

Article

Prediction of the Atmospheric Dustiness over the Black Sea Region Using the WRF-Chem Model

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Abstract: To make a reliable forecast for the level of dust, many external factors such as the wind energy and the soil content in the moisture must be considered. The numerical prediction of the Black sea region's content of dust is the focus of this study, and for this purpose, the WRF-Chem model is used. The investigation is based on the statistics of the prediction coincidence and the actual result extracted from the data of the backward trajectories of AERONET and aerosol stratification maps in the atmosphere constructed with the help of the CALIPSO satellite. A comprehensive set of data was collected, and a comparative analysis of the results was carried out using machine learning techniques. The investigation identified 89% hits in the prediction of dust events, which is a very satisfactory result.

Keywords: air quality; dust aerosol; WRF-Chem; AERONET; aerosol optical thickness; CALIPSO



Citation: Papkova, A.; Papkov, S.; Shukalo, D. Prediction of the Atmospheric Dustiness over the Black Sea Region Using the WRF-Chem Model. *Fluids* **2021**, *6*, 201. <https://doi.org/10.3390/fluids6060201>

Academic Editors: Xinguang Cui, Ali Farnoud, Saikat Basu and Mohammad Mehdi Rashidi

Received: 30 April 2021
Accepted: 25 May 2021
Published: 27 May 2021

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1. Introduction

As environmental issues are becoming a dominant concern in our lives, the numerical prediction of the dust particles and their strength in the surrounding atmosphere has become an area of intense research activity all over the world. The research interest in this area will continue to grow amongst the scientific community, as expected. The presence of dust aerosol in the atmosphere affects the quality of satellite data which often require additional atmospheric correction [1]. The wide range of scales often used and the lack of suitable observations available for assimilation make it difficult to forecast the measure of atmospheric dust and many of the numerical models have a number of problems due to their complexity, causing difficulties in the system implementation [2].

In the current work, WRF-Chem is used as the basic component in the forecasting model. The Weather Research and Forecasting Model is abbreviated as the WRF-Chem model as it has mixed chemistry. The focus of this model is to study the transfer or emission of gaseous impurities and chemical conversions inside the aerosols and how they are linked with the meteorology. This model can be effectively used to study air quality on a regional scale. [3,4]. It can also be used as a supplement when identifying the place of origin of dust aerosol, which is very useful in studying the physicochemical properties of aerosol [5]. Additional investigations have shown that the GSF (an abbreviation of Ginoux Source function) is well known and in the models of WRF-Chem is used, and as a result, in some parts of Western Asia, it has resulted in large number of errors. [6]. In recent studies, a number of errors in the dust forecast model were identified and some were eliminated. It was found that 0.1 to 0.46 μm radius containing dust particles are sometimes not added in any analysis of the aerosols while studying their optical characteristics and in this way, can lead to an underestimation of the thickness of aerosol optics (AOT). By accounting for the particles with radius $\geq 0.1 \mu\text{m}$, the error was rectified later. In this case, 0.1 stands for the first GOCART trash can [7].

This paper evaluates the numerical prediction of dust content using the WRF-Chem (specifically its online application—WRF-Chem model), for the Black Sea region based on the statistics of the prediction coincidence and the actual result. AERONET 7-back trajectories of atmospheric aerosol generation and aerosol typing maps provided by CALIPSO satellite algorithms were used as the source of information and subsequent data. It was noted that overestimated concentrations of mineral dust in the atmosphere are annually or yearly recorded in the region of Black Sea. The main source of dust for this region is the Sahara Desert. The greatest number of Sahara dust outbreaks regularly occurs in the summer season (May–October) [8]. Also, this period is sufficient for the main assessment of the results, for example, in [9], the correlation between the results of overestimated MODIS AOT and overestimated dust concentrations (WRF-Chem) in the 6-month period of 2011 (spring–summer) was studied. Earlier, a similar study was conducted over the central Mediterranean, the model of WRF-Chem with the dust simulation and overbreak of dust particles was observed and another term was used by the authors. This term is MODIS-Terra, which generally comprises of the photometers and sensing information and it is known as AERONET. The model has the ability to reproduce the AOT in horizontal field as shown in the study and in time, its evolution is considered as a coefficient of temporal correlation with 0.85 of the AERONET [10].

