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IDENTIFICATION OF OPTIMAL SATELLITE DATA FOR USE IN THE AIR QUALITY MODELING SYSTEM BGCWFS

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Abstract: *In this work we present an investigation of finding and processing of optimal satellite dataset for assimilation in the air quality modeling system BgCWFS. The modeling system BgCWFS simulates the transport and chemical transformation of air pollutants over five different nested domains with different spatial resolution and the optimal satellite datasets for each of them are different. We show that data from MetOp satellites is optimal for use in Europe and, Balkan domains while Sentinel 5P data is better for two other ones - Bulgaria and Sofia district*

ИЗБОР НА ОПТИМАЛНИ СПЪТНИКОВИ ДАННИ ЗА ИЗПОЛЗВАНЕ В СИСТЕМАТА ЗА АТМОСФЕРНО ЗАМЪРСЯВАНЕ BGCWFS

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Ключови думи: *дистанционни изследвания, атмосферни замърсявания*

Резюме: *В настоящата работа е представено изследване на избора и обработката на спътникови данни за асимилиране в BgCWFS.. Моделната система BgCWFS симулира разпространението и химическите трансформации на различни атмосферни замърсители в пет различни, вложени една в друга области с различна пространствена разделителна способност. Така оптималните спътникови данни за различните области са различни. Показали сме, че данните от спътниците MetOp са подходящи за областите Европа и Балкански полуостров, докато данните от Sentinel 5P са по-добри за използване в други две такива – България и София област..*

Selection of satellite data for use in BgCWFS

The satellite data to be used by the Bulgarian Chemical Weather Forecast System (BgCWFS), [1, 2] should have proper spatial and temporal resolution. The focus is on free data mainly from European satellites.

The modeling system BgCWFS operates over five different nested domains with different spatial resolution - Europe (81 x 81 km), Balkan Peninsula (27 x 27 km), Bulgaria (9 x 9 km), Sofia region (3 x 3 km) and Sofia city (1 x 1 km). The satellite data assimilation will be only in the first three domains.

In the perfect case we must use satellite data with the same space resolution and coverage of the whole areas of interest. There is no such kind of satellite data.

We decided to use data mainly from GOME-2 and TROPOMI instruments with space resolution 40 x 40 (40 x 80) km and 3.5 x 7 km respectively.

Data from GOME-2 are suitable for use in the first two model domains and TROPOMI data – for the two other domains.

There are three satellites – *MetOp A, B and C* respectively, with the same instrument GOME-2. Data from the first two satellites are used in the current investigation. They lay on the same orbit, placed on opposite sides of the Earth as it is shown in Fig. 1.

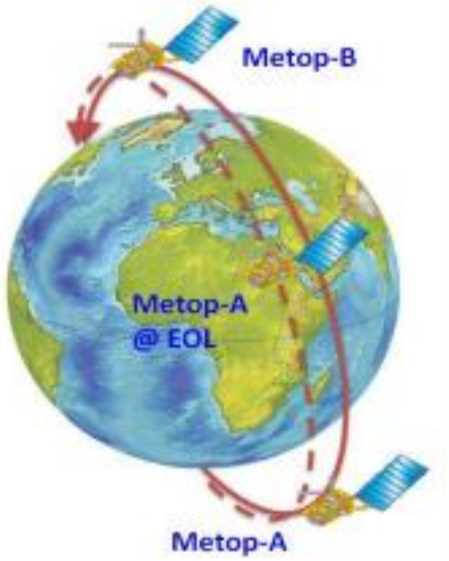

Fig. 1. The Orbit positions of MetOp A and B satellites

Metop-C has been placed in same orbit as *Metop-A* and *B* and at equal distance to both platforms, with LT equator crossing at 9:30 UTC, the same as for *Metop-A* and *B* (a '*Tristar* ' configuration – see Fig. 2, left)

During the course of commissioning, and based on the early data-user feedback, the decision will be made to either remain in a tristar phasing configuration or to shift *Metop-C* 180 degrees opposite *Metop-B* (original A/B configuration from Fig. 1) with *Metop-A* in-between ("*Trident*" configuration – see Fig. 2, right) [3]. At the moment (October 2019) three MetOp satellites are in Tristar position.

Combining data from two or from all three of satellites, it is possible to obtain better space resolution and have the possibility to use such data even in the third area in BgCWFS – Bulgaria domain.

