SEARS

Ship Emissions to Atmosphere Reporting Service

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Contents

List of abbreviations and acronyms

BB	Bay of Biscay
BIRA	Belgian Institute for Space Aeronomy
CF	Cloud Fraction
COT	Cloud Optical Thickness
CP	Cloud Pressure
CTM	Chemistry-Transport Model
ECMWF	European Centres for Medium-range Weather Forecasts
EMS	East Mediterranean Sea
FOV	Field of View
GEMS	Geostationary Environment Monitoring Spectrometer
GMES	Global Monitoring of the Environment and Security
GOME-2	Global Ozone Monitoring Experiment-2
IUP	Institute of Environmental Physics (University of Bremen)
LT	Local Time
MODIS	Moderate Resolution Imaging Spectroradiometer
NS	North Sea
OMI	Ozone Monitoring Instrument
OZA	Observation Zenith Angle
OAA	Observation Azimuth Angle
OMPS	Ozone Mapping Profiler Suite
RAA	Relative Azimuth Angle
SECA	Sulphur Emission Control Area
S4	Sentinel-4
S5P	Sentinel-5 Precursor
SAA	Solar Azimuth Angle
SCD	Slant Column Density
SCIAMACHY	Scanning Imaging Absorption spectrometer for Atmospheric CartograpHY
SNR	Signal-to-noise ratio
STD	STandard Deviation
SZA	Solar Zenith Angle
TEMIS	Tropospheric Emission Internet Service
TEMPO	Tropospheric Emissions: Monitoring of Pollution
TROPOMI	TROPOspheric Monitoring Instrument
VCD	Vertical Column Density
UV	UltraViolet
NIR	Near-infrared
SWIR	Shortwave infrared

1. Introduction

In recent years, space-borne spectrometers, such as GOME, SCIAMACHY, OMI, and GOME-2, have been used to detect and quantify NO_2 pollution due to shipping emissions. Although these satellite instruments are limited in their ability to obtain useful data with a time resolution better than typically one month or longer, they have provided valuable information on the seasonal and inter-annual variability in shipping emissions as well as on their long term trends.

Current shipping NO_2 products are limited by four main factors: signal to noise ratio, spatial and temporal resolution, cloud and/or aerosol contamination, and difficulty to separate shipping NO_2 from other sources of emissions. Improvements on the first three of these points can be expected from future satellite instruments, in particular the Sentinel-5 Precursor (S5P) and the Sentinel-4 (S4) that are planned to be launched during the current decade. Both instruments will have better spatial resolution, comparable or better coverage and better signal-to-noise ratios than current sensors. Better spatial resolution reduces cloud contamination and increases signal for localized sources such as ships. Improved coverage (which will be available over Europe with S4 flying in a geostationary orbit) improves statistics for cloud free pixels and thereby reduces noise. This can even be further improved by combining data from several instruments operating at the same time, e.g., combining S4 data with observations from GOME-2, S5P, and other instruments. Based on these considerations, it is anticipated that future sensors will allow for significant improvement of the time resolution of the shipping NO_2 products therefore matching better the requirements from International Maritime Organizations such as EMSA.

The purpose of this technical report is to investigate more quantitatively the gain to be expected from future sensors. Our focus is on three areas over European waters: The East Mediterranean Sea (EMS), the Bay of Biscay (BB), and the North Sea (NS). These are relatively polluted regions with significant emission contributions from dense ship traffic. A regional chemical transport model (CHIMERE) combined with a high-resolution emission inventory is used to generate NO_2 profile data with high spatial ($10\times10km^2$) and temporal (hourly) resolution. These NO_2 data sets are used to generate pseudo-observations for the future sensors, as well as for OMI as a reference. The pseudo-observation satellite data sets are compared to the existing data records of OMI, and used to assess the potential of future sensors for identifying shipping emissions.

At the start of the project focus was on global NOx emissions. After EMSA user consultation the project was restructured and it was decided to focus the study on the following scientific issues:

1. Derive NO_x shipping emissions based on satellite data over European waters
2. Assess the feasibility of detecting shipping in SO_2 emissions using satellite data
3. Assess the potential of future instruments in detecting NO_x shipping emissions.

The document is set up as follows:

- Section 2 summarizes the user requirements
- Section 3 summarizes the used models and data
- Sections 4, 5, and 6 summarize the results and conclusions as described in D2, D3 and D4

- Section 7 provides the lessons learned and reported in D6 and a possible roadmap for service delivery.

2. User requirements

The kind of shipping emission products useful for EMSA in fulfilling its mandate was established during a joint meeting in April, 2012 between the SEARS team and EMSA's representatives.
EMSAs requirements are based on current directives and legislations pertinent to shipping emissions. In order to enforce the legislations and to measure their effectiveness, EMSA would need a tool for monitoring shipping emissions. The currently available in-situ measurement techniques are cumbersome and can only be carried out in harbors or during dedicated fly-bys. Emissions from ships in transit are not monitored on a regular basis.

