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Evaluation of NASA's Remote-Sensing Capabilities in Coastal Environments



U.S. Department of the Interior Bureau of Ocean Energy Management Sterling, VA



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ABSTRACT

This work represents the second part of a two-part study set up by the National Aeronautics and Space Administration (NASA) and Bureau of Ocean Energy Management (BOEM) in 2017. The study summarizes a three-year investigation on the feasibility of using satellite remote sensing to monitor emissions of oil and gas operations over the outer continental shelf (OCS) to determine if they have negative impacts on coastal air quality (AQ). The target pollutant is nitrogen dioxide (NO₂), for which BOEM conducts regular emissions surveys. The major data source for this report is a May 2019 oceanographic cruise ("SCOAPE" = Satellite Coastal and Oceanic Atmospheric Pollution Experiment) conducted in the Gulf of Mexico (GoM) off Louisiana with the Research Vessel Point Sur, loaded with a suite of trace-gas analyzers and a direct-sun remote sensor Pandora spectrometer that measures column NO₂. The SCOAPE cruise, augmented by in situ NO₂ and Pandora measurements at Cocodrie (Louisiana; 29.25° N, 90.66° W) showed that (1) under cloud-free conditions, satellites can detect elevated column NO₂ amounts near isolated large platforms and from clusters of smaller operations; (2) satellite (the European Space Agency's TROPOspheric Monitoring Instrument [TROPOMI]) total column (TC) NO₂ agrees well with TC NO₂ from ground-based Pandora spectrometers (to 11-18%), with the satellite biased low when pollution levels are higher; (3) in general, NO_2 measured in situ and in column amounts by Pandora or TROPOMI is greater over coastal Louisiana than over the OCS: (4) the extent to which Pandora or satellite measurements correlate with surface NO₂ is highly variable.

It is recommended that BOEM and NASA continue to work together on collecting ground-truth NO₂ data and on interpreting remote sensing data for BOEM's AQ requirements. Specific recommendations:

- BOEM and NASA should work together to analyze the 2019 SCOAPE data more thoroughly, including conducting studies with tracers, ancillary satellite data, trajectories, and appropriate chemical transport model output to more firmly establish the magnitude of oil and natural gas influences on GoM AQ. Because remote-sensing measurements (satellite- and ground-based) do not provide ambient NO₂ concentrations, these studies must be conducted to determine the column-surface NO₂ relationship. NASA POC: anne.m.thompson@nasa.gov
- 2. Coastal monitoring along the GoM with NASA and the Environmental Protection Agency (EPA) using Pandora Spectrometer Instrument and other instruments would establish better statistics and contribute to the ongoing improvements in OMI (Ozone Monitoring Instrument) (mature algorithm) and the still evolving TROPOMI. Co-location with BOEM's coastal project, aiming to begin in late 2020 at a remote unpolluted location in Louisiana, would greatly benefit BOEM. Daily overpass comparisons of OMI and TROPOMI TC NO₂ with a Pandora instrument would give BOEM more complete statistics than the 5-week exploratory dataset of April–May 2019. Comparisons of the in situ and column NO₂ amounts, along with other pollutants being measured, would further our understanding of the relationship of chemical transformation and interactions with dynamical processes in the boundary layer. NASA POC:

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Acronym/Name	Phrase/Description		
Chemical Species			
CH4 CO CO2 HCHO NO2	Methane Carbon Monoxide Carbon Dioxide Formaldehyde, a VOC Nitrogen Dioxide		
NO _x O ₃ SO ₂ VOC	Nitrogen Oxides ($NO_x = NO + NO_2$) Ozone Sulfur Dioxide Volatile Organic Compound		
Instruments			
MODIS OMI PSI TEMPO TROPOMI VIIRS	MODerate resolution Imaging Spectrometer Ozone Monitoring Instrument Pandora Spectrometer Instrument Tropospheric Emissions: Monitoring of Pollution TROPOspheric Monitoring Instrument [ESA] Visible Infrared Imaging Radiometer Suite		
Agencies/Programs			
BOEM EPA ESA HAQAST KNMI NASA NIST NOAA	Bureau of Ocean Energy Management Environmental Protection Agency European Space Agency NASA Health and Air Quality Applied Sciences Team Royal Dutch Meteorological Office National Aeronautics and Space Administration National Institute of Standards and Technology National Oceanic and Atmospheric Administration		
Other			
AQ AQS CBBT CEMS CONUS CS GoM HDA HMI KORUS-AQ/OC LaRC LOOP LUMCON OCS ONG OWLETS SCOAPE TC NO ₂ TropC NO ₂ VCD	Air Quality U.S. Air Quality System Chesapeake Bay Bridge Tunnel Continuous Emission Monitoring System CONtinental United States Case study Gulf of Mexico heavy density area Hart Miller Island Korea-U.S. Air Quality/Ocean Color campaign Langley Research Center Louisiana Offshore Oil Port Louisiana Universities Marine Consortium Outer Continental Shelf Oil and Natural Gas Ozone Water–Land Environmental Transition Study Satellite Coastal & Oceanic Atmospheric Pollution Experiment Total Column NO_2 = atmospheric column Tropospheric Column NO_2 = tropospheric column Vertical Column Density = the total number of molecules between the satellite and Earth's surface per unit area, such as molecules/cm ² .		

List of Abbreviations and Acronyms

1 Introduction

1.1 Background

The Outer Continental Shelf Lands Act (OCSLA) requires the Bureau of Ocean Energy Management (BOEM) to ensure compliance with the National Ambient Air Quality Standards (NAAQS) so that Outer Continental Shelf (OCS) oil and gas exploration, development, and production do not significantly impact the air quality (AQ) of any state. In July 2015, BOEM personnel first approached the National Aeronautics and Space Administration (NASA) to inquire if satellite data could be used to help monitor offshore AQ in BOEM's jurisdiction, that portion of the OCS west of 87°30' West longitude in the Gulf of Mexico (GoM) Region and the Chukchi and Beaufort Sea Planning Areas in the Alaska Region. An interagency agreement was signed in 2017 to begin a feasibility study on the use of NASA and related satellite data for BOEM's requirements.

The feasibility study consists of two parts. First is a review of satellite observations that can be applied to BOEM's needs, including capacity-building tools and case studies, as described in Duncan (2020). This document reports on the second part of the feasibility study: the design and execution of a field campaign for validation of satellite NO₂ columns and evaluation of surface instrumentation that will be useful to BOEM as it moves forward with satellite measurements aimed at quantifying the impacts of oil and gas (ONG) activity on coastal AQ. The field effort, designated as the Satellite Coastal and Oceanic Atmospheric Pollution Experiment (SCOAPE), was carried out in May 2019. This report begins with a review of coastal field experiments in 2016–2018 that are related to SCOAPE (**Section 2**), followed by a summary of findings from the SCOAPE oceanographic cruise (**Section 3**).

1.2 Remote Sensing of NO₂ for BOEM's Requirements

The first part of this study, as reported in Duncan (2020), reviews the basic principles of satellite detection of pollution and lists several atmospheric constituents of relevance to BOEM's AQ requirements that NASA and other organizations monitor from space. Chief among these is the important ozone precursor nitrogen dioxide (NO₂) that has been observed by satellite since 1995 (Burrows et al., 1999). Over polluted regions of the globe, nearly all the total column (TC) of NO₂ resides in the troposphere so satellite observations represent an ideal method for measuring NO₂ emissions. Considerable effort has been put into algorithm development, validation and applications (Lamsal et al., 2008; Duncan et al., 2014; Lamsal et al., 2015; deFoy et al., 2016; Krotkov et al., 2017) for tracking pollution NO₂, especially related to the Dutch-Finnish OMI instrument on NASA's Aura satellite that has been in orbit for 16 years (Levelt et al., 2018). Since late 2017, ESA has flown the TROPOMI instrument that is now being heavily used for AQ applications, for example, recording reduced NO₂ during the COVID-19 pandemic (Bauwens et al., 2020). Because oil and gas activity, both direct emissions from platforms (Wilson et al., 2017; Wilson et al., 2019) and from associated transportation, emit NO₂, NO₂ is the atmospheric constituent of focus for this report. (The primary product of combustion, of course, is NO, which is in chemical equilibrium with NO₂; together NO + NO₂ = NO_x; the latter parameter is what BOEM and most Agencies use for emission inventories). Remote-sensing instruments measure and report NO₂ in column amounts of number of molecules called Dobson Units (1 DU = $2.69 \times 10^{16} \text{ cm}^{-2}$).