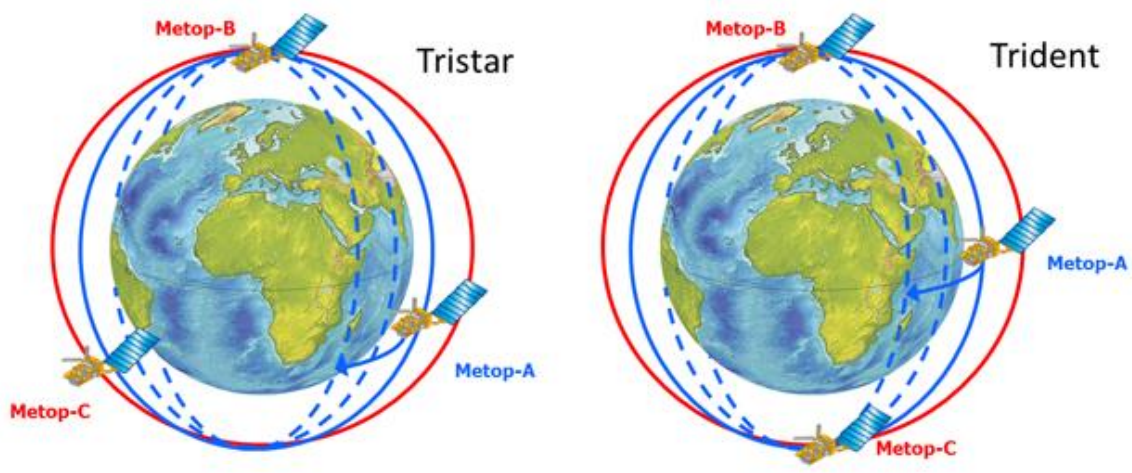

Fig. 2. The Orbit positions of *MetOp A, B* and *C* satellites

The time difference between two orbital passes of the same satellite is about an hour and forty minutes (about 100 minutes) as it is shown in Fig. 3.

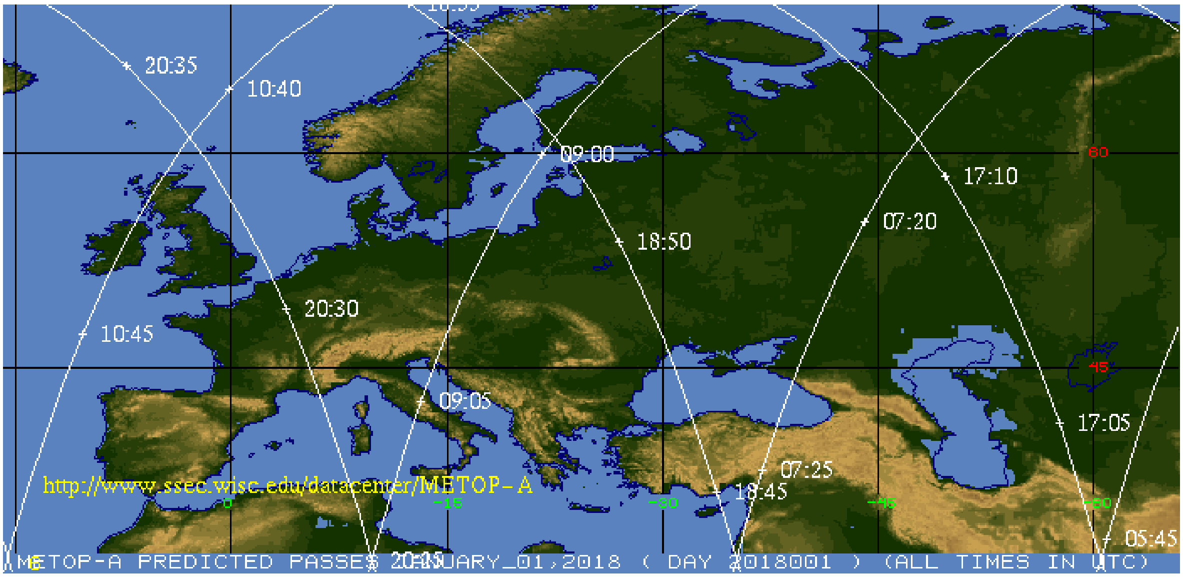

Fig. 3. Time difference between *MetOp* orbit tracks

If we use all three satellites in *Tristar* configuration, we will have time difference between their passes less than 70 minutes, so we can use them together. If the satellites are in a *Trident* position, the time difference will be about 50 minutes.