EMSA is primarily interested in a means of monitoring SO_2 emissions in European waters. Identifying SO_2 emissions from individual ships would provide a tool for legislation enforcement as the SO_2 emitted can be directly linked to the sulphur content of the fuel used. A comprehensive SO_2 trend analysis in SECAs would be valuable for evaluating the effectiveness of legislation. However, ship SO_2 emissions have never been observed from satellites, except in a very recent study analyzing long-term averages of OMI measurements. Even in the case of NO_2 it is not possible to distinguish emissions from individual ships given the relatively low resolution of satellite data and the signal-to-noise ratio.

NO_x emissions are regulated via engineering standards for vessel engines, not via emission thresholds. The enforcement of the legislation happens in ports by checking the engine specifications; therefore EMSA is less interested in a monitoring tool for NO_x emissions.

There is a clear contrast between EMSA's needs and the capabilities of current satellite instruments. Nevertheless a list of products and study areas were identified which would both benefit EMSA and are feasible given the current capabilities of satellite instruments. The resulting user requirements and the degree of involvement of EMSA in SEARS are summarized in sections 2.1 and 2.2 below.

2.1. User requirements

Shipping NO_x emissions
Even though current regulations on NOx emissions from shipping are in the form of engineering standards, estimates of NOx emissions from shipping could still be useful for EMSA. Such a product can help with the political decision making process, can be used to estimate trends and to identify over-polluted areas. Given EMSA's European mandate, NOx emission products should be developed for the major shipping lanes in European territorial waters.

Shipping SO_2 emissions
EMSA's main interest is in the monitoring of SO_2 emissions. However, as described before, SO_2 emissions from shipping emissions can hardly be observed from satellites. EMSA is interested in knowing what the detection limits of satellites are and if detecting shipping SO_2 emissions from space is at all possible.

Capabilities of upcoming instruments
There are several upcoming European satellites dedicated to the monitoring of atmospheric composition, including the Sentinel-5 precursor, Sentinel 4, and Sentinel 5. EMSA is

interested in knowing what can be achieved with these instruments with respect to the detection of shipping emissions.

2.2. Degree of involvement

The degree of involvement of EMSA in the project was determined and EMSA agreed to collaborate with the SEARS team in the following areas:

- Contribute to establishing the study requirements;
- Review reports and provide input where needed;
- Take part in the milestone meetings.

3. Modelling and data

3.1. Modelling

In this study a meteorological and a chemistry transport model are coupled to simulate NOx and SO_2 vertical profiles over 4 areas with dense shipping. Results are produced for each season in 2007. Concentration maps are used to construct pseudo satellite data for comparison with existing satellite observations and to assess potential of future missions.

3.1.1. Meteorological modelling

The numerical weather prediction model used in this study is the so-called Weather Research and Forecasting (WRF) model [Skamarock et al. 2008]. The WRF model is a state-of-the art regional atmosphere model and is used by many institutes around the world, both for research and operational purposes.

The model comes with a large number of physical parameterisation schemes. The model makes use of a surface layer scheme, a planetary boundary layer scheme, a cumulus parameterisation scheme for resolutions above 5 km, and a microphysics scheme allowing for the formation of ice, snow, graupel, and rain.

WRF is a regional atmosphere model which means it cannot run without boundary conditions. Here, both the initial conditions and boundary conditions are supplied by NCEP FNL (Final Analysis) data. The WRF model was set up with two nested domains: an outer domain with a 27 km resolution and an inner domain at 9 km resolution.

In this project runs have been made for 4 areas: Indian Ocean, eastern Mediterranean Sea, Bay of Biscay and the Baltic Sea. The domain setup for these areas is shown in Figure 3.1 and Figure 3.2. The WRF model was run for the year 2007. After a 48-hour period it is re-initialised using NCEP FNL data and a six-hour long spin-up window is used before the start of each 48-hour period.

The data are available with a temporal resolution of one hour. The primary weather model variables that are passed on to the chemistry-transport model are: temperature (3D), pressure (3D), humidity (3D), wind speed and direction (3D), Incoming and outgoing, radiation, precipitation and planetary boundary layer height.