Both Ozone Monitoring Instrument (OMI) and TROPOspheric Monitoring Instrument (TROPOMI) data are included in this report. OMI has a more mature and time-tested algorithm and is used to compare current views of NO₂ pollution with the past, e.g., Figure 3 in Duncan (2020); Duncan et al. (2016); McLinden et al. (2016). TROPOMI has higher resolution, which will be shown to give superior views (**Section 2**) but is less well-developed for some applications.

Evaluation of satellite NO₂ columns is typically done with ground-based instruments such as MAX-DOAS (Piters et al., 2012) or aircraft versions of the ground instruments or other sensors meant to simulate the satellite (Lamsal et al., 2017; Nowlan et al., 2018; Judd et al., 2019). A relatively recent addition to the constellation of ground-based instruments is the Pandora spectrometer (or PSI, Pandora Spectrometer Instrument) that was developed about 15 years ago by scientists working at NASA/Goddard Space Flight Center (Herman et al., 2009). The PSI has been deployed in several coastal AQ investigations (Reed et al., 2013; Tzortziou et al., 2015; Martins et al., 2016; Kollonige et al., 2018). A major series of hardware and software upgrades was being made to the PSI as the joint NASA-BOEM research study was beginning in 2017. Thus, at NASA we viewed a GoM study as an ideal opportunity to evaluate OMI and TROPOMI NO₂ products for BOEM and to further optimize the Pandora instrument for coastal applications.

2 Findings from Previous Field Campaigns

The relationship of satellite TC NO₂ and TropC (tropospheric column) NO₂ to surface NO₂ can be complex. Thus, there is a need for independent verification of the satellite column amount and parallel measurement of surface NO₂. Among a number of ground-based spectrometric approaches to TC NO₂ is the Pandora instrument (Knepp et al., 2015; Reed et al., 2015; Martins et al., 2016; Kollonige et al., 2018). In this section, we present new analysis of data collected during recent (2016–2018) coastal field campaigns. Both satellite and spectrometric NO₂ are assessed in terms of capability for monitoring AQ over open water and coastal environments.

2.1 South Korean Coastal Pollution Study: KORUS-OC 2016

Overall, the atmospheric-related goals of the joint venture between NASA and the Korean Institute of Ocean Science and Technology (KIOST), KORUS-OC (Korea-United States Ocean Color), were to (1) characterize dynamics in surface air pollution and the variability of TC measurements of gases over the South Korean coastal environment, (2) determine onshoreoffshore gradients in the region, and (3) link in situ and remotely sensed land and water observations to understand both the spatial and temporal variability of trace gas distributions. Essentially, these goals are similar to those of SCOAPE, but for a different region.

Here, we analyze a set of surface and TC NO₂ observations aboard the *R/V Onnuri* that operated from May–June 2016 to investigate coastal and offshore AQ near South Korea (Tzortziou et al., 2018; Thompson et al., 2019). **Figure 1** shows the *R/V Onnuri* ship track as it sailed on the East and Yellow Seas along the South Korean coast from 20 May 2016 to 5 June 2016. Data gaps in territorial waters are depicted as missing segments of the track. A temporary malfunction of OMI operation precluded comparisons between OMI and Pandora after 29 May 2016, so statistics on satellite-spectrometer comparisons in Tzortziou et al. (2018) are somewhat limited. Thompson et al. (2019) focused on Pandora TC NO₂ comparisons with in situ NO₂ measurements on the *R/V Onnuri* to investigate factors influencing the relationship (good or poor correlations) between the Pandora ("PSI" in **Figure 2**) columns and shipboard NO₂

measurements. **Figure 2a** is the time series of in situ and Pandora TC NO₂, taken along the R/V Onnuri track. Coincident surface NO₂ and PSI TC NO₂ measurements presented as a scatterplot with linear least squares best-fit lines for Case Studies 1 (red), 2 (black), and 3 (cyan), appear in **Figure 2b**.

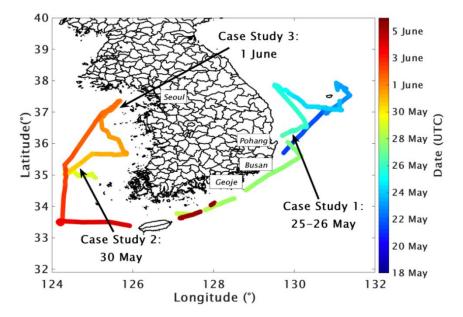


Figure 1. KORUS-OC case study map.

Color scale by date; case study regions marked by arrows. Source: Thompson et al. (2019).

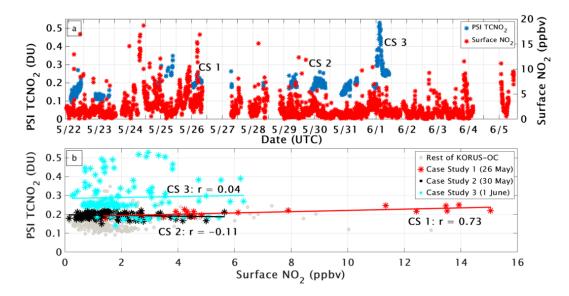


Figure 2. KORUS-OC in situ and Pandora TC NO₂ on the *R/V Onnuri*. Case studies (CS) marked. Source: Thompson et al. (2019).

The relationship between surface AQ and shipboard TC NO_2 observations over open water varied considerably throughout KORUS-OC as indicated in the three case studies (**Figure 2**). Observations from Case Study 1 (CS 1, 26 May 2016, in **Figure 2**) took place as the ship sailed toward the city of Pohang on the East Sea. In the presence of a well-mixed boundary layer in a coastal environment, Pandora (PSI) observes near-surface pollution with a good correlation

between TC and near-surface NO₂ (r=0.73, red stars in **Figure 2b**). (Note that all observations except those recorded during the three case studies appear in light gray in **Figure 2b**). Under certain lower atmospheric conditions (i.e., one or more stable layers), the vertical distribution of NO₂ can vary sharply with height throughout the column and limit the satellite and/or PSI's capacity for detecting near-surface NO₂. Stable-layer conditions prevailed in the other cases (**Figure 2b**) and consequently there is poor correlation: CS 2, 30 May 2016; black symbols; CS 3, 1 June 2016, in cyan.

⇒ Relevance to BOEM: Overall, conclusions from the KORUS-OC South Korea coastal study:

(1) Near-surface meteorology and transport can affect comparisons between TC NO_2 observations and near-surface NO_2 measurements over coastal and open waters,

(2) Agreement between column and in situ NO₂ depends on atmospheric stability near surface (i.e., stable layers affecting the vertical distribution of trace gases), and

(3) A well-mixed lower atmosphere with local pollution shows the best correlation between the surface Pandora column and in situ NO_2 observations in coastal waters.

In the next section, results are presented from a campaign similar to KORUS-OC but conducted with a suite of measurements called the Ozone Water–Land Environmental Transition Study (OWLETS). OWLETS focused on land-water ozone and ozone precursor gradients along the U.S. Mid-Atlantic coast and the Chesapeake Bay region.

2.2 Mid-Atlantic and Chesapeake Bay Ozone Study: OWLETS 2017

Past investigations into understanding poor AQ and pollution events at land-water interfaces in the U.S., particularly near major urban centers, include the Lake Michigan Ozone Study (LMOS) in 1991 (Dye et al., 1995) and 2017 (https://www-air.larc.nasa.gov/missions/lmos/), Texas Air Quality Study (TexAQS) in 2000 (Daum et al., 2003), TexAQS/GOMACCS in 2006, and Great Salt Lake City Ozone Study in 2015 (Blaylock et al., 2017). Within each of these land-water investigations, and especially within the Chesapeake Bay, differences in emissions, mesoscale meteorology, cloud coverage, and aqueous deposition rates compared to nearby continental land masses drive gradients in ozone and other pollutants (Goldberg et al., 2014).

In addition to typical mobile sources (e.g., automobiles and other transport vehicles) and point sources (e.g., power plants), the air pollution of the Chesapeake Bay is complicated by recreational marine and large ship-produced emissions (Ring et al., 2018). OWLETS was a two-part campaign focused on the complexity of the water–land transition in the Chesapeake Bay during two summer periods:

- (1) In 2017 in the Tidewater Virginia area with two "super-site" locations at NASA Langley Research Center (LaRC) and Chesapeake Bay Bridge Tunnel (CBBT) Third Island site (Figure 3)
- (2) In 2018 in the Baltimore Harbor region with the University of Maryland Baltimore County (UMBC) campus and Hart Miller Island (HMI) as "super-sites"

During OWLETS 2017, LaRC and CBBT were the "over-land" and "over-water" locations, respectively, following a similar setup as the Chemistry And Physics of the Atmospheric Boundary Layer Experiment (CAPABLE; Martins et al., 2012; Knepp et al., 2015). These supersites integrated a combination of remote sensors, including ozone lidars and Pandoras, with

surface and balloon-borne instrumentation. To better characterize the fundamental processes at the water–land interface and pollutants gradients, ongoing investigations use observations at the super-sites along with mobile (airborne, ship-based, and vehicular) observations connecting the two sites (Sullivan et al., 2018). Note, for example, the elevated ozone (**Figure 3a**) and NO₂ (**Figure 3b**) as measured from a coastal research vessel operated by SERC, the Smithsonian Environmental Research Center. The Bay sampling illustrates the complexity of emissions and their interaction with the complicated Chesapeake coastline (cf. Stauffer et al. 2012; Stauffer and Thompson, 2013).