Unite data from *MetOp A, B* and (in future) *C* satellites

Satellite data with small and middle space resolution (such as *MetOp*) are appropriate for the investigation of continental scale processes. So we can use such kind of data only to register and study pollution distribution over the region of Europe.

Initially it was planned to use data from a single satellite to be sure that all measurements are made with the same instrument. However, *MetOp A* satellite is older and its scanning width becomes smaller. Its spatial resolution is 40 x 40 km, while *MetOp B* satellite has a resolution of 40 x 80 km. So, we decided to unite data from both of them.

After launching of *MetOp C* satellite at the end of 2018, we have the opportunity to use together data from all three satellites.

Even if we use two or three satellites, to cover the whole European area we must use at least two orbital passes of each of them. Fig. 4 shows the first domain of BgCWFS (domain Europe) and the corresponding area covered by one track of *MetOp A* and one of *MetOp B* satellites with pointed centres of their measurement cells.

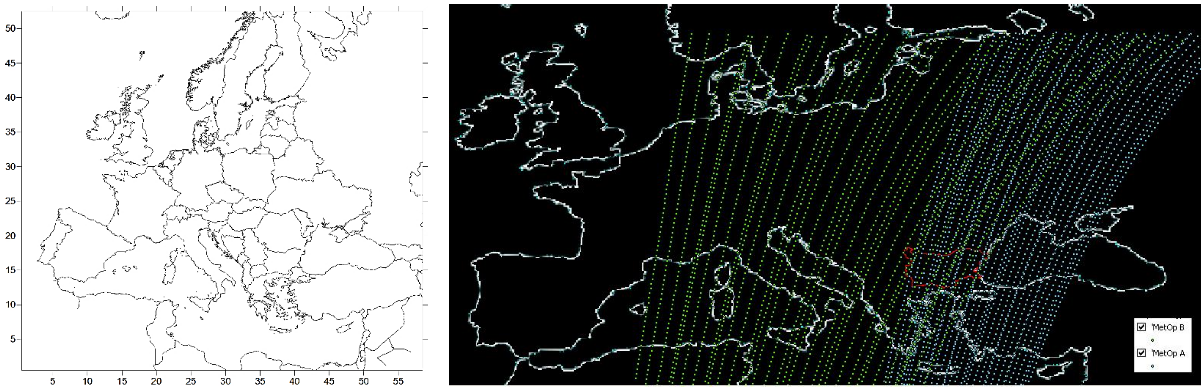

Fig. 4. The European domain in BgCWFS (left) and coresponding area covered by one track of *MetOp A* (blue dots) and one track of *MetOp B* (green dots) satellites (right)

The purpose of using satellite data in BgCWFS is better air quality predictaions through downscaling towards smaller domains and the area of interest is the Balkan region. Thus, more important is to use satellite data in the second domain of BgCWFS. Its horizontal grid resolution of 27 x 27 km is appropriate to the resultant space resolution of the combined data from the two MetOp satellites. Figure 5 shows the second modelling domain of BgCWFS and the corresponding area covered by one track of *MetOp A* and one track of *MetOp B* satellites with pointed centres of their measurement cells.