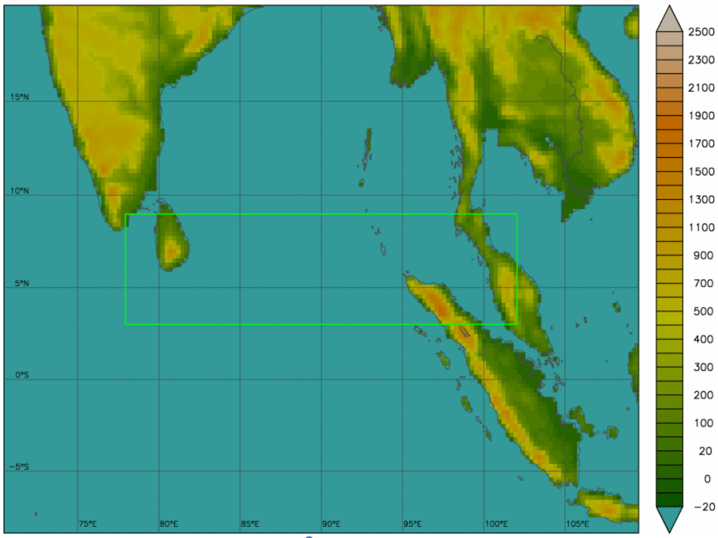

Figure 3.1: The outer, 27 x 27 km^2 resolution outer WRF domain covering the northern part of the Indian Ocean. The green rectangle marks the location of the 9 x 9 km^2 resolution inner domain. The colour bar indicates surface elevation in m.

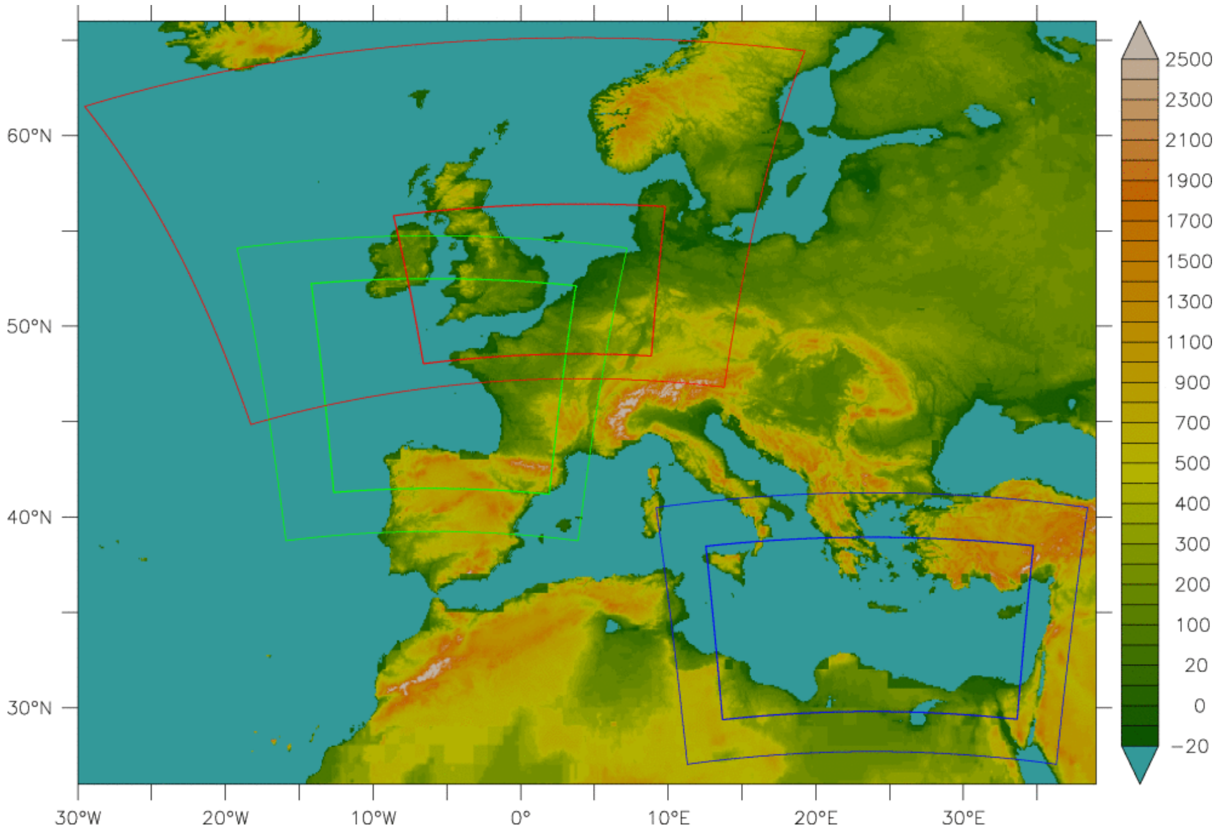

Figure 3.2: The WRF domain covering the North Sea (red), Bay of Biscay (green) and eastern Mediterranean Sea (blue). The outer rectangle marks the 27 x 27 km^2 resolution WRF domain. The inner bold rectangle marks the location of the 9 x 9 km^2 resolution domain.

3.1.2. Air quality modelling

The chemistry transport model used in this study is CHIMERE, which is developed and maintained under the lead of researchers from the École Polytechnique near Paris in France. (see *http://www.lmd.polytechnique.fr/chimere*).

