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Dust Emission Calculation and Forecasting using CALPUFF and GCM models

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ABSTRACT

Dust is an important atmospheric phenomena that occurs in spring and summer in many regions, including Iran and its neighboring countries. Considered one of the most important challenges of the last century, this phenomenon occurs on a global scale in arid and semi-arid regions. Because of changes in climate and vegetation as well as progressive processes of soil erosion and the disturbances resulting from them, the sensitivity of regions to rapid erosion will have important reactions on the region's climate and desertification. Therefore, the current research investigated the concentration and distribution of fine dust under the influence of meteorological parameters using the GCM climate model and attempted to determine the effect of climate change on the concentration of the relevant pollutant in the coming years. In this study, the CALPUFF model considered the temporal and spatial effects of weather conditions on the transfer, transformation, and removal of atmospheric pollutants. The emission rate of the PM10 pollutant was estimated. The results indicated that the increase in greenhouse gas emissions and changes in climate variables in the near future will cause the distribution of suspended particles one of the important pollutants to increase significantly. The results also revealed a significant relationship between the degradation of air quality and the trend of air warming during the period 2046-2065.

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INTRODUCTION

The CALMET/CALPUFF modeling system is more and more commonly used around the world in evaluations of impacts on air quality, including determining the shares of particular emission sources in shaping the level of air pollutant concentrations, especially in areas characterized by highly diversified landscape. Significant factors in these evaluations are the method of describing topography and land cover as well as the resolution of the computational grid. The impact of topography on the modeling results of atmospheric dispersion using this model system has already been noted (Oleniacz, R.; Rzeszutek, M., 2014). Special attention should be paid to Digital Elevation Model data—Shuttle Radar Topography Mission (SRTM), (Shuttle Radar Topography Mission (SRTM), 2018). It is timely that a new dust emission frequency point source (DPS) database is available and has been used with the albedo-based dust emission model (AEM) to circumvent the assumptions about sediment entrainment and supply (Hennen, Chappell et al., 2021). A detailed spatiotemporal analysis of the Aral Sea dust

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emissions-transport process is a necessary contribution to promote the understanding about the global dust cycle and its response to climate change (Zhang et al., 2020). GCM modeling studies that include fully interactive dust lifting processes typically represent saltation by way of wind stress threshold parameterizations, whereby dust is lifted when a threshold wind stress is exceeded (Chow et al., 2022). In recent decades, global and regional climatic models (GCMs and RCMs, respectively) have been widely used to simulate different climatic phenomena (Armstrong et al., 2019; Patlakas et al., 2019). Dust storms in Sistan are associated with serious impacts on atmospheric environment, ecosystems, human health, and the local economy (Yousefi et al., 2020).

Nature is a serious source of airborne particles in the world, including dust from arid regions and marine aerosols (Shahsavani et al., 2020; Alizadeh-Choobari, Ghafarian, and Owlad, 2016). Dust storms, usually originating in arid and semi-arid areas, are considered primary sources of mineral dust (Salmabadi, Khalidy, and Saeedi, 2020). Strong and turbulent winds ordinarily cause the phenomena of sand and dust storms (SDS), blowing over desert or aridisol surfaces and depleting visibility. Large quantities of dust particles are carried into the air and transported hundreds or thousands of kilometers away (Zoljoodi, Didevarasl, and Saadatabadi, 2013). Soil erosion by wind (wind erosion) happens in dry conditions when the soil is exposed to wind and creates a major environmental problem (Borrelli et al., 2017). Some weather conditions such as high wind speed and temperature, low rainfall, low soil moisture, and low relative humidity could cause areas to become uninhabitable, directly damage human health (Cao et al., 2015), and strengthen the level of PM (atmospheric particulate matter) to ambient air quality standards and health indices (Marsham et al., 2013; Shahsavani et al., 2020). An excessive level of PM is associated with increased cardiopulmonary morbidity and mortality (Kang et al., 2012). Cyclone rotations and Shamal winds in the Middle East add to the dust creation, which is especially exacerbated when such conditions occur over Syria and Iraq. Because Iran is located in Southwest Asia, i.e., within the Earth's "dust belt," it is often significantly affected by severe dust episodes (Alizadeh-Choobari, Ghafarian, and Owlad, 2016). Summer and spring dust storms typically occur in Iran, north-eastern Iraq and Syria, the Persian Gulf and southern Arabian Peninsula (Liu et al., 2004). Northern Iraq and the Iraq-Syria border host the main dust origins. This phenomenon is the result of reduced vegetation cover, maximum soil disturbance, increased sediment for emission enhanced by drought, factors that may be linked to land use dynamics and human activity, including conflicts (Modarres and Sadeghi, 2018). The nature of the interactions between surface winds and natural desert surfaces has important implications for aeolian sediment transport (Lancaster, Greeley, and Rasidussen, 1991). Middle East Dust (MED) events increased the PM10 level to the values of 5338 and > 9000 µg/m3 on June 3, 2010 and January 27, 2017, respectively, in Ahvaz, Khuzestan (Al-Taiar and Thalib, 2014). Wind velocity has a positive correlation with the quantity of dust in the air (Kutiel and Furman, 2003). Dust storms result in a considerable amount of topsoil being eroded and subsequently transported thousands of kilometers downwind. The city of Ahvaz, Iran, is ranked as one of the most polluted cities in the world in terms of particulate matter (PM) concentration (WHO, 2016), mainly due to MED episodes.

One major global environmental problem is soil erosion by wind (wind erosion). In dry conditions, wind erosion occurs when the soil is exposed to wind (Borrelli et al., 2017). Particles less than 10 micrometers in diameter (PM10) pose a health concern, because they can be inhaled and accumulate in the respiratory system.

To evaluate the potential health threat from PM10 inhalation, health risk estimates are based on exposure and dose assessments for exposed individuals. However, equally important is the estimation of the effective internal dose via lung deposition, transport, and clearance mechanisms (ICRP, 1994).Wind erosion affects the semi-arid areas of the Mediterranean region as well as the temperate climate areas of northern European countries (Borrelli et al., 2017).

Several reviews have reported that emissions mainly stem from natural and miscellaneous sources such as fugitive dust (unpaved and paved roads) and agricultural and forestry activities.

MATERIAL AND METHODS

Case study and meteorological characteristics

Khuzestan province in southwestern Iran covers 63,213 km2 and is home to 4.7 million inhabitants. It is located between 31 °N and 32 °N latitude and 48 °E and 49.5 °E longitude (Fig. 1, 2). The topographic altitudes change from 0 to 3740 m. The weather ranges from humid to arid. It is interesting to know that while the southern parts experience a tropical climate, the northern side has a cold climate. Summer runs from April to September, and wintertime is from October to March. During the summer, the annual mean maximum temperatures are about 50