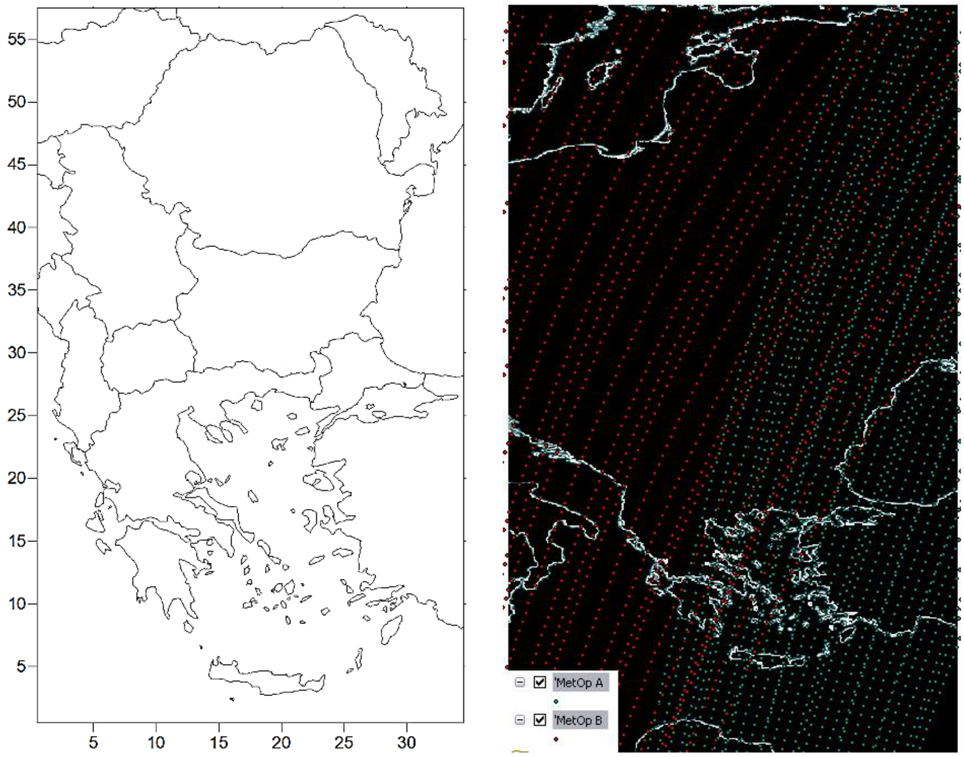

Fig. 5. The Balkan domain of BgCWFS (left) and the corresponding area covered by one track of *MetOp A* (blue dots) and one of *MetOp B* (red dots) satellites with pointed centres of their measure cells (right)

The *MetOp* orbits are in north-east toward south-west directions. The covered area changes from day to day and not-every-day single orbital pass of one satellite covers the whole area. Thus, we have a different spatial resolution of satellite data in the different domains.

Mineral dust is significant source of natural particulate matter. Sand storms from Africa may affect the Balkan region and thus contribute to elevated pollution levels. These sand storms approach Bulgaria mostly from south-west moving towards north-east and this is in good accordance with the *MetOp* tracks. Thus, for the investigation of dust pollution in Bulgaria, it is important to have good coverage of the whole south area of the Balkan domain.

Relevant to SO_2 and NO_2 column densities, we have analysed *MetOp* data for the period - from 2007 till now (more than 10 years). Based only on these data we don't register any significant SO_2 pollution and can't say anything about the tendency of its propagation. On the contrary, we registered a tendency for NO_2 propagation from north-west towards our area of interest. In this case it is more important to have better spatial resolution and coverage for the north-west area of the Balkans.

So, according to the main goal of the investigation, we may choose an earlier or the next orbit of each satellite.

Figure 6 shows the domain Bulgaria of BgCWFS and the corresponding area covered by one track of *MetOp A* and one of *MetOp B* satellites. As it is seen, we have small amount (100–150) of measurement points over the whole area (less than 100 points for *MetOp A* and less than 50 points for *MetOp B*).

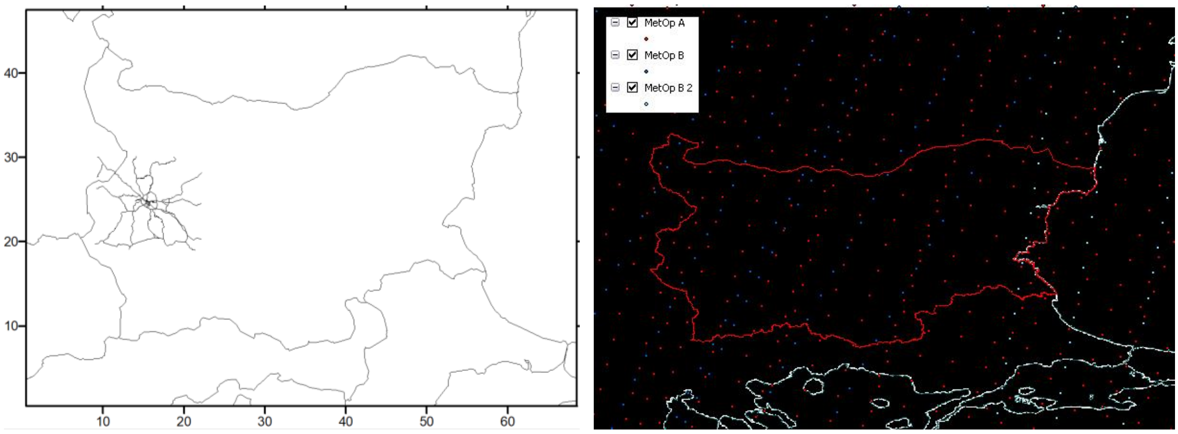

Fig. 6. The domain Bulgaria of BgCWFS (left) and responding area covered by one track of MetOp A (red dots) and two of MetOp B (dark and light blue dots) satellites with pointed centres of their measure cells (right).

