



Analyses of industrial air pollution and long-term health risk using different dispersion models and WRF physics parameters

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Abstract

This study consists of three main sections. The first section delves into a performance analysis centered around modeling PM₁₀, NO_x, and CO emissions from a cement factory. It examines the effectiveness of various factors, including meteorological data, physics models, and air quality dispersion models, in producing accurate results for atmospheric simulations. The second section covers the dispersion direction and concentrations obtained by visualizing the dispersion maps. The third section covers an analysis of heavy metals emitted from the facility, taking into account potential risks in the region such as cancer, acute and chronic effects, and long-term respiratory risks. This study made use of meteorological models (WRF, AERMET, and CALMET), air quality dispersion models (AERMOD and CALPUFF), a health risk analysis model (HARP), and various sub-models (MMIF and CALWRF). Satellite meteorological data were obtained from NCEP and ERA, with the majority of meteorological data based on the Global Data Assimilation System (GDAS)/Final Operational Global Analysis (FNL) from Global Tropospheric Analyses and Forecast Grids used for the WRF model. In the daily results, AERMOD showed the highest concentration values, but CALPUFF had greater concentrations throughout the annual period. The winter season had the highest concentrations of pollutants. Although there are differences among the physics models used in this research, the conclusions produced are consistent. Analysis of the data from the HARP model suggested that cancer risk levels exceeded the threshold of one person per million. However, the proportion of exceedance instances is rather small in comparison to the receptor points.

Keywords PM₁₀ · NO_x · CO · AERMOD · CALPUFF · WRF · HARP · cancer risk

Introduction

Studies on air pollution from past to present revealed that chemical, biological, or organic and inorganic substances released into the air as a result of human activities were extremely dangerous for living things and the environmental ecosystem (Sierra-Vargas and Teran 2012; Dianat et al. 2016; Li et al. 2016; Maleki et al. 2016; Rao et al. 2017; Cipriani et al. 2018; Zhao et al. 2019). Every year, millions of people die from the acute and chronic effects of pollutants in the air as well as extremely fatal health problems such as cancer (Goldberg et al. 2008; Kampa and Castanas

2008; Guarnieri and Balmes 2014; Guan et al. 2016). Emissions released to the environment as a result of the activity of numerous factors, such as industrialization, pandemic, global climate change, and human activities, have become an important topic in terms of air pollution for researchers (IPCC 2007; Zhang and Batterman 2013; Kinney 2018; Fu et al. 2020).

With the increasing number of people living in our world, the need for materials increases as a consequence of the increase in the need for raw materials. Different building materials are used to meet this demand. Among these building materials, cement which, in addition to being a durable, long-lasting, and low-cost building material, meets the needs of many sectors and is widely used, thereby increasing its production. On examination of the cement-producing countries in the world, China, America, and India stand out as the largest producers, while Vietnam and Turkey follow this ranking (USGS 2023). Despite the efforts to keep emissions under control in the cement factories, these factories still

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account for approximately 5–7% of the total carbon dioxide (CO₂) and 3% of the total greenhouse gas effect (Hendriks et al. 1998; Galvez-Martos and Schoenberger 2014; Çankaya and Pekey 2019; Raffetti et al. 2019). It also causes the release of compounds such as sulfur dioxide (SO₂), particulate matter (PM), volatile organic compounds (VOC), carbon monoxide (CO), nitrogen oxide (NO_x), sulfur compounds, ammonium (NH₃), hydrogen chloride (HCl), heavy metals, and hydrogen fluoride (HF) (Chinyama 2011; Schorcht et al. 2013; Mosca et al. 2014; Leone et al. 2016; Shen et al. 2017). PM, which is the main intermediary product in cement production activities, can be found in different sizes depending on the particle size and diameter, especially particles below 10 µm, both causes respiratory diseases and increases the mortality rate (Zanobetti and Schwartz 2009; Stanek et al. 2011; Anderson et al. 2012). NO_x, another gas that has an important role in atmospheric chemistry, is an important pollutant that must be kept under control as it plays a role in the formation of inorganic aerosols and can cause negative effects on human health (Mueller et al. 2004; Wang et al. 2011; Zhao et al. 2013; Salva et al. 2023). Emissions can enter the human body directly through the respiratory tract as a result of their dispersion into the atmosphere, or indirectly through penetration into soil and water (Schuhmacher et al. 2004).

The World Health Organization (WHO) has determined certain limit values to control the damage caused by emissions that may negatively affect the environment and living life. On examination of the studies, Miller and Moore (2020) revealed the climate, health, and economic impact of air pollution emissions caused by cement production. Rauf et al. (2021) emphasized that the health effects of emissions released from a cement factory in Indonesia on the residential areas were below the threshold limits of risk for respiratory non-carcinogenic risks and that studies beware of total suspended emissions (TSP). The study of Leone et al. (2016) compared the simulation of PM₁₀ pollutants originating from two cement factories in Caserta, Italy for a whole year with air quality monitoring station (AQMS) data in the region by means of the Second-order Closure Integrated Puff (SCIPUFF) model and revealed that while both simulation and measured data exhibited high levels in winter, low levels in autumn and spring, and lowest levels in summer and the cement was highlighted to be responsible for the deterioration of air quality in the city of Caserta. Bildirici (2020), in the study conducted on the effects of production, death rate, economic growth, and air pollution relations in China, India, Brazil, America, and Turkey, which are the largest cement-producing countries in the world, mentioned that the air pollution and the mortality rates are increased as a result of the increase in the cement production and highlighted that CO₂ and mortality rates could not be reduced without reducing the cement production. In a study determining the causes and effects of air pollution in

Turkey, Bayram et al. (2006) specified the causes as cement, iron and steel industry, and thermal power plants, also including the transportation and domestic fuel sources, and the importance of the development of renewable energy sources was emphasized.

The best way to reduce pollution and harm caused by pollutants is to keep emissions under control. For this purpose, a number of models have been developed through numerous methods and theories to predict the resulting pollution, and the models are expected to meet criteria such as performance, reliability, and compatibility (Weil et al. 1992). Air pollution has been recognised as a major concern by many studies, and at the same time, meteorological, geographical, and emissions changes affect air pollution on both regional and global scales. (Mayer 1999; Arnold et al. 2004; Ilten and Selici 2008; Fenger 2009; Ramanathan and Feng 2009). Air pollution affects pollutant release depending on the geographical land structure, pollutant type, and the effect of atmospheric events (Kesarkar et al. 2007; Stein et al. 2007). As atmospheric weather events can be affected by many conditions and situations, unlike fixed factors such as geographical conditions, their analysis, and acquirement of realistic results are very difficult. Therefore, various physics models have been developed to analyze weather simulation (Gbode et al. 2019; Tian et al. 2021). A "mesoscale numerical model" was developed to analyze such complex calculations and perform full-time calculations (Molinari and Dudek 1992; Song et al. 2009; Ching et al. 2014; Fustos-Toribio et al. 2022; Valappil et al. 2023). An example of these models, the Weather Research and Forecasting (WRF) model, is a medium-scale weather forecasting model that enables researchers around the world to obtain past, future, and instantaneous meteorological data (Skamarock et al. 2019). On examination of the studies prepared with the WRF model, the model seems to be used in many different fields and studies such as hurricanes, floods, precipitation, heat wave, wind, and solar energy (Davis et al. 2008; Lara-Fanego et al. 2012; Efstathiou et al. 2013; Eltahan and Magooda 2018; Fustos-Toribio et al. 2022; Tuy et al. 2022; Valappil et al. 2023).

In this study, we modeled PM₁₀, NO_x, and CO emissions released from a cement plant. We compared the performance of meteorological data, physics models, and air quality dispersion models to determine which option yielded the best results in atmospheric simulations. Additionally, we examined the long-term risks posed by heavy metals and PM₁₀ emissions from the plant, as well as the potential cancer, acute, and chronic respiratory risks in the vicinity.