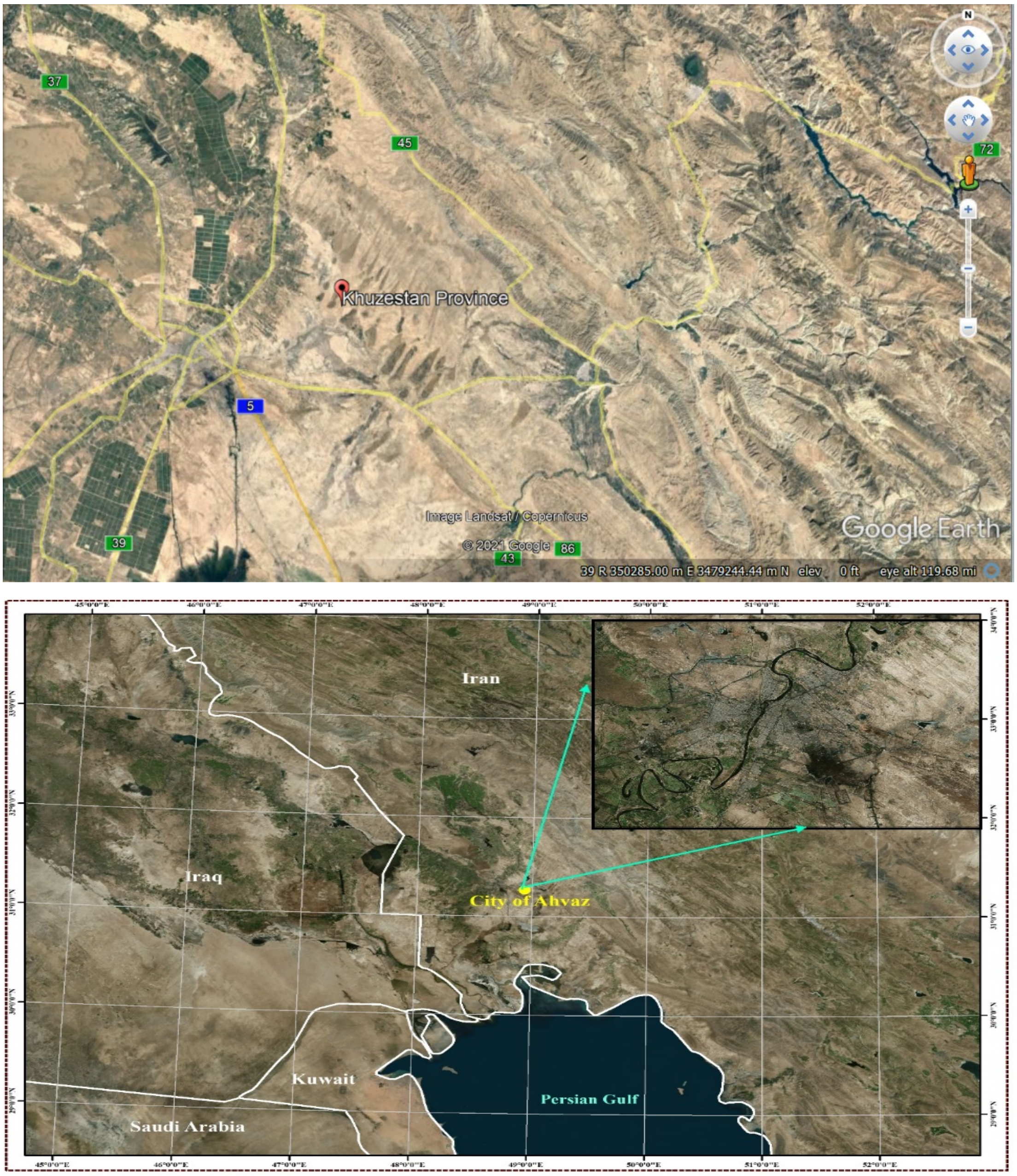

Fig. 1. Khuzestan province and Ahvaz city location

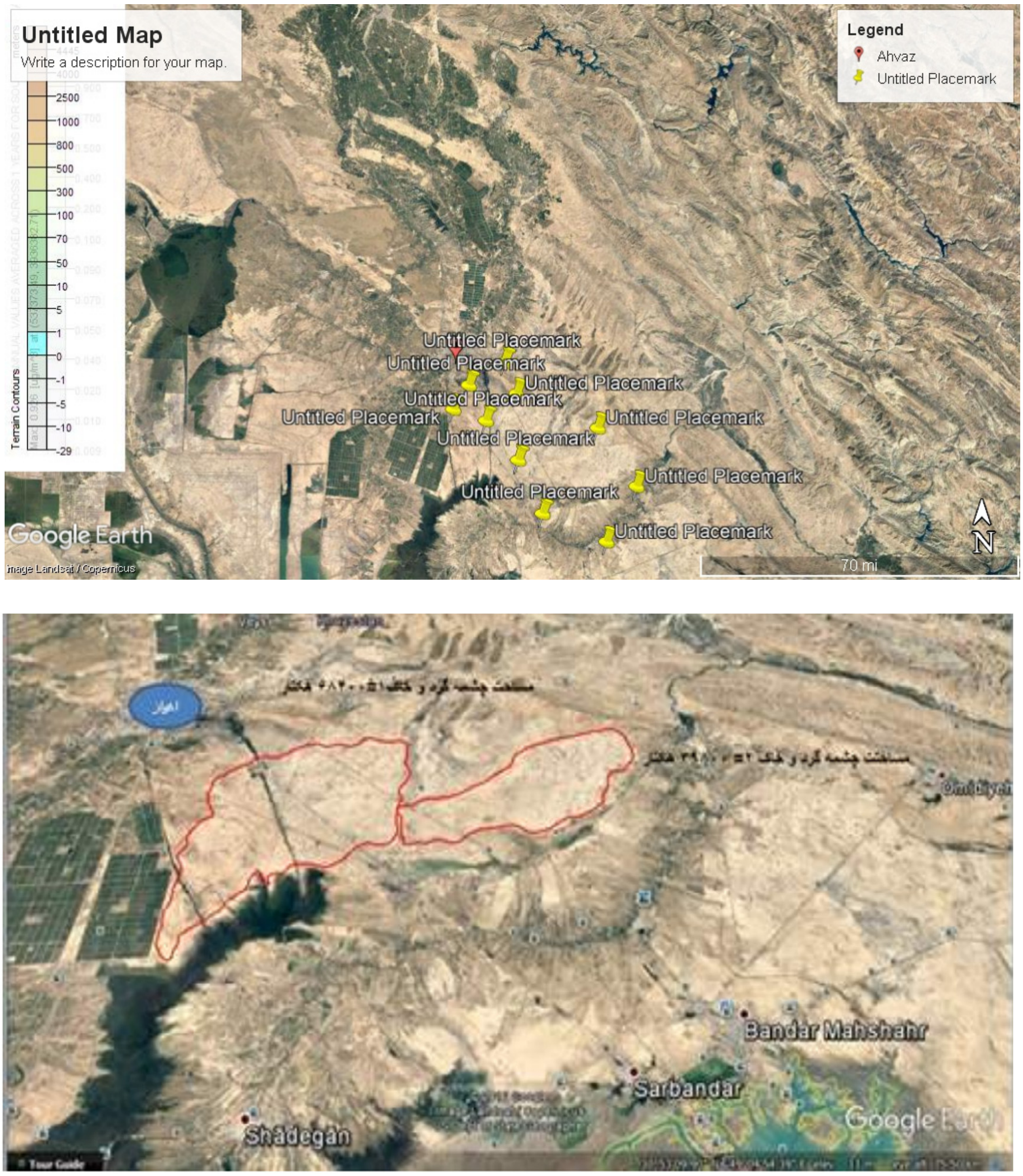

Fig. 2. Location of study area in Ahvaz

°C, and the minimum value is seen in March (9 °C). Annual precipitation levels are 995-1100 mm in the north and 150-256 mm in the south. Roughly 70% of annual rainfall occurs from February to April. The annual amount of evaporation is 2000-4000 mm. The direction of the prevailing wind speeds are W→E and NW→SE (Zarasvandi et al., 2011).