Primary OWLETS Ground Sites With SERC Vessel Measurements on 17-18 July 2017

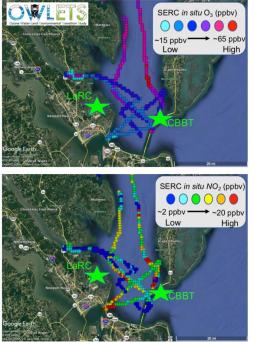


Figure 3. OWLETS 2017 map of the primary ground sites. Primary ground sites marked in green stars: NASA LaRC and CBBT. Ship data marked in colors; see key.

Our OWLETS 2017 analysis focuses on the differences in TC NO₂ measured by Pandora and OMI (satellite-based) over the "land" and "water" locations. Over 20 days of OWLETS observations, there were 11 and 17 coincidences between OMI and Pandora for LaRC and CBBT, respectively. Of these comparisons, each site had 11 total instances where percent differences were greater than 10% between OMI and Pandora. A histogram of the percent differences between the two instruments over both sites (**Figure 4**) demonstrates that the "overwater" site, CBBT (in green), is shifted to the left with better OMI-Pandora agreement than at LaRC and with a mean difference of ~15%. At LaRC (in blue), with readings during cloud cover > 30% excluded, the "over-land" percent satellite-PSI offsets range from 10% to > 50% with a mean of ~30%. This result is not surprising. Other studies of OMI-Pandora comparisons in the Chesapeake Bay region have shown that in more polluted areas on land there are larger offsets between the satellite and ground-based instruments (Flynn et al., 2014; Reed et al., 2015; Tzortziou et al., 2015). The main reasons: (1) differences in OMI vs Pandora field of view (i.e., whether Pandora "represents" the same air as OMI samples); (2) due to its relatively coarse horizontal resolution, OMI column TC NO₂ readings are usually lower than those of Pandora.

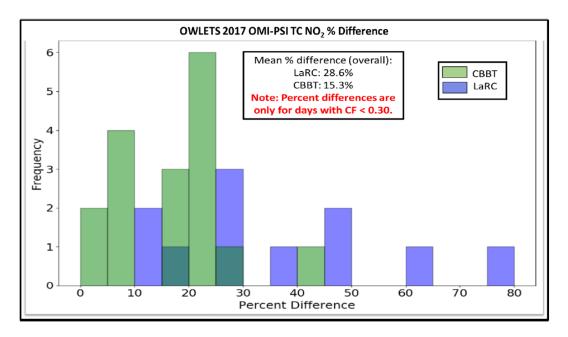


Figure 4. Histogram of OWLETS 2017 OMI-PSI % differences for LaRC (Pan 37) and CBBT (Pan 19). Mean percent differences on the figure do not include days with greater than 30% cloud fraction when offsets ranged near 50–75%.

⇒ Relevance to BOEM: Analyses of OMI and Pandora data at LaRC and CBBT pointed to four factors influencing the column NO₂ comparisons. These factors, listed in order of importance based on frequency during the OWLETS 2017 time period, are the following:

- 1) Cloud cover,
- 2) Satellite pixel size and/or location with respect to the ground site,
- 3) Mixing height versus boundary layer height differences, and
- 4) A combination of cloud cover and satellite pixel size/location.

The OMI Cloud Fraction product was used to determine cloud influence during each OMI-PSI coincidence. Cloud cover alone affected only ~20% of the comparisons at both CBBT and LaRC. However, cloud cover appeared to have a larger impact on LaRC, causing OMI-PSI differences as large as 70% or more. However, in 55% of the CBBT comparisons (36% for LaRC), the size of the OMI pixel and/or the location of that pixel with respect to the ground site (and/or the Pandora Field of View [FOV]) is the dominant factor contributing to larger percent differences between the two instruments. When high cloud cover is also a factor that degrades agreement, 64% of the comparisons at both sites also had large OMI-PSI differences. **Figure 5** shows an example of OMI "good" (on 18 July) and "bad" (on 24 July) pixel size location with respect to the CBBT ground site. On 24 July, the OMI pixel size was three times larger than its nominal horizontal resolution at nadir (13x24 km²); this can happen at the edges of the satellite instrument swath. The difference between OMI and Pandora on July 24 was ~40%, the largest single offset observed at CBBT.

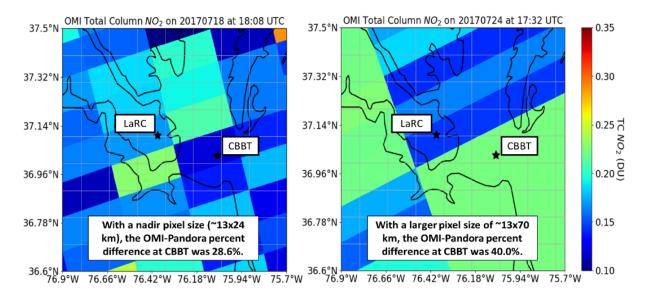


Figure 5. OWLETS 2017 OMI pixel size examples.

OMI smaller pixel size (left) leads to closer OMI-Pandora TC NO₂ agreement at LaRC and CBBT than for larger OMI pixel size (right, 24 July 2017).

From these results, we conclude that the magnitude of OMI-Pandora disagreements for the OWLETS 2017 Tidewater region is most sensitive to

(1) Geographical complexity of the Chesapeake Bay land-water interface

(2) OMI-PSI coincidences, with best agreement when the super-sites are closely aligned with nearly overhead satellite

⇒ Things to Know: Based on the findings above, we assume that with the higher spatial resolution satellite data provided by TROPOMI NO₂ in 2018, there is better potential for good satellite-PSI agreement than was possible for OMI in 2017. Figure 6 presents an image of TropC NO₂ over the OWLETS 2017 LaRC and CBBT sites taken by TROPOMI during summer 2018 (9 July). As expected, the retrieval problems inherent in OMI, i.e., large pixel size (Figure 5), are less serious for TROPOMI than for OMI. Furthermore, TROPOMI discriminates NO₂ differences between land and water. In Figure 6, values of TropC NO₂ near CBBT are lower (mostly blue pixels in the area) than over land, where, for example, TropC NO₂ near LaRC is higher (mostly green in the area) than over the nearby Bay. The polluted Norfolk region (orange-red colors for TropC NO₂), southwest of CBBT, is also distinct from the super-sites.

⇒ Relevance to BOEM: Higher spatial resolution observations from TROPOMI demonstrate a distinct land-water gradient in TC NO₂ in the Tidewater area that was not well-resolved by OMI during OWLETS 2017. For the GoM Region, it was expected that the complications in trying to validate satellite column NO₂ that were encountered during OWLETS 2017 would be reduced by having access to TROPOMI NO₂ data during the 2019 SCOAPE cruise. However, based on our OWLETS 2017 and KORUS-OC results, high amounts of cloud cover and various properties of the marine mixed layer over water could still complicate surface and TROPOMI TC NO₂ comparisons.

The next section focuses on preliminary evaluations of Pandora, OMI, and TROPOMI during OWLETS 2018 in the northern Chesapeake Bay area and the Baltimore Harbor region.

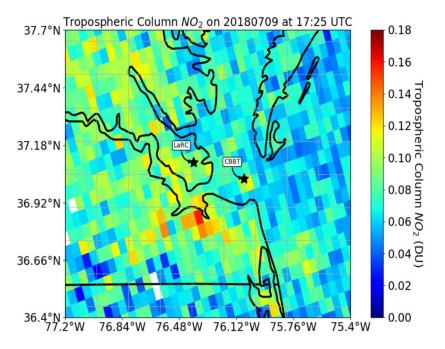


Figure 6. Map of TROPOMI TropC NO₂ over LaRC and CBBT on 9 July 2018. Compare this to 2017 OMI views in **Figure 5**.