For the Figures 4, 5 and 6 we used information for different days of March, 2018 in order to show the differences in satellite data coverage from day to day.

GOME 2 Data processing

When satellite data will be used on daily basis it is important to obtain and process data quickly and almost automatically.

The data from the *MetOp* – GOME-2 instrument are in h5 format [4] (Level 2 products) [4], Near real time product contain the data for AAI and NO2 and offline - for AAI, NO_2 and SO_2 in one file. In the same file there are other interesting variables such as clouds, other pollution ingredients, water column etc.

Data processing starts with obtaining the needed track for both *MetOp A* and *B* satellites. Then, from the files of each satellite we extract data for AAI, NO_2 and SO_2 only at geographical points (lat-lon coordinates) from one single orbit (Latitude from -90 to 90 degree). Then we import data in ArcGIS and define our area of interest (the Balkans in this case). The next step is to convert the data to one-and-the-same units as needed for BgCWFS. The last step is to unite the data from both satellites.

The AAI values from *MetOp A* satellite are much smaller than those from *MetOp B* satellite.

The values for NO_2 and SO_2 from both satellites are fully comparable.

The AAI data are in dimensionless units, but not from 0 to 1 as AOD. Data for NO_2 are in [molecules/cm^2] and data for SO_2 are in DU (Dobson units) [5].

The data conversion we use is as follows:

$$\text{If } NO_2>0 \text{ then } NO_2\,[\mu g/cm^2] = NO_2\,[\text{molecules}/cm^2] \times 7.636 \times 10^{-17}$$

$$\text{If } SO_2>0 \text{ then } SO_2\,[\mu g/cm^2] = SO_2\,[DU] \times 2.14$$

For AOD we use the following relationship:

$$\text{If } AAI > 0.5 \text{ then } AOD = AAI/10 \text{ for } \textit{MetOp B}$$

$$\text{If } (AAI \neq -1) \text{ and } (AAI + 3 > 0.5) \text{ then } AOD = (AAI + 3)/10 \text{ for } \textit{MetOp A}$$

The two wavelengths that constitute the AAI wavelength pair are set to 340 and 380 nm, respectively [6, 7].

These relationships between AAI and AOD are based on previous comparison of data for AOD and AAI from AURA satellite and data for AAI from *MetOp B* and for AOD from Terra, Aqua and Aura satellites [6, 7].

Comparing data for AAI (340 and 380 nm) and AOD (550 nm) from the same OMI instrument for past periods, we found that relationships between values for these two characteristics are close to linear. Values for both of them are dimensionless, but have different spatial resolution. The AOD (550 nm) from Terra and Aqua have average values for the period from January to March 2018 about 10 times higher than AAI form *MetOp* values. Further in this analysis we obtained the maximal value of AAI from *.h5* files for the period February–April 2018 and found that AAI not exceeds the value of 8.5 even in the regions above Sahara at moments of stronger sand storms.

Thus, the above relationship for increasing AAI value from *MetOp A* was derived comparing *.h5* data and the official *.nc* data, provided for this satellite from ESA [4, 7].

If the value of any pollution ingredient is negative, the value is treated as error.

Usage of Sentinel 5P data

The data from *MetOp* satellites is not appropriate for investigation of local pollution processes. For such kind of processes is better to use satellite data with finer space resolution such as the data provided by *Sentinel 5P* (3.5 x 7 km)

Sentinel 5P- TROPOMI instrument provides data for aerosol index AI (the same as absorption aerosol index AAI) in two different diapasons – 340–388 nm and 380–354 nm in one file and, in another separate file for NO_2 and SO_2.

For our purposes we may use the data provided in the Copernicus Scientific Hub [8] for the region, as it is shown in Fig. 7.

