comparison. Hence, the xylene concentration from MWDOAS is defined as the sum of the measured m- and p-isomers and the inferred o-isomer from associated MeFTIR or canister speciation.

The MWDOAS system has been used in previous campaigns with good results. For instance, during the 2013 DISCOVER-AQ campaign [Johansson, 2013b] in Houston, Texas, the system was run in parallel to a mobile Proton Transfer Mass spectrometer (PtrMS) lab as a validation check. The results of benzene, toluene and styrene was compared and showed good agreement, with the PtrMS showing slightly elevated benzene concentrations compared to the MWDOAS. The sensitivity of MWDOAS is better than 1 ppb for benzene, better than 3 ppb for toluene, ethylbenzene and m-xylene and 0.5 ppb for p-xylene.

Since the distribution of the BTEX constituents varies with source we will also present the benzene to alkane ratio to facilitate the calculation of benzene flux and identify specific benzene sources.

Note that all concentrations are enhancements above the reference/background.

Wind Measurements and Auxiliary Data

Wind LIDAR

A wind LIDAR (Light Detection and Ranging, ZephIR ZX300) is used to measure vertical wind profiles of wind speed and direction. The LIDAR provides wind profiles in the vertical range of 10 m up to 200+ m above ground, and wind speed accuracy of 0.1 m/s. The system records 1-s data, and 1-minute averages are typically used for flux calculations. The principle of detection is based on the Doppler shift of the infrared pulse that the instrument sends out and retrieves.



Figure A 6. Wind LIDAR ZX300 installed on the bed of a pick-up truck.

Wind Masts

Meteorological parameters are also measured at selected sites using a portable 3-10 m mast. This mast is equipped with a calibrated RM Young 05108 “prop and vane” anemometer and a Campbell Scientific CR5000 data-logger, see Figure A 7.



Figure A 7. The FluxSense mobile wind mast with an RM Young anemometer mounted on top. The mast was raised to 10 m height.

Airmar (Mobile Weather Station)

A sonic wind meter (Airmar WeatherStation 200 WX) is installed on the roof of the measurement vehicle to complement the other wind measurements and give local ground winds at the vehicle. The wind information from the car-based Airmar is not used for flux calculation since the wind field can be heavily disturbed and turbulent. The Airmar is only used as a real-time aid to keep track of the plume directions when making the gas emission measurements. The Airmar provides wind speed and direction relative to true north (compensating for vehicle position), as well as air temperature, pressure and relative humidity. It also provides GPS positions that may be used as a backup for the other GPS-antenna.

GPS

The FluxSense vehicle is equipped with two standard USB GPS-L1 receivers (GlobalSat BU-353S4) hooked up to the SOF and MWDOAS-computers. They are placed horizontally on the roof and by the windscreen for optimal reception. The receivers give the position at a rate of 1 Hz.

Principal Equations

The primary methods in this project is the direct flux measurements from SOF and SkyDOAS. In the secondary method BTEX and alkene fluxes are measured indirectly from MWDOAS/MeFTIR or canister gas mass ratios.

DIRECT FLUX MEASUREMENTS:

The emission mass flux (Q) of species (j) measured by SOF for a single transect (T) across the plume (P) along path (l) can be expressed by the following integral (SI-units in gray brackets):

$$Q_T^j [\text{kg/s}] = \bar{v}_T [\text{m/s}] \cdot \int_P C_l^j [\text{kg/m}^2] \cdot \cos(\theta_l) \cdot \sin(\alpha_l) dl [\text{m}]$$

Where,

\bar{v}_T = the average wind speed at plume height for the transect,

C_l^j = the measured slant column densities for the species j as measured by SOF or SkyDOAS,

θ_l = the angles of the light path from zenith ($\cos(\theta_l)$ gives vertical columns),

α_l = the angles between the wind directions and driving directions

dl = the driving distance across the plume

Note that SOF and SkyDOAS have different light paths, where the SkyDOAS telescope is always looking in the zenith direction while the SOF solar tracker is pointing toward the Sun. Hence, the measured SOF slant column densities will vary with latitude, season and time of day.

To isolate emissions from a specific source, the incoming/upwind background flux must be either insignificant or subtracted. If the source is encircled, the integral along l is a closed loop and the flux calculations are done with sign.

INDIRECT FLUX MEASUREMENTS:

The indirectly measured flux (indirectly measured emission, IME) is computed using a combination of SOF and MeFTIR/MWDOAS measurements. The indirect mass flux (\hat{Q}^i) for species (i) are calculated from MeFTIR and/or MWDOAS gas mass ratios integrated over the plume (P) along path (l) are given by (SI-units in gray brackets):

$$\hat{Q}^i [\text{kg/h}] = \bar{Q}^j [\text{kg/h}] \cdot \frac{1}{k} \sum_k \frac{\int_P N_l^i [\text{mg/m}^3] dl [\text{m}]}{\int_P N_l^j [\text{mg/m}^3] dl [\text{m}]}$$

Where,

\bar{Q}^j = the average flux of species j from multiple transects as measured by SOF,

N_l^i = the number density concentrations of species i as measured by MWDOAS or MeFTIR,

N_l^j = the number density concentrations of species j as measured by MeFTIR,

k = the number of gas ratio measurements

Note that the IME operates on average values since simultaneous SOF, MWDOAS and MeFTIR measurements are not always performed and because individual gas ratios are more variable and uncertain than the average. Although not necessarily simultaneously measured, SOF and MeFTIR/MWDOAS measurements must represent the same source plumes. Note also that gas ratios do

not intrinsically depend on complete plume transects (like for direct flux methods) as long as the emission plume is well mixed at the sampling distance.

Uncertainties and Error Budget

A summary of the typical performance of the FluxSense measurements is presented in Table A. 2.

In addition, for each site the statistical error is calculated. It corresponds to the random error but in addition there could be systematic errors. For instance, in the used wind speed due to the errors in estimated height of the plume and spectral calibration errors. The statistical error is given by the 95 % Confidence Interval (CI) for the mean, \bar{x} , according to:

$$CI = \bar{x} \pm t_{.025} \frac{s}{\sqrt{N}}$$

Here t is Student's T distribution and s corresponds to sample standard deviation:

$$s_x = \sqrt{\frac{\sum_{i=1}^N (x - \bar{x})^2}{N - 1}}$$

Table A. 2. Performance of FluxSense measurement methods.

Measurement Parameter	Analysis Method	Accuracy	Precision
SOF column concentrations alkanes, alkenes, NH ₃	QESOF spectral retrieval	±10%	±5%
SkyDOAS column concentrations NO ₂ , SO ₂ , H ₂ CO	DOAS spectral retrieval	±10%	±5%
MeFTIR concentrations CH ₄ , VOC*, NH ₃ , N ₂ O, C ₂ H ₄	QESOF spectral retrieval	±10%	±5%
MWDOAS concentrations BTEX, Benzene	MWDOAS spectral retrieval	±10%	±5%
Wind Speed (10 m)	R.M. Young Wind monitor	±0.3 m/s or 1%	±0.3 m/s
Wind Direction (10 m)	R.M. Young Wind monitor	±5°	±3°
LIDAR Wind Speed (10-200+ m)	Doppler LIDAR	±0.1 m/s	-
GPS position	USB GPS receiver	±2m	±2m
SOF mass flux Alkanes, alkenes, NH ₃	SOF-Report flux calculations	±30%	±10%
SkyDOAS mass flux SO ₂ , H ₂ CO, NO ₂	SkyDOAS flux calculations	±30%	±10%

* MeFTIR measures concentrations of total VOCs as observed by C-H-stretch absorption in the 2700-3100 cm⁻¹ wavenumber region.

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B - Wind data

Figure B 1 through Figure B 6 show wind speed data acquired by a ZX300 wind LIDAR between 10 m - 300 m height above ground, for the period 10 May - 21 May, 2021. Figure B 7 to Figure B 17 show wind speed and wind direction data both at different height levels and as composite wind profiles over the course of the day.

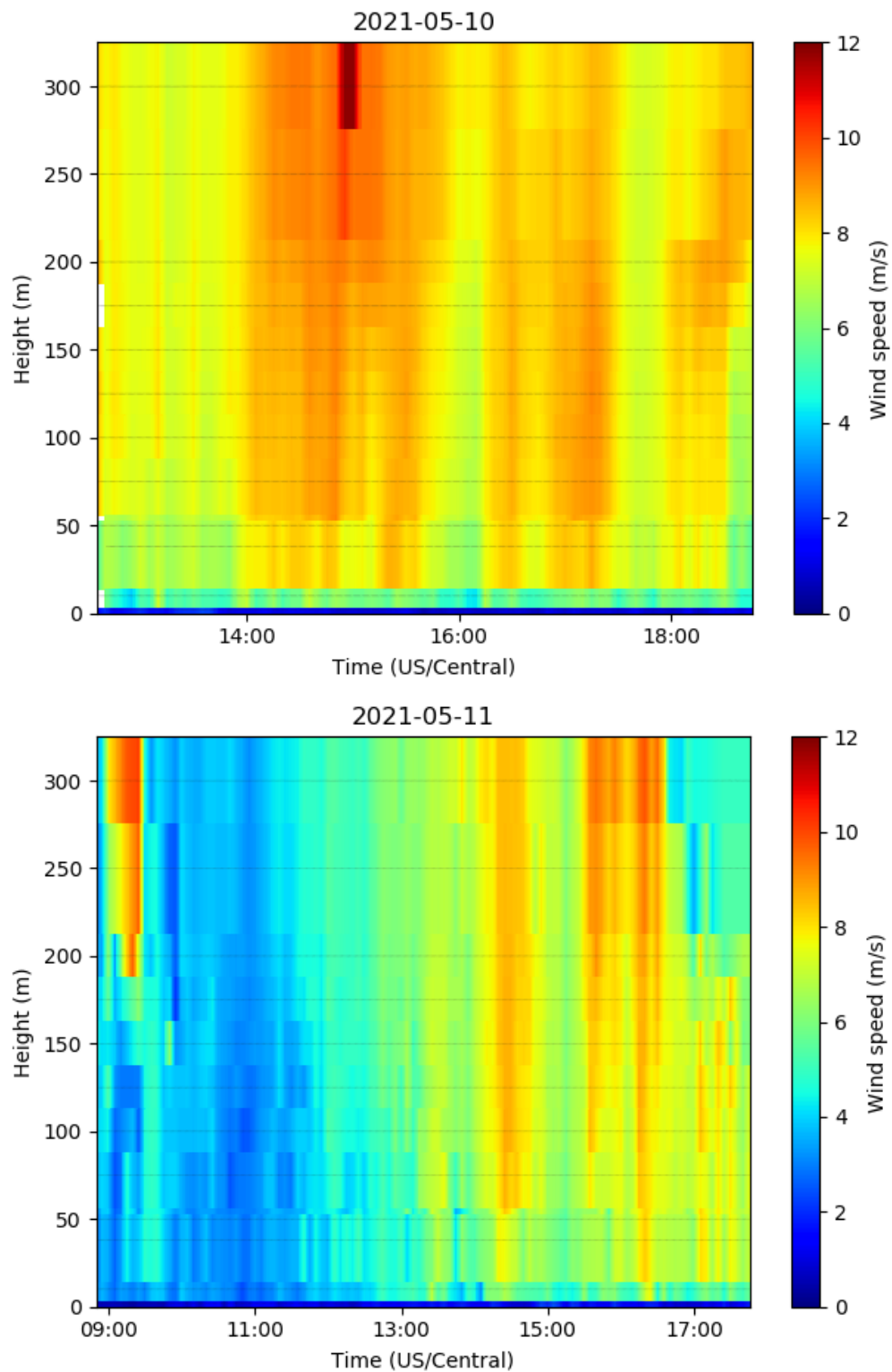


Figure B 1. Wind LIDAR wind speed data from 10 May (top) and 11 May (bottom), 2021.