Study area

The study was conducted in the Balıkesir region, located in the northwestern region of Turkey. Balıkesir is a city that hosts multiple activities such as tourism, agricultural, and industrial activities. The city, with approximately 1.3 million people, has a higher population in the summer months due to being a tourism region (TUIK 2023). The general characteristics of the Balıkesir region include a continental climate in the inner regions and a Mediterranean climate in the coastal area. In addition to hosting Turkey's most important mountains, the city center is surrounded by mountains in the north, northwest, and southwest parts due to its unique geographical structure, as seen on the relief map in Fig. 1. As an effect of such land conditions, the warm air rising from the ground encounters hot air higher than itself, preventing the air coming from the lower level from dispersing and remaining suspended. Consequently, the so-called inversion layer emerges and can lead to serious health problems (Ahrens 2015; Trinh et al. 2019). In particular, consumption of fossil fuels and industrial activities increase this risk for settlements in mountainous terrain such as the central region of Balıkesir (MOEUCC 2020; Mutlu and Bayraktar 2021). The long-term dominant wind direction of the region was

emphasized to be northern winds by studies (Mutlu and Bayraktar 2021). Two AQMS measure the composition of existing air in the city center. This study referred to these stations as A-AQMS (Central Station) and B-AQMS (Bahçelievler Station). The stations were established to test the air quality of Balıkesir City Centre and measure the limit exceedances. Considering the placement of stations, the Central AQMS is positioned inside the residential center region, therefore monitoring background emissions from domestic heating and vehicles. In this station, PM_{10} , NO_x , and CO ambient concentrations have been monitored by employing "Environment SA-MP101M", "Environment-SA-AC32e", and "Environment-SA-CO12e". In addition, the instruments measure PM, NO_x , and CO using beta-ray, chemiluminescence, and non-dispersive infrared (NDIR) methods, respectively. The second station, Bahçelievler, is distant from downtown, the major route, and mostly sources concerned with background and heating emissions. The "Metone BAM1020" and "Teledyne API 200E" instruments are utilized at the Bahçelievler station to measure ambient concentrations using the same method as Central AQMS for PM_{10} and NO_x . Both AQMS are situated in the upwind region of the facility, with the center midpoint of the facility being assessed in this study positioned at a distance of 4.6 km for the center AQMS and 3.2 km for the Bahçelievler AQMS.

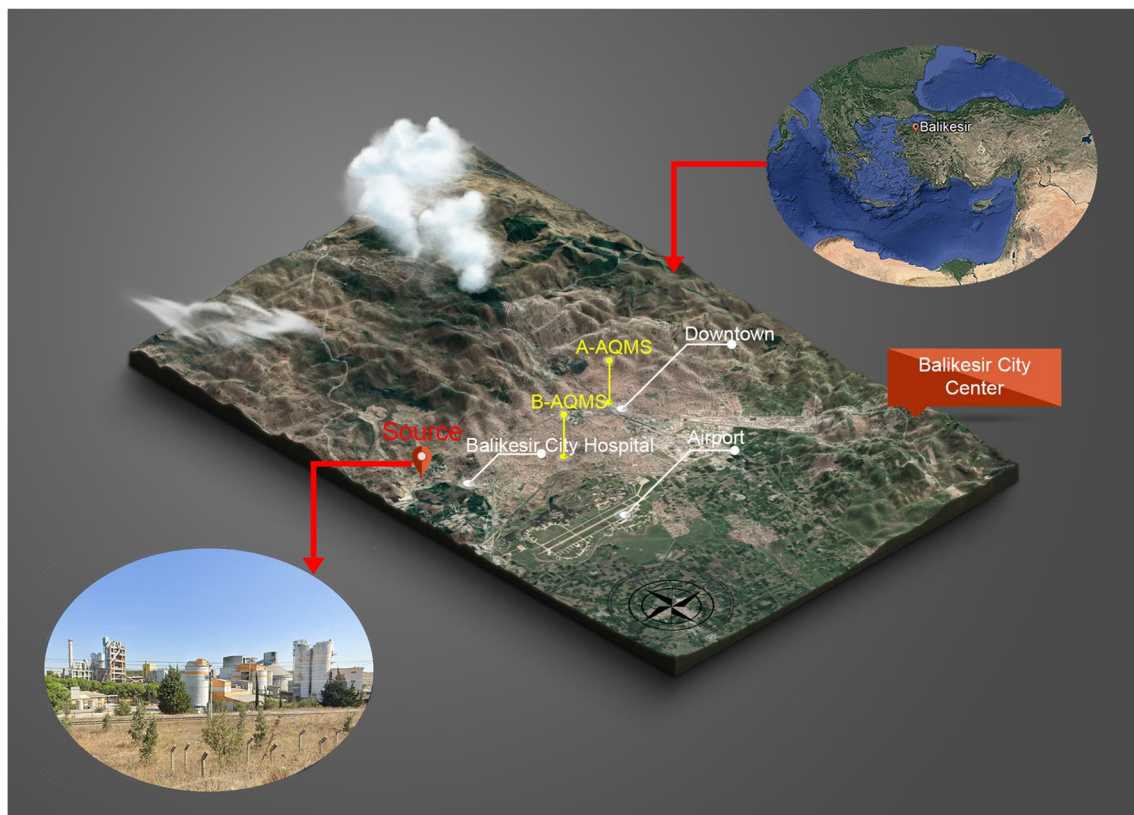


Fig. 1 Study area

While the facility is located in the center of Balıkesir province in the Marmara region of Turkey, it continues its operations in the south of the city center. There are residential areas and a 500-bed Balıkesir Central Hospital approximately 1 km away from the facility. The facility blends clay, limestone, gypsum, and iron ore raw materials from cement production quarries through certain processes, and consequently produces, packages, and ships the final product. The facility produces approximately 2 million tons of clinker and cement and sells the same to the domestic and foreign markets (EIA Report 2014). The facility possesses an open area of 1,140,000 m² and a closed area of 25,630 m². The facility runs full-time throughout the year and employs around 150 people. During its operation, PM₁₀, NO_x, CO, and heavy metals are emitted from the plant owing to these activities.

Data and methodology

Emission inventory

Cement manufacturing processes emit PM, NO_x, CO, SO₂, VOCs, and heavy metals pollutants. (Zhang et al. 2015; Wang and Chen 2016; Li et al. 2018; Adeniran et al. 2019; Parlak et al. 2023). This study measured emission data of PM₁₀, NO_x, CO, SO₂, and heavy metals from the facility. Background emission input was not included in this study. Emission measurements were carried out at regular intervals between February 16 and 23, 2021. The simulation period in this study was also 2021. SO₂ was neglected for this investigation because SO₂ concentrations did not exceed the official limits levels. Modelled and measured NO_x pollutants at the plant are the sum of NO and NO₂. Flue gas

basic parameters of the ISO 10780 method were utilised to measure basic parameters. Emission sources were monitored utilising the PM₁₀ “EPA 40 Part 50”, NO_x “EPA CTM 022”, and CO “ISO 12039” techniques for this investigation. The air quality model utilized three distinct emission types in this study: point, line, and area sources. The facility under investigation comprises a total of 45 active chimneys, with primary emissions originating from the farine mill (Stack 1), coal mill stack (Stack 2), and vertical cement mill (Stack 3). The remaining 42 chimneys exhibit significantly lower emission levels. Therefore, 42 operational chimneys were integrated with a representative stack (Stack 4) to develop air quality models for this study (Mutlu 2020). Additionally, storage, bulk, and loading activities were considered part of the area’s sources. Vehicles facilitate the transportation of raw materials within the facility, covering an estimated distance of 820 meters from the source line. Various measures such as bag filters, dust collector cyclones, electrostatic dust collectors, and watering of plant roadways are employed to mitigate PM emissions released by the facility. The study presents annual emissions data for carcinogenic heavy metals, fine dust (PM₁₀), and other pollutants (NO, NO₂, and CO) from point emission sources in Table 1. Furthermore, Table 2 provides information on emissions from other line and area sources.