2.3 Baltimore Harbor and Chesapeake Bay Pollution Study: OWLETS 2018

OWLETS 2017 was designed to investigate ozone and other pollutant behavior in the lower Chesapeake Bay. OWLETS 2018 (Sullivan et al., 2020) was a follow-on study to better understand behavior of ozone and related trace gases across the water–land transition zone in the upper Chesapeake Bay near Baltimore, Maryland. Two "super-sites," located at UMBC on the west side of Baltimore and at HMI to the east side in the Bay, served as collection points to obtain data simultaneously over land and water from June 6 to July 6, 2018. Instrumentation included two ozone lidar systems, Pandora Spectrometer Instruments, multiple wind and aerosol lidars, ozonesondes, research aircraft, and a suite of standard AQ measurements at other locations (**Figure 7**), some of which are State of Maryland monitoring sites.

With the newly available TROPOMI data, OWLETS 2018 facilitated the first comparisons of TROPOMI/OMI/Pandora TC NO₂ over an urban and coastal environment during summer. Our comparisons include the two super-site locations, UMBC and HMI, as well as measurements from NASA Goddard Space Flight Center (GSFC) illustrated in **Figure 7** where sampling extended from June to August 2018. Clearly, TROPOMI is more effective than OMI at capturing localized pollution sources and gradients (example: a distinct NO₂ gradient between Baltimore and Washington, D.C. on July 9, 2018 in **Figure 8**). This is because only 1–2 OMI pixels covered the three ground sites with OMI (left side of **Figure 8**) compared to the multitude of TROPOMI pixels over HMI, UMBC, and GSFC (right side of **Figure 8**).

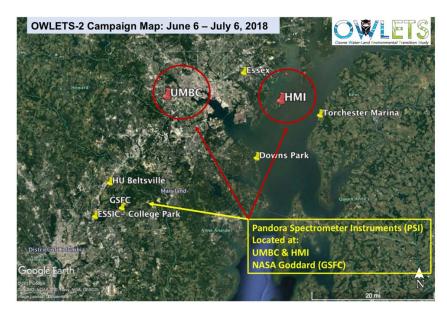


Figure 7. Map of OWLETS-2 (2018) "super-sites". Super-sites circled in red; Pandora Spectrometer Instruments also operated at GSFC and Beltsville.

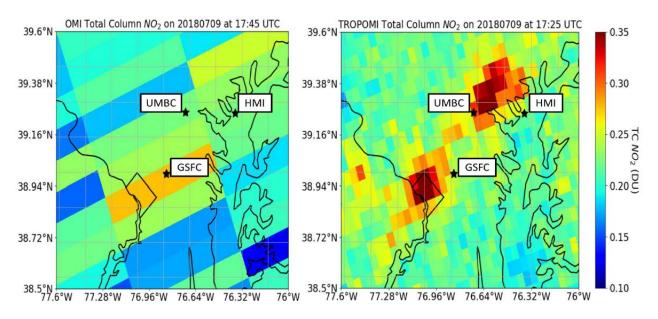


Figure 8. OMI (left) and TROPOMI (right) TC NO2 images in OWLETS 2018, 9 July 2018.

We find that OMI and Pandora have little to no correlation in their TC NO₂ observations at the three marked sites (left panel of **Figure 9**), with mean differences at GSFC ~20% and at UMBC ~50% (left panel of **Figure 10**). However, the mean difference between TROPOMI and Pandora TC NO₂ at GSFC is ~9% (right panel, **Figure 10**) compared to a ~20% OMI-Pandora discrepancy. For TROPOMI, the comparisons with Pandoras are much improved with correlations ~0.7 and ~0.8 at HMI and GSFC, respectively (**Figure 9**, right). These findings are consistent with early TROPOMI-Pandora correlations (Griffin et al., 2019) based on measurements taken at Fort McKay in the Canadian oil sands in Alberta, Canada.

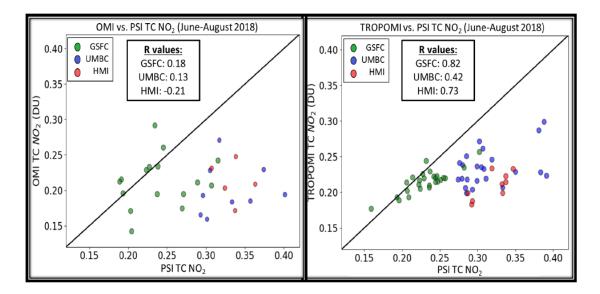


Figure 9. OWLETS 2018 satellite vs. Pandora comparisons. Satellite (y-axis) vs Pandora (PSI) TC NO₂ comparisons for cloud fraction < 0.3. OMI (left), TROPOMI (right).

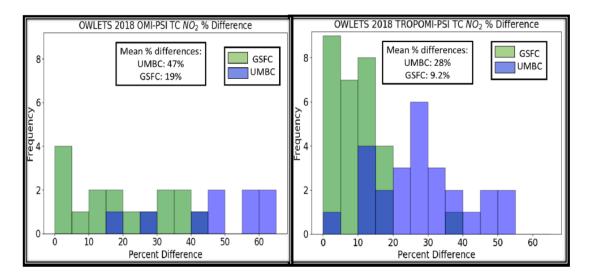


Figure 10. OWLETS 2018 satellite-PSI differences, based on same data as Figure 9.

A lower correlation and higher percent TROPOMI-Pandora TC NO₂ differences observed at UMBC (relative to the other sites) was caused by Pandora capturing some highly polluted days where TROPOMI was biased low. More analysis is needed to further investigate this bias. Differences in the vertical distribution of NO₂ (i.e., pollution closer to ground and to Pandora) among the ground sites may be significant. HMI is in the Bay and subject to complex flows (cf. bay-breeze influences characterized by Stauffer et al., 2012; Stauffer and Thompson, 2013); UMBC is generally the most frequently polluted of the three sites in terms of NO₂. The pattern of satellite-Pandora offsets increasing in magnitude as the TC NO₂ absolute values increase has been noted in other field campaigns, e.g., Herman et al. 2018; Herman et al., 2019.

 \Rightarrow Relevance to BOEM: Preliminary comparisons between TROPOMI and Pandora TC NO₂ during OWLETS 2018, as in Griffin et al. (2019) over the Canadian oil sands, demonstrate the

effectiveness of the higher-resolution TROPOMI in capturing localized pollution gradients relative to OMI. This is what was expected for the SCOAPE cruise assuming GoM sampling would be relatively free of cloud contamination or a stratified lower atmosphere.

3 SCOAPE Cruise

3.1 Background: Emissions and Meteorological Conditions in Gulf of Mexico

Figure 11, with imagery from January 2019, illustrates the first promising satellite data obtained over the GoM prior to the SCOAPE cruise. Figure 11a displays the TropC NO₂ measured midday from TROPOMI. The black circles in the image are the locations of the 200 highestranked NO_x emitting platforms based on BOEM's 2014 inventory (Wilson et al., 2017). Regions of white are too cloudy for a retrieval. The GoM segment displayed here is clear as are the adjacent portions of Louisiana, Mississippi, and Alabama. The dominant high TropC NO₂ features are seen over the industrial coastal regions, consisting of Baton Rouge, New Orleans, ports, and petrochemical operations. The red-outlined region over the GoM in Figure 11a is shown in expanded scale in **Figure 11b**. The NO₂ pollution in this region is elevated above background, represented by very low TropC NO₂ (~0.03 DU). The enhanced TropC NO₂ is depicted by orange-red colors, 0.08–0.10 DU. Checking the locations of these features in Figure 11b—each pixel is ~7x3.5 km²—reveals them to coincide with the large and closelypositioned platforms Allegheny, Brutus, and Genesis; elevated TropC NO₂ is also observed farther east at the Mars and Olympus platforms. The presence of elevated NO₂ in satellite imagery mostly signifies combustion, of which there are various sources on an operating platform: flaring and different types of engines. There are often ships stationed near large platforms that also emit NO₂. There are natural and other anthropogenic NO₂ sources, notably lightning (Pickering et al., 2016), agricultural fires, and soils; these are mostly, but not always, observed over the continent, as shown in Section 3.2.

In **Figure 11c**, a different satellite, the Suomi-NPP VIIRS, with a white area at the location of Mars and Olympus, detects elevated temperature anomalies associated with flaring. The images displayed in **Figure 11** were the first confirmation of the feasibility of using satellites to observe offshore pollution at the relatively fine-scale over the GoM regions of interest to BOEM.