Data

Datasets of dust storms for use in the current study were obtained from the Iran Department of Environment (https://www.doe.ir/portal/home(. The dataset for the frequency of dust storm events in Iran was obtained from reports from synoptic stations throughout the country for the period 2020 to 2021 (https://www.irimo.ir/far/index.php). These reports are available from the Islamic Republic of Iran Meteorological Organization (IRIMO).

Model description

The Weather Research and Forecasting with CALPUFF (WRF/CALPUFF) regional model was applied to simulate dust events in Khuzestan province, Iran.

The Guidelines for Environmental Impact Assessment-Atmospheric Environment (hereinafter "Guidelines") published by the Ministry of Environmental Protection recommend AERMOD, ADMS, and CALPUFF modeling systems for predicting atmospheric environmental impacts. CALPUFF (American Meteorological Society/Environmental Protection Agency Regulatory Model) can be applied for an assessment range of 120 km, making it advantageous compared to the other systems. The prediction objects for CALPUFF modeling include point, area, and volume sources. In addition, CALPUFF has an extensive application range, including rural and urban areas, simple and complex terrains, and elevated and low sources. Based on the characteristics and pollutant sources of the study area, CALPUFF was chosen as the prediction software. CALPUFF can be applied on scales of tens to hundreds of kilometers. The input data of CALPUFF consist of meteorological, topographic, and pollution data.

Meteorological data extraction from the WRF model

The WRF model is a set of numerical models (NWP) that deals with forecasting and predicting weather conditions.

The WRF advanced modeling system is a medium-scale model and a flexible system with many capabilities that can be used to simulate different atmospheric conditions. It determines the meteorological parameters for each grid point (surface, sea, etc.) in three dimensions at all altitudes. Therefore, in the present research, the output data of this model was used to obtain the information required by the CALMET software. Weather prediction models numerically solve the hydrostatic equations of the atmosphere. In other words, extrapolation models such as CALMET call the data of weather prediction models and compare and correct them with other data, including geophysical and weather station data.

Geophysical data consists of two main parts: terrain and land use.

These two parameters are very decisive and important in that they form the basis of modeling

Represents the trend diagram of the WRF-CALMET-CALPUFF modeling system (Figs. 3) and (Tables. 1 to 4).

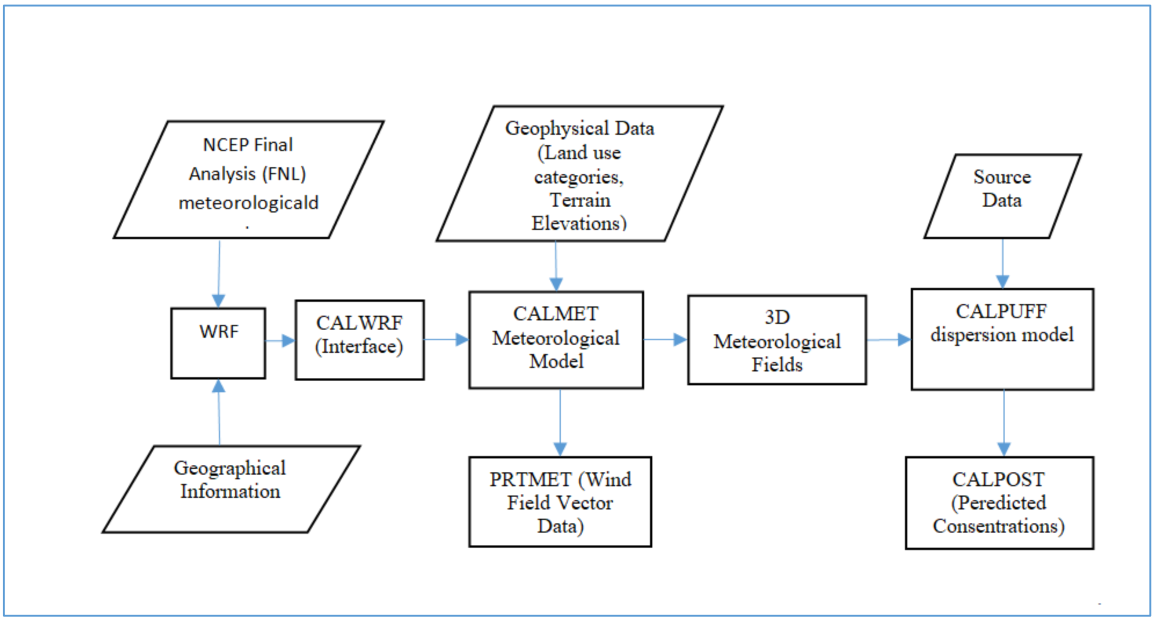

Fig. 3. Trend diagram of the WRF-CALMET-CALPUFF modeling system

Table 1. Surface meteorological information

Variable No	Description
1	Beginning year of data
2	Beginning Julian day
3	Beginning time (hour 00-23)
4	Beginning time (second 0000-3599)
5	Ending year of data
6	Ending Julian day
7	Ending time (hour 00-23)
8	Ending time (second 0000-3600)
9	Wind speed (m/s)
10	Wind direction (degrees)
11	Ceiling height (hundreds of feet)
12	Opaque sky cover (tenths)
13	Air temperature (degrees K)
14	Relative humidity (percent)
15	Station pressure (mb)
16	Precipitation code

Table 2. Output file of upper air data

YEAR	MONTH	DAY	JUL.DAY	HOUR-ENDING(GMT)	NO. LEVELS EXTRACTED
2019	1	1	1	0	30
2019	1	2	2	12	31
2019	1	3	3	0	28
2019	1	4	4	12	30
2019	1	5	5	0	24
2019	1	6	6	12	23
2019	1	7	7	0	22
2019	1	8	8	12	18
2019	1	9	9	0	38
2019	1	10	10	12	38
2019	1	11	11	0	20
2019	1	12	12	12	14
2019	1	13	13	0	15
2019	1	14	14	12	16
2019	1	15	15	0	18

Table 3. schematic Land use format

Grid Points	1	2	3	4	5	6	7	8	…..
1	0.000	0.167	0.000	0.000	0.333	0.000	0.000	0.333	….
2	0.000	0.167	0.000	0.143	0.333	0.000	0.167	0.000	…..
3	0.000	0.167	0.000	0.143	0.333	0.000	0.167	0.000	…..
4	0.000	0.167	0.000	0.000	0.333	0.000	0.167	0.000	……
5	0.000	0.167	0.000	0.000	0.333	0.000	0.000	0.333	……
6	0.000	0.167	0.000	0.000	0.333	0.000	0.167	0.000	……
7	0.000	0.167	0.000	0.000	0.333	0.000	0.000	0.333	……
8	0.000	0.167	0.000	0.000	0.333	0.000	0.167	0.000	……
….	…..	……..	………	……..	…….	……	……..	……	……

Table 4. Grid Specifications in CALPUFF and CALMET

No. of Grids in X direction	No. of Grids in Y direction	Ref. Point X coordinate	Ref. Point y coordinate	No. Vertical Layers	ZFACE
190	180	218	3316	10	0.,20.,40.,80.,160.,300.,600.,1000.,1500.,2200.,3000.