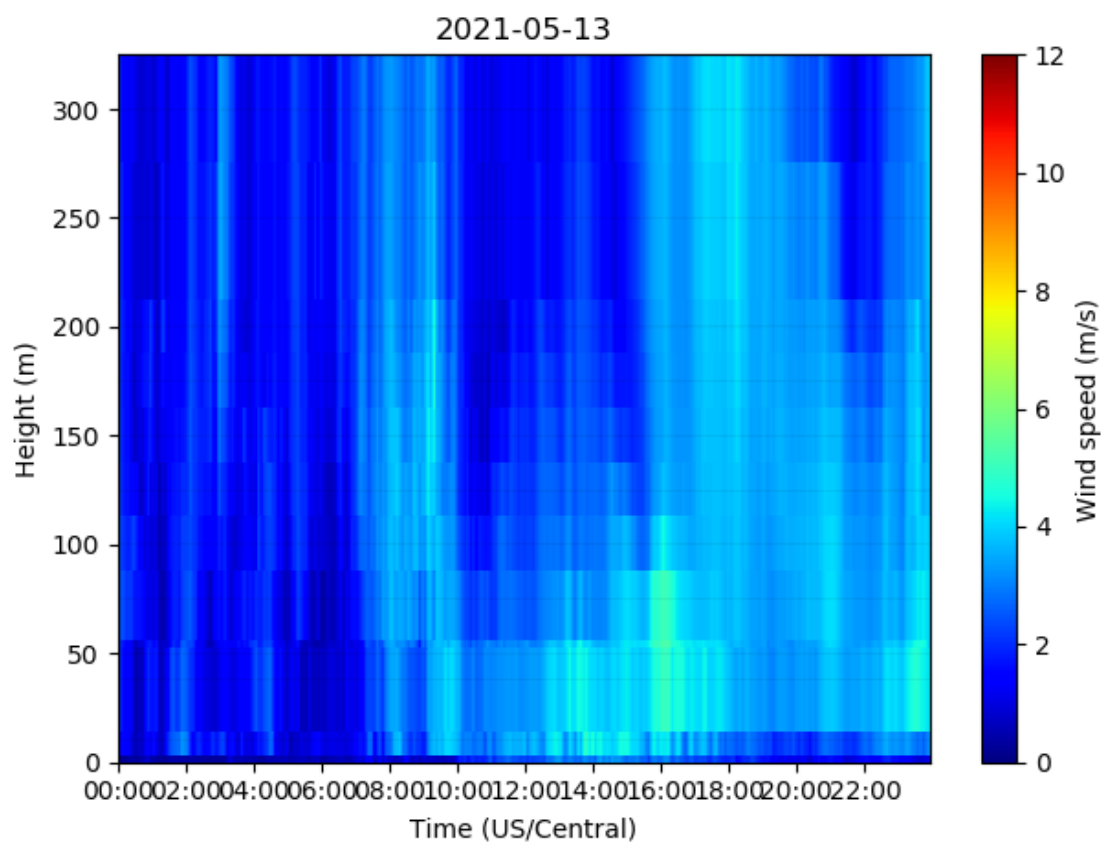
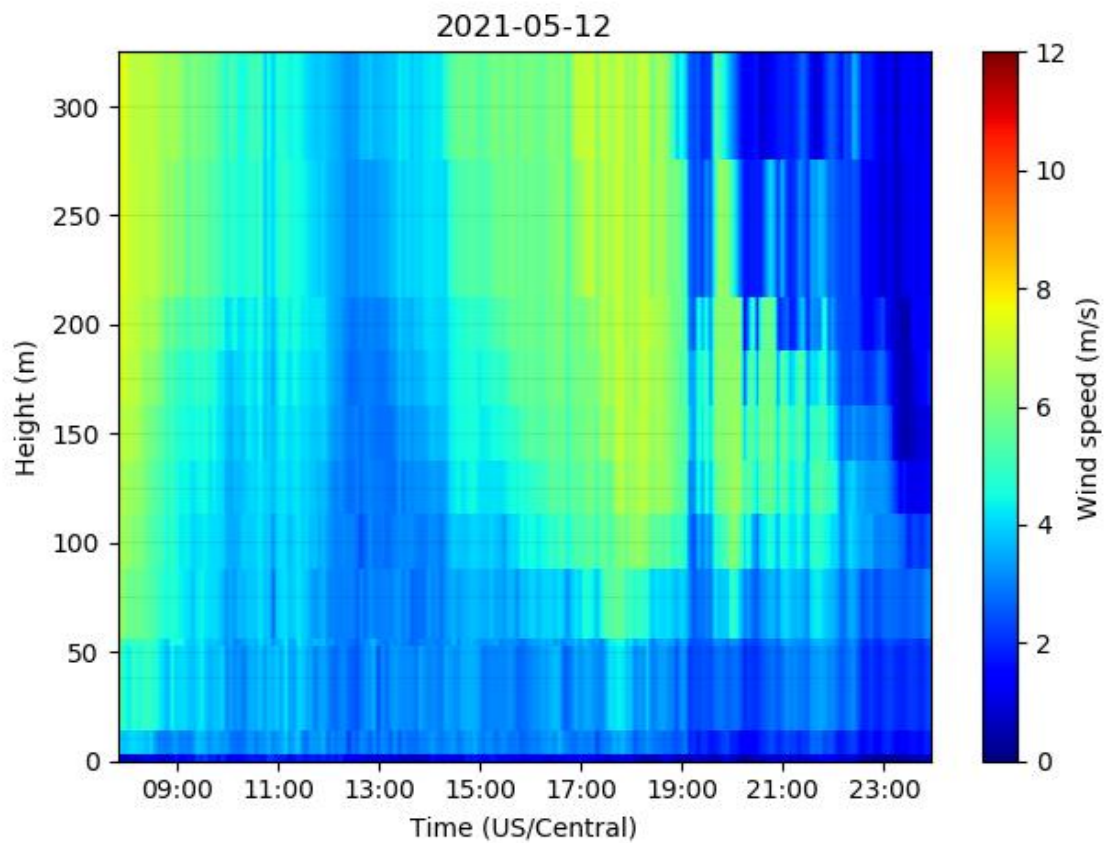


Figure B 2. Wind LIDAR wind speed data from 12 May (top) and 13 May (bottom), 2021.

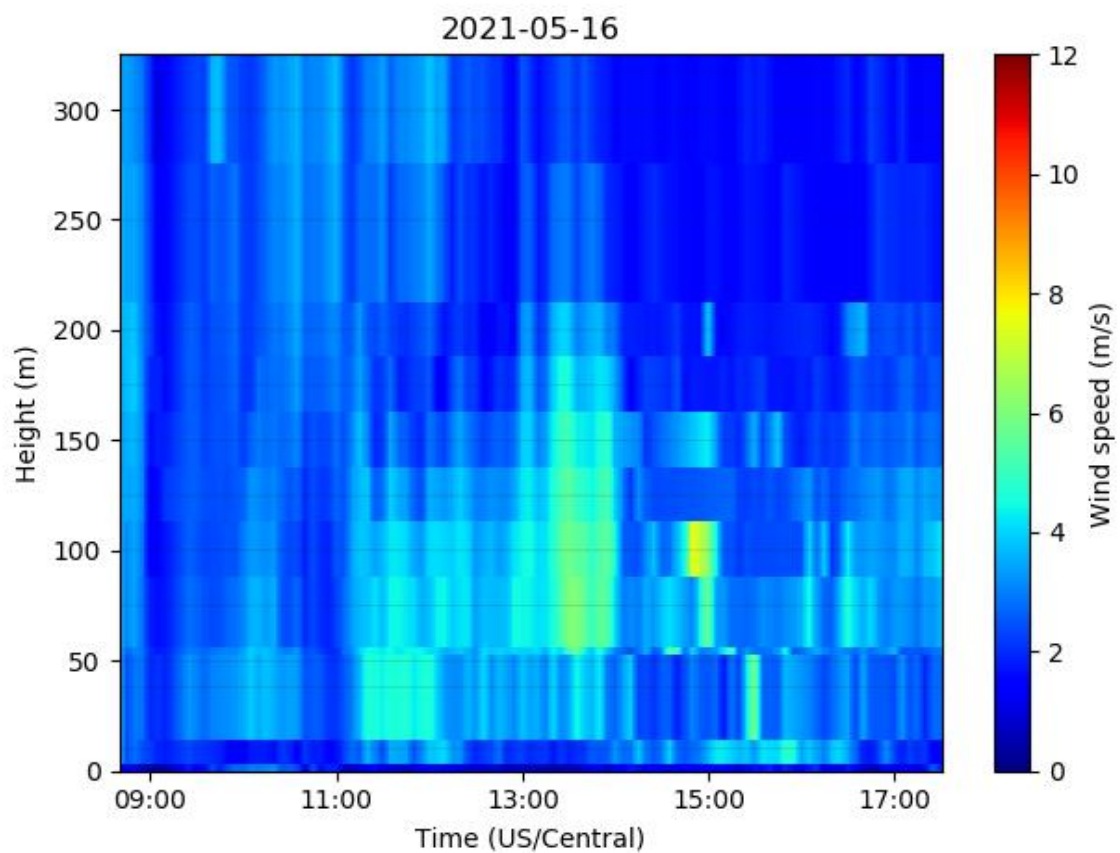
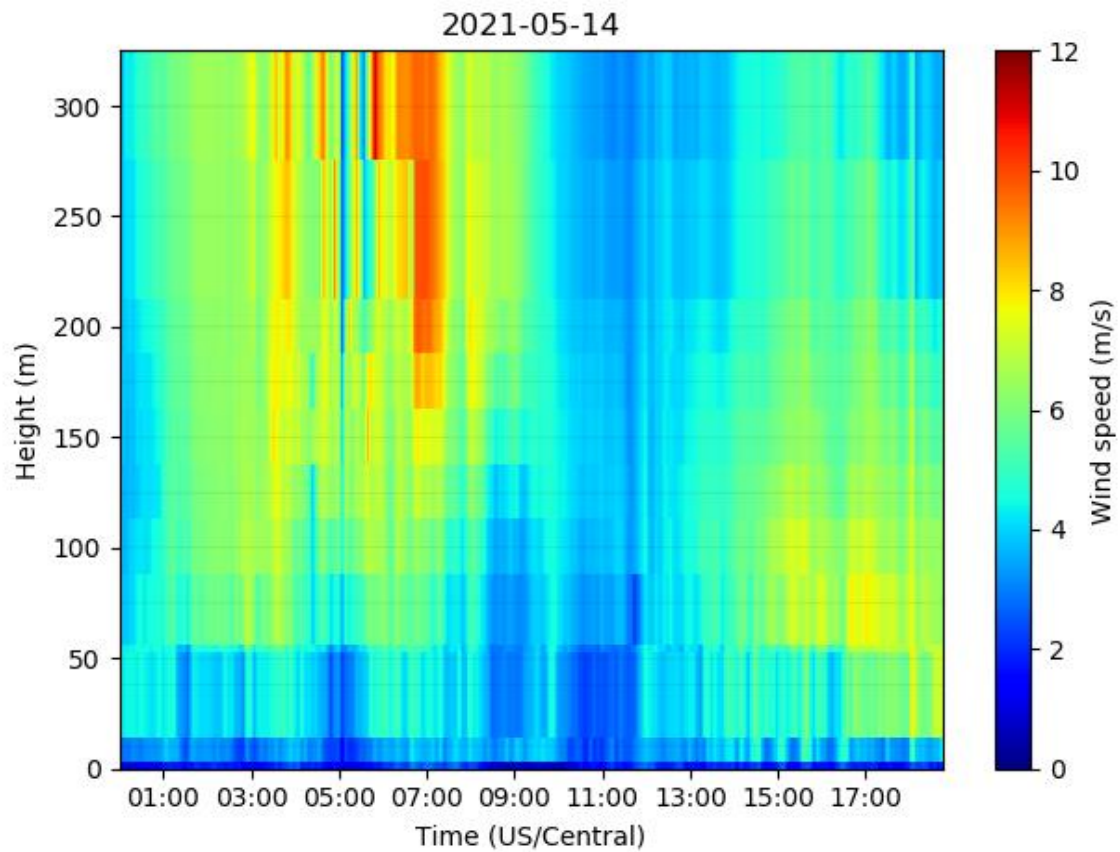


Figure B 3. Wind LIDAR wind speed data from 14 May (top) and 16 May (bottom), 2021.