Previously, a reliability analysis of the WRF-Chem model was carried out by comparing the AOT and extinction coefficient from different dust emission schemes over the northern Africa region during the summer of 2006. The model showed its capability to broadly reproduce the dust source regions, the dust AOT and extinction profile observed by the CALIOP and AERONET. It is worth noting that as a result of this study, there were significant differences between the three WRF schemes (GOCART, AFWA, and UoC). The authors assume that these differences are related to the calculation of the threshold wind speed in each scheme, which indicates the necessity to continue improving the WRF-Chem model to reduce uncertainties in the representation of dust plumes [11].

Also, this model is often used to track (simulate) the movement of dust clouds in single episodes. Ref. [12] describes the case of the dust process in northwest China during May 2018, where the process was simulated using satellite-retrieved and observational data, including aerosol optical depth (AOD), extinction coefficient and dust index, as well as observational wind field, precipitation, and particulate matter with particle size mass concentration at the surface [12].

Interesting results were obtained in the study of the evaluation of WRF-Chem Predictions for Dust Deposition in Southwestern Iran during 2014–2015. The strongest positive correlation between the WRF-Chem model results and monthly recorded ground deposition rates (GDR) data was found for the concentration in the spring (correlation coefficient of 76%) and in the winter (80%). The authors note that this combination is an important data source and can be a relevant subject for studies in this field [13].

In Ref. [14] demonstrated the assessment of WRF-CHEM forecasting using reanalysis, satellite data, and ground-based observations (i.e., MERRA-2, MODIS-Terra, Aura-OMI, CPCB) over the Arabian Peninsula. From the statistical analysis it was noted that there was a consistent underestimation of the simulated dust by WRF-Chem as compared to the observational data sets. Thus, it was noted that on an average the probability of the detection of a dust event is about 77% and false alarm ratio is about 15% with an overall accuracy of 76% [14].

The first step in this study is the modelling of the trajectory of movement of aerosol clouds (particles) from the African continent and some Asian countries by using the WRF-Chem model. Subsequently, using the reverse AERONET trajectories and the results of the CALIPSO algorithm model coupled with the degree of reliability of the WRF-Chem model, forecasts for the region of interest is estimated. The optical density and thickness of aerosol AOT is used as well and for the state of atmosphere, it is considered as one of the key optical features. Aerosol turbidity is also indicated inside the atmosphere and the air

basin's ecological state is determined [8]. To evaluate the predicted outcomes this solution allows highly accurate results be obtained with ease.

The relevance of the study is fully justified by the fact that the overestimated concentrations of absorbing aerosol particles generated from organic aerosol and anthropogenic pollutants will surely have a negative impact on human health and exacerbate chronic cardiopulmonary diseases [15]. Timely and reliable forecasting will make it possible to warn the public about possible risks to their health, and importantly, appropriate preventive measures can be suitably adopted in advance.

2. Materials and Methods

2.1. WRF-Chem

The WRF (Weather and Research Forecasting) model is used for the mesoscale prediction of the weather. The model was designed specially to serve the requirements of atmospheric tasks needs and operational forecasting [16]. In [17], the detailed WRF model along with its descriptions is given. Along with the calculation model for the dynamics of weather, the WRF model can be used to estimate the presence of dust particles in the atmosphere. The physical parameters for dust detection in the model of WRF-Chem are similar to the GOCART model. The WRF modeling system software (including chemistry) installation is straight forward on the ported platforms. The WRF-Chem code development and maintenance is conducted at the NOAA/ESRL/GSD in strong collaboration with other research groups at NOAA/ESRL, NCAR, PNNL, NASA and ERDC and many other institutes. You can download the software, as well as find out any additional information at the link (<https://ruc.noaa.gov/wrf/wrf-chem/> (Accessed on 15 May 2020)). The term GOCART is an abbreviation of Georgia Tech/Goddard Global Ozone Chemistry Aerosol Radiation and Transport model. WRF-Chem is a non-hydrostatic model running once daily at the National Observatory of Athens (1200 UTC cycle). More information about model domain, configuration, chemistry component, and sensitivity tests for the WRF-Chem in the Athens National Observatory can be found in [9]. One domain is used covering a large part of Sahara (main source of mineral dust), the Mediterranean and Black Seas, and Europe, with 20 km horizontal grid increment. In the WRF-Chem model, there are 5 dust size bins (mean radius of bins 0.6, 1.2, 2.4, 4.5, and 8.0 μm , respectively), the same as the boundaries of the GOCART dust bins. The dust emission for each size bin is calculated by taking into account a number of geophysical parameters such as the factor of erosion, soil particle fraction, and surface wind velocity. The threshold velocity of wind erosion is also included. The threshold velocity is a function of the distribution of particle size and density, taking into account soil moisture [18]. Ultimately, the WRF-Chem online application program provides prediction maps for the concentration of dust aerosols above the earth's surface.