GCM Model

Numerical models (general circulation models or GCMs), representing physical processes in the atmosphere, ocean, cryosphere, and land surface, are the most advanced tools currently available for simulating the response of the global climate system to increasing greenhouse gas concentrations, while simpler models have also been used to provide globally- or regionally-averaged estimates of the climate response. Only GCMs, possibly in conjunction with nested regional models, have the potential to provide geographically and physically consistent estimates of regional climate change which are required in impact analysis, thus fulfilling this criterion.

GCMs depict the climate using a three-dimensional grid over the globe (see below), typically having a horizontal resolution of between 250 and 600 km, 10 to 20 vertical layers in the atmosphere, and sometimes as many as 30 layers in oceans. Their resolution is thus quite coarse relative to the scale of exposure units in most impact assessments, hence only partially fulfilling criterion 3. Moreover, many physical processes, such as those related to clouds, also occur at smaller scales and cannot be properly modeled. Instead, their known properties must be averaged over the larger scale in a technique known as parameterization. This is one source of uncertainty in GCM-based simulations of future climate. Others relate to the simulation of various feedback mechanisms in models concerning, for example, water vapor and warming, clouds and radiation, ocean circulation, and ice and snow albedo. For this reason, GCMs may simulate quite different responses to the same force, simply because of the way certain processes and feedbacks are modeled.

METHOD OF DUST EMISSION ESTIMATION

Windblown Dust from Vacant lands

Fugitive dust from the wind erosion of agricultural and vacant lands represents a significant source of particulate matter emissions, particularly throughout the Western US. For agricultural windblown dust, emission factors may be estimated using the USDA wind erosion equation (WEQ) (ARB, 1997), which relates the PM_{10} emission factors to various parameters characterizing the specific crops, soil erodibility, surface roughness, vegetative cover, and climatic factors. PM10 emissions are obtained by multiplying the resulting emission factor by the total crop acreage in units of tons/acre/yr. For non-agricultural vacant lands, numerous wind tunnel studies have been conducted to estimate appropriate emission factors based on soil types, surface conditions and threshold friction velocities.

Windblown fugitive dust emissions have not been estimated by the EPA in previous national emission inventories. ENVIRON recently completed the development of a windblown dust model for use in WRAP regional haze modeling efforts (Mansell et Al., 2006). A description of the model development and most recent results for WRAP states can be found at http://www.wrapair.org/forums/dejf/fderosion.html. The model estimates fugitive PM dust emissions from vacant lands given wind speed data. All vacant land types except mechanically disturbed lands, e.g., agricultural tilling, are considered. The current version of the model is set up to use regional-scale land use databases to characterize vacant lands and also requires specification of soil characteristics, specifically soil texture. The model provides hourly gridded emission estimates that can be easily summarized on a county level. A complete detailed description of the model development and requisite input databases is included in the project final report and related documentation (Mansell et al., 2006).

Regional dust storms and other phenomena such as stable weather conditions and inversion can increase ambient PM levels. In our study, dusty days affected by regional dust intrusion were statistically separated from non-dusty days by analyzing the air pollutant levels. The threshold value of 120 μg/m^3 for PM_{10} concentration was applied to distinguish the dusty days from regular days suggested by others (Escudero et al., 2007; Givehchi et al., 2013).

Dust source identification is one of the most crucial factors in studying dust storms. Many studies have focused on dust source determination using vastly different methods including ground-based measurements (Cao et al., 2015), remote sensing data (Ginoux et al., 2012; Moridnejad et al., 2015a; Nabavi et al., 2016; Prospero et al., 2002; Yu et al., 2018), and numerical models (Gherboudj et al., 2017). Several investigations have suggested that there are many dust regions with different productivity in the Middle East, and they yield different main areas of dust entrainment and uplift.

Magnitudes and locations of estimated PM_{10} emissions depend on the estimated extent of disturbed vacant lands, on the measured or estimated erodibility of the soil surfaces, and on the intensity, duration and frequency of erosive wind events.

PM_{10} emission rates at sites with wind erosion are related to dust suspension (Roney and White, 2006)

Categorizing Vacant Land

Vacant land within the study area must be categorized based upon the potential of the parcels to emit fugitive dust during wind events. Many wind tunnel studies have been conducted in the western United States, and the vacant land descriptions of the wind tunnel test areas should be used to categorize the vacant land within the study area. Wind tunnel tests conducted with particulate size determinations will be very helpful when preparing PM_{10} and $PM_{2.5}$ emission inventories.

When soil survey data is not available for the study area, other sources of approximation may suffice, e.g., data on geology, topography, vegetation, and climate, together with Land Remote Sensing Satellite (LANDSAT) images. Soils of like areas should be identified and the probable classification and extent of the soils determined. If the study area is limited, it may be practical to conduct a stratified random sampling.

Categorization of land types will be beneficial when determining where focus is needed. Two key elements will be of value in making this determination: land-use category percentage of total acreage within the study area and the applicable emission factors. Ultimately, the focus will relate to the volume of the emissions and the duration of the emissions generated within land-use categories.

For the area to be studied, hourly average wind speeds, rainfall, and (if available) peak wind gust data should be gathered. If a study area is particularly large, several different meteorological data sets may need to be gathered.

PM_{10} Emission Rate

Defining the vertical flux of PM_{10} concentration with the concept of turbulent mixing was difficult due to the steep gradients of vertical PM_{10} concentration profiles, as used in Equation1, because the wind-speed profiles beneath the canopy did not follow the law-of-the-wall profile. Thus, the concept of mass balance in a control volume was used to determine PM_{10} emission rates. A mass balance across the boundaries is given by the integral for the hexahedral control volume in the wind tunnel:

The existing formula and the coefficients of A and B were modified. In addition, this formula can be used to predict dust production:

$$E = \frac{1}{D}\int_0^h \left(c_e u_e - c_i u_i\right) dz \tag{1}$$

where **E** is emission rate of PM_{10} concentration in ($1/ML^2/T$) dimensions, **D** is distance between inlet and outlet boundaries of the control volume, **h** is the height of the control volume, **c** is local PM_{10} concentration as measured by the TSI DustTrak, **u** is local mean wind speed, **z** is vertical coordinate, and subscripts **e** and **i** represent exit and inlet, respectively.

The fifth-order polynomial of the wind speed profile and an exponential for the PM_{10} concentration profile were used for each case to evaluate this integral relationship. Note that the quantity E determined from Equation (1) is referred to as the PM_{10} emission rate, while F from Equation (4) is referred to as the PM_{10} vertical flu. Figure 4 shows the distribution of PM_{10} emission rates for various vegetation coverages as a function of reference wind speed. Significant increases in PM_{10} emission rates are observed when the reference wind speed, U0, is greater than about 7 to 10 m/s. For reference wind speed less than 10 m/s, PM_{10} emission rates of vegetated surfaces are observed to be as high or even greater than the unvegetated surfaces (See Figure 4). Note that the "crossover" of the two curve-fit lines of Cv =0 and Cv = 0.55 at speeds less than 8 m/ s the emission rate of Cv = 0.55 is greater than Cv = 0, yet its contributions to the total emission rate are negligible, as they are over two orders of magnitude less than the emissions occurring at 15 m/s. This suggests that enhanced turbulent mixing and oscillation of the stems causes a "sweeping" like action of the plant, thus creating an albeit small addition to the emissions from the soil surface. Furthermore, PM_{10} material on leaves and stalks may be dislodged and entrained into the flow (Fig. 4).