The timing of the SCOAPE cruise was chosen to optimize viewing conditions favorable for observing scenes such as those in **Figure 11**. Winter was avoided due to weather, ship schedule limitations and reduced likelihood of pollution buildup offshore. Early to mid-spring was chosen for an expected prevalence of onshore flow, relatively low cloud cover, and avoidance of hurricanes that occur in the latter part of the pollution season. A plethora of weather-related satellite imagery and customized model output for AQ was available to the ship and onshore scientific complement (**Section 3.2**; see also Duncan, 2020). This meant, for example, that the NASA AQ forecasts showed us ahead of time the contrasting regimes through which the *R/V Point Sur* sampled (**Figure 12**). The CO forecast for 12 May 2019 depicts a sharp gradient between the eastern and western part of the nearshore GoM.

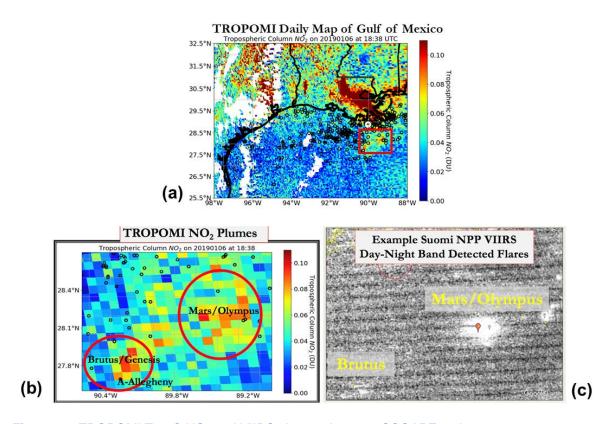


Figure 11. TROPOMI TropC NO₂ and VIIRS observations pre-SCOAPE: 6 January 2019. Example: (a) and (b): TropC NO₂ (DU) on 6 January 2019. Black circles indicate the 200 most highly emitting platform operations according to BOEM's 2014 inventory (Wilson et al., 2017). In (c) the image is from the Suomi-NPP satellite on 6 January 2019. The VIIRS instrument operates in the thermal infrared; white regions are elevated thermal anomalies detected in its Day-Night Band. The red marker denotes a flaring signature near the Mars/Olympus complex. Copernicus Sentinel data processed by ESA (<u>https://doi.org/10.5270/S5P-s4/jg54</u>).

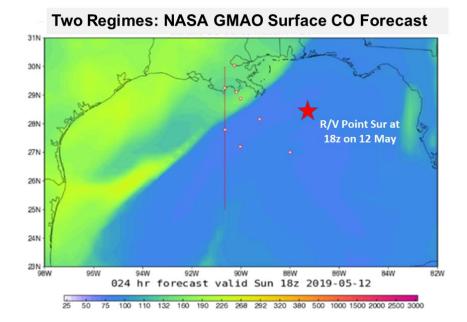


Figure 12. Two AQ regimes during SCOAPE: NASA surface CO forecast. CO forecast is for 12 May 2019 at 18Z (midday).

At the location of the ship on 12 May, CO mixing ratios were 50–75 ppbv, which are very low, almost tropical, marine values. To the west, in a region traversed by the ship a day or so later, CO mixing ratios were predicted to be 150–190 ppbv, more representative of onshore conditions in southern Louisiana. Indeed, all the atmospheric constituents sampled on the *R/V Point Sur* reflected two distinct regimes over the nine days of the cruise (illustrated in **Section 3.2**). The contrast of the two regimes was captured very well by the TROPOMI TropC NO₂ (**Figure 13**). Cloud cover precluded extensive retrievals over much of the GoM coast and GoM itself on 13 May. However, what was observable displayed very low levels of TropC NO₂ (**Figure 13a**); only a few pixels of elevated TropC NO₂ (> 0.05) are seen over the New Orleans-Baton Rouge areas. Two days later, extensive regions onshore and in the adjacent GoM register readings from 0.05 DU to greater than 0.09 DU in TropC NO₂ (**Figure 13b**). **Section 3.2** illustrates contrasts in a number of other pollutants under the influence of onshore and offshore air masses. The signature of changing AQ regimes is reflected in TC NO₂ as measured by the shipboard Pandora instrument.

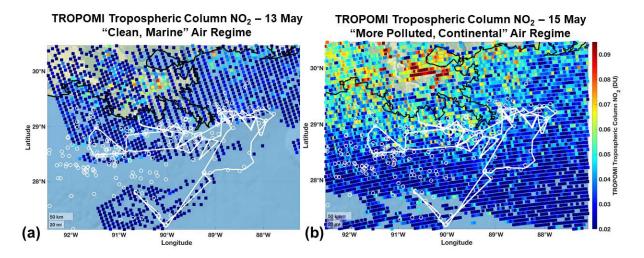


Figure 13. TROPOMI TropC NO₂ daily observations of marine vs. continental air during SCOAPE. TROPOMI TropC NO₂ (DU) over SCOAPE cruise region on (a) 13 May 2019 and (b) 15 May 2019. White open circles are the locations of the top 500 NO_x-emitting platforms from BOEM's 2014 inventory (Wilson et al., 2017). The white solid line marks the *R/V Point Sur* cruise track. Source: Thompson et al. (2020).

3.2 Onshore and Offshore SCOAPE Instrumentation and Plan

There were two objectives in choosing instrumentation (**Tables 1 and 2**) for the SCOAPE cruise. The first was to use newly designed Pandora spectrometer instruments (PSI) to ground-truth TC NO₂. We planned to do this on the ship sampling around the GoM and at a reference near-coastal site in Cocodrie, LA, (29.26°, -90.66°) at the Louisiana Universities Marine Consortium (LUMCON) facility, the departure port for the *R/V Point Sur*. In addition, to test the precision of the new Pandora we deployed three instruments, Pandoras 66, 67 and 68, at LUMCON starting on 10 April and continuing for four weeks prior to the cruise (**Figure 14**). Two of the instruments remained at LUMCON during the cruise; the third one, Pandora 66, specially outfitted for operations on a rolling platform, was installed on the *R/V Point Sur*. At both LUMCON and on the *R/V Point Sur*, a standard NO₂ analyzer was operated in order to examine the relationship between column and ambient ("nose-level") NO₂. At LUMCON, low-cost sensors (i.e., "NO₂-sondes"; Sluis et al., 2010; Duncan, 2020) were operated and occasionally deployed at remote coastal sites when the *R/V Point Sur* was a few tens of km offshore (**Table 2**). During

these coastal coincidences, whole-air samples were taken by flask sampling onshore and on the ship (**Figure 15**). The whole-air samples were collected in specially prepared flasks and analyzed by the D. R. Blake group (Blake et al., 1992) for a range of VOC (e.g., alkanes, alkenes, and aromatics), halogenated carbon species, CO, CH₄, dimethylsulfide (a biogenic marine tracer), and others.



Figure 14. View of Pandora spectrometers deployed pre- and during cruise.

(Left) The three Pandora spectrometers (PSI) during the calibration and intercomparison period at LUMCON, 10 April through 7 May. On 8 May, the PSI #66 was moved to the bow of the *R/V Point Sur* (Right). Credits: R. M. Stauffer



Figure 15. Pictures of *R/V Point Sur* sampling and ONG operations during SCOAPE. (Left) Canister sampling and Pandora on the *R/V Point Sur*. (Right) Heavy-Density Area platforms. Credits: A. M. Thompson. Second, to characterize AQ over the GoM, a complement of standard analyzers for ozone, CO, CH₄, and CO₂ were chosen for continuous sampling on the *R/V Point Sur* (**Table 1**). The carbon species act as tracers for the air masses being sampled. Unfortunately, the shipboard CO instrument malfunctioned so CO readings were provided only through the whole-air samples; there were 27 of those total. Flask sampling on the *R/V Point Sur* was normally coordinated with a platform encounter. For large platforms, when a plume downwind was intercepted, as denoted by simultaneous NO₂ and CO₂ spikes, a flask was exposed. The platform was circled to get an upwind sample. For smaller operations closer to shore (marked Heavy Density Area, HDA) in **Figure 16**, right), plumes were more frequent and there was no contrast sampling. Several flasks were filled during a circling of the LOOP on 16/17 May.

For meteorological information, the *R/V Point Sur* was instrumented with a standard set of temperature, wind speed/direction and humidity sensors. One-two radiosondes were launched each day on the *R/V Point Sur* from 11–18 May for vertical information on pressure-temperature-humidity, wind speed, and direction; these give detailed information on boundary layer and tropopause characteristics. Ten ozonesondes were launched with the radiosondes; the ozone mixing ratios provide vertical information on pollution structure and stratospheric influences on tropospheric ozone. Continuous information on boundary layer characteristics came from one ceilometer at LUMCON and one on the *R/V Point Sur* (**Tables 1 and 2**).