Apart from the cement factory located in Balıkesir, which has been selected for this research, there are structured industrial zones and numerous firms as well as residential neighbourhoods in the region. It is revealed that, while looking at the downtown location in Fig. 1, domestic settlements are more concentrated in the city center and B-AQMS locations. Therefore, air pollution produced by heating occurs in this location, and it was noted that CO and SO₂ pollutants

Table 1 Annual air emissions from the analyzed point emission sources

Type of pollutants	Name of pollutants	Point sources			
		Stack 1 (kg/yr)	Stack 2 (kg/yr)	Stack 3 (kg/yr)	Stack 4 (kg/yr)
Heavy metal	Antimony	14.1	-	-	1.4
	Arsenic	22.2	0.9	0.5	11.8
	Copper	10	1.8	0.5	15
	Cadmium	-	0.9	-	0.5
	Cobalt	7.7	-	0.5	2.3
	Chromium	43.5	0.5	0.5	16.3
	Lead	35.8	3.2	0.5	11.3
	Mangan	7.7	1.8	0.9	43.1
	Thallium	-	1.4	-	0.5
	Vanadium	21.3	1.8	0.5	10.4
Emission	PM ₁₀	7621	754	797	17695
	NO	721824	90404	-	-
	NO ₂	11826	2190	736	-
	CO	377206	47041	-	-

Table 2 Area and line sources

Name of pollutants	Type of process	Type of sources	Emission rates (kg/yr)
PM ₁₀	Area	Storage area	2745
		Bulk area	8451
		Loading area	8451
	Line	The transportation of raw materials to the facility	32050

had the maximum values in February, which was the heating season (Mutlu and Bayraktar 2021). Linear emissions from vehicles, an average of 4600 vehicles pass through the downtown location during the morning peak hours (Mutlu 2019). At the same time, A-AQMS is positioned in this location, where the heaviest traffic passes. In addition, B-AQMS is distant from the city center's main road line. The industrial zones in the centre of Balikesir can be classified into two places. The industrial zone is situated in the northeast of the Downtown area, while the other is located in the southwest relative to the site of the cement factory utilised for the study in Fig. 1. At the time of this study, insufficient research existed regarding the air pollution emanating from these structured industrial zones; consequently, they were not included in the model inputs.

Meteorological data and WRF domain

Meteorological data were obtained from satellite data for the WRF-ARW model and local stations for the AERMET and CALMET models. Surface meteorological data were obtained from Balikesir Airport station, which was 4.5 km away from the center of the cartesian for chosen grids, and wind speed, wind direction, temperature, pressure, humidity, cloud cover, and cloud height data sources were provided hourly. Upper air meteorological data were obtained from Istanbul Kartal Regional Station, approximately 180 km away, with pressure, altitude, temperature, wind speed, and wind direction data in 12-hour periods. Meteorological data from the stations were prepared using AERMET and CALMET models. Meteorological data from the satellite were obtained from NCEP and ERA. The majority of meteorological data was used for the WRF model from Global Tropospheric Analyses and Forecast Grids (ds083.3) data via the Global Data Assimilation System (GDAS)/The Final Operational Global Analysis (FNL) (NCEP 2015). Although the data set was from NCEP, which measured nearly 35 meteorological parameters in 0.25 grid and 6-hour periods, due to the absence of sea surface temperature (SST) data in the ds083.3 meteorological data set, this data was obtained through the Fifth Generation of European Re-Analysis (ERA5). ERA5, developed by the European Center for

Medium-Range Weather Forecasts (ECMWF), produces a dataset containing atmospheric, surface, and ocean climate data (Hersbach et al. 2020; Muñoz-Sabater et al. 2021). The model domain area is divided into two types: internal and external domains, taking Balikesir City center as the origin point. The outer domain of the model was kept as wide as possible and more data sets were tried to be included in the model. The outer domain was created with a total of 70 grids in an area of 2100 x 2100 km with a distance range of 30 km². The inner domain was created with a total of 40 grids in an area of 400 x 400 km with a grid distance of 10 km². The meteorological model domain area is presented in Fig. 2.

WRF model and physics

The WRF model, which was developed as a result of the collaboration of many institutions and organizations such as the National Center for Atmospheric Research (NCAR), the National Centers for Environmental Prediction (NCEP), the National Oceanic and Atmospheric Administration (NOAA), the Forecast Systems Laboratory (FSL), the Air Force Weather Agency (AFWA), the University of Oklahoma and the Federal Aviation Administration (FAA), and the Naval Research Laboratory, is still being developed and new versions continue to be developed (Michalakes et al. 2005; Afzali et al. 2017). In its simplest definition, the model tries to approximate weather events in the atmosphere to real data through numerical calculations. The occurrence of atmospheric weather events depends on many factors and conditions. It is, therefore, difficult to follow and examine weather events. Researchers have developed various physics methods by introducing specific calculation methods to analyze such events. Microphysics (MP), cumulus, and planetary boundary layer (PBL) were emphasized to be important for predicting weather events in terms of achieving realistic prediction and simulation (Boadh et al. 2016; Gbode et al. 2019). Many academics have worked with WRF to improve the results of the model and optimize it for the desired purpose. Bukovsky and Karoly (2009) analyzed the 4-month precipitation period via the convective parameterization scheme using SST data, and as a result, the simulations used with SST data achieved the best results; additionally, while many researchers benefited from SST data as well (Jung et al. 2012; Shimada et al. 2015; Martinez et al. 2019; Tuy et al. 2022). Evans et al. (2012) analyzed the physics options suitable for the region by using different PBL, cumulus, short wave (SW), long wave (LW), and MP schemes to analyze the rain season in Australia. Duzenli et al. (2021) achieved realistic results with the WRF model by using different physics options, ERA5, and, Global Forecast System (GFS) data for the analysis of flood events taking place in the summer and autumn periods in the eastern Black Sea

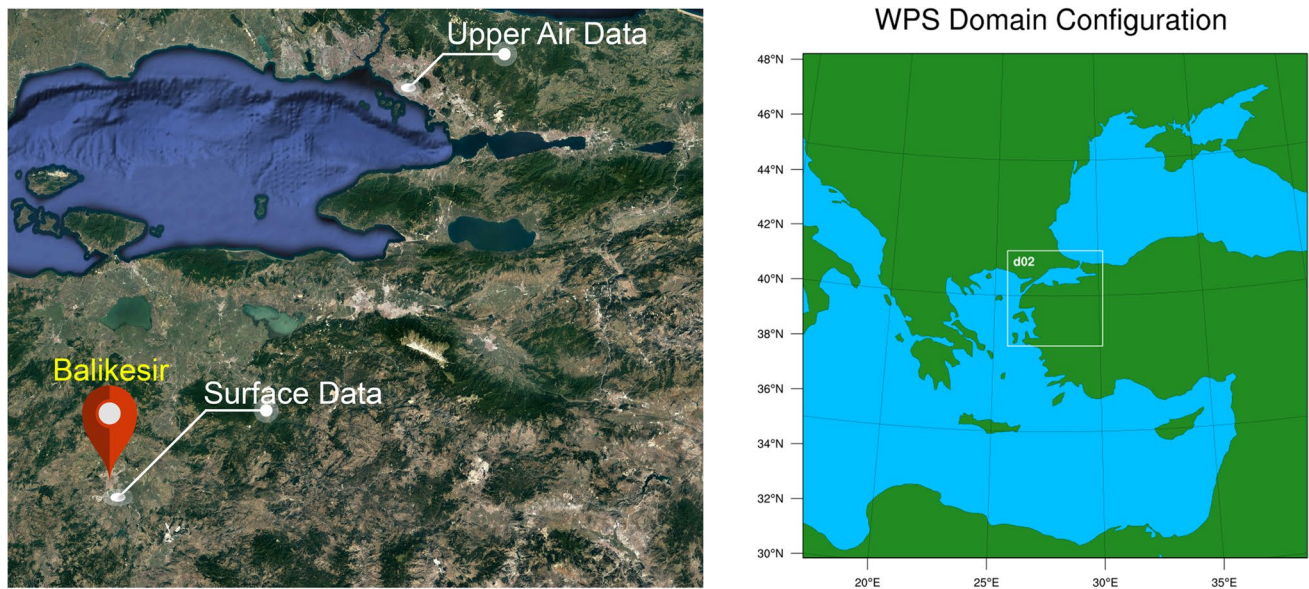


Fig. 2 Meteorological stations and WRF domain

and Mediterranean regions in Turkey, despite stating the possibility of reaching better results with SST data. Boadh et al. (2016) stated that PBL had an important place in wind circulation for transporting energy in the atmosphere, and suggested Yonsei University (YSU) and Mellor-Yamada-Nakanishi and Niino Level 2.5 PBL (MYNN2) for studies that can be used for air pollution dispersion. Afzali et al. (2017) examined the air quality dispersion of the region with AERMOD, using PM_{10} , NO_2 , and SO_2 pollutants released as a result of multiple industrial activities in Malaysia as well as surface and upper air meteorological data obtained from the WRF model. Rzeszutek et al. (2023) studied the WRF model with other air quality dispersion models (AERMOD, ADMS, and CALPUFF) for under 50 km as a consequence of temperature and wind speed simulations that were sensitive to the location of the grid area, and the WRF domain size created less inaccuracy with high resolutions.