CHIMERE is capable of calculating the changes in air pollutant concentrations due to transport, turbulent diffusion, chemical transformations and deposition. The model requires several input data sets: information on meteorological conditions, boundary conditions (either from climatology or large-scale air quality models), land use data, biogenic emissions, and finally the locations and strengths of anthropogenic emission sources. The meteorological input data are generated in the SEARS project using the WRF model (see previous section).

Like the WRF model, CHIMERE can be applied on a wide variety of spatial scales from local (km or sub-km resolutions) to regional (hundred km resolution). The model can run with several vertical resolutions and with a wide range of complexity. It can use a simplified or a more complete set of chemical mechanisms; it can include or exclude aerosol and organic chemistry. There are also options to include dust uptake by wind, deep convection, urban heat island effects, etc. The temporal resolution of the model is typically one hour.

The CHIMERE model needs the average emissions for each species, per month, per day type (work days, Saturdays and Sundays), and for each hour of the day. The emission data is provided with 6 vertical layers representing pollutants emitted at various altitudes (road surface, chimneys).

3.1.3. Emission database

A chemistry transport model requires input from an emission database. The CHIMERE model was designed to use the EMEP data. However, the emissions in the EMEP database are not available for all project target areas and the 50 x 50 km^2 resolution is too coarse for modelling shipping lanes in the vicinity of land. The EDGAR emission database turned out to be more suitable. For application in this project this database was converted to become EMEP compatible, i.e. format was adapted and activity sectors were remapped.

The following species are available in the global EDGAR database: CH_4, CO, NH_3, NMVOC, NO_x, and SO_2.The data are available in the form of yearly averages, in units of $kg/m^2/s$. The data are gridded and have a resolution of 0.1° x 0.1°. To bring the EDGAR data in line with the EMEP data, the SO_2 emissions were converted to SO_X using a linear relation.
Redistribution of emissions based on land-use was not applied for the Edgar data, because the resolution is already good enough.
As an example the annual mean NOx emissions available in the EDGAR database are shown in Figure 3.3. Shipping lanes are clearly visible. The range of colours is chosen to enable viewing of shipping emissions. As a result the colour scale saturates often for over land areas.

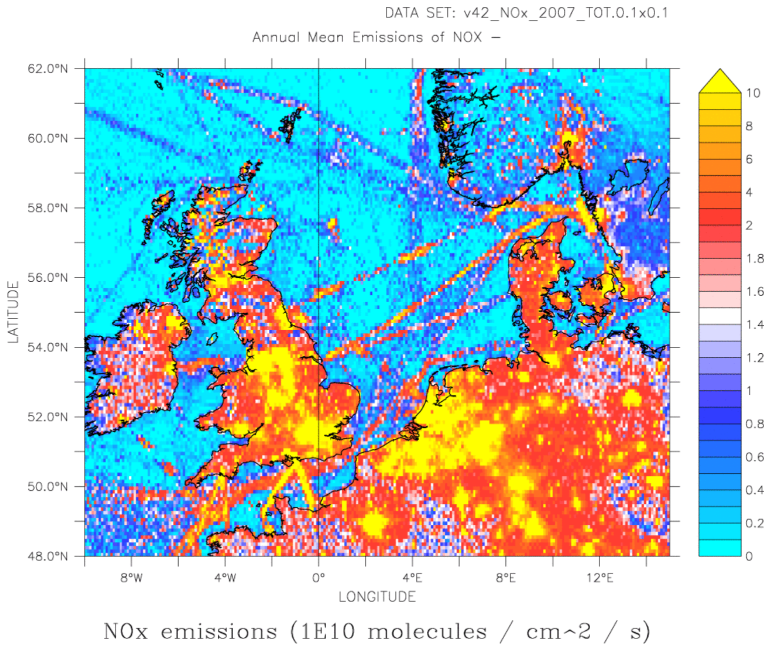

Figure 3.3: The annual NO_x emissions according to the EDGAR database.

3.2. Satellite data

Model results have been compared with observations from past and current missions and used to simulate future missions. Past and current missions are GOME, SCIAMACHY, OMI and GOME-2. OMI and GOME-2 data are used in this study.
The potential of future missions is studied for the UVN spectrometer to be carried by Sentinel-4 and TROPOMI carried by the Sentinel-5 Precursor mission. The concentration data produced by WRF/CHIMERE have been used to construct a set of pseudo observations for Sentinel-4 and Sentinel-5.

3.2.1. GOME

The Global Ozone Monitoring Experiment (GOME), launched in 1995 provided the first global view of tropospheric NO_2. In 2004 Beirle et al. (2004) detected a line of NO_2 from India to Indonesia that matched the position of ship tracks. No other ship tracks could be detected, mainly due to the very large pixel size of GOME (320 x 40 km^2).