2.2. AERONET Network

AERONET (Aerosol Robotic Network) is a worldwide network that has a potential to monitor the optical characteristics of the state of the atmosphere and surface sea layer with high spatio-temporal coverage. There are more than 200 stations located in different parts of the world and all the needed estimations are taken with great accuracy. The advantage of this network is that it uses the same type of automatic photometers and standardized calibration procedures and data processing. All stations are usually installed with Cimel-318 (CE-318) multi-channel automatic sun photometers manufactured by CIMEL Electronique (Paris, France). The stations are equipped with photometers function for a relatively long period (from a year to several decades). Over the entire period of work and within the AERONET network, the Black Sea region is represented by 4 regular measuring stations: Sevastopol ($44^{\circ}61' \text{ N}$, $33^{\circ}51' \text{ E}$), Gloria ($44^{\circ}60' \text{ N}$, $29^{\circ}36' \text{ E}$), Galata_Platform ($43^{\circ}04' \text{ N}$, $28^{\circ}19' \text{ E}$) and Eforie ($44^{\circ}07' \text{ N}$, $28^{\circ}63' \text{ E}$). Since 2019, the Gloria station has been replaced by an analogue of Section-7_Platform ($44^{\circ}54' \text{ N}$, $29^{\circ}44' \text{ E}$) [19]. In this paper, the daily average AERONET measurement data will be the resource for retrieving the AOT data.

In this work, we use 7-day back trajectories of aerosol transfer, calculated with the support of the BAMGOMAS project (Reverse trajectories, AERONET, MODIS, GOCART, MPLNET Aerosol Synergism). Twice a day at present times, the 7 back trajectories are analyzed and these are recorded to be as 00Z and 12Z. The images are generated in two sets as well, more information can be found in [20]. It is worth noting that currently the backward trajectories are still calculated for stations that have stopped functioning, for example, Sevastopol (44°61'N, 33°51' E) and Gloria (44°60' N, 29°36' E). These trajectories make it possible to track the movement of aerosol particles in the atmosphere and draw conclusions about the place of origin of these particles, which in most cases makes it possible to more accurately assess their optical and microphysical characteristics.

2.3. CALIPSO Mission

The Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observation (CALIPSO) satellite provides new insight into the role that clouds and atmospheric aerosols (airborne particles) play in regulating Earth's weather, climate, and air quality. CALIPSO is a joint U.S. (NASA) and French (Centre National d'Etudes Spatiales/CNES) satellite mission that has been in operation for four years. The calculations of the CALIPSO algorithms are based on the measurements of the CALIOP lidar. The incident polarization is used to scatter the changes in the atmosphere and in this way; the depolarization extent can be measured as well. By doing this, we can obtain plenty of information about the particles and their nature. This model also offers an idea about the geometry of these particles and atmospheric aerosols and optical features. The coefficients of depolarization and AOT are the examples of it. In built algorithms, the model CALIPSO is used, and it offers the maps of the atmosphere by entering the flight path in the corresponding satellite [8]. The algorithms and methodology for constructing the data of the atmospheric aerosol subtypes are described in detail in [21]. The older version of the algorithm is described in [22].

3. Results and Discussion

The territorial feature of the Black Sea region is such that the frequent dustiness of the atmosphere in the region is clearly apparent, which established the need for the investigation. Dust bursts were tracked by the authors from May 2020 to October 2020 to carry out the investigation. The tracking was performed using WRF-Chem based dust load maps showing hourly concentrations and movements of the dust cloud (see Figure 1).

