SEARS

Ship Emissions to Atmosphere
Reporting Service
Contract No. 400104295

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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
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
RAA	Relative Azimuth Angle
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
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. 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 provide a critical review of the SEARS project results: what has been achieved, which factors limit application of NOx and SOx observations by future instruments. Finally, SEARS project results are compared with user expectations. Note that “D5 – Utility review report” has been integrated in the current D6 report.

The document is set up as follows:

- Section 2 summarizes the user requirements
- Section 3 summarizes the problems encountered while working on
  D2 – Prototype NOx product development
  D3 – Assessing the potential of satellite instruments to detect and quantify SO_2 from ships
  D4 – Potential of future instruments to detect NO_2 from ships over European water
- Section 4 provides the lessons learned and recommendations for product improvement.
- Section 5 provides assessment on meeting user expectations

2. User expectations

Four users were identified at the start of the SEARS project: EMSA, scientists, EU, and ESA. These four user groups have different requirements, translating into different questions to the SEARS project:

EMSA

- can NO_2 and SO_2 measurements from space be used to support operational work on shipping emissions in European waters?

Science:

- can we detect and quantify NO_2 and SO_2 from ships using satellite observations?
- can we convert observed NO_2 and SO_2 columns into ship emissions of NOx and SO_2?

EU: can NOx and SOx retrievals enabled by satellite measurements be used to:

- assess effectiveness of regulations,
- assess effectiveness of work by EMSA
- assess trends in NOx and SOx emissions by shipping

ESA:

- SEARS will give insight in capabilities of current missions to measure NOx and SOx shipping emissions. Current missions: GOME, GOME-2, OMI, SCIAMACHI
- SEARS will give insight in capabilities of planned missions, i.e. sentinel S4, precursor.
- SEARS will give recommendations on changes for the planned missions.
- SEARS will give recommendations for follow-on missions

It should be noted that, 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.

3. Critical SEARS result summary

3.1. Satellite data

For retrieval of NOx and SO_2 shipping emissions data of four spectrometers was used: GOME, GOME-2, SCIAMACHY and OMI. Characteristics of these four instruments are presented in table 5. Each instrument is in a 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

To assess potential of future instruments two cases are studied, Sentinel-4 and Sentinel-5

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

3.2. Modelling

To calculate concentrations and vertical profiles of SO_2 and NOx use was made of the WRF weather forecast model and the CHIMERE chemistry transport model. WRF wind results determine the transport of SO_2 and NOx, where CHIMERE calculates the chemical interactions. The shipping emissions used as input for the modelling have been obtained from the EDGAR database.
Radiative transfer modelling was applied to link the modelled 3D concentrations of SO_2 and NO_2 to instrument characteristics and orbits of Sentinel-4 and 5 in order to create realistic S4 and S5 SO_2 and NO_2 maps. For this purpose tabulated results from the SCIATRAN radiative transfer model were used. The resulting pseudo observation datasets were used to study the potential of future instruments.

3.2.1. Emission data

To model the shipping signals, emissions of SO_2 and NOx from the EDGAR database have been used. EDGAR is a global emission dataset, including European waters and the Indian Ocean. Spatial resolution of the emission data is 5 km, which is fine enough to distinguish between shipping emissions and land based emissions for near shore shipping lanes.
An alternative emission database is EMEP. Shipping emission values provided by EMEP are likely better. However, EMEP is limited to European waters, and its spatial resolution of 50 km is too coarse for shipping lanes in the Dutch coastal zone.