Fig. 7. The *Sentinel 5P* area for the maps in Fig. 8 and Fig. 9

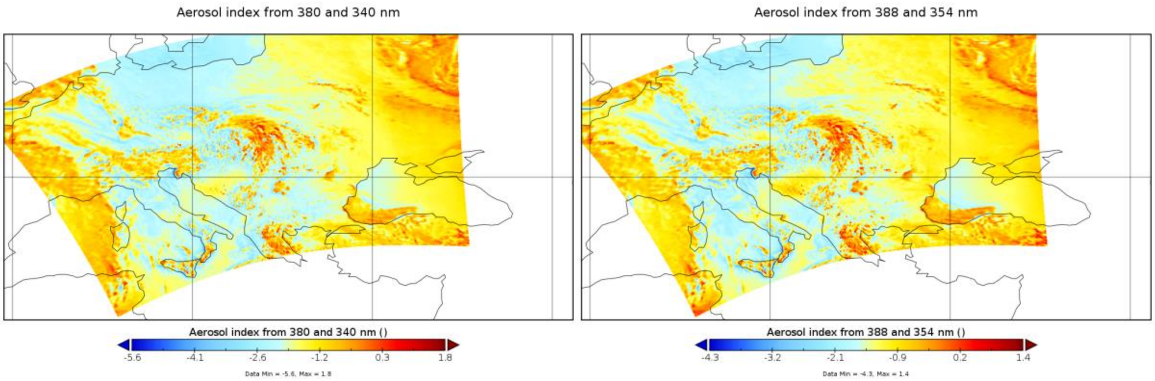

Fig. 8. The Aerosol Index in 340-380 (left) and 354–388 (right) nm - *Sentinel 5P* for the area shown in Fig. 7 on April 6th 2019

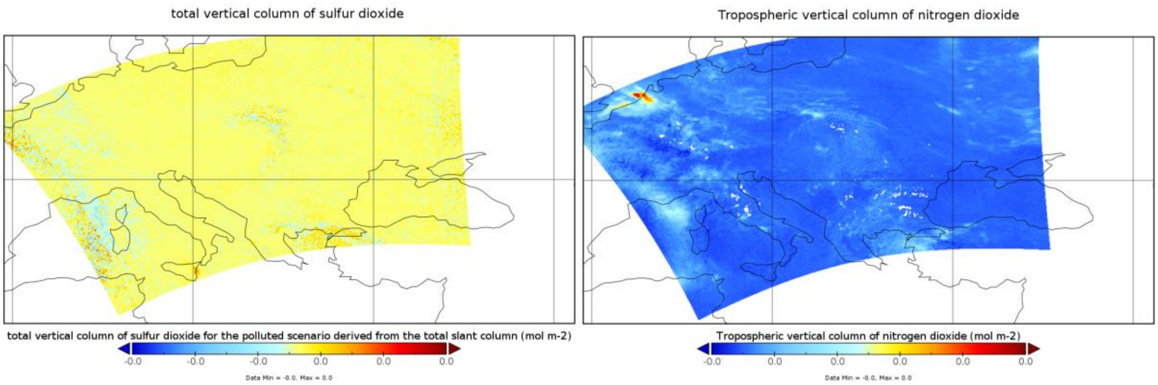

Fig. 9. SO_2 (left) and NO_2 (right) - *Sentinel 5P* for the area, shown in Fig. 7 on April 6th 2019

In Fig. 8 and 9 the spatial distribution of the AI estimated for two diapasons, and the vertical columns of NO_2 and SO_2 are shown for 6.04.2019 in the region marked in Fig. 7.

We can notice small differences between the two Aerosol Indexes (Fig. 8)

Before using of TROPOMI aerosol data as input to some of the domains of BgCWFS, an analysis of the conversion AI – AOD has to be performed.

However, Sentinel 5P data will be used also for other tasks in the project and we are working on data-set preparation for the purposes of WP3.

Data from other satellites

Except *MetOp* and *Sentinel 5P* data, we inspected other sources of satellite air quality related data.

Data are available from MODIS spectrometer on *Terra* and *Aqua* satellites directly for AOD with spatial resolution of 3 x 3 or 10 x 10 km in 540 nm [9]. But these satellites do not provide data for other pollutants. Moreover, these data are often missing in case of clouds.

There are data from OMI instrument of *Aura* satellite. The data provided include all the pollutants - SO_2, NO_2, AAI and AOD measured together. The spatial resolution is the same as of *MetOp. GOME 2* instruments are placed on three *MetOP* satellites *(A, B* and *C),* while *OMI* instrument is placed only on board of one and a much older *AURA* satellite.