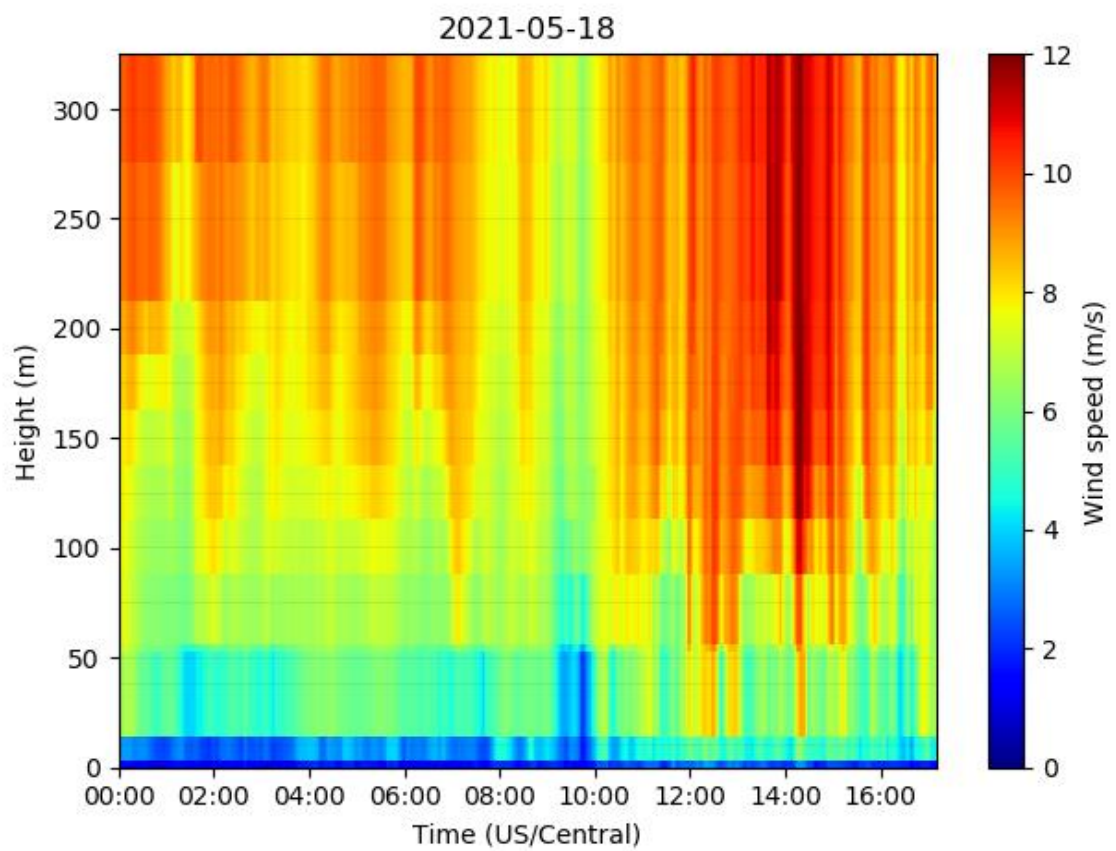
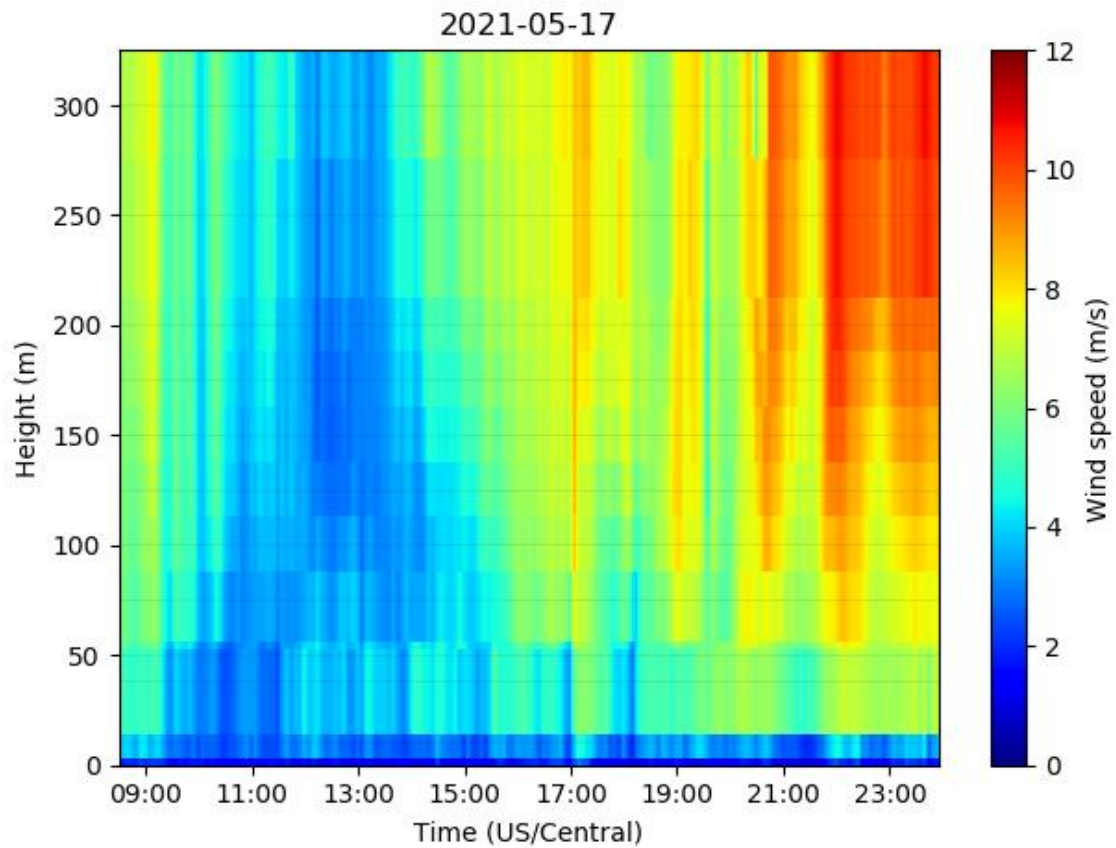


Figure B 4. Wind LIDAR wind speed data from 17 May (top) and 18 May (bottom), 2021.

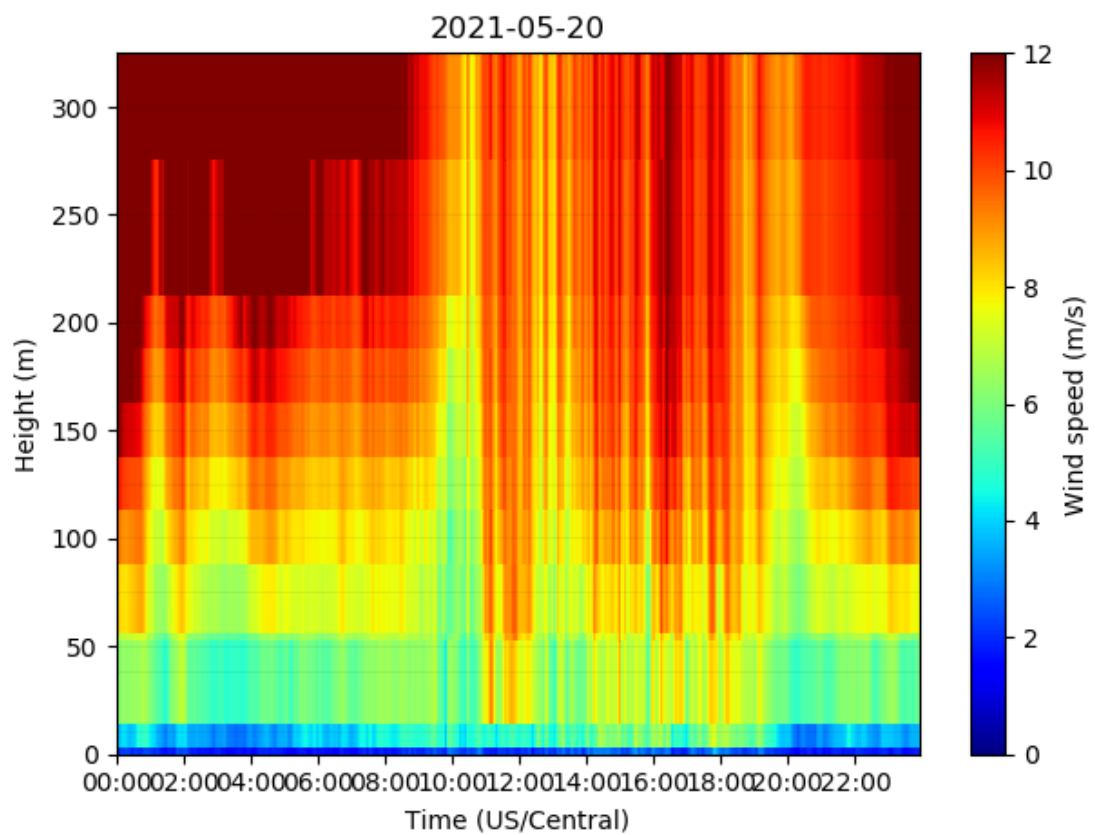
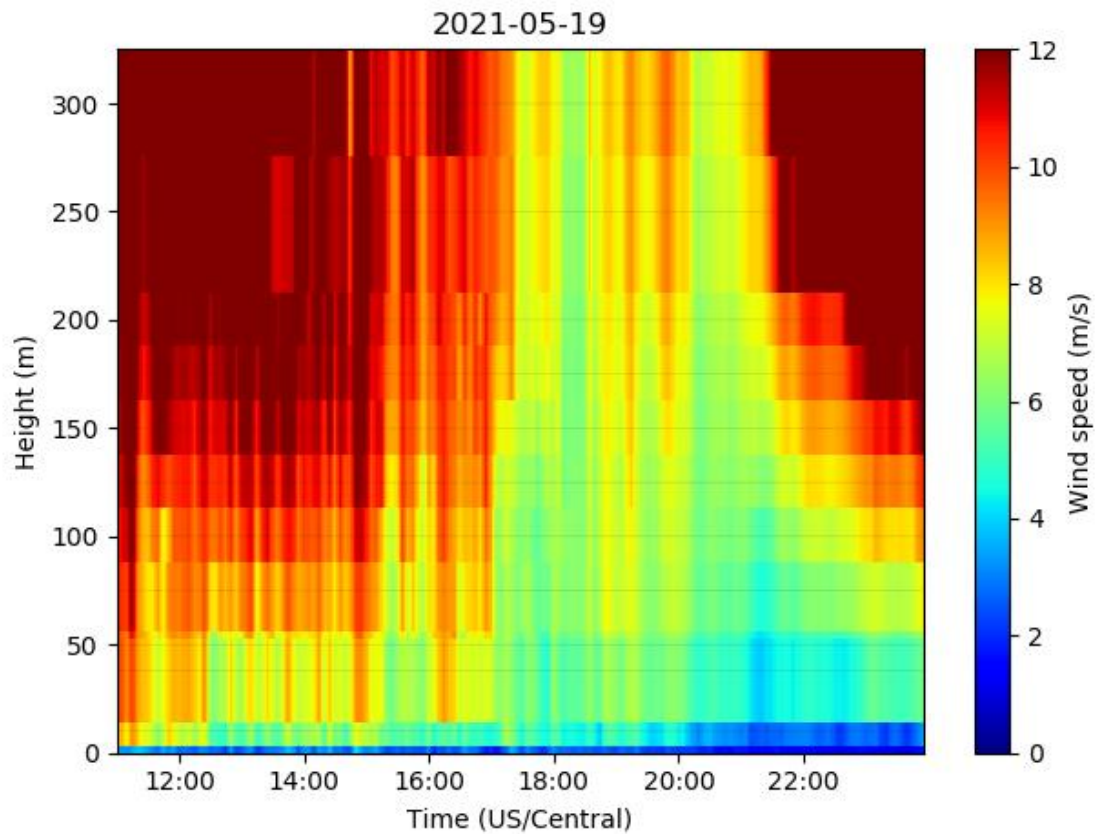


Figure B 5. Wind LIDAR wind speed data from 19 May (top) and 20 May (bottom), 2021.

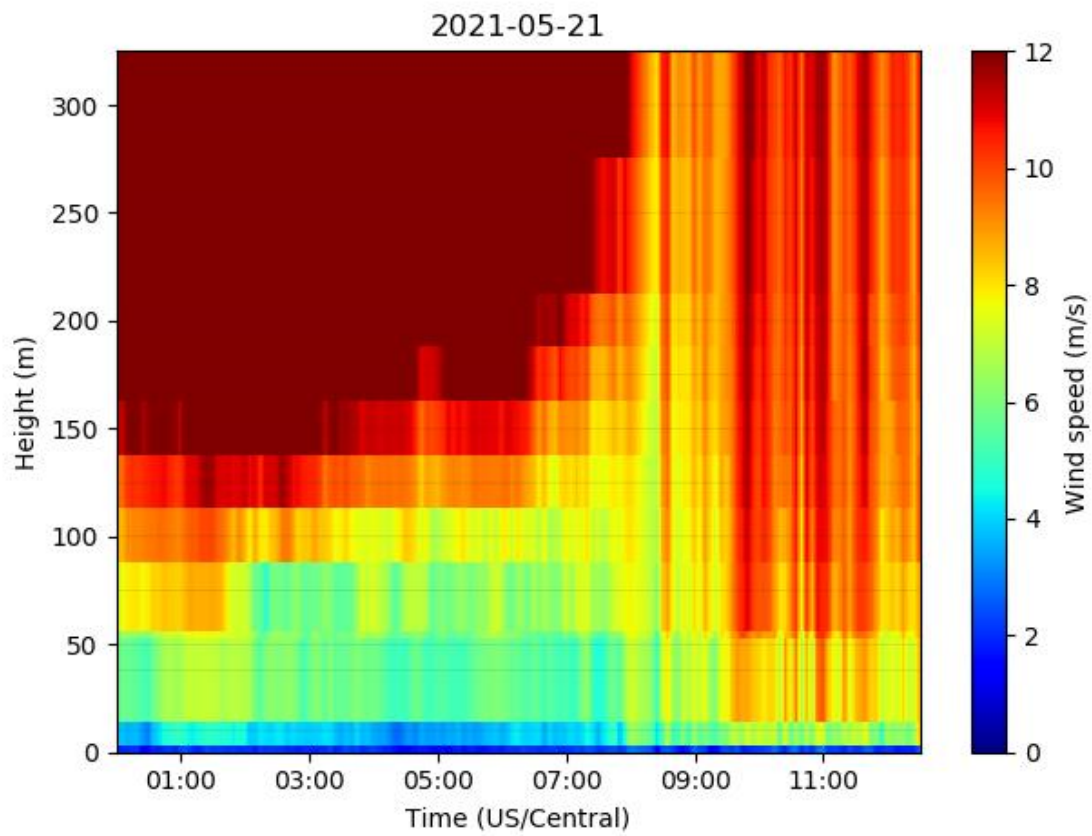


Figure B 6. Wind LIDAR wind speed data from 21 May, 2021.