This study aims to obtain the best results for the study area by testing different physics options with the WRF

model. Depending on this situation, simulations were carried out on seven different scenarios. While selecting physics options, previously used physics infrastructures with the best results were used and studies conducted in the same geography were also included. The scenarios were prepared for the WRF model. The selected physical properties and the rationale based on previous studies according to the ensemble numbers (EN) provided in Table 3 are as follows: No. 1: The Thompson microphysics option, which was used as Contiguous United States (CONUS) in the WRF user guide and the WRF model input file "namelist.input" by default after model installation, was preferred and used in a variety of studies (Lo et al. 2008; Wyszogrodzki et al. 2013; Ryu et al. 2019; Ünal et al. 2019). No. 2: The WSM6 Class microphysics option recommended by "NCAR" in the 10-30 km grid range, specified in the WRF user guide regional climate was used (NCAR 2017; Skamarock et al. 2019). It was also preferred because Turkey was the region of this study and it had a frequently preferred physics infrastructure

Table 3 Physical options

Ensemble no (EN)	Microphysics	Planetary boundary layer/ Surface layer	Cumulus physics	Shortwave/Long-wave radiation physics
1	Thompson "CONUS"	MYJ/ETA	Tiedke	RRTMG/RRTMG
2	WSM6 "NCAR"	YSU/MM5	KF	CAM/CAM
3	GD	MYJ/ETA	BMJ	RRTMG/RRTMG
4	MY	MYJ/ETA	BMJ	RRTMG/RRTMG
5	Eta Ferrier	MYJ/ETA	KF	Dudhia/RRTMG
6	WSM3	YSU/MM5	Grell	RRTMG/RRTMG
7	LIN	Bougeault/ETA	Grell	RRTMG/RRTMG

for different studies (Patel et al. 2019; Özen et al. 2021). No. 3: Gbode et al. (2019) compared 27 different physics combinations to analyze the African monsoon rain regime and used Goddard (GD) microphysics, one of the options that provided the best value in terms of model skill score, while Hines and Bromwich (2008) used MM5 and WRF models and GD microphysics for polar weather research as the same physics model. No. 4: Morrison and Milbrandt (2011) examined precipitation, storm, and cold pool strength activities between Morrison and Milbrandt-Yau microphysics using the WRF model. No. 5: Efstathiou et al. (2013) carried out large-scale simulations for heavy rainfall situations, especially by evaluating different microphysics options and using Eta Ferrier microphysics. No. 6: Mahala et al. (2015) and Eltahan and Magooda (2018) used WRF-single-moment-microphysics Class 3 (WSM3) for atmospheric events such as excessive rain and severe storm formation. No. 7: Patel et al. (2019) evaluated different physics options to predict floods in the coastal region and stated that Lin and Grell's physics options significantly reduced the bias rate. The physics schemes prepared for this study are presented in Table 3.

Due to the width of the study area and the density of the resulting data set, WRF outputs are in compressed files. Libraries developed from programming languages such as WRF-python help to extract data from these files. As another option, sub-models have been developed to make the necessary data for the models ready for use. Especially, models such as The Mesoscale Model Interface Program (MMIF) and CALPUF-WRF (CALWRF) are useful tools for air quality dispersion models to capture the meteorological data needed for AERMOD and CALPUFF and the data prepared in the WRF model. For this study, MMIF and CALWRF models were used and converted into a data set format that air quality dispersion models can understand. In addition, CALMET has been used to re-run the CALWRF outputs. CALMET has optimized the discrepancies between the WRF and CALPUFF meteorological domain areas because they differ from one another in this study. The required bases for the simulation were WRF pre-processing system (WPS), version 4.3.1 and WRF-ARW, version 4.3.3.

Air quality dispersion models

While many different models have been used for many fields and purposes from past to present for air quality dispersion models, models have been developed with new methods and technological developments (Hanna et al. 2001; Gulliver and Briggs 2011; Holnicki et al. 2016; Ruiz-Arias et al. 2016). While these predictions were prepared with manual calculations and limited data sets in the past, with technological developments today, it has become possible to obtain meteorological data from satellites and results closest to reality with different methods and calculation methods.

Consequently, different air quality dispersion models have been developed depending on the needs of different institutions, organizations, and researchers. Examples of these models include AERMOD and CALPUFF. Both models are used by many researchers and validated by organizations (US EPA 2000; FLAG 2010; De Melo et al. 2012; Tartakovsky et al. 2013; US EPA 2019). Although both types fundamentally perform the same job, they have variances based on the region of application and method of function.

AERMOD model is generally used for distances between 0–50 km whereas the CALPUFF model is mainly used to represent lengths of 50 km or greater. The EPA does not recommend < 50 km as near-field applications for the CALPUFF model (Harnett et al. 2008; Jitra et al. 2015). On the other hand, the CALPUFF model has also been used in near-field applications for long-term dispersion models where complicated flows caused by complex terrain and land use variations are considered significant with emphasis on model performance, validation, and exposure levels (MacIntosh et al. 2010; Cui et al. 2011; Dresser and Huizer 2011; Ghannam and El-Fadel 2013). When the near-field applications using the CALPUF models were examined, there were variances in the study distances utilised for the models; they were used to estimate emission distributions for research regions under 50 km in many studies (Scire et al. 2000; Abdul-Wahab et al. 2011; Tartakovsky et al. 2013; Gulia et al. 2015; Afzali et al. 2017; Demirarslan et al. 2017; Rzeszutek et al. 2023; Zeydan and Karademir 2023). On examination of these studies, Emert et al. (2024) analysed the air quality distributions of PM₁₀ and PM_{2.5} pollution from beef cattle feedlots using the CALPUFF model, which included the hot months and indicated that modelled pollutants exceeded the safe limit values for humans. Eslamidoost et al. (2023) investigated a gas refinery in Iran, which has a capacity of approximately seven hundred twenty billion cubic metres of gas, using the AERMOD model and concluded that there was no exceedance of the EPA limit value. In the same region, Rashidifard et al. (2018) simulated CO emissions using AERMOD and CALPUFF models from a steel industry in Iran and found that AERMOD had better results than the CALPUFF model. In another research, Gulia et al. (2015) emphasised that AERMOD, which used a plume dispersion model, was less successful in calm weather conditions compared to CALPUFF.

AERMOD (AMS/EPA Regulatory Model), a prediction model that uses the algorithm based on the plume model dispersion and the Gaussian dispersion, is a model developed by the American Meteorology Society (AMS) and the United States Environmental Protection Agency (US EPA). It also has a sub-model that prepares data for AERMOD. The model, with its 2 sub-models AERMAP and AERMET, makes the terrain and meteorological data set ready for the AERMOD, and finally, the model is run after the processing

of specific inputs such as building evaluation, study area, grid distances, and pollutant features through AERMOD (US EPA 2019). The CALPUFF (California Puff Model) model, developed together with the California Air Resource Board and Sigma Research Corporation, uses the Lagrangian Puff dispersion model method. The model contains multiple sub-models within itself. The fundamental models consist of TERREL, CTGPROC, MAKEGEO, and CALMET. Sub-models prepare the parts where the geographical land data set, vegetation, and meteorological data are processed for the CALPUFF model. The CALPUFF model is also an EPA-recommended model (US EPA 2000).

Risk analysis model

Hotspots Analysis and Reporting Program (HARP), developed by the California Air Resource Board and Office of Environmental Health Hazard Assessment (OEHHA), is a program that can perform toxicity analysis depending on air quality and emission characteristics (OEHHA 2009; OEHHA 2015). The HARP model is a model originally developed to control air quality and take precautions against possible risks of emissions released into the air from facilities. In addition, the HARP model was used to analyse health risk assessment using air quality models (Environ Australia 2008; Donoghue and Coffey 2014). The model calculates possible risk scenarios using AERMOD outputs and toxic pollutants. In addition, the model includes different scenario options such as respiration, soil, skin, breast milk, drinking water, fish, and small and large livestock farming. The model consists of Emission inventory, Air Dispersion Modeling, and Risk assessment tools. The model can produce the required outputs with its own AERMOD module, and the dispersion results produced by AERMOD can also be separately incorporated into the HARP model. Since the model outputs are in the plot file (PLT) data type produced by the AERMOD model, it is possible to prepare and use different data sets or different air quality dispersion models in this format. After the study area inputs are processed for risk analysis by the model, pollutant emissions that pose a health risk are input. After processing the operating characteristics, air quality dispersion results, and toxic characteristics of the pollutant required by the model, the exposure level (25, 35, 70 years (lifetime), etc.), analysis type (cancer, acute and chronic risk), and risk type are selected.