A general empirical equation is developed to predict the amount of PM_{10} emission, E, as a function of vegetation cover and wind speed. It is given as:

(2) $E = Au_{10}(1 - Cv) \exp [B (u10 - ut) (1 - Cv)2]$

where E is PM_{10} emission rate ($\mu g/m^2/s$), u10 is wind speed at 10-m height (m /s), u_t is a PM_{10} emission threshold wind speed at 10-m height (m /s), and CV is vegetation coverage defined in Equation (7). The dimensional constants A and B are determined from the data (i.e., empirical input). The dimension of A is of density in units of ($\mu g/m^3$), and the dimension of

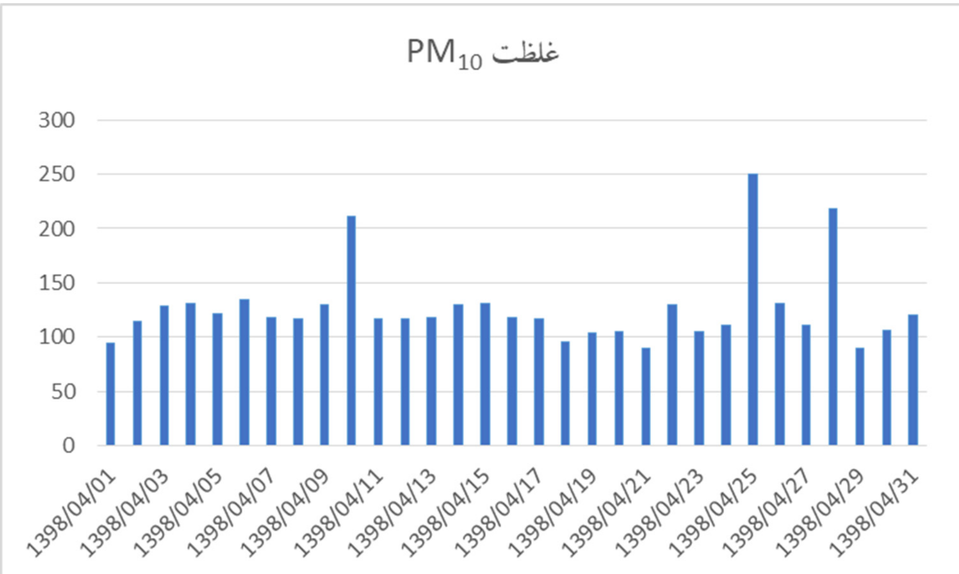

Fig. 4. Emission of PM_{10}

B in the exponent is the inverse of friction velocity in unit of (m/s). Values of A = 0.27 µg/m^3 and B = 0.37 m/s were determined from the Owens lakebed soil and salt grass vegetation data. The parameter u_t was found to be equal to 11.8 m /s. This is considered the speed at which significant increases of PM_{10} emissions were observed to occur.

RESULTS AND DISCUSSION

On June 15th, 2019, a dust storm occurred in vacant lands around Ahvaz city. The duration of the occurrence of dust storm was short, just as the similar occurrence in 2018; the zones of occurrence of dust were clear, and dust forecasting model was being used, considering that the hourly pollutant concentration is predicted by the hourly measurement data (Fig.5 to 13).