3.2.2. SCIAMACHY

The SCIAMACHY (SCanning Imaging Absorption spectroMeter for Atmospheric CartograpHY) was carried by ENVISAT, launched in 2002. SCIAMACHY data have better spatial resolution (60 x 30 km^2), enabling the detection of shipping NO_2 also in the Red Sea, the Persian Gulf and from Indonesia towards Japan and China (Richter et al., 2004).

3.2.3. OMI

The OMI instrument, launched in 2004, has even better spatial resolution of 13 x 24 km^2 and much better coverage. Consequently additional NO_2 from ships has been observed in the Mediterranean in OMI data (Marmer et al., 2009). Improved filtering techniques have enabled the detection and quantification of shipping NO_2 in the Bay of Biscay, the North Sea and the Baltic Sea (Vinken et al., 2014) and an additional ship track in the Baltic Sea was reported by Ialongo et al., 2014. The very first identification of SO_2 emissions from ships in the Persian Gulf has been also obtained from OMI in a recent study (Theys et al., 2015).

3.2.4. GOME-2

The latest UV/visible instrument providing NO_2 data is the GOME-2, launched on Metop-A in October 2006 and on Metop-B in September 2012. Although it has reduced spatial resolution (80 x 40 km^2), the good signal-to-noise ratio of these data has resulted in detection of NO_2 from shipping from Europe, around Africa towards Indonesia (Richter et al., 2011). Franke et al. (2009) investigated the temporal evolution of the NO_2 signal from India to Indonesia using data from all available instruments, finding large seasonality, an upward trend, and also interannual variability. A closer look on the temporal evolution of shipping NO_2 and the link to international trading volume was presented in de Ruyter de Wildt (2012), highlighting the reduction in shipping NO_2 signal during the 2008 crisis visible in several shipping lanes observed by GOME-2, OMI and SCIAMACHY. In all cases, averages over one month or longer were used to achieve appropriate signal-to-noise ratios.

3.2.5. Sentinel-4

The Sentinel-4 mission will consist of an UVN (Ultraviolet-Visible-Near-Infrared) spectrometer accommodated on Meteosat Third Generation Sounder (MTG-S) platforms operating in geostationary orbits. Two missions are planned for the S-4 UVN payload: the first one in 2019 and the follow-up mission in 2027.

The mission objective of the Sentinel-4 is the continuous monitoring of atmospheric composition and air quality in Europe (O_3, NO_2, SO_2, HCHO, and aerosol optical depth) at a fast revisit time of ~1 hour. The spectral resolution of the UVN instrument will be 0.5 nm in the UV/visible and 0.12 in the NIR. Spatial sampling will be 8 km at 45°N.

With its geostationary orbit, Sentinel-4 UVN will for the first time provide hourly observations over Europe, increasing measurement statistics, reducing sensitivity to clouds, and enabling studies of the diurnal variation of emissions, chemistry, and transport of pollutants. As the spatial coverage of UVN is limited to Europe, it will be operated in combination with low earth orbiting instruments such as S5P and S5.

3.2.6. Sentinel-5 Precursor

The measurement principle of TROPOMI/ Sentinel-5 Precursor is similar to that of OMI. The instrument images a strip of the Earth on a two dimensional detector for a period of 1 second (2 seconds for OMI) during which the observed swath moves by about 7km along its orbit. The field of view of the imaging system is large (~114°) and approximately corresponds to a swath width of 2600km. The ground pixel size at nadir position is about 7×7km^2 (along × across track) for TROPOMI. In fixed binning mode (such as OMI), the pixel size in the swath-direction increases with the viewing angle, and the across-track size at the most outer swath-angle (57°) is approximately 5 times larger than the pixel size at the nadir viewing angle. In contrast, TROPOMI adopts a variable binning factor (van Geffen et al., 2013); the binning factor is reduced by a factor of 2 and 4 at the point in the swath where the ground pixel size has doubled and quadrupled in comparison to the nadir pixel size.

The instrument characteristics of the above instruments are summarized in Table 3.1 and Table 3.2. In Table 3.3 other instruments relevant for future service development are presented. See also section 7 Roadmap.