In this model, HARP uses several fundamental inputs to the working principle of the model, and the first necessary data is the air quality dispersion model in PLT format. In addition, background emission inputs may be combined with air quality inputs in the model. The model needs input emissions inventory (a "HARP database" for the emission risk ratio) and health risk assessment factors. Pollutant sources need their parameters (stack height and internal diameter,

gas exit velocity, and UTM coordinates). Pollutant source features are also incorporated into the model (stack height and inside diameter, gas exit velocity, and coordinates). In regard to the working time of the facility, it is important to examine the health risks related to the exposed time period. Finally, the model risk scenario is chosen to examine health concerns. As a consequence, the model creates the analysis-type situations specified by the user. The computation of the model configuration differs according to the specified research scenario. Model scenarios and calculation methods are included in the guidebook, and the equation is presented below (OEHHA 2015). Daily inhalation dose ($Dose_{air}$) and residential inhalation cancer risk ($RISK_{inh_res}$) were used to calculate the inhalation-risk scenario. The other equalities are formulas, concentration in air (C_{air}), daily breathing rate normalised to body weight (BR/BW), inhalation absorption factor (A), exposure frequency (EF), inhalation cancer potency factor (CPF), age sensitivity factor for a specified age group (ASF), exposure duration (ED), averaging time for lifetime cancer risk (AT), and fraction of time spent at home (FAH) (OEHHA 2015).

$$Dose_{air} = C_{air} * \left\{ \frac{BR}{BW} \right\} * A * EF * 10^{-6} \quad (1)$$

$$RISK_{inh-res} = Dose_{air} * CPF * ASF * \frac{ED}{AT} * FAH \quad (2)$$

This study used calculation methods for the inhalation-risk scenario, but ASF , FAH , and BR/BW inputs were missing. Therefore, these inputs were utilised as the default data of the HARP model. The latest available version of the model is HARP 2, and the most current version was used for this study.

Model methodology

This study made use of meteorological models (WRF, AERMET, and CALMET), air quality dispersion models (AERMOD and CALPUFF), health risk analysis model (HARP), and various sub-models required for these models (MMIF and CALWRF). Meteorological, topographic, vegetation, and emission inputs were used as data input. The meteorological data set was provided in two different ways, i.e., satellite and local station. The majority of meteorological data sets from satellites were obtained through "NCEP GDAS/FNL 0.25 Degree Global Tropospheric Analyses and Forecast Grids". However, since SST data is not included in GDAS data, it was obtained through ERA. Both data sets available through ERA and NCEP were compatible with the WRF model and no preliminary correction was required. Due to the missing data in the local meteorological station data set, the deficiencies were eliminated by using the

meteorological data of the last 5 years from surface stations that belong to 2017-2021. The completed data sets were made compatible with the air quality dispersion model with sub-models, the sub-units of the models. The Shuttle Radar Topography Mission (SRTM3) 90 m data was used for topography data in both models. Due to the differences between the models, the vegetation was processed manually in AERMOD and this dataset was used as a raster 100 m via CORINE for CALPUFF. CALPUFF is different from AERMOD in that it includes a chemical transformation process. CALPUFF can simulate secondary fine particles formed by chemical reactions in atmospheric transports (Scire et al. 2000; Zhou et al. 2003). In this study, the utilization of secondary emission input was not incorporated into the CALPUFF model. Using the satellite and local meteorological data and AERMET, CALMET, and WRF models together with the air quality dispersion models of AERMOD and CALPUFF, we prepared eight different dispersion models, that is, the eight meteorological inputs (7 WRF + 1 Local) used by each model.

While the main emission sources released as a result of the operation of the facility were the pollutants of PM₁₀, NO_x, and CO, heavy metal emissions took place as well. The models consist of line, area, and point source as source types. Air quality dispersion models were prepared on an hourly, daily, and annual basis for the entire year 2021. Model-specific input of air quality models was arranged as a Cartesian grid within an area of 15 x 15 km in 500 m grids. The model was run after the arrangement of the data for the AERMOD and CALPUFF models. Correlation analysis was carried out between the forecast data produced as a result

of the simulation and the data obtained from the measurement stations at A and B-AQMS locations in Fig. 1. In the data from the stations, PM₁₀, NO_x, and CO pollutants were measured with A-AQMS, while PM₁₀ and NO_x were measured with B-AQMS. As a result, the relationship between air quality models along with meteorological models and physics models was examined.

In the last stage, the HARP model was used to analyze the health risks of the model outputs. PLT pollutant data, which are CALPUFF and AERMOD model outputs, and heavy metal data released from the facility were added to the model as source output in Table 1. Then, within the HARP model, a risk assessment was made at a total of 962 recipient points, including possible cancer through the respiratory tract, acute and chronic risks, 70-year (lifetime) exposure, 95th risk effect, and sensitive points such as Balikesir Central Hospital. The general flow scheme of the model is presented in Fig. 3.

Data analysis results

Model-observation comparison

The model simulation content prepared for this study was prepared to cover the entire year. Since the WRF model domain used to provide meteorological data does not allow the computer hardware to operate over a long period, the one-year study period was divided into three parts, creating 4-month intervals. Sixteen different results were obtained in this period, with model outputs being created with eight

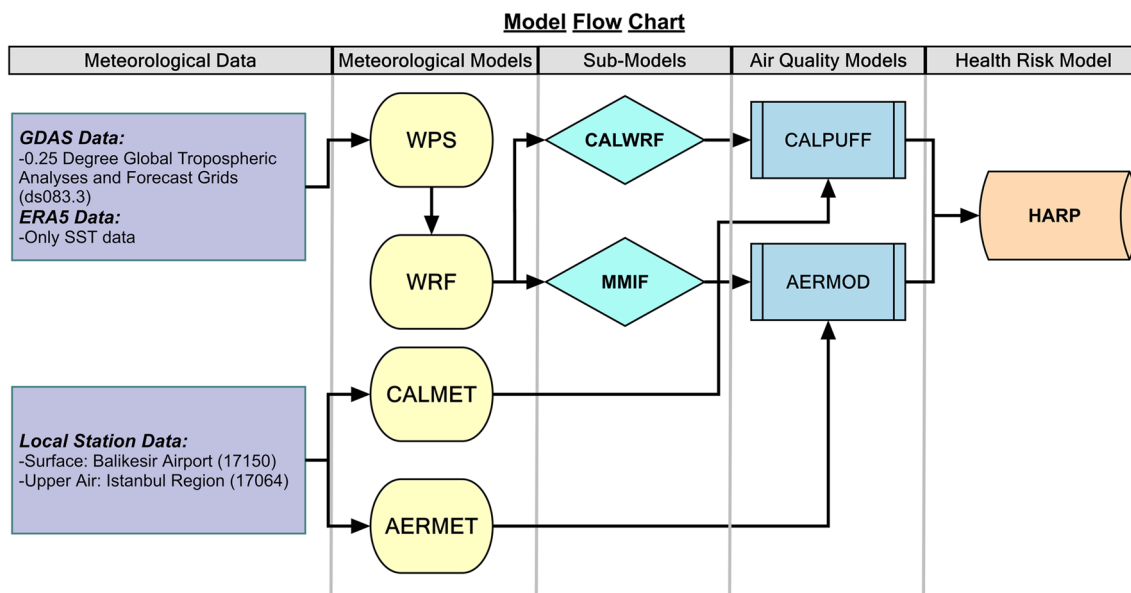


Fig. 3 Model flow chart

different meteorological inputs, i.e., hourly, daily, and annual, and two different air quality dispersion models. Within the scope of the aims of the study, the pollution levels were determined and the results between the models and the physics options were compared. There are two stations in Balikesir city center: Central Station and Bahçelievler Station. Among these stations, PM₁₀, NO_x, and CO pollutants were measured at Central Station, while PM₁₀ and NO_x pollutants were measured at Bahçelievler Station. The characteristics of the sixteen model simulations are presented in Table 4.