A considerable amount of data (152 values) was collected, and the results were analyzed and compared with those using the actual AERONET and CALIPSO data. For each of the dates, the reverse trajectories of the origin of atmospheric aerosol were tracked for the three Black Sea stations of the AERONET network (Gloria (Romania), Eforie (Bulgaria), Sevastopol (Russia)). The correlation of the values of aerosol optical thickness (AOT) and the main optical characteristic of atmospheric turbidity, together with dust transfer events, were also investigated. Earlier, it was proven that the direct influence of overestimated dust aerosol concentrations overestimated the AOT values [23]. Usually, on the days of dust transport, AOT exceeds the monthly average values by more than 2 to 3 times, depending on the seasonality. The end level collaboration, as mentioned, is in the 1.5 level and hence for the AERONET the returning of the trajectories is considered for the optical thickness estimation of the aerosols, which confirmed the presence of 33 dust transfers towards the Black Sea. AERONET provide spectral AOT for each station, for example, Figure 2 shows the spectral AOTs constructed from Section_7 platform observations for the studied dates.

One case confirmed the need to take into account the AOT in this problem, since the backward trajectory of aerosol origin did not confirm the dusty nature of the aerosol, while the AOT values and the corresponding distribution of course and mode particles confirmed the presence of an absorbing coarse aerosol on August 1 with an increase in AOT by more than 1.5 times (see Figure 3).