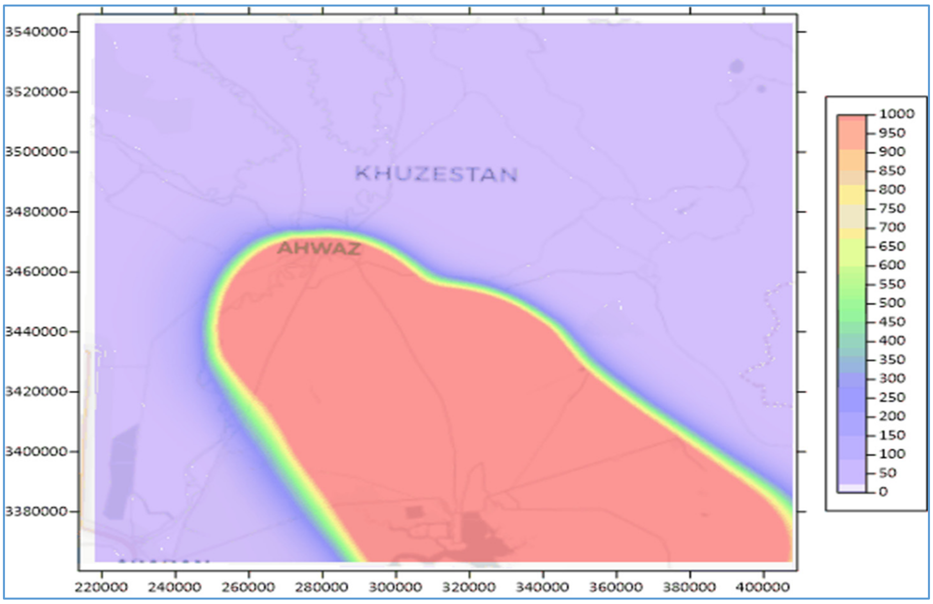

Fig. 5. Pollutant distribution in the study area

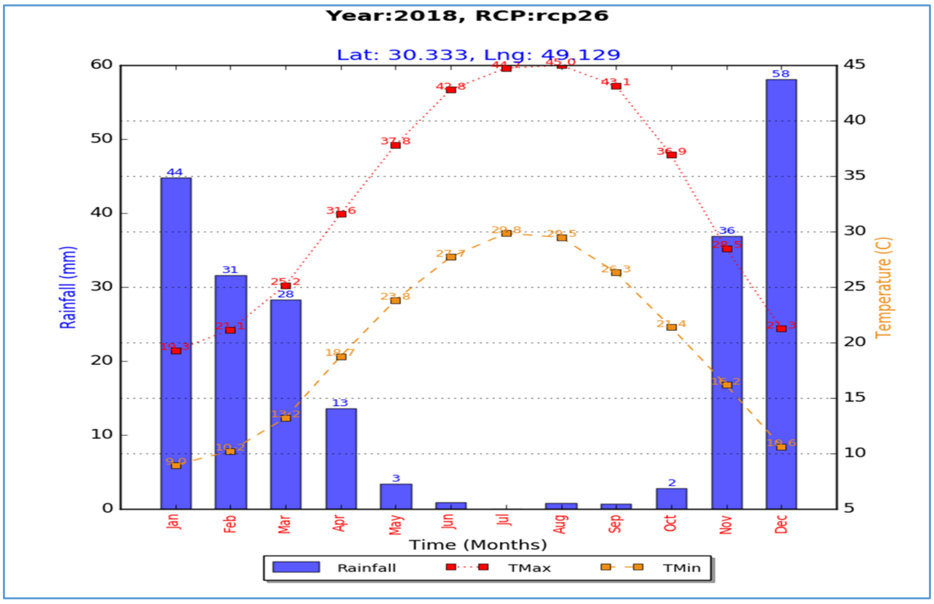

Fig. 6. GCM climate change model output in 2018

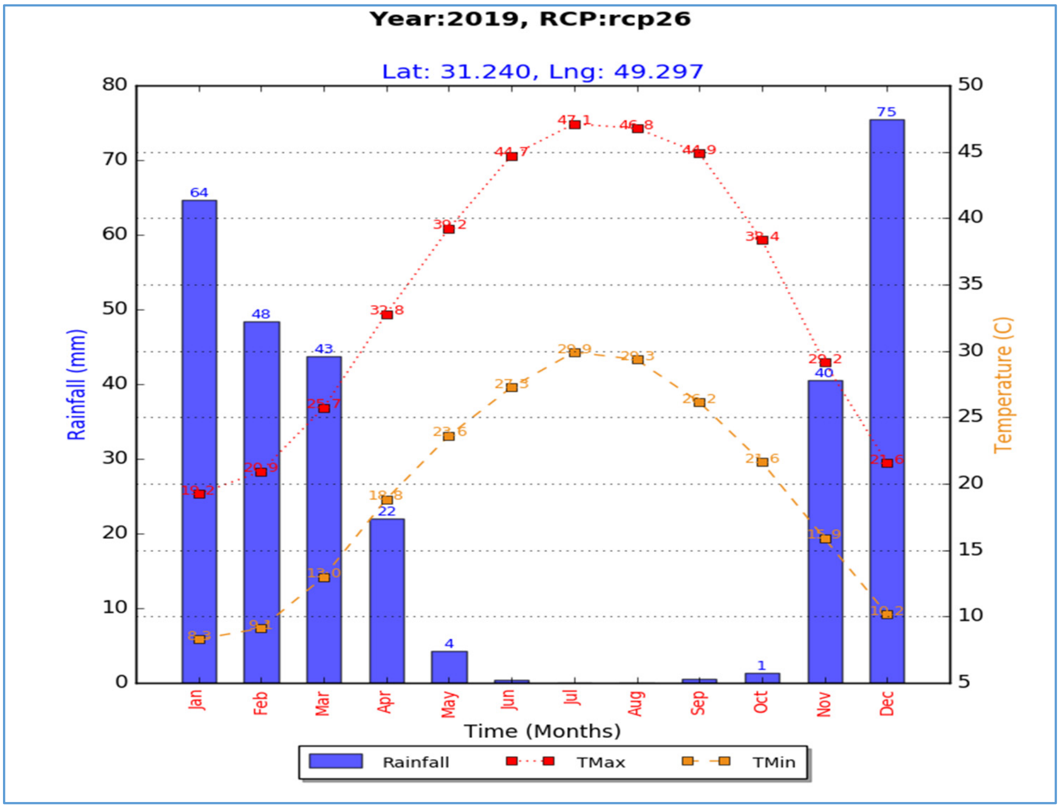

Fig. 7. GCM climate change model output in 2019

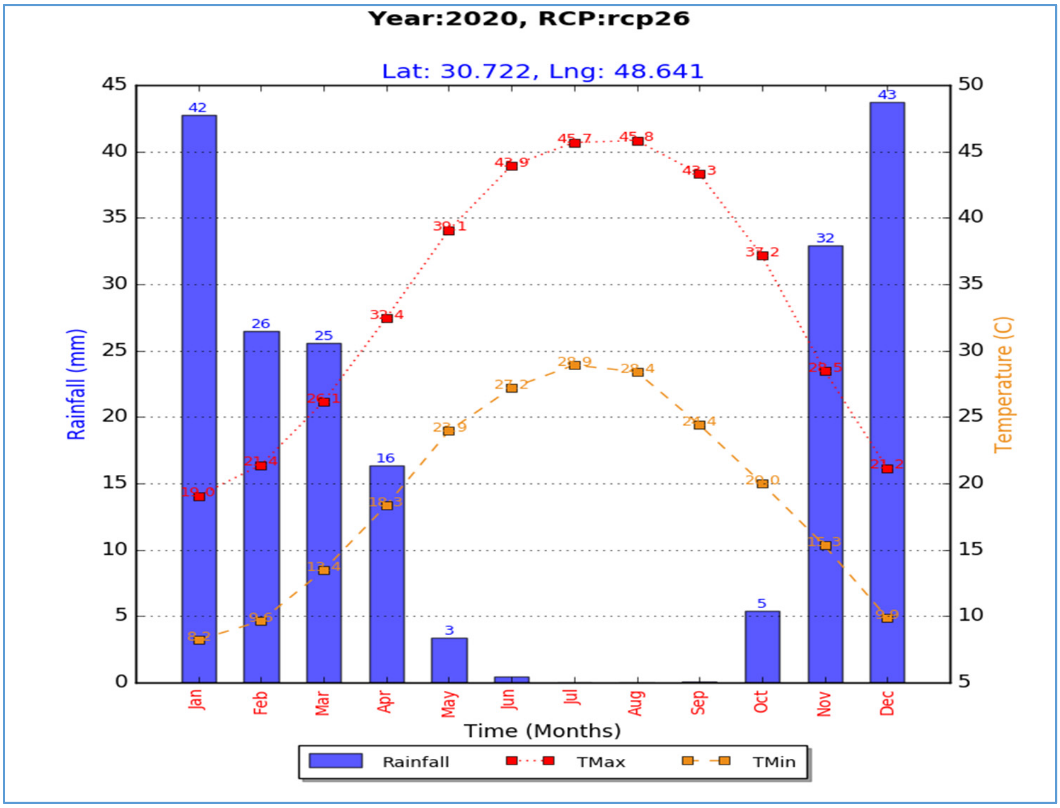

Fig. 8. GCM climate change model output in 2020

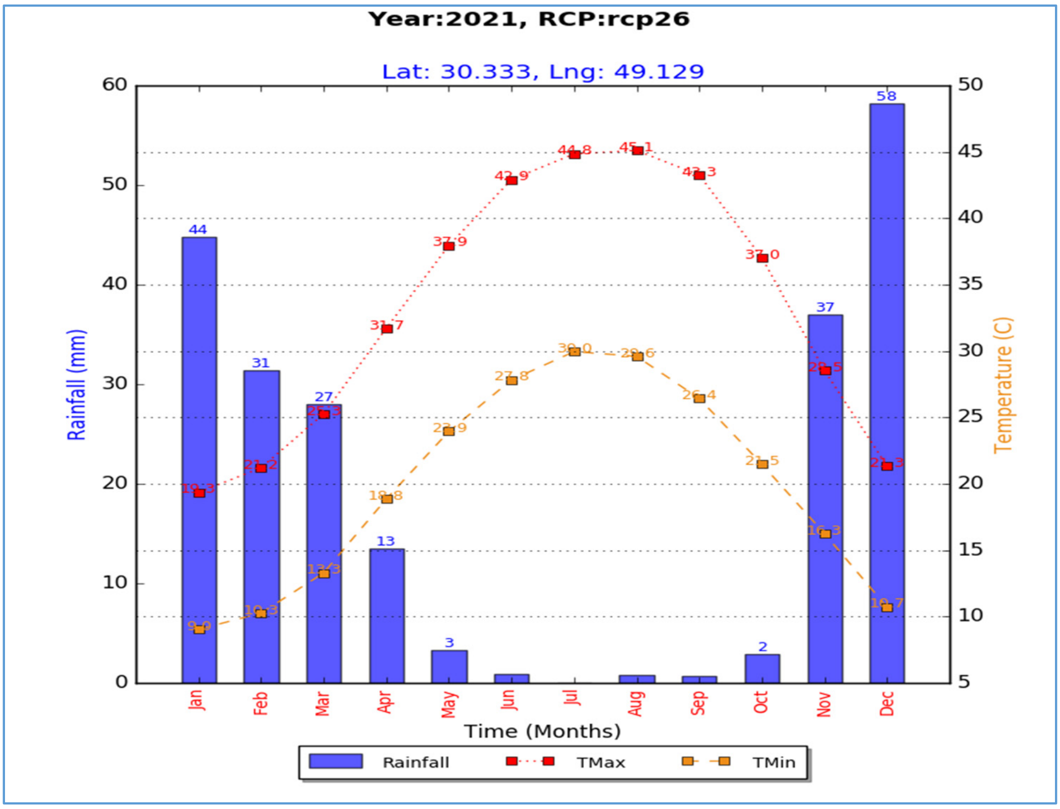

Fig. 9. GCM climate change model output in 2021

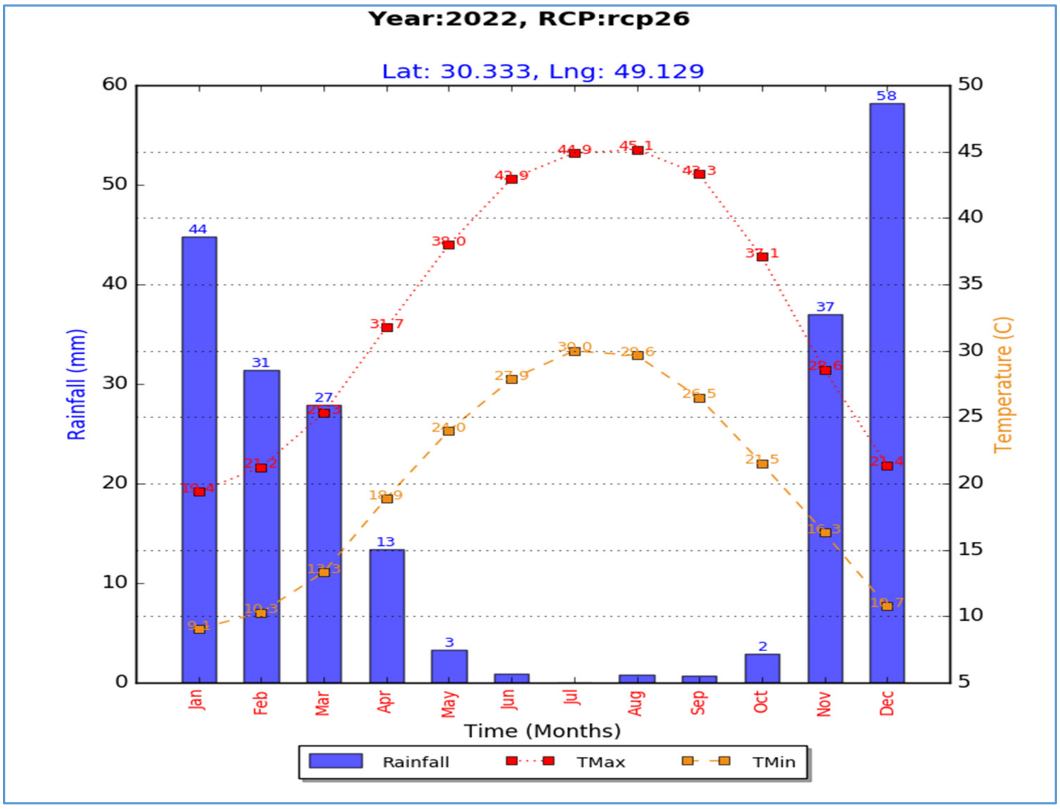

Fig. 10. GCM climate change model output in 2022

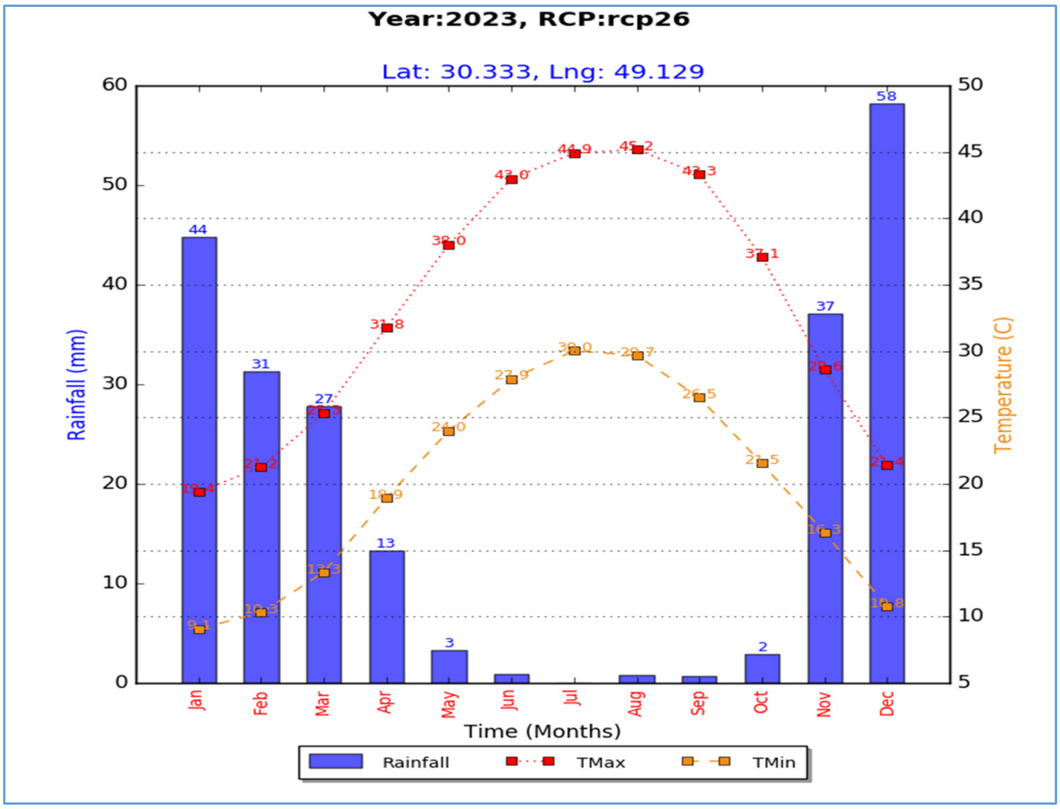

Fig. 11. GCM climate change model output in 2023

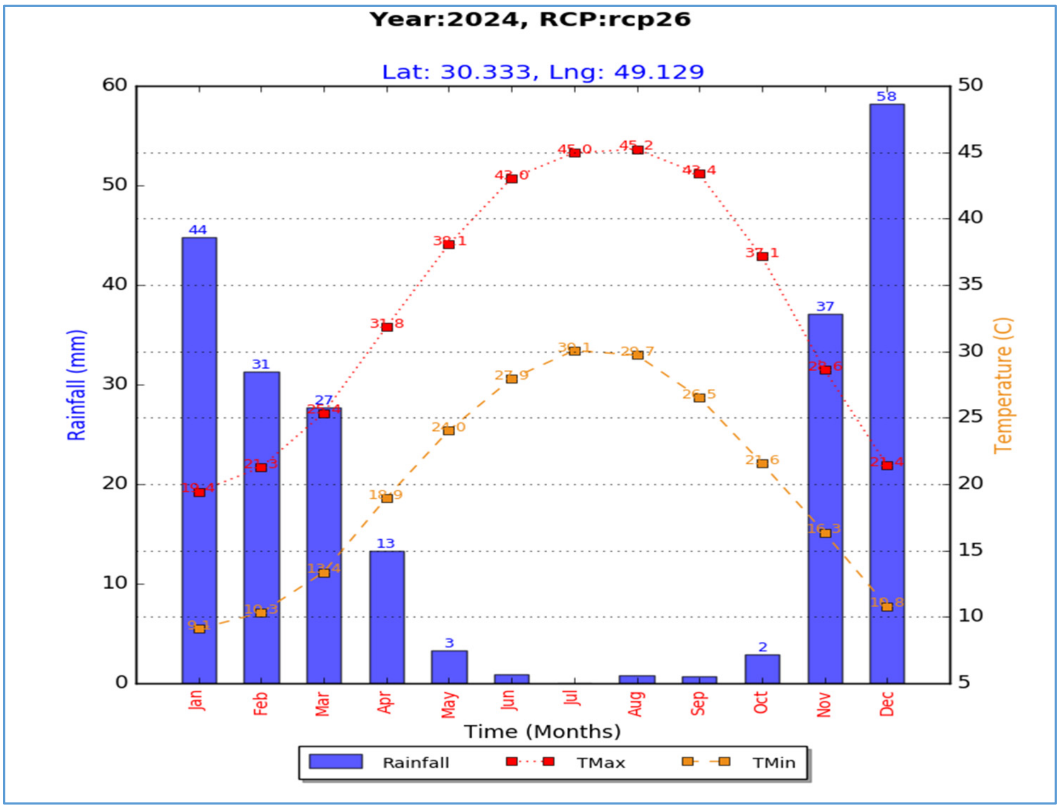

Fig. 12. GCM climate change model output in 2024

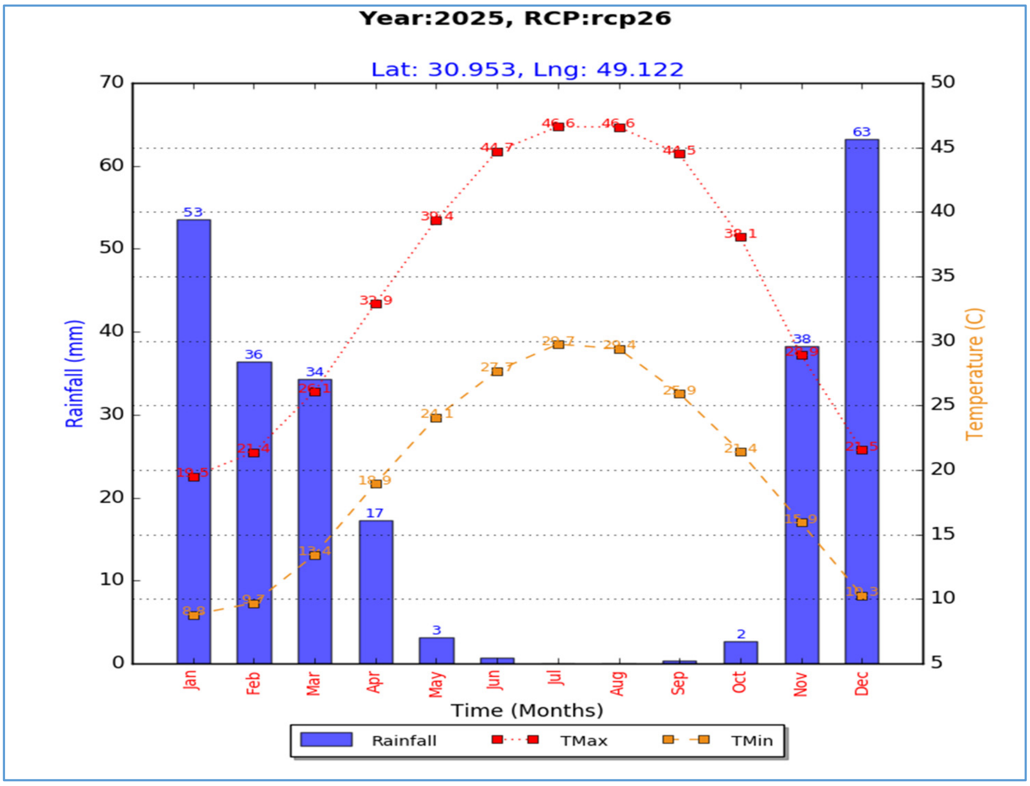

Fig. 13. GCM climate change model output in 2025

Graph 1. Increasing level of dust production

CONCLUSION

According to the output concentrations of the model and comparison with the data of the monitoring stations in this study, it is possible to calculate the pollutant production rate of suspended particles measuring less than 10 microns in any point of the country that has dust occurrences in order to manage air quality. The strategy of controlling and evaluating the capacity of pollutant transfer and providing methods of controlling dust centers inside the country and controlling dust centers are used.