3.2.2. WRF/CHIMERE models

The WRF/CHIMERE model suite has been used to perform runs for the Indian Ocean and European Waters, i.e. East Mediterranean, Gulf of Biscay and North Sea. The Indian Ocean was studied because here best conditions are found to retrieve NO_2 and SO_2 from current satellite data, and because this region has been the focus of several previous studies. European waters were modelled to meet the user request by EMSA.
The WRF / CHIMERE model suite produced NO_2 and SO_2 concentration fields at 9 km resolution, comparable with the resolution of the future satellite data. Runs were performed for 2007, with emphasis on the months January, April, July and October.
The CHIMERE runs for eastern Mediterranean posed some problems. The program crashed many times, resulting in loss of data. In particular 20 days in July could not be processed.
The CHIMERE model has been tested extensively using EMEP emission data. The resolution of EMEP data covering Europe only is coarser than the resolution of the global EDGAR emission data using for the SEARS project, i.e. EMEP resolution is 50 km whereas EDGAR resolution is 5 km. Probably the combination of a finer grid and higher emissions due to less strict environmental regulations are causing the program instabilities. To remove instabilities, a shorter time step and a spreading of emissions by high intensity point sources were considered. However, the effort required for implementation of both solutions exceeded project resources, and the decision was taken to use the data as is.
The WRF/CHIMERE simulation activity resulted in NO_2 and SO_2 concentration data at 5 km horizontal resolution in 15 vertical layers suited for ingestion in the radiative transfer software to simulate remote sensing scenes.
The WRF time-step is adapted to the maximum value that can support the underlying horizontal and vertical motions. This assures mode stability and leads to a shorter total run-time as compared to a static time-step. A time-step that is too long will cause model instability and simulation failure, whereas a time-step that is too short will require unnecessary computing power.

Due to the stiffness of the chemical system to solve, the CHIMERE model does not allow for an adaptive time step.

3.2.3. Radiative transfer modelling

The future S4 and S5 instruments will measure electromagnetic radiation associated with the atmospheric composition. Here atmospheric composition is calculated using WRF and CHIMERE. The interaction of the atmosphere and the radiation can be modelled using radiative transfer code. For SEARS the SCIATRAN (Rozanov et al., 2014) and LIDORT radiative transfer software packages have been used or at least tabulated results. Use of lookup tables speeds up calculations by orders of magnitude.

The available tables were constructed for instruments in a sun synchronous orbit. Entries for these lookup tables are a limited number of sun azimuth, sun elevation, viewing azimuth and viewing elevation angles. While appropriate for S5P simulations, this set of viewing angles turns out to be unsuited for instruments in a geo-stationary orbit and calculations for the S4 instrument had therefore to be done using on-line calculations, limiting RTM simulations to a few full days. The RTM data were then applied for all days of the month, neglecting the small seasonal changes in solar geometry but fully accounting for chemistry and the diurnal cycle of observation geometry.

3.3. NO_x shipping emissions based on satellite data over European waters

Fast conversion of satellite observed NO_2 columns to shipping NOx emissions relies on assuming a local linear relationship between the two quantities which can be derived from the model data and can thus be performed only for low wind speed conditions where transport can be neglected or by using averaged data. Proper estimation of shipping NOx emissions requires a full scale inversion and many model runs to assess the best estimate of the emission distribution and to account for the nonlinear relation between NO_2 amount in the atmosphere and the column observed by the satellite. The CHIMERE model selected here for its accurate chemical modelling is too slow for this purpose. By eliminating chemical processes irrelevant for NOx and/or SO_2 modelling it should be possible to speed up calculations significantly, potentially enabling online inversion in the future.

3.4. Feasibility of detecting shipping in SO_2 emissions using satellite data

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 a recent optimised version of the scientific OMI SO_2 product from BIRA, the shipping lane in the Red Sea and in the Mediterranean Sea close to Gibraltar can be detected but only in a 5 year average, highlighting the potential of OMI data (Theys et al., 2015).

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 for favorable observation conditions (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.

3.5. Potential of future instruments in detecting NO_x shipping emissions

The gain to be expected from future sensors has been investigated more quantitatively, focusing on three areas over European waters: The East Mediterranean Sea (EMS), the Bay of Biscay (BB), and the North Sea (NS). 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 3.5.1 expected improvements from TROPOMI and Sentinel-4 relative to existing sensors are presented and section 3.5.2 describes capabilities of the future instruments for shipping NO_2 retrieval. Improvements are due to the better spatial resolution, comparable or better coverage and better signal-to-noise ratios than current sensors.