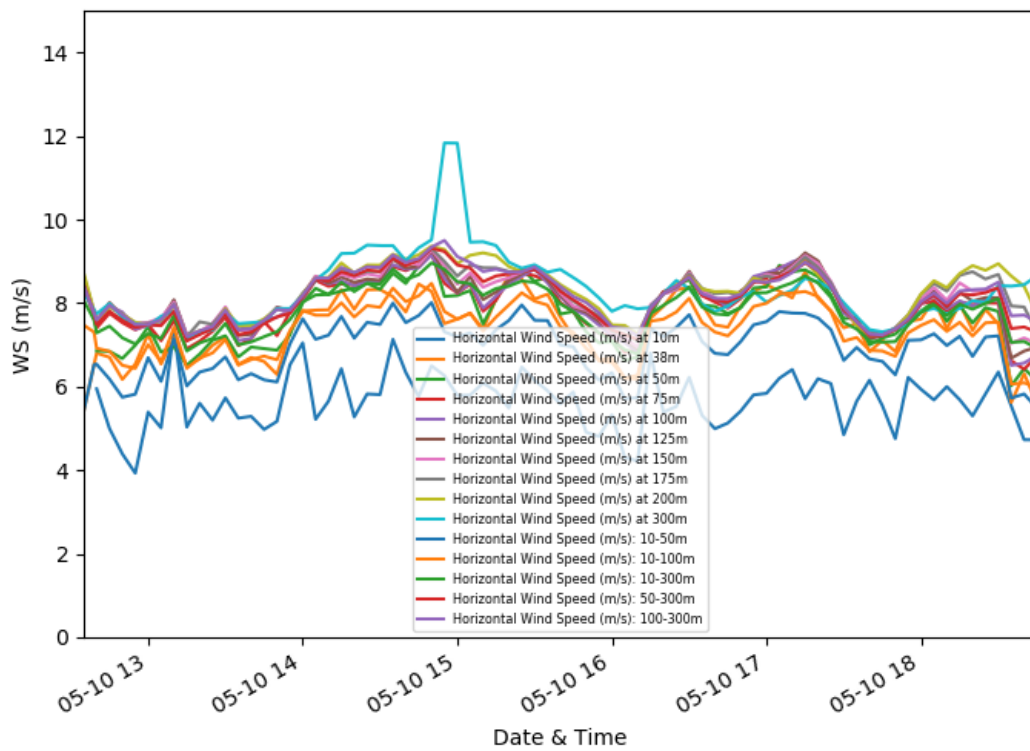
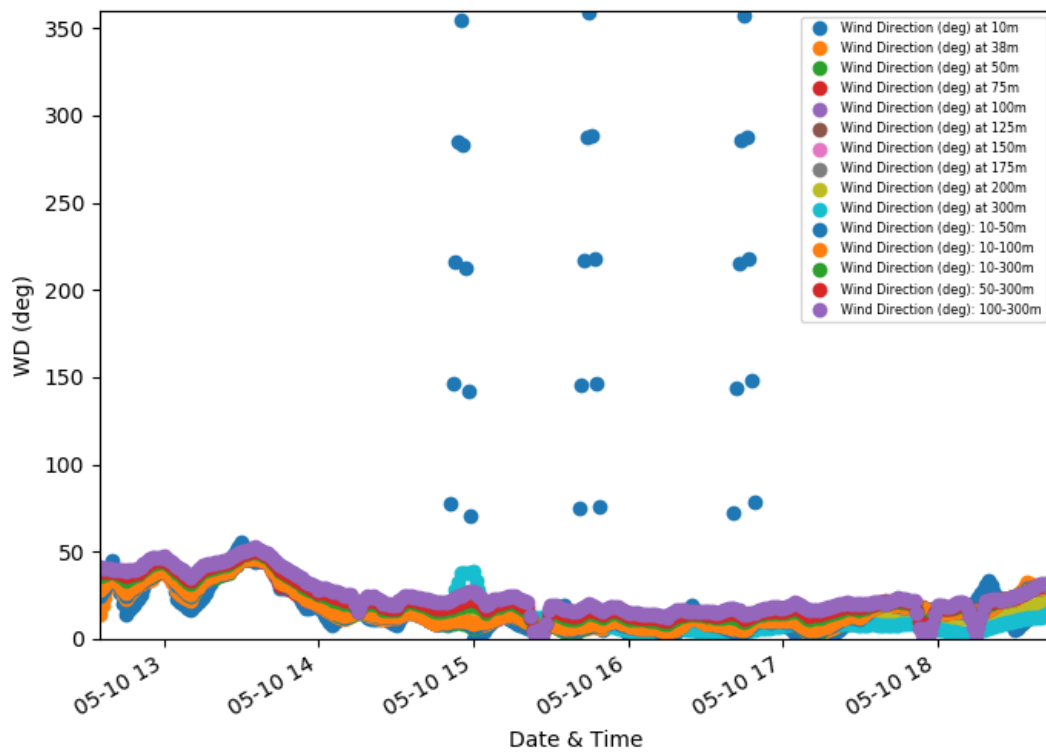


Figure B 7. Wind LIDAR wind direction (top) and wind speed data (bottom), 10 May 2021, showing both data at specific heights and composite wind profile data.

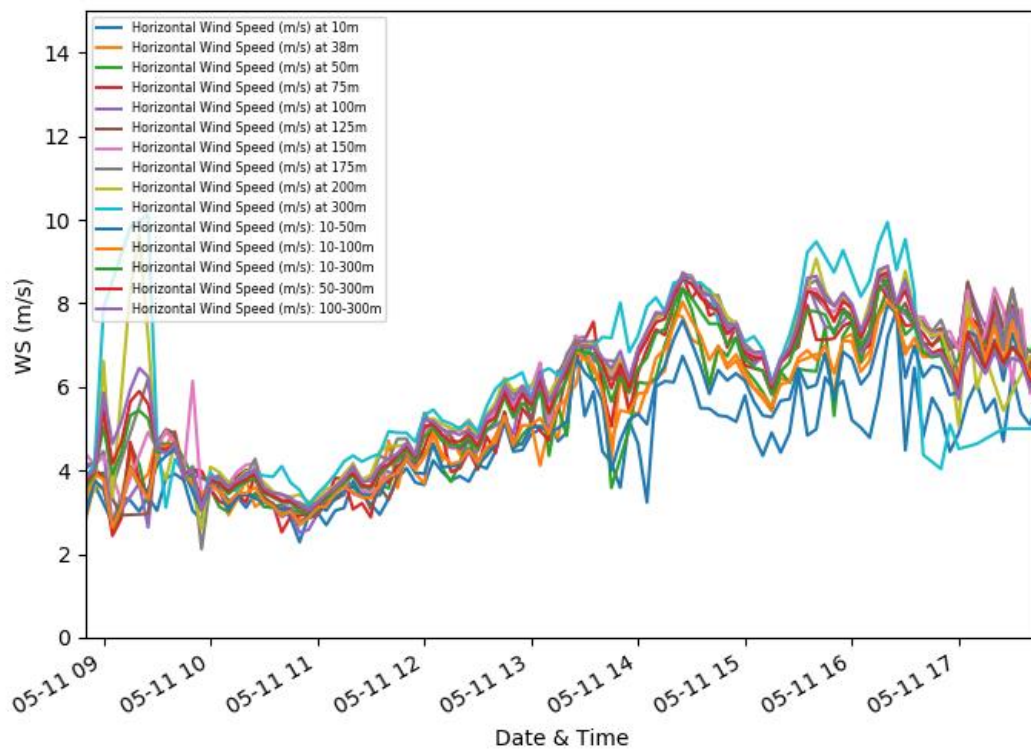
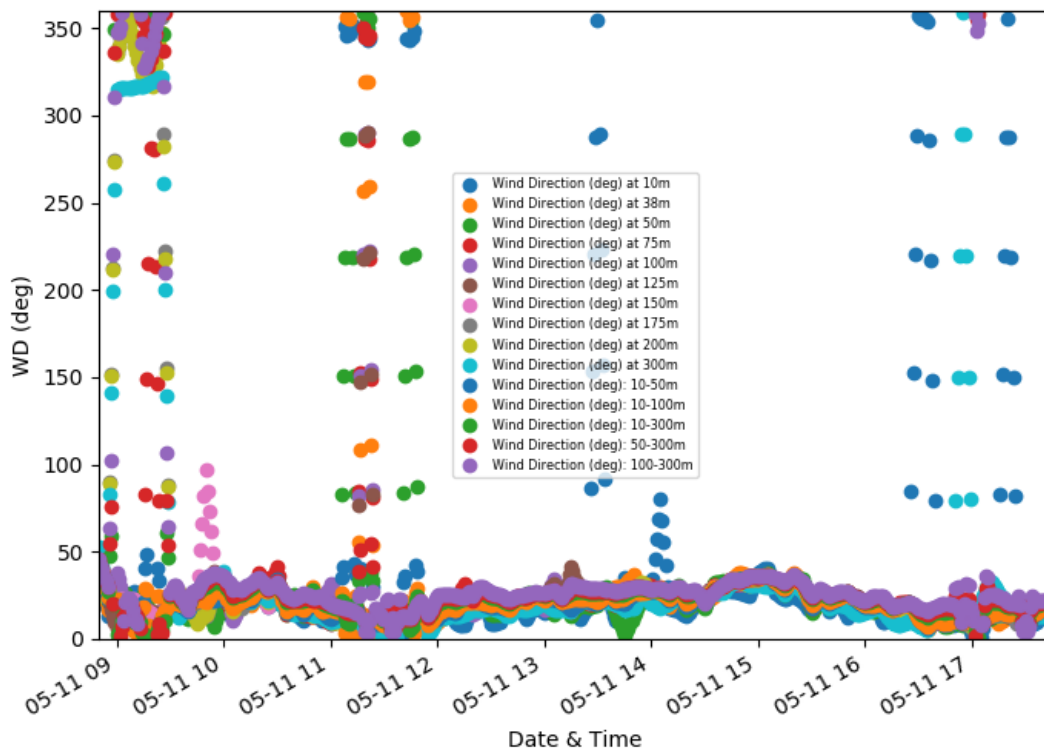


Figure B 8. Wind LIDAR wind direction (top) and wind speed data (bottom), 11 May 2021, showing both data at specific heights and composite wind profile data.

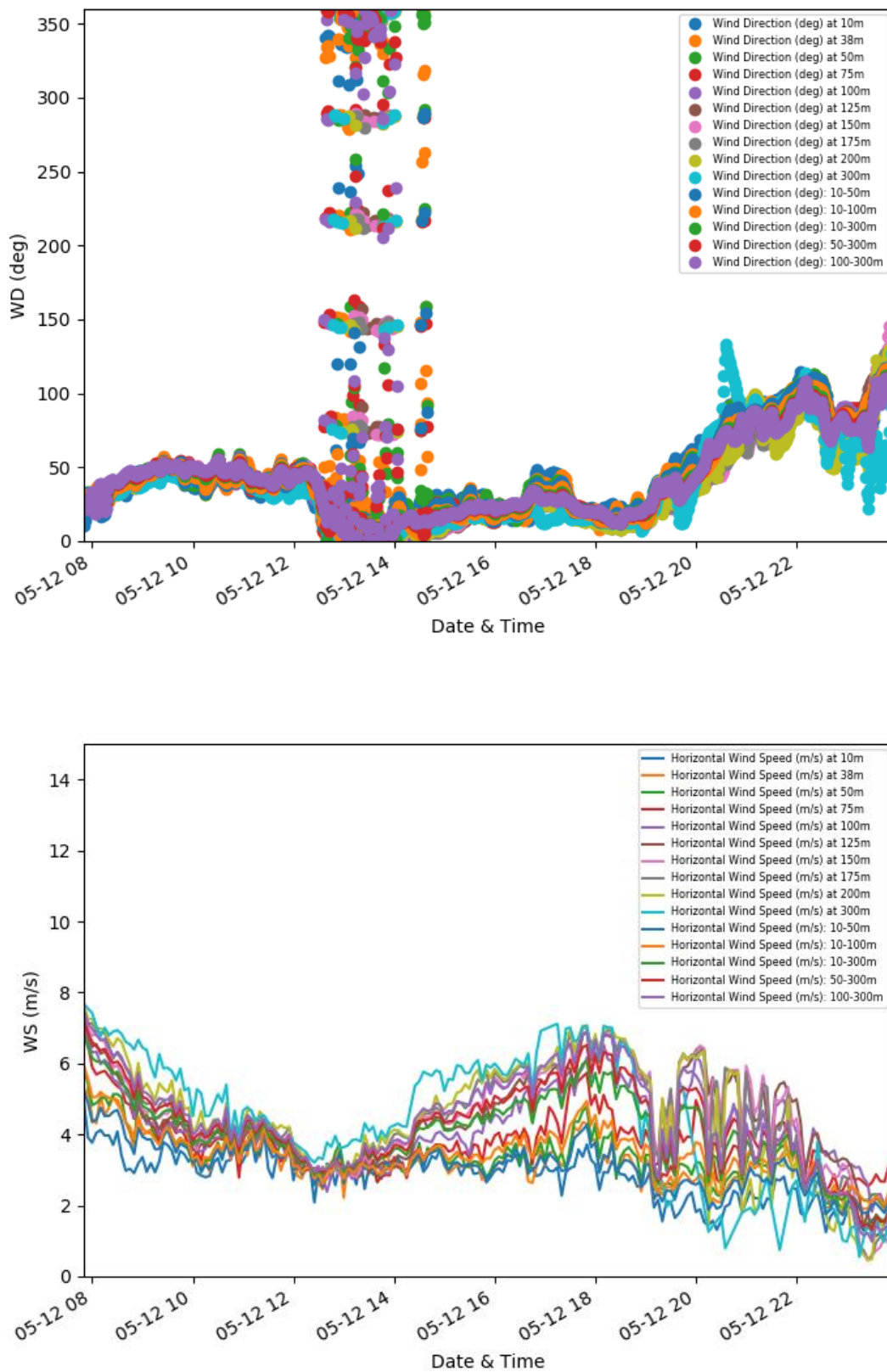


Figure B 9. Wind LIDAR wind direction (top) and wind speed data (bottom), 12 May 2021, showing both data at specific heights and composite wind profile data.