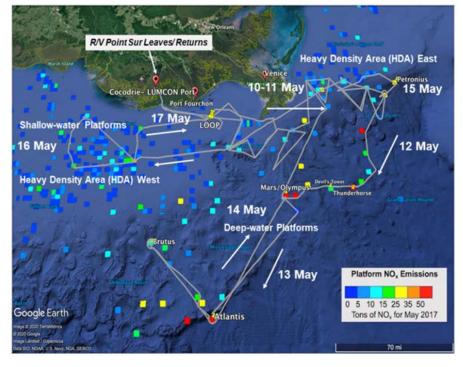


Figure 16. SCOAPE cruise *R/V Point Sur* track with onshore sampling locations. Gray indicates the track of the *R/V Point Sur* between 10 and 18 May 2019. Details given in text.

Species	Instrument	Collaborator	
NO ₂ (and calibrator)	In situ	NASA GSFC	
Column NO ₂	Pandora (PSI)	NASA GSFC (Swap*)	
O ₃	In situ Ozonesondes	NASA GSFC	
Temperature, RH, etc.	Met system	R/V Point Sur	
Aerosol (AOD) & O ₃ columns	Microtops Columns	NASA GSFC	
VOCs (plus CO & CH ₄)	In situ canisters	UCI (Blake)	
НСНО	In situ (Aeris)	NASA GSFC (Hanisco)	
PBL height	Ceilometer	UMBC (Delgado)	
Black carbon	Aethalometer	NIST (Conny)	
CH4, CO2, H2O	In situ (Picarro)	GSFC (Kawa / Hanisco)	

Table 1. Offshore instrumentation on R/V Point Sur during SCOAPE cruise.

* Collaborators for loaned instruments in parentheses.

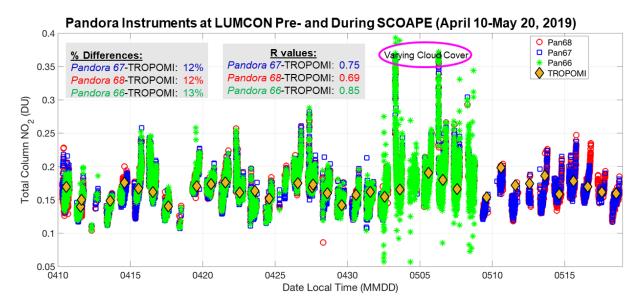
Table 2. Onshore instrumentation during SCOAPE cruise.

Species	Instrument	Collaborator	
NO ₂	In situ analyzer	NASA GSFC (Sullivan)	
NO ₂	Mobile in situ (NO2 sonde)	KNMI (Stein-Zweers/den Hoed)	
Column NO ₂	Pandora	NASA GSFC (Swap)	
VOCs (plus CO & CH ₄)	In situ canisters	UCI (Blake)	
PBL height	Ceilometer	U Houston (Flynn)	

The cruise track for the *R/V Point Sur*, superimposed on a Google Earth Map, with major land and platform locations and color-coded NO_x emissions (Wilson et al., 2019), is shown in **Figure 16.** The *R/V Point Sur* departed LUMCON at midnight starting 10 May and headed east, sampling in the region labeled HDA-East (Heavy Density Area East) before heading south and southwest toward the deepwater platforms. The 10 May sampling was conducted by automated instruments only; it was stormy, and seas were too rough for deck work. Clouds continued through 12 and 13 May. The farthest south point was near the Atlantis platform; an excursion to Brutus and back to Atlantis followed. Deepwater sampling concluded after a return to Mars/Olympus, followed by the track east and north to Petronius. HDA-East was sampled again along with the region near the entry to the Port of New Orleans ("Venice" on the map) followed by LOOP and HDA-West before the return to LUMCON in the afternoon (local time) of 18 May.

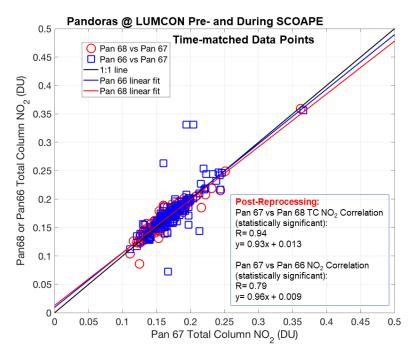
3.2.1 Onshore Observations

Figure 17 and **Figure 18** display comparisons of the three Pandora instruments inclusive of the pre-cruise period along with Pandoras 67 and 68 during the cruise period. Overpass comparisons for TROPOMI and OMI are also shown. **Figure 17** presents the TC NO₂ readings from all three Pandoras pre-cruise at LUMCON followed by the two LUMCON Pandoras during the cruise. TROPOMI overpass measurements (gold diamonds) with coincident TC NO₂ are also illustrated. R-values for comparisons with TROPOMI appear in legends within **Figures 17** and **18** and mean Pandora-TROPOMI TC NO₂ offsets are displayed. The latter are 12–13%, with the Pandora measuring higher column amounts than the satellite. There is more scatter among the three PSI during a cloudy period before the cruise on 4 through 8 May 2019. The R-values for the TROPOMI TC NO₂ relative to the Pandoras range from 0.69–0.85 (**Figure 17**).





TC NO₂ as measured by Pandoras 66, 67, and 68 prior to the SCOAPE cruise, from 10 April through 8 May with TROPOMI overpass readings in gold diamonds. After the Pandora 66 was installed on the R/V Point Sur; only Pandoras 67 and 68 recorded TC NO₂ at LUMCON. Source: D. E. Kollonige.





Time-matched data from Pandora 66 (blue squares) and 68 (red circles) referenced to Pandora 67 at LUMCON from 10 April–8 May 2019. Linear best-fit lines are blue and red respectively with 1:1 black line for reference. Source: D. E. Kollonige.

The reproducibility of the three Pandora instruments during their 4-week test period at LUMCON (**Figure 17**) is illustrated by referencing Pandoras 66 and 68 to Pandora 67. **Figure 18** shows the comparability of the three co-located Pandoras during the LUMCON test period. Agreement in terms of slope and offset of the best-fit lines, as shown in the box at lower right in **Figure 18**,

is excellent for both Pandora 66 and 68 relative to Pandora 67. The R-factor is lower for Pandora 66 because, as the blue symbols show, the latter instrument is noisier than the other two.

3.2.2 Offshore Observations: AQ Indicators on the SCOAPE Cruise

Examples of AQ forecasts and satellite products described in **Section 2.5** illustrate the complexity of pollution detection and attribution in the GoM. For example, the 11 September 2019 flare detected by VIIRS described by Duncan (2020) did not coincide with elevated NO₂ from satellite as did the early January 2019 examples shown in **Figure 11**. The SCOAPE cruise encountered pollution from Mexican agricultural fires with some of the trace gases on 14 May influenced by fires upwind of the *R/V Point Sur*. The tagged fire sources (**Figure 19**) show that correctly interpreting satellite and in situ NO₂ is not yet complete. Accurate NO₂ source attribution will require examining tracers, e.g., VOC, isotopes of CH₄ and meteorological parameters from the ship.

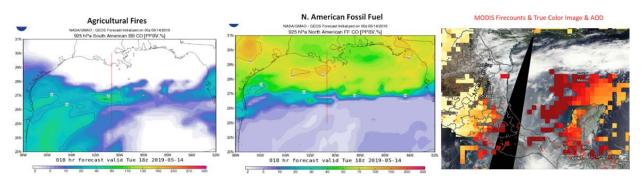


Figure 19. Imported pollution during the SCOAPE cruise on 14 May 2019.

(a) and (b) Tracers of fire pollution from Mexican origin, denoted as CO-fires and CO-fossil fuel, respectively, from the GEOS-CF model forecast for 14 May 2019; (c) MODIS images showing fire locations on 14 May 2019. Discriminating pollution sources on 14 May will require further analysis of both data and model output.

Figure 20 displays confirming evidence for the complexity of AQ encountered by the *R/V Point Sur*. In addition to the fire pollution episode, there were two general meteorological regimes with distinct chemical compositions. Late on 13 May, there was an abrupt transition in wind direction from mostly southerly and southwesterly directions to north/northeast (**Figure 20a**). Surface ozone increased from 20 ppbv or less to more than 40 ppbv, with a peak of 70 ppbv on 16–17 May. Shipboard ozone concentrations over the course of cruise (**Figure 20b**) show that these high levels near the final days of the cruise occurred in the westernmost segment (red colors in **Figure 20b**). The lowest ozone values (in blue near the coast) were measured at the beginning of the cruise. The days of the cruise up to the wind shift (10–13 May) are referred to as having air of "marine" origins. After that the air is designated as "continental," with the understanding that the air from Mexican fires is included in that label.