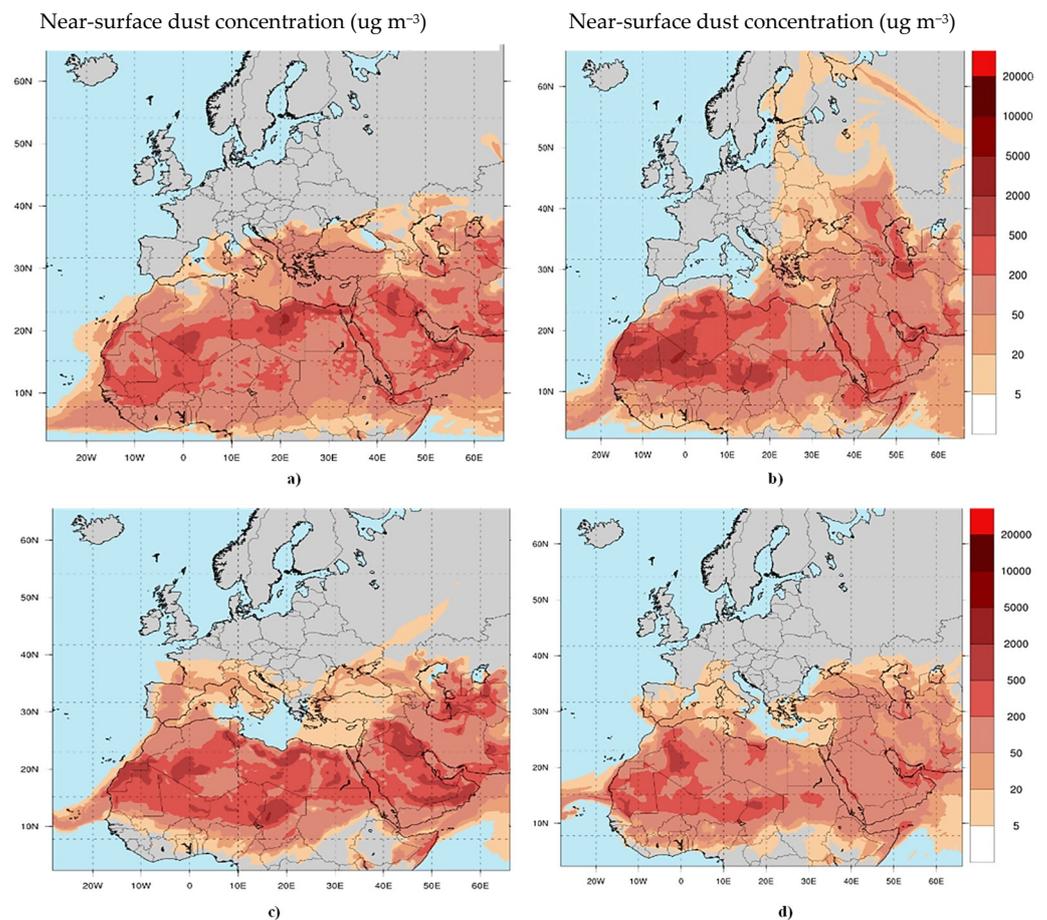


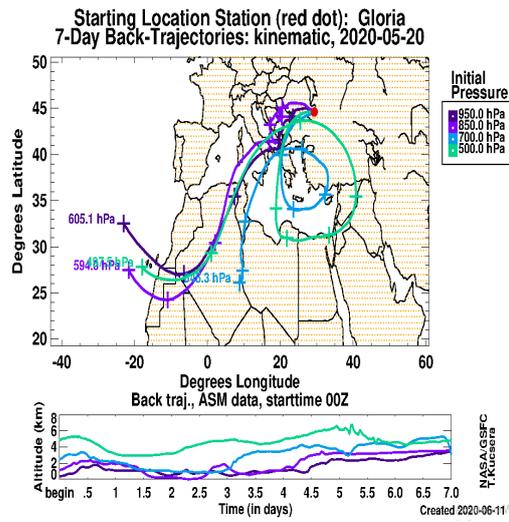
Figure 1. Maps for dust aerosol prediction using the WRF-Chem model for 20.05.2020 (a) 10.06.2020 (b) 30.07.2020 (c) and 13.09.2020 (d).

In general, the averages of the daily average *AOT* changes during the study period (from May 2020 to October 2020) are shown in Table 1. These studies were carried out for different wavelengths at the Section-7_Platform (44°54' N, 29°44' E) AERONET station. These results revealed a high degree of correlation between overestimated dust aerosol concentrations and changes in the *AOT*, especially in the long-wavelength range (more than 2 times) (Table 1).

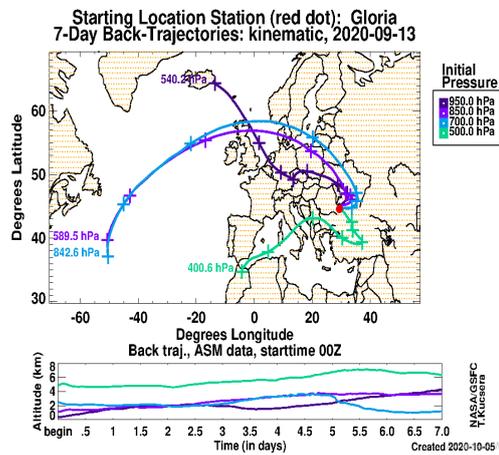
Table 1. Values of average aerosol optical thickness on the days of WRF-Chem dust forecast during May 2020 to October 2020, taking into account the mean deviation.

	<i>AOT</i> ₁₀₂₀	<i>AOT</i> ₈₆₅	<i>AOT</i> ₆₆₇	<i>AOT</i> ₅₁₀	<i>AOT</i> ₄₉₀	<i>AOT</i> ₄₄₃
<i>Dust</i>	0.15 ± 0.07	0.16 ± 0.07	0.19 ± 0.06	0.25 ± 0.05	0.25 ± 0.05	0.28 ± 0.05
<i>Clean</i>	0.06 ± 0.02	0.07 ± 0.02	0.09 ± 0.03	0.14 ± 0.04	0.14 ± 0.05	0.16 ± 0.05

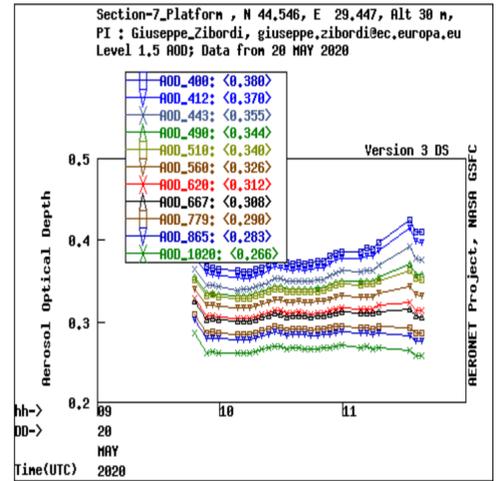
As an additional independent source, a dust identification coincidence analysis with the CALIPSO satellite was carried out, noting that the effectiveness and reliability of the results of the CALIPSO for the Black Sea were previously established. A comparative analysis of CALIPSO maps and AERONET results identified 86% coincidence of identification of the presence of dust aerosol over the Black Sea region (14% of the data was not provided by CALIPSO for the corresponding coordinates). An example of CALIPSO dust identification on 13.09.2020 is shown in Figure 4.