Accurately calculating and determining the production rate of air index pollutants in areas affected by dust phenomenon has always been considered a basic step for making decisions related to air pollution management programs in order to prevent environmental destruction. To manage air quality, for example, to develop a control strategy, and to evaluate the capacity of transferring pollutants in the region, the amount and manner of the spread of these pollutants in the region should be considered.

According to the results of the current study, with the increase in greenhouse gas emissions and changes in climate variables in the near future in the summer season, the distribution of suspended particles measuring less than 10 microns (as one of the important pollutants of Ahvaz city) will increase significantly. It is noteworthy that the results of studies conducted in Portugal and at the University of North Carolina both showed that according to CAMx and CAM5 air quality models in the future period until 2050 and according to RCP8.5 scenarios, the annual concentration of PM10 will increase in the city of Porto and in North Carolina. Moreover, according to the results of the estimation of other air pollutants in Portugal (especially in the city of Porto), the degradation of air quality has a significant relationship with the trend of air warming during the periods of 2046-2065. A study conducted in 2007 for the city of Pune, India, also reported that the concentration of PM_{10} particles in the central areas of the city of Pune had increased compared to the surrounding areas, while the results of the current research in the city of Ahvaz have revealed that the distribution of PM_{10} particles concentration in the centers of Ahvaz is more concentrated and will increase more than in the past.

According to another study conducted in America to investigate the effects of climate fluctuations and changes on air pollution and its relationship with health, atmospheric chemical processes at local and global scales are affected by temperature, precipitation, humidity, and cloud parameters, wind speed and direction, and greenhouse gas emissions. The results of the current research in Ahvaz city also showed that considering the changes in climate parameters and greenhouse gas emissions according to two scenarios RCP2.6 and RCP8.5 in the coming years and assuming the stability of the concentration of air pollutants, the concentration and distribution of pollutants of suspended particles smaller than 10 microns will be affected.

GRANT SUPPORT DETAILS

The present research did not receive any financial support.

CONFLICT OF INTEREST

The authors declare that there is not any conflict of interests regarding the publication of this manuscript. In addition, the ethical issues, including plagiarism, informed consent, misconduct, data fabrication and/ or falsification, double publication and/or submission, and redundancy has been completely observed by the authors.

LIFE SCIENCE REPORTING

No life science threat was practiced in this research.

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