The contrast of the marine and continental air is evident in the CH₄ and CO₂ time series (**Figure 20c**). The tropical marine (unpolluted) air averages ~1.90 ppmv CH₄ and is only occasionally punctuated by high-CH₄ plumes. With the transition to continental air (dashed vertical line in **Figure 20c**), the mean CH₄ mixing ratio is ~2.00 ppmv, with several extended peaks close ~2.05 ppmv. Many of the latter observations were made close to shore in the HDA regions near natural gas operations. The time series of CO₂ (**Figure 20c**) is opposite of the other constituents shown in **Figure 20.** CO₂ levels decreased under the influence of continental air in mid-spring due to greening up of vegetation with an uptake of CO₂. In **Figure 20d**, the highest surface NO₂

measurements are more prevalent near shore, but elevated NO₂ measurements were also found between Brutus and Atlantis and southwest of Mars/Olympus.

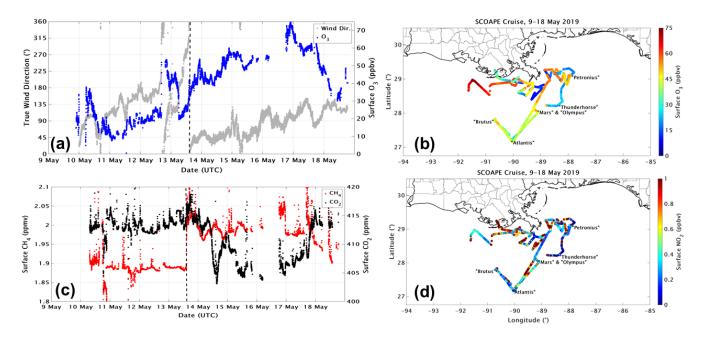


Figure 20 *R/V Point Sur* trace gas time series (a, c) and along-track maps (b,d). Concentrations of trace gases measured over the course of the SCOAPE cruise on the *R/V Point Sur*. (a) ozone and

Concentrations of trace gases measured over the course of the SCOAPE cruise on the *R/V Point Sur*. (a) ozone and wind direction, the latter measured by the ship's instrumentation; (b) ozone mixing ratio time series along the ship track, 9–18 May; (c) as (b) except for CH_4 and CO_2 ; (d) as (b) except for NO_2 . Source: R. M. Stauffer.

The ozone vertical structure (**Figure 21**) shows the complex nature of the ozone columns sampled during the cruise. During the "clean marine" phase the sharp ozone gradient seen at 15 km on 12–14 May is typical of a tropopause in subtropical or tropical air. The low-ozone layer between 10 and 14 km may originate from convective redistribution of air from the surface to cloud-outflow level that occurs frequently in the tropics (Petropavlovskikh et al., 2010; Thompson et al., 2010; Thompson et al., 2012). The continental air in contrast, appears to have a tropopause closer to 10 km and ozone greater than 80 ppbv is pervasive above 3 km.

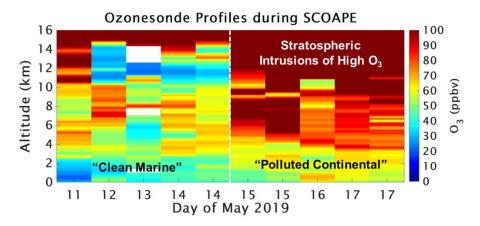


Figure 21. Ozonesonde profiles during SCOAPE.

Based on 0.25 km resolution data. Mixing ratios to 16 km are illustrated; layers with > 80 ppbv may signify stratospheric influence. Source: R. M. Stauffer.

A snapshot of marine vs continental influences for CH₄, CO, CO₂, and dimethylsulfide (DMS) concentrations, based on the 27 flask samples taken on the *R/V Point Sur*, appears in **Figure 22.** DMS is of marine biogenic origin; comparisons of species with continental biogenic origin (isoprene, α - and β -pinene) exhibit the opposite pattern, not shown.

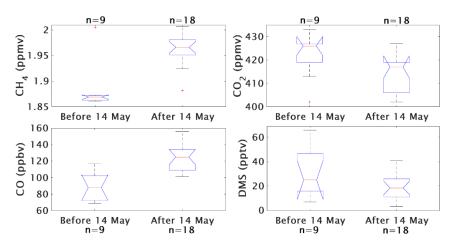


Figure 22. Summary of carbon-containing gases and DMS from *R/V Point Sur* flask samples. Box and whisker panels for CH₄, CO, CO₂, and dimethylsulfide (DMS) before (left side of each panel) and after 14 May (right side of each panel). Sample numbers indicated at the top of each panel. Red line denotes median values, blue box denotes 25th and 75th percentile, and whiskers (dashed bars) are 95th percentile. Source: R. M. Stauffer.

As the examples in **Figure 20–Figure 22** demonstrate, throughout the cruise, there is considerable variability in all the constituents measured. One of the more extreme examples was captured in a whole-air sample near a shallow-water platform at 1612 hr Central Daylight Time on 16 May. A CH₄ spike to 16 ppmv was observed by the Picarro instrument. Concentrations of representative carbon-containing compounds in the flask exposed at that time appear in **Table 3**. The CH₄ increase in the flask was a factor of ~3, signifying leaks from gas production. CO₂ was nearly identical to the cruise flask mean. However, ethane, *n*-propane and benzene amounts were 75, 130, and 45 times higher, respectively, than their cruise averages.

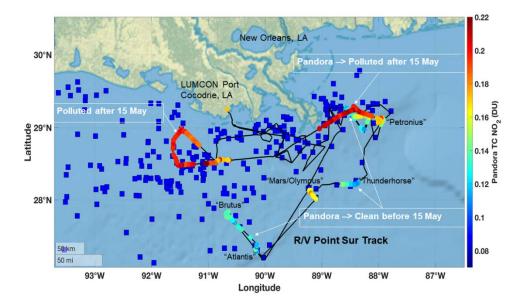
VOC Can Species	Cruise Median	16 May Plume Can	Notes
CH ₄ (ppmv)	1.96	5.71	Deepwater platforms flare this off
CO ₂ (ppmv)	415	418	No combustion, likely just leaky pipes
Ethane (ppbv)	2.1	145	C ₂ H ₆ ; second largest component of fossil gas after CH ₄
Propane (ppbv)	0.7	90.1	C ₃ H ₈ ; byproduct of fossil gas processing
n-Butane (ppbv)	0.3	29.9	C ₄ H ₁₀ ; i-Butane had similar concentrations
Benzene (ppbv)	0.04	1.88	C ₆ H ₆ ; known carcinogen

Table 3. Extreme AQ condition	ns on 16 Mav near	shallow-water platform.	28.9795°91.4760°.

3.2.3 Satellite, Pandora and Surface NO₂ Comparisons on the SCOAPE Cruise

Figure 23–Figure 25 illustrate NO₂ variability during the SCOAPE cruise, with observations from Pandora 66, TROPOMI and the *R/V Point Sur* trace gas analyzer. In **Figure 23** the entire ship track is shown with Pandora TC NO₂ columns for segments before 15 May 2019 mostly below 0.18 DU. After 15 May Pandora 66 records several segments with higher TC NO₂. These occurred near large platforms like Petronius as well as in extended regions within the natural gas platforms in HDA-East and West (orange to red in **Figure 23**). Overall, both TC NO₂ and the

in situ NO₂ measurements along the cruise track follow the two-regime pattern of the other constituents described above (**Figure 24**). Both Pandora 66 TC NO₂ and surface NO₂ increase an average of 50% between the clean marine and continental regimes. The increase in TROPOMI TC NO₂ is not as large. This is similar to the pattern observed in the OWLETS campaigns where, as pollution measured at the ground increased, the satellite appeared to be less sensitive to it (**Figure 9**). In other words, at higher TC NO₂, the deviation of the satellite reading was further from the 1:1 line; that tendency also appears in **Figure 26** for both OMI and TROPOMI comparisons.





Blue squares mark the locations of platforms that fall into the category of the top 200 NO_x emitters according to the 2014 BOEM inventory (Wilson et al., 2017). Black is the *R/V Point Sur* track from 10–18 May 2019. The cleaner air portion of the cruise as described above, was sampled prior to 14 May, more polluted air masses after 14 May. Source: D. E. Kollonige.

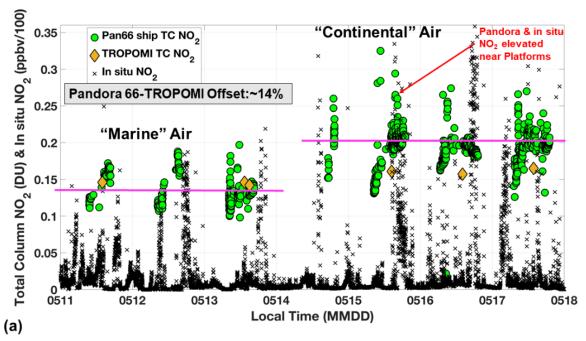


Figure 24. Time series of TROPOMI, Pandora, and in situ NO₂ during SCOAPE cruise. Pandora TC NO₂ measurements and in situ data are 5-min averages. Source: Thompson et al. (2020).