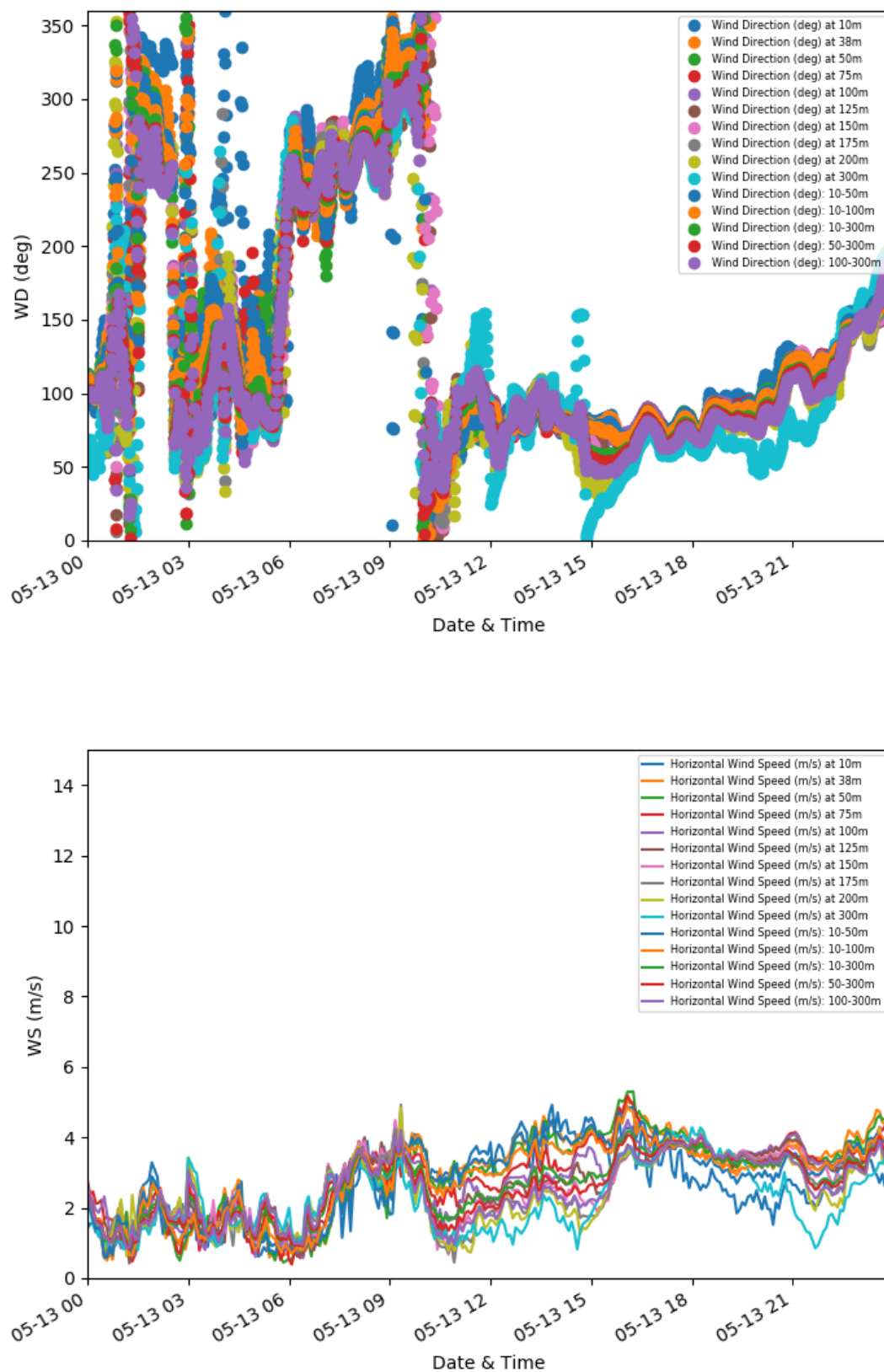


Figure B 10. Wind LIDAR wind direction (top) and wind speed data (bottom), 13 May 2021, showing both data at specific heights and composite wind profile data.

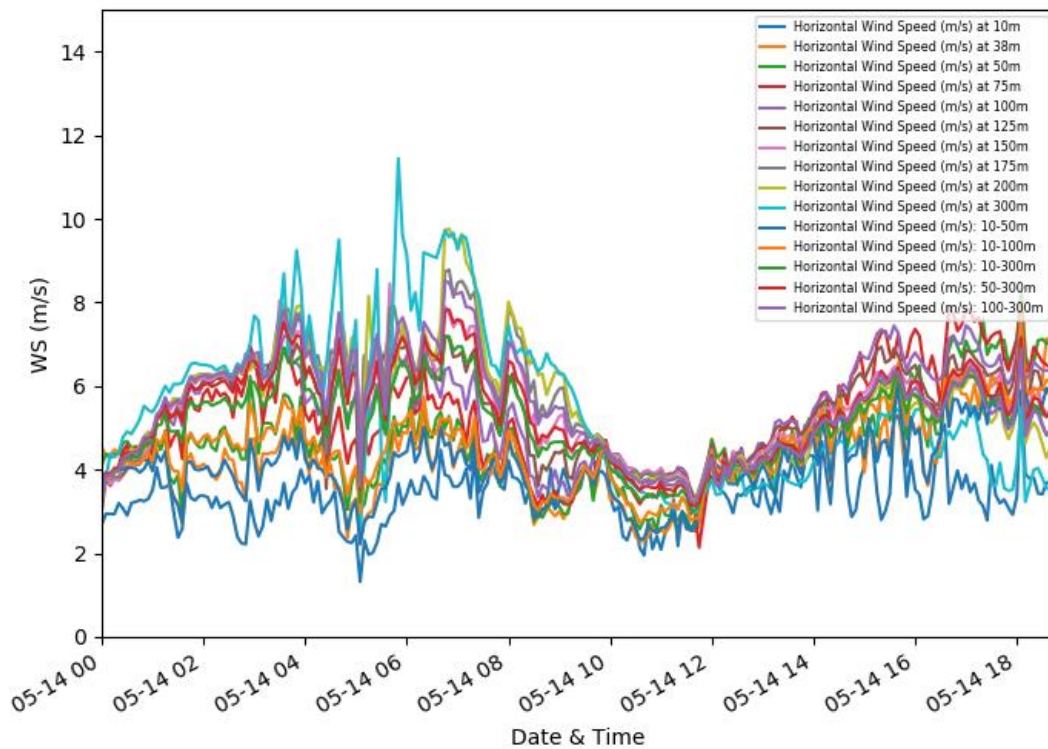
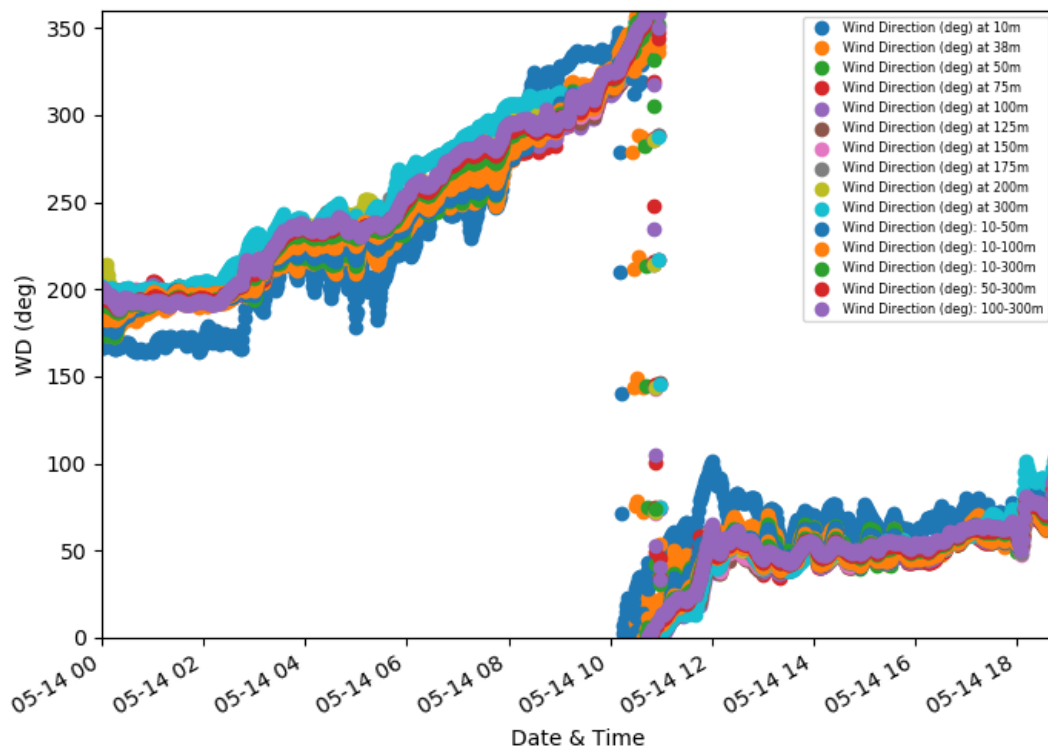


Figure B 11. Wind LIDAR wind direction (top) and wind speed data (bottom), 14 May 2021, showing both data at specific heights and composite wind profile data.

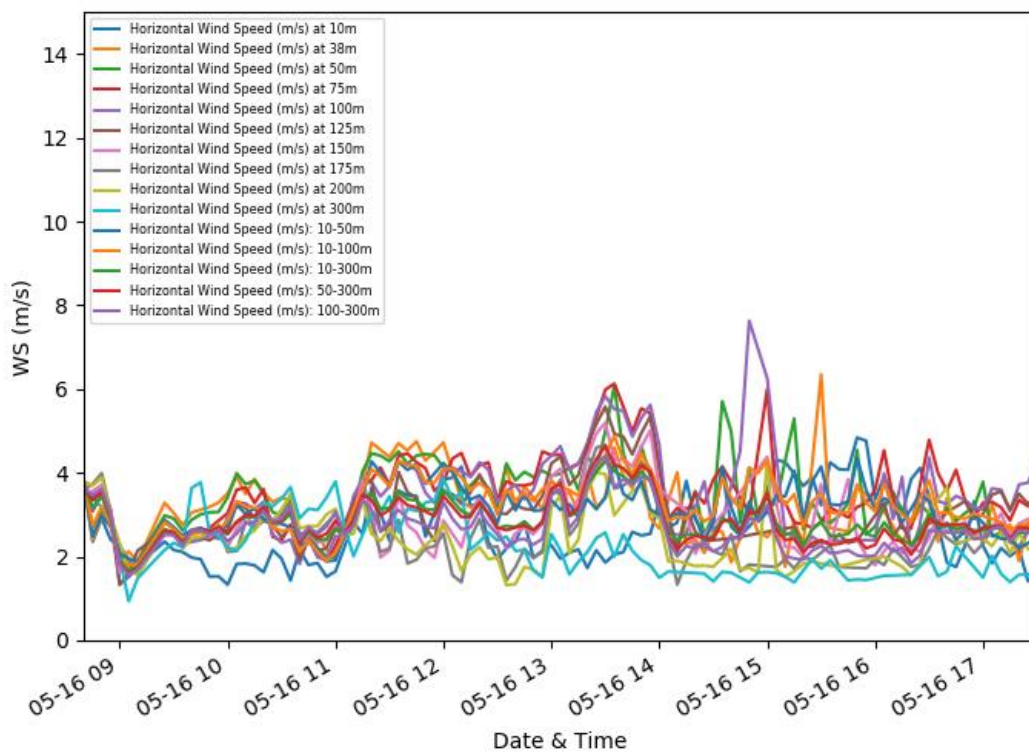
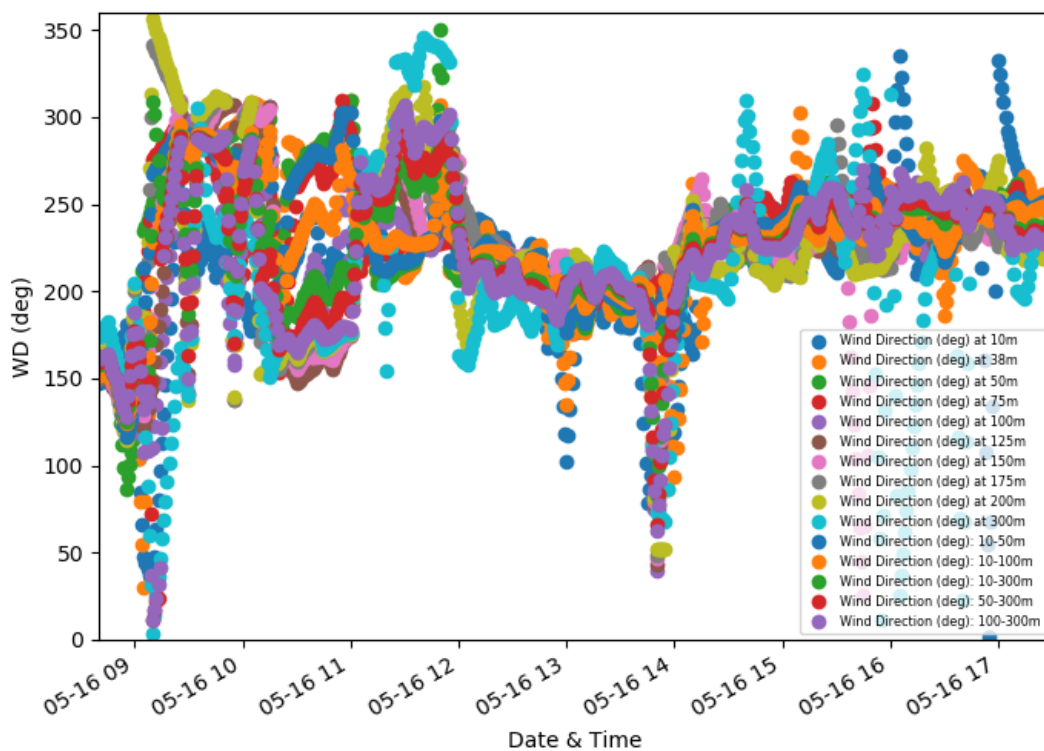


Figure B 12. Wind LIDAR wind direction (top) and wind speed data (bottom), 16 May 2021, showing both data at specific heights and composite wind profile data.