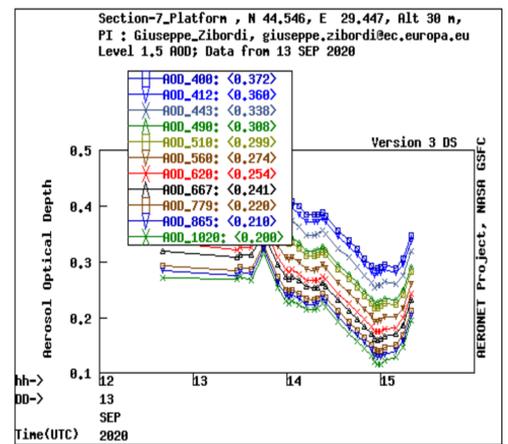
(a)



(b)



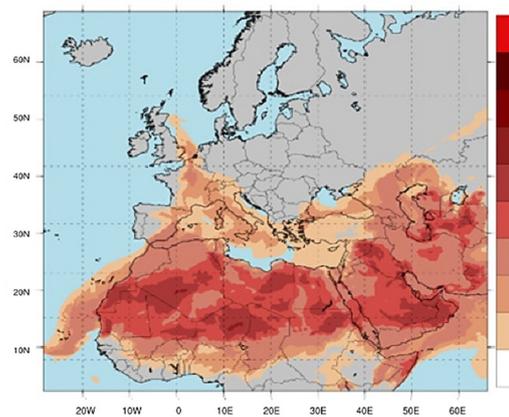
(c)



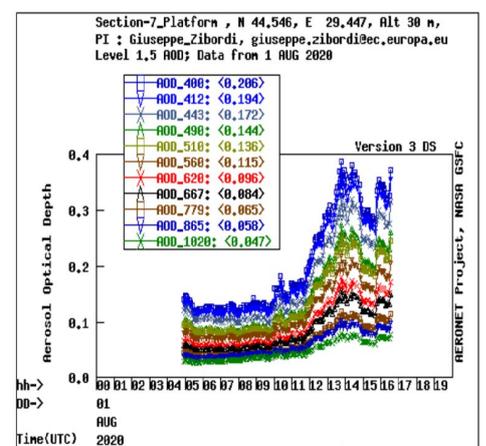
(d)

Figure 2. Backward trajectories of AERONET (20.05.2020 (a), 13.09.2020 (b)) and the corresponding dynamics of the change in the AOT on the days of dust transport predicted by the WRF-Chem model (20.05.2020 (c), 13.09.2020 (d)).

Near-surface dust concentration ($\mu\text{g m}^{-3}$)



(a)



(b)

Figure 3. WRF dust load forecast for 01.08.2020 (a) and the corresponding dynamics of the change in the AOT (01.08.2020 (b)).

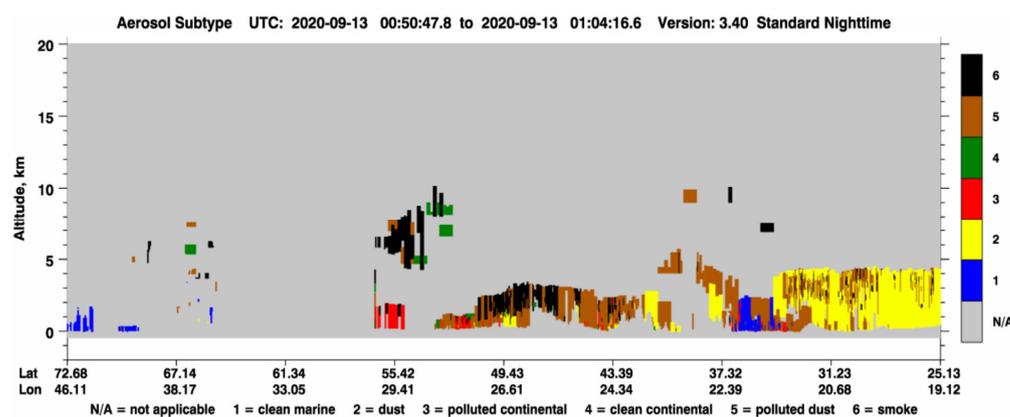


Figure 4. Detection of dust aerosol over the Black Sea region by CALIPSO methods for 13.09.2020.

MODIS Aqua satellite data can also be used as an additional data source. In most cases, this problem requires the use of more complex algorithms for determining the homogeneity of the sea brightness coefficients and aerosol optical thickness. The presence of clouds and discarding data on the optical characteristics of dust as an error is very often interfering with visual determination. The figure below shows a satellite image for one of the cases of a dust event, a dust flow along with cloudiness, due to a large number of error flags, produces white pixels, in which parameters such as chlorophyll concentration, remote sensing reflectance (R_{rs}), AOT and e.t. are not calculated in the future (see Figure 5).