Table 3.1: Instrument characteristics of European platforms in sun-synchronous orbit

Instrument	GOME	SCIAMACHY	OMI	GOME-2
Platform	ERS-2	Envisat	Aura	Metop-A/Metop-B
Launch date	April 1995	March 2002	July 2004	October 2006/November 2012
Status / end	July 2011	April 2012	operational	operational
Altitude [km]	785	800	705	705
Spatial resolution [km x km]	40 x 40 to 40 x 320	30 x 30 to 30 x 60	13 x 24 to 13 x 128	40 x 80
wavelength range [nm]	240 - 790	240 – 1700 and 2000 – 2400	270 - 500	240 - 790
wavelength resolution [nm]	0.2 – 0.4	0.2 – 0.5	0.14 – 0.63	0.2 - 0.5
viewing geometry	nadir	nadir, limb, occultation	nadir	nadir

Table 3.2: Instrument characteristics of future European systems

Instrument	Sentinel-5P/UVNS (TROPOMI)	Sentinel-4/UVN	Sentinel-5/UVNS
Platform	Sentinel-5 Precursor	MTG-S	Metop-SG-A
Launch date	2016	2019 / 2027	2020
Orbit type	Sun-synchronous	Geo-stationary	Sun-synchronous
Altitude [km]	824		817
Spatial resolution [km x km]	7 x 7	8 km at 45^{o}N	7 x 7
wavelength bands	UV-Vis-NIR-SWIR	UV-Vis-NIR	UV-Vis-NIR
wavelength resolution [nm]	0.5 – 1.0 (UV1) 0.55 (UV2Vis) 0.5 (NIR) 0.25 (SWIR)	1 (UV1) 0.5 (UV/Vis) 0.12 (NIR)	1 (UV1) 0.5 (Vis/NIR) 0.25 (SWIR)
revisit time	daily	1 hour	daily
coverage	global	Europe (UVN)	global

Table 3.3: Instrument characteristics of non-European systems

Instrument	OMPS	GEMS	TEMPO
Platform	NPP	GEO-KOMPSAT-2B	TEMPO
Country/Agency	US/NOAA	Korea/KARI	US/NASA
Launch date	2011	2018	2018
Orbit type	Sun-synchronous	Geo-stationary	Geo-stationary
Altitude [km]	824	35786	35786
Spatial resolution (nadir) [km x km]	50 x 50	8 km at 45^o	2 x 4.5
wavelength bands	UV	UV-Vis	UV-Vis
wavelength resolution [nm]	1.0	0.6	0.6
revisit time	daily	1 hour	1 hour
coverage	global	5000 km x 5000 km centred around Korea	Mexico, US, Canada 18 N – 58 N
viewing geometry	nadir, limb	nadir	nadir

4. Prototype NO_x product development

The potential of satellite observed tropospheric NO_2 columns to be used for the estimation of shipping NOx emissions has been evaluated. First, in a series of sensitivity studies, a number of approaches have been evaluated to improve the detection of NO_2 signal from ships. The main results are that:

- The use of a **larger fitting window** in the NO_2 retrieval reduces the noise of the shipping NO_2 signal
- The noise of the data can further be reduced by applying an **improved gridding algorithm** based on a fine sub-grid sampling and subsequent averaging on the final grid. By careful adaptation of the final grid size to the geophysical dimensions of the NO_2 ship track an optimum in detectability and low noise can be obtained.
- **Cloud contamination** is a problem for any tropospheric NO_2 product, and this is also the case for shipping signals. Depending on region, limitation to cloud free observations increases the observed shipping signal albeit at a loss of the number of satellite measurements included in the averages. The effect is particularly pronounced in the Bay of Biscay region.
- Observations taken under **sun-glint** geometry provide higher sensitivity to the boundary layer NO_2. Consequently, the shipping signal is larger in GOME-2 and OMI data if only sun-glint geometries are used for the averages. However, the number of these observations is limited spatially and temporally in European waters, and cloud contamination imposes additional limitations.
- Limitation to **low wind speeds** increases the observed shipping signal in some regions as dilution by wind as well as contamination by NO_2 from land-based sources is reduced. However, in particular in the North Sea region, the number of calm situations is small, reducing the data base for averaging and therefore the signal to noise ratio of the resulting averages.
- **Spatial filtering** can be applied to detect and quantify shipping NO_2 in ocean regions in an automatic and objective way. In order to improve the detection and to reduce occurrences of negative side lobes, an iterative approach is needed in which detected shipping regions are removed from the data set used for background determination applying a threshold technique. As in all filtering techniques, the choice of cut-off value is critical and using too little smoothing in the filter will artificially reduce the shipping signal. More work is needed to determine optimal choices of this parameter for all shipping regions.
- Conversion of NO_2 columns to **NOx emissions** relies on accurate modelling of atmospheric NO_2 over shipping lanes. While the agreement between CHIMERE modelled columns produced in this study and satellite data is reasonable, differences in the seasonality and spatial distribution are a problem for the conversion of NO_2 columns to NOx emission strengths.

5. Potential of satellite instruments to detect and quantify SO_2 from ships

CHIMERE simulations of SO_2 from ship emissions for the ship track between India and Indonesia which is the most visible in satellite NO_2 data predict relatively small SO_2 columns of 0.3 – 1.5×10^{15} molec cm^{-2}. As result of the longer atmospheric lifetime of SO_2, the ship track is less localised in SO_2 than in NO_2 fields, making detection more difficult. According to model results, changes in meteorology lead to a strong seasonal variation in shipping related SO_2 columns.