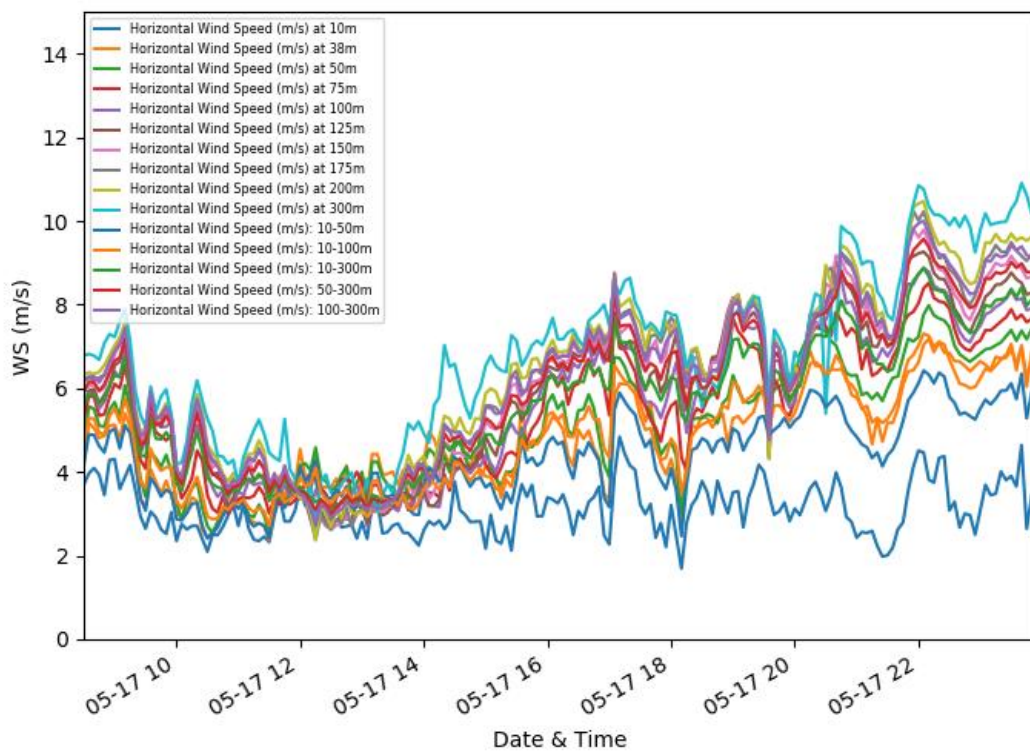
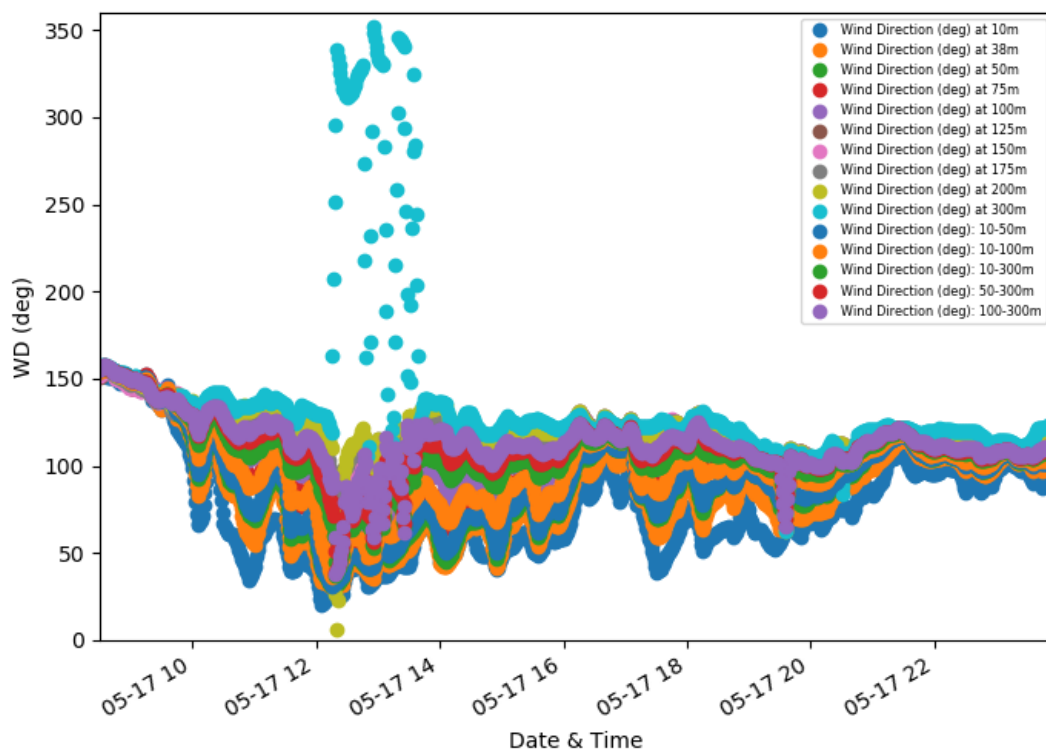


Figure B 13. Wind LIDAR wind direction (top) and wind speed data (bottom), 17 May 2021, showing both data at specific heights and composite wind profile data.

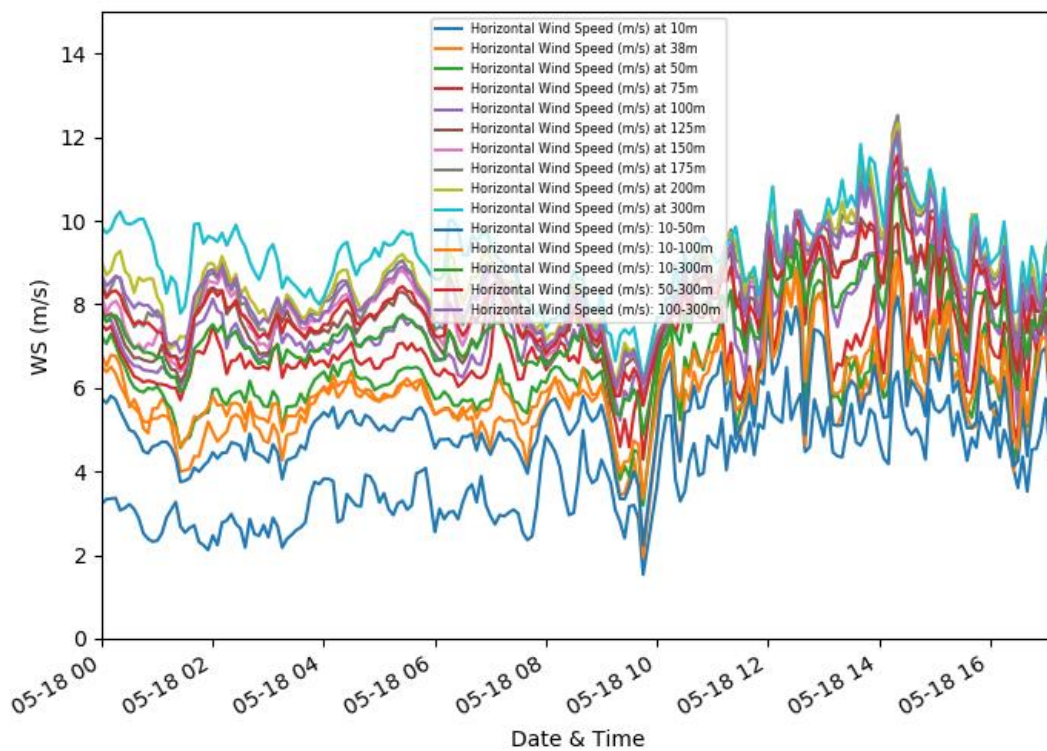
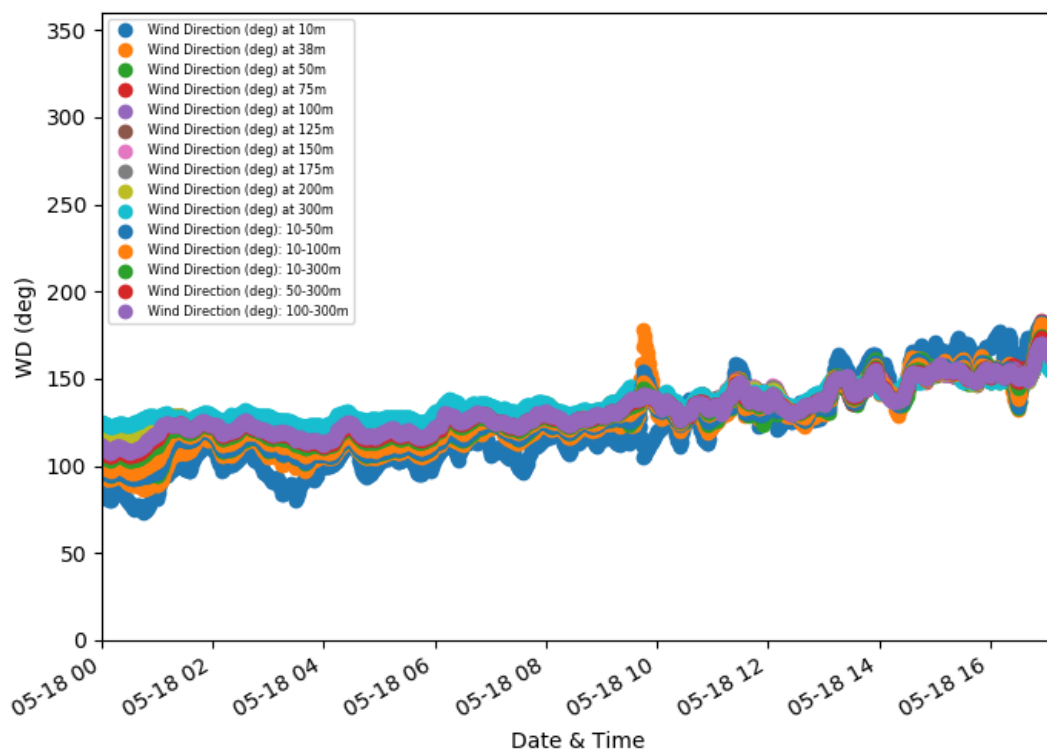


Figure B 14. Wind LIDAR wind direction (top) and wind speed data (bottom), 18 May 2021, showing both data at specific heights and composite wind profile data.

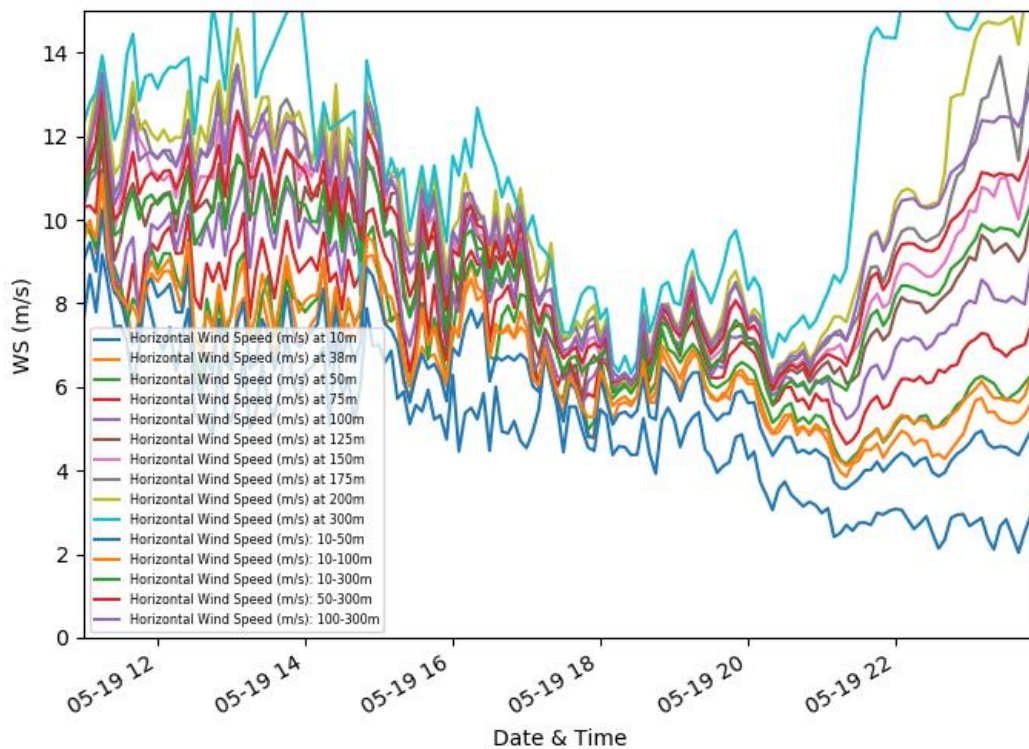
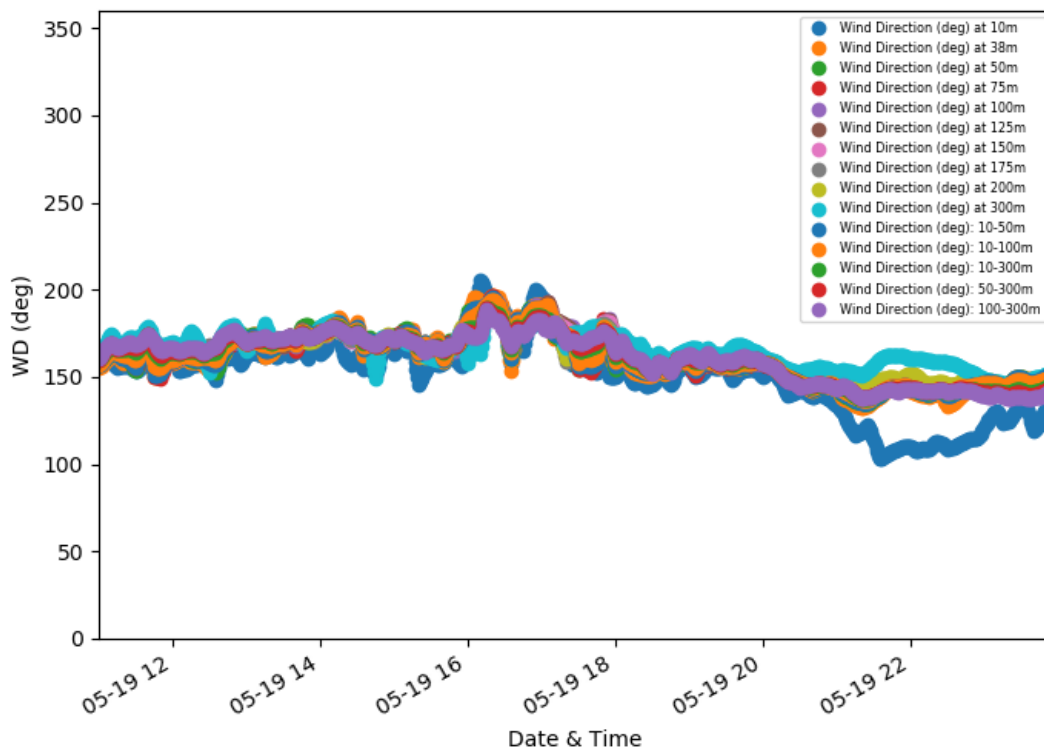


Figure B 15. Wind LIDAR wind direction (top) and wind speed data (bottom), 19 May 2021, showing both data at specific heights and composite wind profile data.