On examination of the pollutant source and AQMS locations used in this study, these were observed to be located in the north and northwest of the source. In this study, Spearman correlation analysis was used because the model outputs did not exhibit normal distribution (Bishara and Hittner 2012) and was also used in many studies from CALPUFF and AERMOD (Zou et al. 2011; Ghannam and El-Fadel 2013; Hoinaski et al. 2017; Bezyk et al. 2021; Eslamidoost et al. 2022). Therefore, the location of the facility in the upwind region may cause differences between the modelled and measured station data. On examination of the correlation analysis between model results and AQMS, daily measurements at both stations exhibited higher significance than hourly measurements. The highest correlation values among pollutants were observed in the daily period. The highest correlation value among concentration was seen in NO_x concentrations, followed by PM₁₀ and CO, respectively. In A-AQMS, the highest correlation of daily concentrations of NO_x were measured at 0.72, while in B-AQMS, they were slightly lower at 0.62. For hourly predictions, the highest correlation of NO_x concentrations were 0.44 in A-AQMS and 0.39 in B-AQMS. Likewise, highest correlation of daily predicted PM₁₀ levels were 0.70 in A-AQMS and 0.41 in B-AQMS, with corresponding hourly predictions of 0.43 in A-AQMS and 0.30 in B-AQMS. Maximum correlation of daily predicted CO concentrations were 0.60 in A-AQMS and 0.43 in B-AQMS. Upon evaluation, it was noted that among the WRF physics options, models No. 3 (GD) and No. 4 (MY) for daily predictions, along with model No. 5

(ETA) for hourly predictions, exhibited stronger correlation values. Conversely, models utilizing local meteorological data demonstrated lower correlation values. When the models were compared, although CALPUFF achieved better results than AERMOD, the AERMOD model also produced good results. In the correlation results, the AERMOD-NO_x correlation of Bahçelievler AQMS was observed as the negative correlation of meteorological inputs. In this situation, it is anticipated that several possibilities, such as calm conditions, low wind speed, different models, chemical reactions, emission sources, and the specific factor of AQMS, may be offered as examples. Hourly and daily correlation results are presented in Fig. 4 and Fig. 5.

Chang (2003), Chang and Hanna (2004), and Hanna and Chang (2012) extensively examined the calculation procedure of model validation parameters in the performance analysis. The validation parameters, such as fractional bias (FB), assess systematic biases between observed and predicted values. A positive FB suggests an under-prediction, while a negative FB signifies an over-prediction by the model (Chang 2003; Chang and Hanna 2004; Hanna and Chang 2012). The normalized mean square error (NMSE) is the total error of the standardized values between the measured and modeled data. The factor of two (FAC2) represents the accuracy of estimating parameters within a range of two times the observed value (Hanna and Chang 2012; Irwin 2014). The normalized absolute difference (NAD) is a metric that quantifies the fractional area for mistakes according to Hanna and Chang (2012). Additionally, a "good model" must satisfy at least one component within their acceptance intervals. Thus, the acceptance intervals for these control parameters are shown in Table 5. The data utilized for validation were acquired after eliminating irrelevant and missing data to compute validation parameters such as FB, NMSE, FAC2, and NAD. In the model performance of Tables 5 and 6, accepted parameters are indicated in bold type.

In this study, air quality distribution models were created using the AERMOD and CALPUFF algorithms, incorporating hourly and daily measurements of PM₁₀ and NO_x from the Bahçelievler AQMS, as well as CO, PM₁₀, and NO_x

Table 4 Model properties

Meteorological data	Meteorological models	Ensemble no	Air quality models	
			AERMOD	CALPUFF
GDAS/ERA5	WRF	1-CONUS	✓	✓
		2-NCAR	✓	✓
		3-GD	✓	✓
		4-MY	✓	✓
		5-Eta Ferier	✓	✓
		6-WSM3	✓	✓
		7-LIN	✓	✓
Local	AERMET/CALMET	8-Surface/Upper air	✓	✓

Fig. 4 Central AQMS correlation results

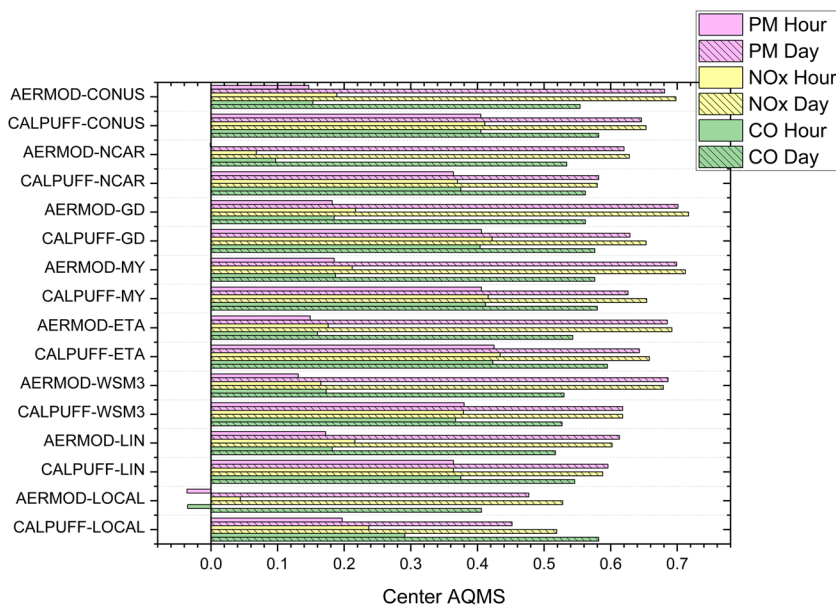
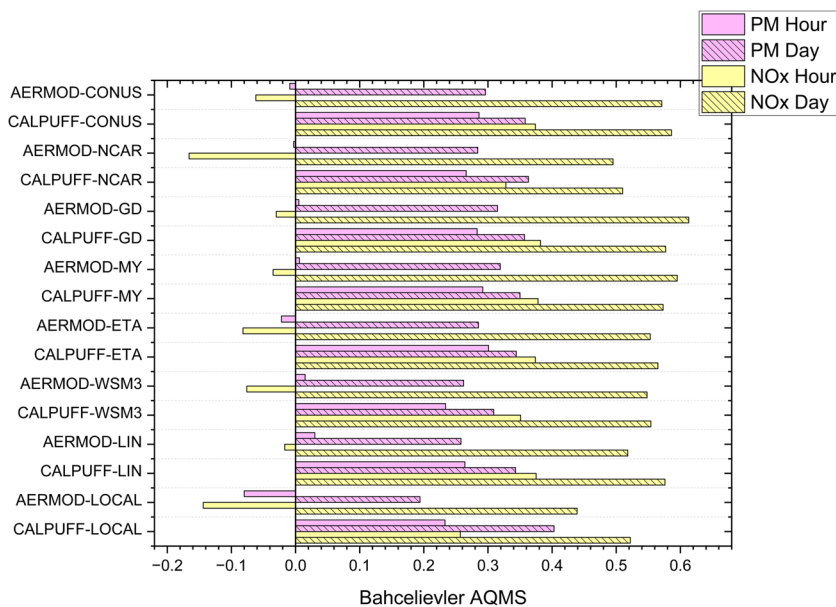


Fig. 5 Bahcelievler AQMS correlation results



pollutants measured with the Central AQMS, along with previously selected physical parameters and meteorological data. The normalized measured and modeled results were statistically analyzed to evaluate model performances. The analysis results of model performances are presented in Table 5 and Table 6 for both AQMSs.

According to the model validation results, less favorable values were observed for the FB validation parameter. On the other hand, FAC2, defined as a robust validation parameter by Chang (2003) because it is not affected by the minimum and maximum values in the datasets, is shown to be compatible with both AERMOD and

CALPUFF. It has been determined that the AERMOD and CALPUFF models are more compatible with validation parameters in daily time intervals in pollutant distributions. It was found that the CO pollutant did not show intensive compatibility in modeling results like other pollutants. Further studies are required to address this issue. According to the model validation analysis results, it was determined that local meteorological data showed the least compatibility with the distribution models. It was concluded that the majority of the selected physical parameters are compatible with both AERMOD and CALPUFF.