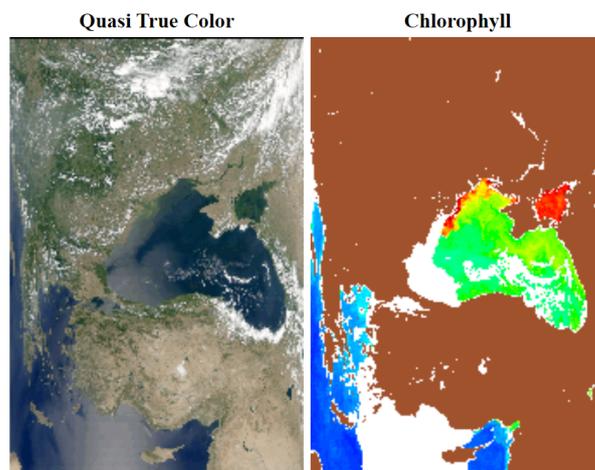


Figure 5. Satellite images from the MODIS Aqua platform during the day of the predicted dust transport over the Black Sea region for 30.07.2020.

Thus, dusty events (days) were identified as follows: (1) Analysis of back trajectories by BAMGOMAS (AERONET) confirmed the presence of aerosol transfer from the Sahara, that is, the aerosol origin points are located in or near the desert; (2) CALIPSO maps of aerosol subtypes also showed the presence of dust/polluted dust over the Black Sea region; (3) A sharp increase in AOT on the days under study compared to the monthly average values of AOT (usually the difference is about 1.5–3 times); threshold values were not used as they vary greatly depending on seasonality. Thus, three sources served as the main criteria for determining the fact of dust transport over the Black Sea region: reverse trajectories, CALIPSO aerosol subtype maps, and variability of the AOT . If 2 out of 3 criteria corresponded to the presence of mineral dust, then this prediction was considered correct. In most cases, to fully understand the effectiveness of the forecast model, it is not enough just to calculate the probability of model hitting. To describe the result, this work proposes the use of precision and recall metrics which are well known in machine learning. The

conclusions of the WRF-Chem forecasting model can be considered as recommendations whereas the mathematical approach for describing recommender systems is generally suitable for a specific task. Traditionally, the following concepts are used in machine learning: positive-advice (the model said “yes”) is divided into: TP (true positive) is the model answered “yes” and guessed it, FP (false positive) is the model answered “yes” and was wrong and negative answers are divided in the same way: TN (true negative) is the model answered “no” and it was correct, and accordingly FN (false negative) is “no” and this is an error [24]. As noted earlier, the measurements were carried out between 20.05.2020 to 18.10.2020. In this way, a data array of 152 values was collected. Based on the calculation of results, the corresponding parameters for our specific task were derived as shown in Table 1 with the following interpretation: TP (the WRF-Chem model correctly predicted dust transport) is 33 values, TN (the WRF-Chem model did not correctly predict dust transport) is 111 values, FN (the WRF-Chem model did not predicted actual dust aerosol transport) is 4 values, FP (WRF-Chem model predicted transport that was not there). Thus, the confusion matrix, a summary of prediction results on a classification problem, looks like this:

In Table 2 the variable \hat{y} is the response of the algorithm on the object and the variable y is the true label on that object. One of the most common metrics is the percentage of correct algorithm responses (accuracy) for this model can be written as:

$$\text{accuracy} = \frac{\text{TP} + \text{TN}}{\text{TP} + \text{TN} + \text{FP} + \text{FN}} \quad (1)$$

Table 2. Confusion matrix of WRF-Chem forecasting for Black Sea region from 20.05.2020 to 18.10.2020.

	$y = 1$	$y = 0$
$\hat{y} = 1$	33	4
$\hat{y} = 0$	4	111

In our case this indicator is 0.94. To assess the quality of the algorithm on each class separately introduce the metric precision (accuracy) and recall (completeness). These parameters can be calculated as:

$$\text{precisios} = \frac{\text{TP}}{\text{TP} + \text{FP}}, \quad \text{recall} = \frac{\text{TP}}{\text{TP} + \text{FN}} \quad (2)$$