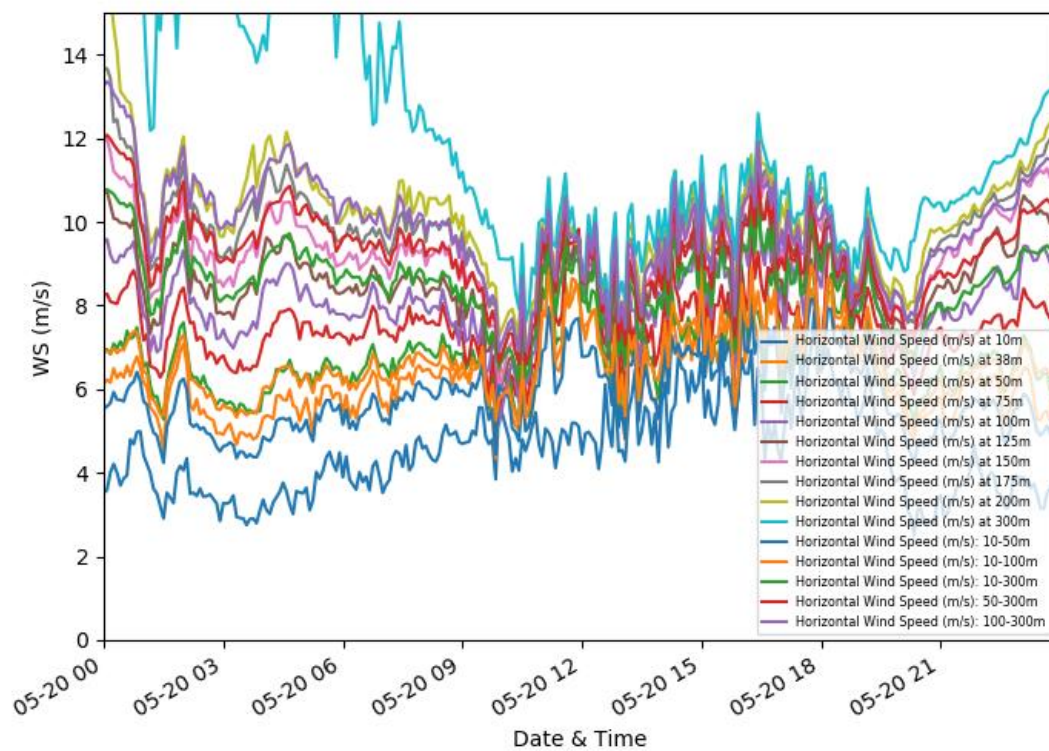


Figure B 16. Wind LIDAR wind direction (top) and wind speed data (bottom), 20 May 2021, showing both data at specific heights and composite wind profile data.

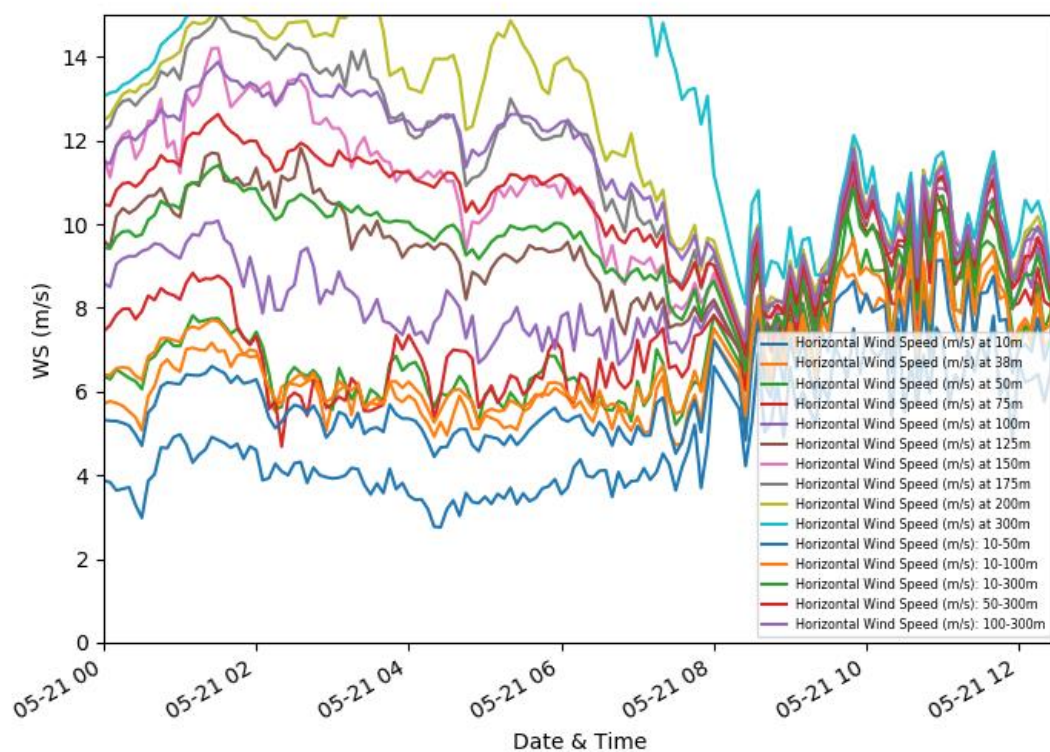
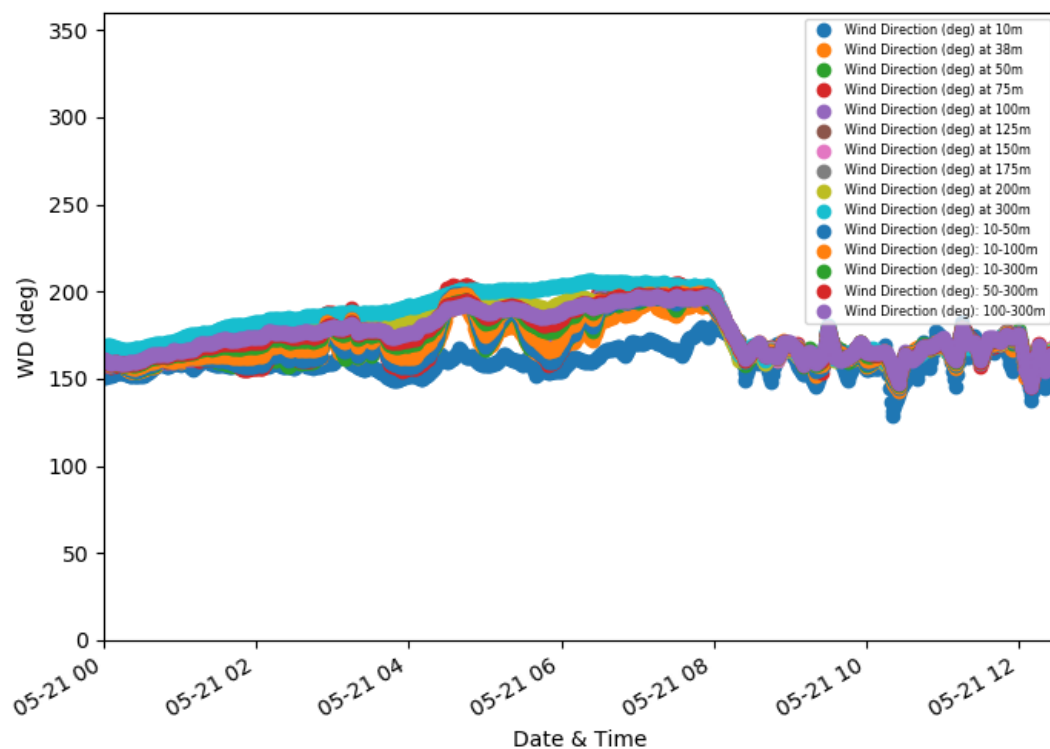


Figure B 17. Wind LIDAR wind direction (top) and wind speed data (bottom), 21 May 2021, showing both data at specific heights and composite wind profile data.

C - Canister data

Canister samples were analyzed at the accredited lab of Swedish Environmental Institute (IVL) in Gothenburg Sweden. Samples were analyzed using FID and MS detectors, and results reported by Annika Potter, IVL. The canisters (Entech Instruments Inc make, Silonite coated, 1.4 L volume with micro-QT valves) were cleaned and prepared at FluxSense lab in Gothenburg, Sweden using Entech Instruments oven and cleaning system run with nitrogen of scientific purity grade (6.0). The following tables Table C 1 to Table C 5 report the canister sample analysis results.

Table C 1. Canister sample data. Concentrations in $\mu\text{g}/\text{m}^3$. *p* denotes production mode and *np* non-production. The less than sign (<) indicates the detection limit, and that the sample concentration was below it.

Can. ID	Sample location	Sample date	Ethane	Ethene	Propane	Propene	Iso-butane	n-Butane	t-2-Butene
3135	Upwind process	16 May 2021	4.2	0.2	1.6	0.2	0.6	1.9	<0.11
3146	Upwind process	18 May 2021	5.9	0.4	3.8	0.3	1.9	6.1	0.2
1036	Fenceline	16 May 2021	3.1	0.5	0.9	0.2	0.3	0.5	0.1
3156	Fenceline	16 May 2021	3.9	0.2	1.4	0.2	0.8	1.5	<0.11
1043	Fenceline	16 May 2021	3.9	0.2	2.4	0.5	0.5	1.4	0.1
3152	Fenceline	16 May 2021	5.5	0.4	3.4	0.2	0.7	2.7	<0.11
3153	Fenceline	18 May 2021	7.8	0.4	3.6	0.5	0.8	1.6	0.2
3157	Fenceline	18 May 2021	8.9	0.5	3.0	0.3	1.3	2.6	0.1
3165	Fenceline	18 May 2021	8.5	0.4	2.1	0.3	1.1	2.5	0.1
3162	Fenceline	18 May 2021	4.1	0.5	1.3	0.2	0.6	1.3	0.1
3160	Fenceline	18 May 2021	14.9	0.7	5.7	1.0	2.7	4.3	0.3
3150	PCM charge	14 May 2021	28.5	6.3	6.9	1.5	1.2	6.0	0.2
3139	PCM charge	14 May 2021	3.8	0.6	4.1	0.3	2.3	5.2	0.2
3145	PCM push	14 May 2021	72.3	18.5	26.1	12.9	3.5	11.5	1.2
3143	PCM push	14 May 2021	13.3	4.4	16.0	1.9	0.8	13.2	0.3
1044	CEMS ^{np}	17 May 2021	2.4	0.7	1.5	0.1	0.8	2.2	<0.11
1046	CEMS ^p	17 May 2021	2.4	1.0	1.8	0.2	1.1	2.4	<0.11
1153	CEMS ^{np}	17 May 2021	4.2	0.5	1.1	<0.09	0.6	1.2	<0.11

Table C 2. Canister sample data. Concentrations in $\mu\text{g}/\text{m}^3$. *p* denotes production mode and *np* non-production. The less than sign (<) indicates the detection limit, and that the sample concentration was below it.