Table 5 AERMOD and CALPUFF modeling performances on the selected physical parameters (Central AQMS)

Validation parameters	Pollutants	Periods	AERMOD/Physical parameters										CALPUFF/Physical parameters									
			CONUS	NCAR	GD	MY	ETA	WSM3	LIN	LOCAL	CONUS	NCAR	GD	MY	ETA	WSM3	LIN	LOCAL				
[FB ≤ 0.67]	FB	PM ₁₀	1.8	1.7	1.8	1.82	1.8	1.82	1.84	1.87	1.1	1.6	1.6	1.1	1.1	1.57	1.3	1.58				
		Day	0.8	1	0.84	1.2	1.05	1	1.2	1	1.2	0.51	1.2	0.85	0.5	0.24	0.5	0.83				
	NOx	Hour	0.98	0.64	0.83	-0.16	0.97	0.33	0.2	1.13	0.8	0.55	0.8	0.3	0.73	0.7	1	0.8				
		Day	0.93	1.04	0.83	0.81	1.16	0.9	0.5	0.88	1.56	1.6	1.6	1.57	0.93	0.61	0.87	1.06				
[NMSE ≤ 6]	CO	Hour	1.15	1.55	1.5	1.45	1.18	1.47	1.3	1.8	1.01	0.82	0.97	0.96	1.13	0.84	1.1	1.24				
		Day	1.14	1.3	1.05	1	1.18	1.12	0.76	1.1	7.2	17.5	18.2	7.3	6.9	16	9.3	17.5				
	NMSE PM ₁₀	Hour	38.1	26.4	37.8	44.5	38.5	43.3	48.7	67.7	1.7	4.3	2.8	1.8	1.47	1.9	2.03	3.7				
		Day	3.6	4.1	3.9	5.5	4.7	4.6	4.4	6.8	13.3	15.1	14.6	13.8	13.9	16.2	17.8	22.1				
[FAC2 ≥ 0.3]	NOx	Hour	7.7	15.5	14.4	14.2	14.8	13.3	11.8	23.5	2.5	2.2	2.45	2.3	3.1	2.2	3.2	5.4				
		Day	3.9	4.01	3.4	3.3	4.2	3.5	2.51	3.8	13.8	17.5	15.9	14.2	14.9	15	20.6	20				
	CO	Hour	7.3	13.9	11.6	10.6	7.2	11.2	8.4	37.6	2.7	2	2.5	2.5	3.4	2.1	3.3	5.7				
		Day	4	4.5	3.4	3.2	4.3	3.6	2.1	3.9	0.3	0.1	0.1	0.3	0.3	0.12	0.2	0.12				
[NAD ≤ 0.5]	PM ₁₀	Hour	0.05	0.08	0.06	0.05	0.05	0.05	0.04	0.03	0.6	0.3	0.4	0.6	0.79	0.6	0.5	0.4				
		Day	0.4	0.32	0.4	0.24	0.31	0.3	0.33	0.27	0.6	0.6	0.4	0.6	0.46	0.47	0.3	0.43				
	NOx	Hour	0.3	0.5	1.2	1.2	1.1	0.7	0.9	0.3	0.6	0.6	0.4	0.74	0.46	0.53	0.39	0.31				
		Day	0.36	0.32	0.42	0.42	0.35	0.38	0.6	0.39	0.12	0.1	0.11	0.12	0.11	0.12	0.1	0.09				
[FAC2 ≤ 0.5]	CO	Hour	0.27	0.13	0.14	0.16	0.27	0.15	0.21	0.05	0.33	0.42	0.35	0.35	0.28	0.41	0.3	0.24				
		Day	0.27	0.23	0.31	0.32	0.26	0.28	0.45	0.3	0.54	0.8	0.8	0.55	0.55	0.78	0.7	0.79				
	NMSE PM ₁₀	Hour	0.9	0.85	0.9	0.91	0.9	0.9	0.92	0.94	0.8	0.8	0.8	0.8	0.8	0.8	0.8	0.8				
		Day	0.4	0.5	0.4	0.6	0.5	0.5	0.5	0.6	0.25	0.57	0.41	0.3	0.12	0.25	0.3	0.41				
[NAD ≤ 0.5]	NOx	Hour	0.49	0.3	-0.07	-0.08	-0.06	0.16	0.07	0.56	0.22	0.3	0.4	0.15	0.37	0.36	0.5	0.43				
		Day	0.47	0.52	0.41	0.4	0.48	0.45	0.25	0.44	0.4	0.3	0.38	0.37	0.47	0.3	0.44	0.53				
	CO	Hour	0.57	0.77	0.75	0.73	0.58	0.74	0.65	0.9	0.8	0.82	0.81	0.78	0.79	0.79	0.84	0.83				
		Day	0.57	0.62	0.53	0.52	0.59	0.56	0.38	0.54	0.51	0.41	0.48	0.48	0.56	0.42	0.54	0.62				

FB, fractional bias, NMSE, normalized mean square error, FAC2, fraction of predictions within a factor of two of observations, NAD, normalized absolute difference

Table 6 AERMOD and CALPUFF modeling performances on the selected physical parameters (Bahcelievler AQMS)

Validation parameters	Pollutants	Periods	AERMOD/Physical parameters										CALPUFF/Physical parameters									
			CONUS	NCAR	GD	MY	ETA	WSM3	LIN	LOCAL	CONUS	NCAR	GD	MY	ETA	WSM3	LIN	LOCAL				
[FB ≤ 0.67]	PM ₁₀	Hour	1.82	1.76	1.8	1.81	1.85	1.81	1.86	1.82	1.29	1.23	1.59	1.27	1.48	1.39	1.22	1.31				
		Day	1.13	1.25	0.7	0.84	0.98	0.87	0.88	0.7	0.18	0.58	0.47	0.4	0.54	0.14	1.04	1.26				
[NMSE ≤ 6]	NOx	Hour	0.92	1.43	0.82	0.83	1.15	1.36	1.05	1.54	1.42	1.29	1.42	1.27	1.45	1.38	1.49	1.69				
		Day	0.39	0.46	0.44	0.53	0.55	0.68	0.19	0.39	0.19	0.1	0.22	0.21	0.57	0.18	0.36	1.03				
[FAC2 ≥ 0.3]	PM ₁₀	Hour	36.76	26.9	32.9	35.2	42.4	33.2	45.3	40.3	7.65	7.7	13.5	7.6	10.6	9.02	6.8	9.3				
		Day	5.5	6.4	4.6	4.6	5.2	4.5	4.4	4.5	2.08	2.6	2.43	2.4	2.62	2.24	3.7	6.7				
[NAD ≤ 0.5]	NOx	Hour	10.7	18.1	10	10.1	12.3	15.8	10	24.5	16.3	13.4	16.4	12.6	17.7	15	18.3	34.5				
		Day	3.85	3.5	3.45	3.7	3.8	4.2	2.9	3.4	2.4	2.5	2.4	2.3	2.9	2.2	1.9	5.4				
[FAC2 ≥ 0.3]	PM ₁₀	Hour	0.05	0.06	0.05	0.05	0.04	0.05	0.04	0.05	0.21	0.24	0.12	0.22	0.15	0.18	0.24	0.21				
		Day	0.28	0.23	0.48	0.41	0.34	0.39	0.39	0.48	0.84	0.55	0.62	0.67	0.57	0.87	0.32	0.23				
[NAD ≤ 0.5]	NOx	Hour	0.37	0.17	0.42	0.42	0.27	0.19	0.31	0.13	0.17	0.22	0.17	0.22	0.16	0.18	0.15	0.08				
		Day	0.67	0.63	0.64	0.6	0.57	0.5	0.82	0.67	0.83	0.9	0.8	0.81	0.6	0.84	0.7	0.32				
[NAD ≤ 0.5]	PM ₁₀	Hour	0.91	0.88	0.9	0.91	0.92	0.9	0.93	0.91	0.65	0.62	0.79	0.64	0.74	0.7	0.61	0.65				
		Day	0.57	0.63	0.35	0.42	0.49	0.44	0.44	0.35	0.09	0.29	0.24	0.2	0.27	0.07	0.52	0.63				
[NAD ≤ 0.5]	NOx	Hour	0.46	0.72	0.41	0.41	0.57	0.68	0.52	0.77	0.7	0.64	0.7	0.63	0.73	0.69	0.74	0.85				
		Day	0.2	0.23	0.22	0.3	0.28	0.34	0.1	0.2	0.09	0.05	0.11	0.11	0.28	0.1	0.2	0.5				

FB, fractional bias, NMSE, normalized mean square error, FAC2, fraction of predictions within a factor of two of observations, NAD, normalized absolute difference

Inter-model comparison

On examination of the model outputs, despite observing differences in the prediction results produced by each model, the concentration difference between daily models was greater compared to annual models. While AERMOD reached the highest concentration values in daily results, CALPUFF exhibited higher concentration in annual results. Among the models, the peak concentrations of the AERMOD model were obtained with the No. 2 and No. 6 physics models, while the lowest concentration results were obtained with the No. 7 model. On examination of the CALPUFF model, a specific peak physics model was not observed for each emission. On evaluation of the annual model results of both models, the difference between them was seen to have narrowed and produced close results. The days when the models reached peak concentration were mostly during the winter season. The results of the models are presented in Tables 7, 8, and 9.