One way to estimate the model is to do it with help of Equation (2), without being tied to a particular threshold such as AUC-ROC (or ROC AUC) which is the area under the error curve (Receiver Operating Characteristic curve). This curve is a line from (0, 0) to (1, 1) in True Positive Rate (TPR) and False Positive Rate (FPR) coordinates:

$$\text{FPR} = \frac{\text{FP}}{\text{FP} + \text{TN}}, \quad \text{TPR} = \frac{\text{TP}}{\text{TP} + \text{FN}} \quad (3)$$

In the notations of Equation (3) TPR is the object proportion of the negative class is shown by the FPR for the incorrectly predicted algorithm. The proper condition is generally considered as a state where no mistake is made by the classifier. (FPR = 0, TPR = 1), area under curve is obtained which is generally equal to one. In other case, when the output class probabilities are given by the classifier randomly, the AUC-ROC will be around 0.5 as the same number of TP and FP will be operated by the classifier [25].

For the considered specific task, these indicators have precision = 0.89, TPR (recall) = 0.89; FPR = 0.03. Thus, the work of the WRF-Chem model shows highly reliable results that cannot be attributed to random events. It can be ascertained that the investigation carried out has a relatively small margin of error.

This section may be divided by subheadings. It should provide a concise and precise description of the experimental results, their interpretation, as well as the experimental conclusions that can be drawn.

4. Conclusions

To make a reliable regional forecast of aerosol dust content in the atmosphere, to consider the external factors such as wind energy and soil moisture is essential, but it is also important to consider the physical characteristics of aerosol particles. This study made it possible, using various approaches of satellite and ground modeling, to assess the reliability of the WRF-Chem system, namely the online WRF-Chem tool for predicting dust transfers over the Black Sea region.

Based on the statistics of coincidences between the forecast and the actual result extracted from the data of the backward trajectories of AERONET and the aerosol typing maps in the atmosphere according to the models of the CALIPSO satellite, metrics were calculated that revealed the degree of confidence in the predictions (precision = 0.89, TPR (recall) = 0.89; FPR = 0.03). This study identified 89% of the prediction hits for dust events, which can be considered as a satisfactory predictor of results.

Along with this, the thickness of optical aerosols, as the key optical characteristic of aerosols, was assessed during the investigation. A correlation analysis of AOT change from dust transfer is particularly necessary in the absence of other evidence. Additional and alternative means of further planned dust prediction with subsequent comparative analysis can be fruitful and instructive. Further, we will consider the possibilities of using the WRF-Chem in the problems of forecasting fires [26]. Since this problem is also extremely relevant for the Black Sea region [27].

Author Contributions: Conceptualization, A.P. and D.S.; methodology S.P.; validation, S.P. formal analysis, S.P.; investigation A.P.; resources, A.P.; data curation, D.S.; writing—original draft preparation, A.P.; writing—review and editing, S.P.; visualization, D.S.; supervision, S.P.; project administration, D.S.; funding acquisition A.P. All authors have read and agreed to the published version of the manuscript.

Funding: The study was carried out with the financial support of the Russian Foundation for Basic Research, scientific project No. 19-35-90066, and within the framework of the state assignment programs of the Marine Hydrophysical Institute of the Russian Academy of Sciences on the topic No. 0827-2019-0002. The work was carried out within the framework of the State Project No. 0555-2021-0003 “Development of operational oceanology methods based on interdisciplinary studies of the formation and evolution processes of the marine environment and mathematical modeling involving remote and contact measurement data” (code “Operational oceanology”).

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: BTA data (<https://tropo.gsfc.nasa.gov/aeronet/> (Accessed on 15 June 2020)) and the CALIPSO satellite data (https://www-calipso.larc.nasa.gov/products/lidar/browse_images/production/ (Accessed on 25 May 2020)). WRF-Chem (web site: <https://ruc.noaa.gov/wrf/wrf-chem/> (Accessed on 15 May 2020)).

Acknowledgments: The authors thank Tom Kucsera, Brent Holben, and the Gene Feldman team of the National Aeronautics and Space Administration (NASA) for the calculations of the BTA data (<https://tropo.gsfc.nasa.gov/aeronet/> (Accessed on 15 June 2020)) and the CALIPSO satellite data (https://www-calipso.larc.nasa.gov/products/lidar/browse_images/production/ (Accessed on 25 May 2020)). We would also like to express our gratitude to and WRF-Chem group, getting information from WRF-Chem (web site: <https://ruc.noaa.gov/wrf/wrf-chem/> (Accessed on 15 May 2020)).

Conflicts of Interest: The authors declare no conflict of interest.

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