Strong Rayleigh scattering at the UV wavelengths used for the retrieval in combination with the dark surface limit the sensitivity of satellite observations of shipping SO_2 and lead to air mass factors of about 0.5, smaller by a factor of 4 than typical SO_2 AMFs for volcanic SO_2. The small AMFs in the shipping lane and larger AMFs elsewhere further complicate the unambiguous detection of shipping SO_2 and can potentially lead to false positive detection as AMF and assumed a priori ship signal are strongly correlated.

Analysis of the existing time series of GOME-2 and operational OMI SO_2 products show no indication of shipping signals, neither in long-term averages using all data, nor in averages limited to clear-sky scenes or the months with the largest model SO_2 columns. Only when integrating over the ship track area in the long-term global average of GOME-2 data, there is some hint of a shipping signal at the right latitude with about the magnitude predicted by the model, but it is questionable if this result is significant above the noise. In the IASB scientific OMI SO_2 product, the shipping lane in the Red Sea can be detected in a 5 year average (Theys et al., 2015), highlighting the potential of OMI data.

Analysis of the scatter of SO_2 vertical columns from GOME-2 data shows a standard deviation of about 40×10^{15} molec cm^{-2} over a clean tropical region for daily observations in 2007 when applying AMFs appropriate for shipping SO_2. This value then deteriorates over the lifetime of the instrument for GOME-2 and after appearance of the row anomaly for OMI. Based on the 2007 value and the CHIMERE simulations, it is expected that only the along-track integration of the long-term average will have a standard deviation smaller than the expected shipping signal, in agreement with the failure to identify a signal in the data. For OMI, the same calculations predict that SO_2 should just be detectable, in line with the first shipping SO_2 observations in OMI data reported by IASB.

In order to improve on this for future missions, the signal to noise of the measurements needs to be improved by a large factor. For example, for monthly detection to be possible, the SNR needs to be improved by about a factor of 10 which would require an increase in throughput and / or number of measurements by a factor of 100. Further increases would be necessary to move from detection to quantification of SO_2 emissions and their changes.
As all the calculations performed here were performed on the Indian Ocean area where observation conditions are very good (high sun, relatively low cloud frequency, high ship density) the conclusion of one order of magnitude missing in SNR is still optimistic for other regions such as European waters. It is therefore unrealistic to expect a contribution to the shipping SO_2 emission monitoring from satellites in the coming decade which goes beyond the detection of average values in the busiest shipping lanes.

6. Potential of future instruments to detect NO_2

The gain to be expected from future sensors has been investigated more quantitatively. Focus is on three areas over European waters: The East Mediterranean Sea (EMS), the Bay of Biscay (BB), and the North Sea (NS). These are relatively polluted regions with significant contributions from dense ship traffic. A regional chemical transport model (CHIMERE) combined with a high-resolution emission inventory is used to generate NO_2 profile data with high spatial (10×10km^2) and temporal (hourly) resolution. These NO_2 data sets are used to generate pseudo-observations for the future sensors, as well as for OMI as a reference. The pseudo-observation satellite data sets are compared to the existing data records of OMI, and used to assess the potential of future sensors for identifying shipping emissions.
In section 6.1 expected improvements from TROPOMI on Sentinel-5 Precursor relative to existing sensors are presented and section 6.2 summarises the results for UVN on Sentinel-4.

6.1. Sentinel-5 Precursor

We created pseudo-observation datasets for the TROPOMI/ S5P based on data from the high resolution CHIMERE chemical transport model. The geometry and geolocation of TROPOMI observations are simulated by extrapolation of OMI data, and cloud parameters are taken from the MODIS cloud products. Moreover, meteorological data fields from the ECMWF reanalysis are used to investigate wind effects on the NO_2 distribution.

The following conclusions are reached:

A. Owing to its higher spatial resolution compared to OMI, TROPOMI measured NO_2 peaks from the narrow shipping lanes will be 17%(Eastern Mediterranean Sea) / 24%(Bay of Biscay) higher, and the improved SNR will reduce up to 50% the noise level on TROPOMI NO_2 maps.

B. The detection of a shipping NO_2 signal requires at least a few days of TROPOMI measurements. However if integrated along the ship track, the SNR will improve by up to a factor of 10, and detection could be achieved in daily maps. Furthermore, the NO_2 signal from shipping lanes will be more easily detected after suitable binning of TROPOMI pixels, owing to noise reduction at the typical scale of the shipping plumes (broader than TROPOMI pixels).

C. Clouds and meteorology are as important as SNR over Bay of Biscay and North Sea areas, in particular during the cold season, when strong wind and cloudy scenes often happen. In addition, since the atmospheric lifetime of NO_x is longer and the SNR lower due to prevailing low solar zenith angles, it is difficult to detect shipping NO_2 over these regions. These fundamental limitations will also apply to future instruments.