There are data from OMPS instrument of *NOAA* satellites. The spatial resolution is 50 x 50 km and the data flow starts in 2012, while the *MetOp* data we collect is from 2007 till now, thus allowing to make analysis based on longer time period

For illustration of the differences in the AAI data from the mentioned before instruments, we show measurements from all of them for a selected day – 11 March 2019, in Figures 10 and 11.

As it is seen, the measurements from GOME-2 and TROPOMI instruments are of similar order and have similar spatial distribution. The data from OMPS are of lower level of details, while the OMI instrument coverage is very limited.

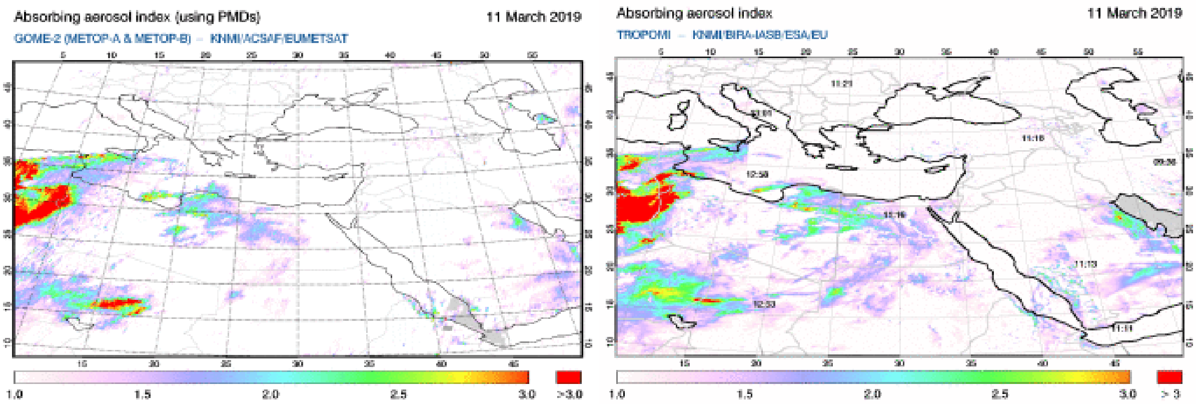

Fig. 10. The AAI from *MetOp A* and *B* satellite (left) and Sentinel 5P (right) on 11.03.2019

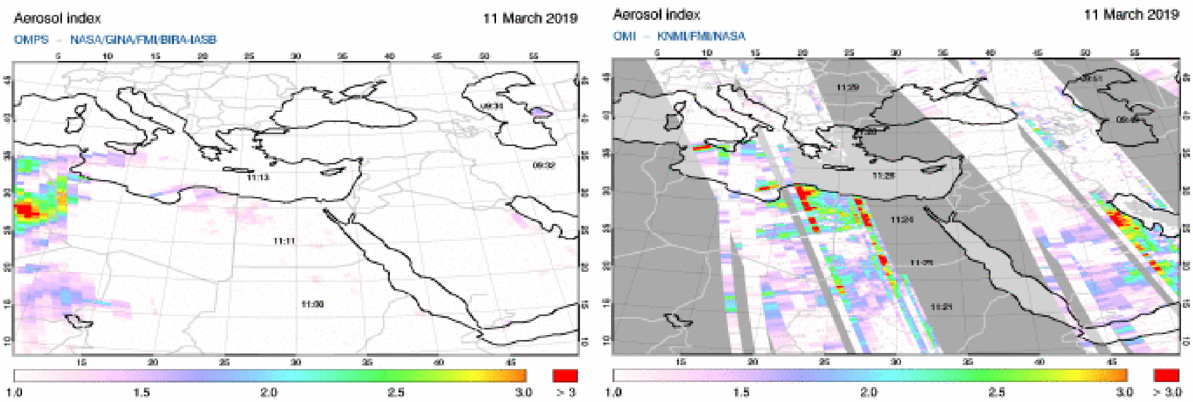

Fig. 11. The AI from OMPS (left) and OMI (right) instruments on 11.03.2019

Conclusions

As a result we can say that it is optimal to use GOME-2 data for the Balkan region either for investigation of past events, or in relation to satellite data assimilation in BgCWFS.

The data from TROPOMI are being collected as they provide information on much finer spatial scale, and might be used for the Bulgarian and near city domains in BgCWFS.

The use of AI for assimilation in BgCWFS is, however, not a trivial task [10] and further analysis based on long – term series of data are needed for proposing such possibilities.

Acknowledgments

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