Can. ID	Sample location	Sample date	1-Butene	c-2-Butene	iso-Pentane	n-Pentane	1,3-Butadiene	t-2-Pentene	1-Pentene
3135	Upwind process	16 May 2021	<0.11	<0.23	0.5	<0.3	<0.44	<0.29	<0.29
3146	Upwind process	18 May 2021	<0.11	<0.23	0.6	0.3	<0.44	<0.29	<0.29
1036	Fenceline	16 May 2021	<0.11	<0.23	0.7	1.5	<0.44	<0.29	<0.29
3156	Fenceline	16 May 2021	0.2	<0.23	0.6	2.0	<0.44	<0.29	<0.29
1043	Fenceline	16 May 2021	<0.11	<0.23	3.9	0.9	<0.44	<0.29	<0.29
3152	Fenceline	16 May 2021	0.1	<0.23	1.0	0.4	<0.44	<0.29	<0.29
3153	Fenceline	18 May 2021	0.2	<0.23	0.5	0.4	<0.44	<0.29	<0.29
3157	Fenceline	18 May 2021	0.2	<0.23	0.8	0.5	<0.44	<0.29	<0.29
3165	Fenceline	18 May 2021	<0.11	<0.23	1.0	1.4	<0.44	<0.29	<0.29
3162	Fenceline	18 May 2021	0.3	<0.23	1.1	2.2	<0.44	<0.29	<0.29
3160	Fenceline	18 May 2021	0.3	<0.23	5.3	0.4	<0.44	<0.29	<0.29
3150	PCM charge	14 May 2021	0.2	<0.23	1.3	1.4	<0.44	<0.29	<0.29
3139	PCM charge	14 May 2021	0.2	<0.23	0.7	0.4	0.5	<0.29	<0.29
3145	PCM push	14 May 2021	4.1	1.1	4.0	4.0	1.3	0.5	1.5
3143	PCM push	14 May 2021	0.4	<0.23	1.3	1.1	<0.44	<0.29	<0.29
1044	CEMS ^{np}	17 May 2021	<0.11	<0.23	0.5	1.7	<0.44	<0.29	<0.29
1046	CEMS ^p	17 May 2021	<0.11	<0.23	<0.3	0.6	<0.44	<0.29	<0.29
1153	CEMS ^{np}	17 May 2021	<0.11	<0.23	<0.3	0.9	<0.44	<0.29	<0.29

Table C 3. Canister sample data. Concentrations in $\mu\text{g}/\text{m}^3$. *p* denotes production mode and *np* non-production. The less than sign (<) indicates the detection limit, and that the sample concentration was below it.

Can. ID	Sample location	Sample date	2-Methyl-pentane	3-Methyl-pentane	Isoprene	n-Hexane	Benzene	Cyklo-hexane	Iso-octane
3135	Upwind process	16 May 2021	<0.21	<0.21	<0.56	<0.35	<0.54	<0.69	<0.28
3146	Upwind process	18 May 2021	<0.21	<0.21	<0.56	0.4	0.5	<0.69	<0.28
1036	Fenceline	16 May 2021	<0.21	<0.21	<0.56	2.8	<0.54	<0.69	<0.28
3156	Fenceline	16 May 2021	<0.21	<0.21	<0.56	0.5	0.8	<0.69	<0.28
1043	Fenceline	16 May 2021	<0.21	<0.21	<0.56	0.5	0.7	<0.69	<0.28
3152	Fenceline	16 May 2021	<0.21	<0.21	<0.56	0.4	0.6	<0.69	<0.28
3153	Fenceline	18 May 2021	<0.21	<0.21	<0.56	0.4	<0.54	<0.69	<0.28
3157	Fenceline	18 May 2021	0.3	<0.21	<0.56	0.5	0.8	<0.69	<0.28
3165	Fenceline	18 May 2021	<0.21	<0.21	<0.56	0.5	0.6	<0.69	<0.28
3162	Fenceline	18 May 2021	<0.21	<0.21	<0.56	0.6	1.3	<0.69	<0.28
3160	Fenceline	18 May 2021	<0.21	<0.21	<0.56	0.7	0.5	<0.69	<0.28
3150	PCM charge	14 May 2021	0.3	<0.21	<0.56	0.8	2.6	<0.69	<0.28
3139	PCM charge	14 May 2021	0.3	0.2	<0.56	0.4	1.6	<0.69	<0.28
3145	PCM push	14 May 2021	1.0	0.7	<0.56	5.1	9.1	1.0	<0.28
3143	PCM push	14 May 2021	0.3	0.3	<0.56	3.7	2.3	<0.69	<0.28
1044	CEMS ^{np}	17 May 2021	<0.21	<0.21	<0.56	2.8	1.0	<0.69	<0.28
1046	CEMS ^p	17 May 2021	<0.21	<0.21	<0.56	0.8	0.8	<0.69	<0.28
1153	CEMS ^{np}	17 May 2021	<0.21	<0.21	<0.56	1.0	0.9	<0.69	<0.28

Table C 4. Canister sample data. Concentrations in $\mu\text{g}/\text{m}^3$. *p* denotes production mode and *np* non-production. The less than sign (<) indicates the detection limit, and that the sample concentration was below it.

Can. ID	Sample location	Sample date	n-Heptane	Toluene	n-Octane	Ethyl-benzene	m+p-Xylen	o-Xylen	n-Nonane
3135	Upwind process	16 May 2021	<0.25	0.7	<0.28	<0.26	<0.26	<0.26	<0.53
3146	Upwind process	18 May 2021	0.4	0.8	<0.28	<0.26	<0.26	<0.26	<0.53
1036	Fenceline	16 May 2021	<0.25	1.0	<0.28	<0.26	0.3	<0.26	<0.53
3156	Fenceline	16 May 2021	0.4	0.8	<0.28	<0.26	0.3	<0.26	<0.53
1043	Fenceline	16 May 2021	0.5	0.7	<0.28	<0.26	<0.26	<0.26	<0.53
3152	Fenceline	16 May 2021	0.4	0.9	<0.28	<0.26	<0.26	<0.26	<0.53
3153	Fenceline	18 May 2021	0.4	0.7	<0.28	<0.26	<0.26	<0.26	<0.53
3157	Fenceline	18 May 2021	0.4	0.9	<0.28	<0.26	0.3	<0.26	<0.53
3165	Fenceline	18 May 2021	0.4	0.8	<0.28	<0.26	0.3	<0.26	<0.53
3162	Fenceline	18 May 2021	0.4	1.0	<0.28	<0.26	0.3	<0.26	<0.53
3160	Fenceline	18 May 2021	0.3	0.7	<0.28	<0.26	<0.26	<0.26	<0.53
3150	PCM charge	14 May 2021	0.6	2.1	<0.28	<0.26	0.8	0.3	<0.53
3139	PCM charge	14 May 2021	0.4	1.0	<0.28	<0.26	0.3	<0.26	<0.53
3145	PCM push	14 May 2021	2.0	10.2	1.4	1.0	5.8	1.9	1.9
3143	PCM push	14 May 2021	0.3	1.4	<0.28	0.1	0.5	<0.26	<0.53
1044	CEMS ^{np}	17 May 2021	1.4	1.3	0.3	<0.26	0.4	<0.26	<0.53
1046	CEMS ^p	17 May 2021	0.9	1.1	0.3	<0.26	0.3	<0.26	<0.53
1153	CEMS ^{np}	17 May 2021	1.2	1.3	0.3	<0.26	0.4	<0.26	<0.53

Table C 5. Canister sample data. Concentrations in $\mu\text{g}/\text{m}^3$. *p* denotes production mode and *np* non-production. The less than sign (<) indicates the detection limit, and that the sample concentration was below it.

Can. ID	Sample location	Sample date	1,3,5-TMB	1,2,4-TMB	1,2,3-TMB
3135	Upwind process	16 May 2021	<0.49	<0.49	<0.49
3146	Upwind process	18 May 2021	<0.49	<0.49	<0.49
1036	Fenceline	16 May 2021	<0.49	<0.49	<0.49
3156	Fenceline	16 May 2021	<0.49	<0.49	<0.49
1043	Fenceline	16 May 2021	<0.49	<0.49	<0.49
3152	Fenceline	16 May 2021	<0.49	<0.49	<0.49
3153	Fenceline	18 May 2021	<0.49	<0.49	<0.49
3157	Fenceline	18 May 2021	<0.49	<0.49	<0.49
3165	Fenceline	18 May 2021	<0.49	<0.49	<0.49
3162	Fenceline	18 May 2021	<0.49	<0.49	<0.49
3160	Fenceline	18 May 2021	<0.49	<0.49	<0.49
3150	PCM charge	14 May 2021	<0.49	<0.49	<0.49
3139	PCM charge	14 May 2021	<0.49	<0.49	<0.49
3145	PCM push	14 May 2021	1.1	1.7	0.4
3143	PCM push	14 May 2021	<0.49	<0.49	<0.49
1044	CEMS ^{np}	17 May 2021	<0.49	<0.49	<0.49
1046	CEMS ^p	17 May 2021	<0.49	<0.49	<0.49
1153	CEMS ^{np}	17 May 2021	<0.49	<0.49	<0.49

D - Coal terminal measurements

Coal terminal area emission measurements

The coal terminal area in the southeast corner of the site, was measured to have an alkane emission of 2.2 kg/h (95% CI: 1.6-2.7 kg/h), Table D 1. Figure D 1 shows a SOF measurement of alkanes on 12 May, 10:35 AM, corresponding to 2 kg/h. Wind was 3.7 m/s from northeast.

Table D 1. VOC emissions (alkane) from Coal terminal area measured by SOF.

Date	Start time	Stop time	Emission (kg/h)	Wind Speed (m/s)	Wind Dir (deg)
210510	144428	144615	3.0	7.7	11
210510	163501	163649	4.0	7	10
210510	165341	165447	0.6	7.4	12
210511	111740	111909	1.9	3.6	351
210511	135823	140009	1.9	5.3	30
210511	140246	140435	0.5	5.2	30
210511	141410	141540	4.0	6.5	30
210511	141806	141917	3.7	7	23
210511	151906	152032	3.4	5.6	38
210512	103933	104113	2.0	3.7	41
210512	105624	105801	2.7	3.4	53
210512	111358	111513	1.0	3.5	43
210512	113345	113509	3.1	3.4	39
210512	113720	113842	1.5	3.4	43
210512	140852	141009	1.4	3.1	23
210512	141242	141404	1.6	2.9	21
210512	154158	154337	0.7	3	25
210513	130256	130422	3.3	3.9	81
210513	130424	130631	3.8	3.9	83
210513	163130	163414	0.6	4.4	83
210513	164536	164739	0.5	3.8	86

Emission average 95% CI: 1.6-2.7 kg/h

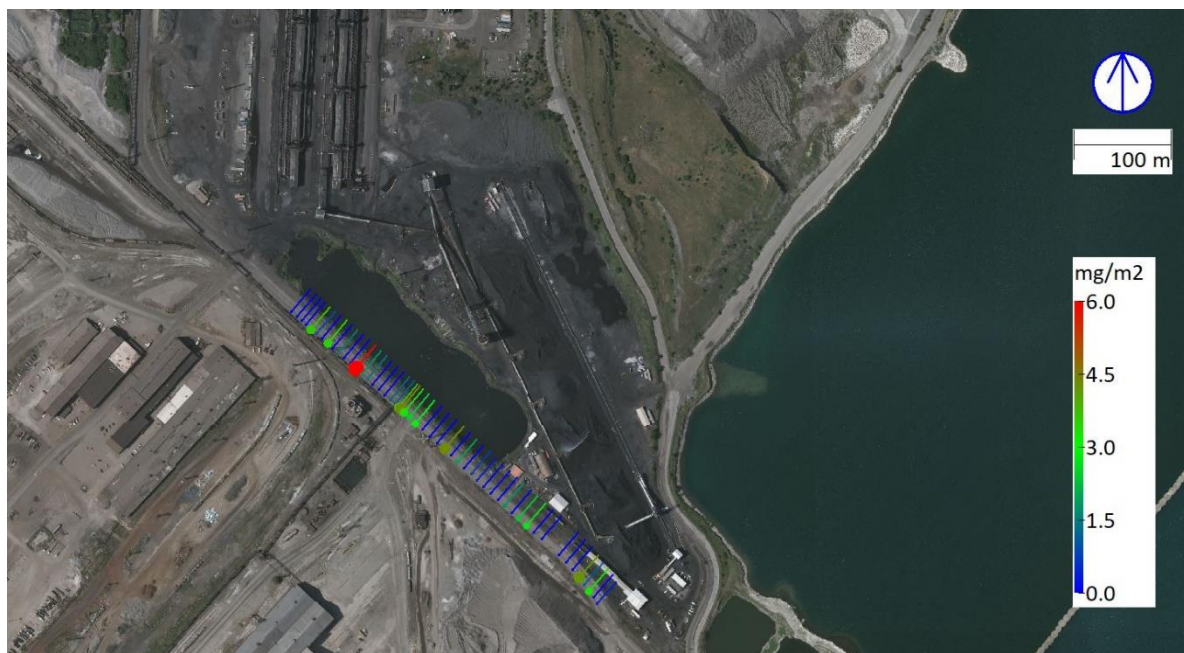


Figure D 1. SOF measurement of alkanes from the coal terminal area on 12 May 2021, 10:35 AM. Wind was blowing from northeast at 3.7 m/s as indicated by the coloured lines (pointing up in wind). The alkane column is colour coded from background (blue) to 6 mg/m². Map from Google Earth™, 2021.

Coal terminal area concentration ratios

For the coal terminal area, Table D 2, a BTEX to alkane mass fraction of 8.6% was obtained from MeFTIR and MeDOAS measurements. Corresponding mass fraction for ethene was 19.2%, Table D 3.

Table D 2. BTEX versus alkane mass fraction integrated across the tested coal terminal area.

Date	Time	N
210512	105648 -154342	2
210513	130351 -164732	2
210514	110022 -110404	1
210516	114324 -140739	3
Mass fraction average 95% CI: 5.0-12.1%		

Table D 3. Ethene versus alkane mass fraction integrated across the tested coal terminal area.

Date	Time	N
210512	103856 -154342	3
210513	130351 -164732	2
210514	110022 -110404	1
210516	113800 -140739	4
210518	113036 -113336	1
Mass fraction average 95% CI: 13.1-25.3%		

The ethene and BTEX mass fractions observed in the coal terminal area tests, indicate that the alkane emission of 2.2 kg/h should be expanded by 28% to also resemble those emissions. This results in an overall VOC estimate of 2.8 kg/h from the coal terminal area, possibly leaving out a small contribution from other compounds when compared to canister speciation in other source plumes.