D. Observations under sun glint geometry increase the shipping NO_2 signals by 15% on average for TROPOMI over EMS during the summer time.

6.2. Sentinel-4

Measurements of the geostationary S4 instrument were simulated using high resolution CHIMERE NO_2 fields, the current specification of the instrument, and dedicated radiative transfer calculations with SCIATRAN. Cloud effects have been included using SEVIRI cloud optical thickness data where available.

The main conclusions from the simulations are

A. The observations of S4 at higher latitudes including the North Sea are performed under large observation zenith angles which will limit the sensitivity to the surface, in particular in winter
B. The improved spatial resolution as compared to GOME-2 and OMI increases the number of measurements for averaging, improving the detection of shipping NO_2
C. The hourly observations of S4 will increase the number of available measurements by about an order of magnitude, reducing the noise of the observations very much.
D. The hourly observations of S4 will also significantly reduce the areas in daily observations of ship tracks for which no data is available due to clouds
E. Monthly observations of the main shipping lanes in the Bay of Biscay and Mediterranean will have good signal to noise. When integrated along ship tracks, the random error will be of the order of a few percent, making it small compared to other sources of uncertainty in the retrievals.
F. Daily observations of shipping NO_2 appear possible when integrating along ship tracks even under unfavourable conditions

7. Roadmap

This chapter describes areas / topics which may benefit from the SEARS research work.

7.1. Emission database

Simulated NO_x vertical column showed some differences with respect to space based measurements. Most pronounced differences concern a shipping lane along the Dutch coast and extending to the Skagerak. Inspection of the EDGAR emission database and comparison with SAR enabled shipping densities showed that the shipping emissions are likely too low.
This procedure can be applied to shipping lanes world-wide and used to identify errors in shipping emission databases.
It is concluded that satellite enabled observations and CHIMERE/WRF modelling is an efficient tool to get better insight in NOx shipping emissions world-wide.

7.2. Ship track detection

Improvements in ship track detection in NO_2 EO data have been investigated and should be applied to the EO data on a regular basis. Proposed improvements are:

- Use of a **larger fitting window** in the NO_2 retrieval
- Application of an **improved gridding algorithm** based on a fine sub-grid sampling and subsequent averaging on the final grid.
- **Avoiding of cloud contamination** by limiting analysis to cloud free conditions
- Use of observations taken under **sun-glint** geometry
- Use of observations taken under **low wind speeds.**
- Applying **spatial filtering** to detect and quantify shipping NO_2 in ocean regions in an automatic and objective way. Optimal filtering parameters should be determined for all shipping regions.

SO_2 signals from ships should be searched for in a systematic way in all existing data including OMI and OMPS. Furthermore, in addition to Sentinel-4, other future geostationary satellites, such as GEMS from Korea, and TEMPO from US, should be used to detect shipping signals with high precision. Although the non-European systems cover regions outside Europe, the data can be used to advance knowledge about shipping signals. Characteristics of the OMPS, GEMS, and TEMPO instruments can be found in Table 3.3.

In this study a pronounced inconsistency between shipping density and NOx concentrations due to shipping emissions was found for a shipping lane along the Dutch coast. It is recommended to perform a systematic comparison of shipping data with satellite data integrated along known ship tracks. This analysis should reveal errors in emission data bases and / or meteorological conditions allowing or blocking proper modelling of shipping lanes.

The EDGAR emission database shows irregular emission variations along ship lanes, see Figure 3.1. This is unrealistic as engine power is mostly constant during a trip. The resulting inconsistencies hamper comparison of shipping emission and satellite data. Future updates of ship emission databases should pay attention to the importance of spatial resolution and consistency of gridding for emission estimates.

The inversion of satellite enabled concentrations to shipping emissions requires further research. The forward modelling, which uses a chemistry transport model to calculate concentrations based on shipping emissions in a database shows some limitations:

1. The spatial and temporal resolution of the database is too coarse to account for the actual distribution of the emission sources. An average emission over an area of 100 km^2 does not take into account the high emissions concentrated at the point like ship engine sources. This hampers accurate modelling of the chemical process in the vicinity of the ships.
2. The CHIMERE model, although it includes advanced chemical processes, does not include plume chemistry and is not able to account for local chemical processes. A first step has been made in a step-wise approach first modelling the plume of the shipping emissions and then a meso-scale chemistry analysis. However, published results show annual averages, and it is not clear if this approach is able to explain the seasonality reported in the SEARS D2 report. Second, inversion of the concentrations to shipping emissions is hampered by transport due to wind. Published results are limited to annual averages, thereby avoiding wind effects. Further research is needed to handle at least moderate wind speed cases more accurately.

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