3.5.1. Sentinel-5

We created pseudo-observation datasets for the 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 NOx 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 Eastern Mediterranean Sea during the summer time.

3.5.2. 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

4. Lessons learned

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

Expected shipping NO_2 product improvements for the Sentinel-5 precursor (S5P) and the Sentinel-4 (S4) instruments due to better spatial resolution, comparable or better coverage and better signal-to-noise ratios than current sensors have been described in section 3.5.

Simulated NOx vertical column showed some differences with respect to space based measurements. Most pronounced difference concerns a shipping lane along the Dutch coast and extending to the Skagerak. Inspection of the EDGAR emission inventory and comparison with SAR enabled shipping densities showed that the EDGAR shipping emissions are likely too low. This procedure can be applied to shipping lanes world-wide and used to identify errors in shipping emission inventories.
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.

The CHIMERE is already a valuable tool to assess relative differences between simulated ship tracks and observations. To get better quantitative results, 2 improvements are proposed:

- First the CHIMERE model lacks plume chemistry and therefore chemical processing occurring in the immediate vicinity of the ship where concentrations are highest might not be modelled properly. Most chemical processes take place within 100 m from a ship. Plume chemistry can be included in CHIMERE or can be added as a separate pre-processing step.
- Second the emission inventories provide average values over grid cells of 10 km x 10 km or larger. Information on the degree of non-uniformity should be added, e.g. the number of ships emitting inside a grid cell.

The geostationary S4 mission is not able to monitor concentrations at high latitudes; sun being too low above the horizon results in too low intensity signals.
As it makes no sense to measure concentrations over dark areas, this time can be used to repeat a scan over lower latitude areas.

Improvements in ship track detection in NOx 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.
- **Avoid Cloud contamination** by limiting analysis to cloud free conditions
- Use observations taken under **sun-glint** geometry
- Use observations taken under **low wind speeds.**
- Apply **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.

5. Meeting user expectation

At the start of the project user expectation was assessed. Below, the SEARS team assessment on meeting their expectations is presented.

EMSA

- can NO_2 and SO_2 measurements from space be used to support operational work on shipping emissions in European waters?

Assessment: No.
SO_2 space based measurements will not be used in the next decade as the detection limit is not good enough.
NO_2 measurements by S4 and S5 might be used occasionally if observation conditions are favourable.

Science:

- can we detect and quantify NO_2 and SO_2 from ships using satellite observations?
- can we convert observed NO_2 and SO_2 columns into ship emissions of NOx and SO_2?

Assessment: Yes for NOx and No for SOx
Measuring SO_2 is at the limits of future instruments but should be doable in favourable cases.
S4 and S5 can be used to measure NO_2, but in the mean time we have to improve modelling capability, for example understand seasonality in NO_2 results, and include plume chemistry. SEARS has resulted in improved air mass factors which can be used for the scientific work. Furthermore, quality of emission inventories has to be improved: by comparison with existing satellite data and by putting special attention to (re)gridding procedures.

EU: can NOx and SOx retrievals enabled by satellite measurements be used to:

- assess effectiveness of regulations,
- assess effectiveness of work by EMSA
- assess trends in NOx and SOx emissions by shipping

Assessment: Yes for NOx, No for SOx.
Current and future satellite enabling NO_2 measurements of shipping lane averaged columns can be used to assess trends in emissions by shipping. These trends can be correlated with regulations and economic factors.

ESA:

- SEARS will give insight in capabilities of current missions to measure NOx and SOx shipping emissions. Current missions: GOME, GOME-2, OMI, SCIAMACHY
- SEARS will give insight in capabilities of planned missions, i.e. sentinel S4, precursor.
- SEARS will give recommendations on changes for the planned missions.
- SEARS will give recommendations for follow-on missions

Assessment: Yes.

- Insight in capabilities of current and planned missions is given.
- Recommendations for changes in instruments are not given, but on processing of the resulting data, i.e. improved fitting window, gridding, spatial filtering, handling of cloud contamination, limit processing to low sun glint and low wind speed conditions.

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