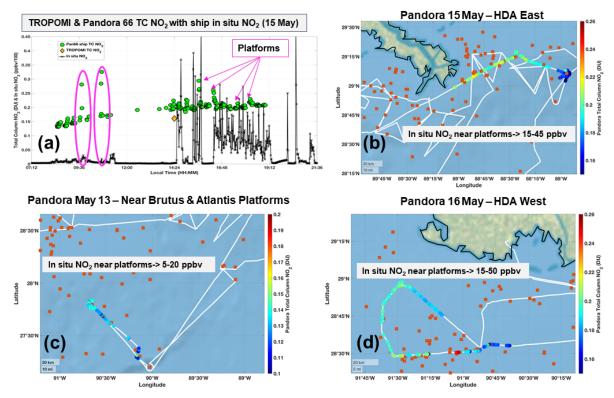


Figure 25. Time series of Pandora and in situ NO₂ on 15 May and along-track Pandora maps. Time series (a) of Pandora 66 (green dots), in situ (black) and TROPOMI (golden diamond) NO₂ on 15 May 2019 at the *R/V Point Sur*. Maps of Pandora NO₂ on (b) 15 May, (c) 13 May, and (d) 16 May provide reference for NO₂ variability along the cruise track. Color bar scales vary to highlight the gradients and elevated NO₂ observed while passing near platforms (marked as orange squares). White line is the *R/V* Point Sur ship track. Source: Thompson et al. (2020).

As described in pre-SCOAPE studies (Section 2) relating the satellite and/or Pandora column NO₂ amounts to surface NO₂ is not straightforward. Generally speaking, when the boundary layer is not well-mixed, i.e., NO_2 may be trapped near the surface, or when much of the NO_2 column is an above-boundary layer residual or is advected from upwind, the column amount does not correspond to the surface (or shipboard) concentration. These discrepancies between in situ and column NO₂ variability are evident in **Figure 25a**, which is a close-up of the 15 May 2019 observations (in local time) during the SCOAPE cruise. Figure 24 shows 15 May to be the day with the greatest range in TC NO₂ values. There is a slow increase in Pandora TC NO₂ during the morning hours and a few spikes for 15 May (magenta highlights in Figure 25a), while surface NO₂ remains well below 5 ppbv. A VOC canister sample, taken at the time of the second Pandora TC NO₂ spike in the morning of 15 May (second magenta circle in Figure 25a), indicates n-butane and i-pentane are ~2-3 times higher than other cruise samples (second highest of the campaign; 16 May example is highest) while passing the Petronius platform. Note: Different processes emit different gases, and this is dependent on the platform's current operation at the time of the ship's measurements. Both species, n-butane and i-pentane. sometimes emitted during the flaring process, are indicators of platform activity.

Midday Pandora TC NO₂ averages ~0.20 DU in the "continental air" (**Figure 24**), approximately 30% higher than the TROPOMI overpass value. However, for 15 May (**Figure 25a**), the Pandora appears to not be sensitive to several pollution plumes (spikes up to > 40 ppbv surface NO₂), one of which is in the vicinity of a large platform in the afternoon ~1,500 LT (first magenta arrow). N-butane and i-pentane are again ~2–3 times higher than other cruise samples, with the exception of the 16 May outlier. More analysis is needed to understand the surface-column NO₂ relationships displayed in **Figure 25a**, but individual NO₂ spikes are enhanced above the daily mean for both when passing platforms on 15 May. This example highlights the value and complexity of taking both surface and column NO₂ measurements in AQ monitoring.

Figures 25b–d illustrate three other regions, summarizing the range of in situ NO₂ readings with the coincident Pandora readings along the track. In these regions there is a wide range of surface NO₂, up to 45–50 ppbv over the HDA regions near shore on 15–16 May and 5–20 ppbv during the leg between Atlantis and Brutus, 13 May (**Figure 25b–d**). There is considerable variation within each region with very low TC NO₂ (dark blue) as well as levels > 0.20 DU. These episodes will be investigated in detail with tracers, ancillary satellite data, air parcel trajectories and, where possible, with model output.

A summary of overpass comparisons from OMI and TROPOMI TC NO₂ relative to the shipboard Pandora 66 appears in **Figure 26.** Although the TROPOMI satellite instrument footprint is smaller than that of the OMI satellite, the offsets with Pandora 66 are nearly the same. Also, in both cases, as TC NO₂ increases, the discrepancy between ground-based and satellite column amounts increases, with the Pandora usually greater. These comparisons are typical for the low to moderate amounts of pollution observed over and near the GoM (see, for example, Herman et al., 2018; 2019).

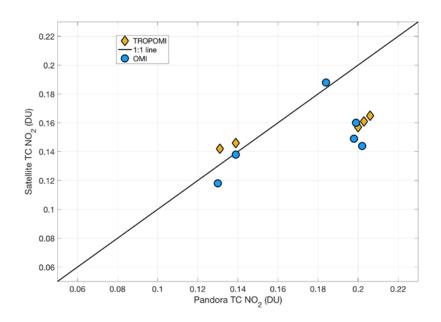


Figure 26. Satellites vs. Pandora 66 TC NO₂ on the R/V Point Sur during the period 10-18 May 2019. OMI (blue circles) and TROPOMI (gold diamonds) are on y-axis versus Pandora 66 on x-axis. Black line is 1:1 line.

4 Summary of SCOAPE Cruise Analysis and Recommendations

SCOAPE set out to answer three important questions for BOEM, and summary answers are as follows:

- Can satellite observations detect emissions from ONG operations, and are the measurements accurate? Using NO₂ as our "Air Quality Proxy," we find, based on the May 2019 SCOAPE cruise, that the operational OMI and TROPOMI satellites are able to detect elevated NO₂ associated with ONG operations. Referenced to both land- and ship-based Pandoras, satellite TC NO₂ was accurate to 11–18%, with the satellite biased low at the higher pollution levels. More analysis of the *R/V Point Sur* PSI and in situ NO₂ measurements using tracers (CH₄, CO₂, other VOC), trajectories, and models is required to better establish uncertainties.
- How reliable are the Pandora instruments used for ground-based remote sensing? During the cruise and four weeks of pre-cruise calibration in coastal Louisiana, comparisons of TC NO₂ readings from the new Pandora instruments showed ~5% precision or better.
- How do pollutant levels measured by satellite over coastal Louisiana and the adjacent GoM compare? From our 2019 sampling, pollution appears to be greater over the continent than the GoM, although both in situ and Pandora measurements during the cruise display prominent NO₂ spikes near platform operations. A comprehensive answer to this question requires continued monitoring of satellite NO₂, as well as coastal observations of NO₂-related pollutants and tracers and models with accurate NO₂ sources.

⇒ Recommendations to BOEM: Based on SCOAPE Results

- 1. BOEM and NASA should work together to analyze the 2019 SCOAPE data more thoroughly, including conducting studies with tracers, ancillary satellite data, trajectories, and appropriate chemical transport model output to more firmly establish the magnitude of ONG influences on GoM AQ.
- 2. Coastal monitoring along the GoM with NASA and EPA using Pandora Spectrometer Instruments and other instruments would establish better statistics and contribute to the ongoing improvements in OMI (mature algorithm) and the still evolving TROPOMI. Colocation with BOEM's coastal project, aiming to begin in late 2020 at a remote unpolluted location in Louisiana would greatly benefit BOEM. Daily overpass comparisons of OMI and TROPOMI TC NO₂ with a Pandora instrument would give BOEM more complete statistics than the 5-week exploratory dataset of April–May 2019. Comparisons of the in situ and column NO₂ amounts, along with other pollutants being measured, would further our understanding of the relationship of chemical transformation and interactions with dynamical processes in the boundary layer.

Neither satellite nor Pandora column amounts provide ambient concentrations of NO₂. By using case studies, of which we have identified a number in the May 2019 SCOAPE dataset, we can establish statistics for the column-surface NO₂ connection and establish environmental conditions under which the relationship is strongest. NASA will continue to conduct this type of analysis as it prepares for the 2022 launch of a geostationary ozone and NO₂ satellite, TEMPO. TEMPO is designed for hour-to-hour pollution monitoring over North America and its coastal waters, including the GoM, Atlantic, and Pacific areas of emerging interest to BOEM.

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