In this study, the legend features and value ranges of daily maximum and annual average dispersion maps were prepared by determining a range for each pollutant. Dispersion models of concentration recipient points were created using SURFER, a surface, a 3D map and a contouring program. Map images were prepared according to the highest pollutant concentration received by the receiving point within the specified period. On examination of the dispersion results of the models, the dispersion of pollutants in the daily model was not distributed in a certain region but had high concentrations in the central region of the pollutant source. On examination of the annual model dispersions, a more pronounced dispersion was observed than the daily model results. In particular, the dispersion of annual model pollutants was observed to be distributed towards the southern location of the source. It is thought that the major cause for this is that the dominant wind direction of the Balikesir region is the northern winds (Mutlu 2020; Mutlu and Bayraktar 2021; Bayraktar 2022; Güğül et al. 2023). When we look at the dispersion between different pollutants, the dispersion direction of NOx and CO pollutants was observed to be towards the south of the source, while the daily and annual dispersions of PM₁₀ pollutants were more dominantly distributed in the center of the source. It is thought that the main reason for this is that the emission sources, which are the transport linear source and the area sources, are 10 m and < 10 m below the emission height, respectively. There are different emission sources from PM₁₀ than the NOx and CO pollutants, such as NOx and CO, which do not have any area or linear type sources. Therefore, different dispersions compared to pollutants can be emphasised in the model distributions. The distributions between the models were analysed, and the daily concentrations of the AERMOD model were higher than the CALPUFF model. Daily distribution

Table 7 Results of simulation models for PM₁₀ pollutant

PM ₁₀	Time	Model	Statistics	Meteorological parameters							
				No 1	No 2	No 3	No 4	No 5	No 6	No 7	Local
Daily	AERMOD (µg/m ³)	Maximum	96.132	177.347	70.153	95.575	87.832	111.644	54.764	73.560	
		Median	2.984	4.901	2.902	2.957	2.746	4.191	2.871	3.885	
		Minimum	0.081	0.094	0.068	0.087	0.096	0.116	0.082	0.043	
Annual	CALPUFF (µg/m ³)	Peak date	06.01.2021	13.04.2021	02.01.2021	02.01.2021	03.04.2021	04.01.2021	02.01.2021	16.09.2021	
		Maximum	74.544	57.576	72.392	78.066	110.2	71.062	76.703	60.364	
		Median	0.634	0.664	0.621	0.618	0.597	0.636	0.612	1.062	
Annual	AERMOD (µg/m ³)	Minimum	0.066	0.043	0.065	0.079	0.051	0.062	0.073	0.208	
		Peak date	08.11.2021	14.11.2021	14.11.2021	20.02.2021	21.12.2021	19.09.2021	23.10.2021	24.09.2021	
		Maximum	8.789	10.986	8.945	8.847	9.008	7.476	8.405	11.484	
Annual	CALPUFF (µg/m ³)	Median	0.129	0.195	0.126	0.123	0.123	0.164	0.104	0.148	
		Minimum	0.004	0.004	0.004	0.005	0.005	0.004	0.004	0.003	
		Maximum	9.127	8.630	9.875	9.376	9.704	8.227	8.248	17.449	
Annual	CALPUFF (µg/m ³)	Median	0.050	0.036	0.043	0.048	0.046	0.038	0.045	0.105	
		Minimum	0.004	0.002	0.003	0.002	0.002	0.002	0.003	0.021	

Table 8 Results of simulation models for NO_x pollutant

Time	Model	Statistics	Meteorological parameters							
			No 1	No 2	No 3	No 4	No 5	No 6	No 7	Local
NO _x Daily	AERMOD ($\mu\text{g}/\text{m}^3$)	Maximum	282.493	369.497	159.912	210.052	242.644	301.776	52.265	103.430
		Median	3.792	3.711	3.757	3.645	3.717	4.084	4.017	2.255
		Minimum	0.375	0.613	0.398	0.500	0.453	0.579	0.523	0.332
		Peak date	02.01.2021	07.02.2021	01.01.2021	03.02.2021	21.05.2021	18.04.2021	01.08.2021	18.09.2021
	CALPUFF ($\mu\text{g}/\text{m}^3$)	Maximum	72.462	103.460	67.041	62.738	67.895	66.295	95.127	166.410
		Median	6.326	6.020	5.025	5.011	5.838	5.886	6.300	7.897
		Minimum	1.437	0.953	0.962	1.202	1.155	1.440	1.049	1.972
		Peak date	05.05.2021	13.12.2021	28.01.2021	18.10.2021	25.04.2021	25.11.2021	05.02.2021	07.05.2021
Annual	AERMOD ($\mu\text{g}/\text{m}^3$)	Maximum	7.913	12.391	7.977	8.266	8.279	8.312	8.577	9.219
		Median	0.222	0.200	0.214	0.209	0.211	0.198	0.231	0.166
		Minimum	0.044	0.039	0.042	0.043	0.046	0.039	0.030	0.033
	CALPUFF ($\mu\text{g}/\text{m}^3$)	Maximum	19.772	14.636	17.309	19.561	19.445	19.558	21.380	11.457
		Median	0.283	0.262	0.253	0.258	0.263	0.251	0.274	0.398
		Minimum	0.051	0.025	0.033	0.033	0.038	0.032	0.049	0.114

Table 9 Results of simulation models for CO pollutant

Time	Model	Statistics	Meteorological parameters							
			No 1	No 2	No 3	No 4	No 5	No 6	No 7	Local
CO Daily	AERMOD ($\mu\text{g}/\text{m}^3$)	Maximum	145.268	190.016	82.235	108.018	124.781	155.187	26.878	53.173
		Median	1.945	1.899	1.923	1.867	1.903	2.092	2.056	1.156
		Minimum	0.192	0.314	0.204	0.256	0.232	0.297	0.268	0.170
		Peak date	02.01.2021	07.02.21	01.01.2021	03.02.2021	21.05.2021	18.04.2021	01.08.2021	18.09.2021
	CALPUFF ($\mu\text{g}/\text{m}^3$)	Maximum	37.250	53.198	34.474	32.129	34.763	34.016	48.927	85.578
		Median	3.286	3.127	2.609	2.596	3.025	3.041	3.275	4.087
		Minimum	0.753	0.502	0.503	0.628	0.606	0.751	0.545	1.041
		Peak date	05.05.2021	13.12.2021	28.01.2021	18.10.2021	25.04.2021	25.11.2021	05.02.2021	07.05.2021
Annual	AERMOD ($\mu\text{g}/\text{m}^3$)	Maximum	4.047	6.371	4.079	4.227	4.257	4.252	4.389	4.714
		Median	0.113	0.103	0.110	0.107	0.108	0.101	0.119	0.085
		Minimum	0.022	0.020	0.022	0.022	0.024	0.020	0.015	0.017
	CALPUFF ($\mu\text{g}/\text{m}^3$)	Maximum	10.132	7.504	9.831	10.023	9.964	10.023	10.960	5.887
		Median	0.147	0.136	0.139	0.134	0.137	0.130	0.142	0.206
		Minimum	0.027	0.013	0.016	0.017	0.020	0.017	0.026	0.060

models have shown variations in distribution compared to annual models in the inter-model distributions. The annual model distribution of pollutants was mostly in southward regions because the prevailing wind direction is north. The daily maximum and annual average PM₁₀ dispersion maps are presented in Figs. 6 and 7.

In this study, especially the NO_x and CO daily model results of the AERMOD model, hot spots were observed in Fig. 8 and Fig. 10. The model outputs of these grids showing high concentrations were analysed, and the results showed that these grids had a high concentration some days. At the same time, the regions of hotspot distribution were also similar between the physics options. Surface and upper air, which are the meteorological inputs utilised in the AERMOD

model, were analysed recently, and low wind speeds were discovered. CALPUFF model provides better outcomes than the AERMOD model under calm conditions and wind speed because CALPUFF can utilise wind speed data on a more precise scale (Scire et al. 2000; Gulia et al. 2015; Mak et al. 2020). However, the puff model used in the CALPUFF model is more successful in estimating concentrations at low wind speeds than using the Gaussian dispersion model in AERMOD (Holmes and Morawska 2006; Qian and Venkatram 2011; Zeydan and Karademir 2023). Although it has been emphasised that the variations in topography utilised for the AERMOD and CALPUFF models may influence the distribution, in this work, SRTM3 data were used for AERMOD and CORINE data for CALPUFF (Demirarslan et al.

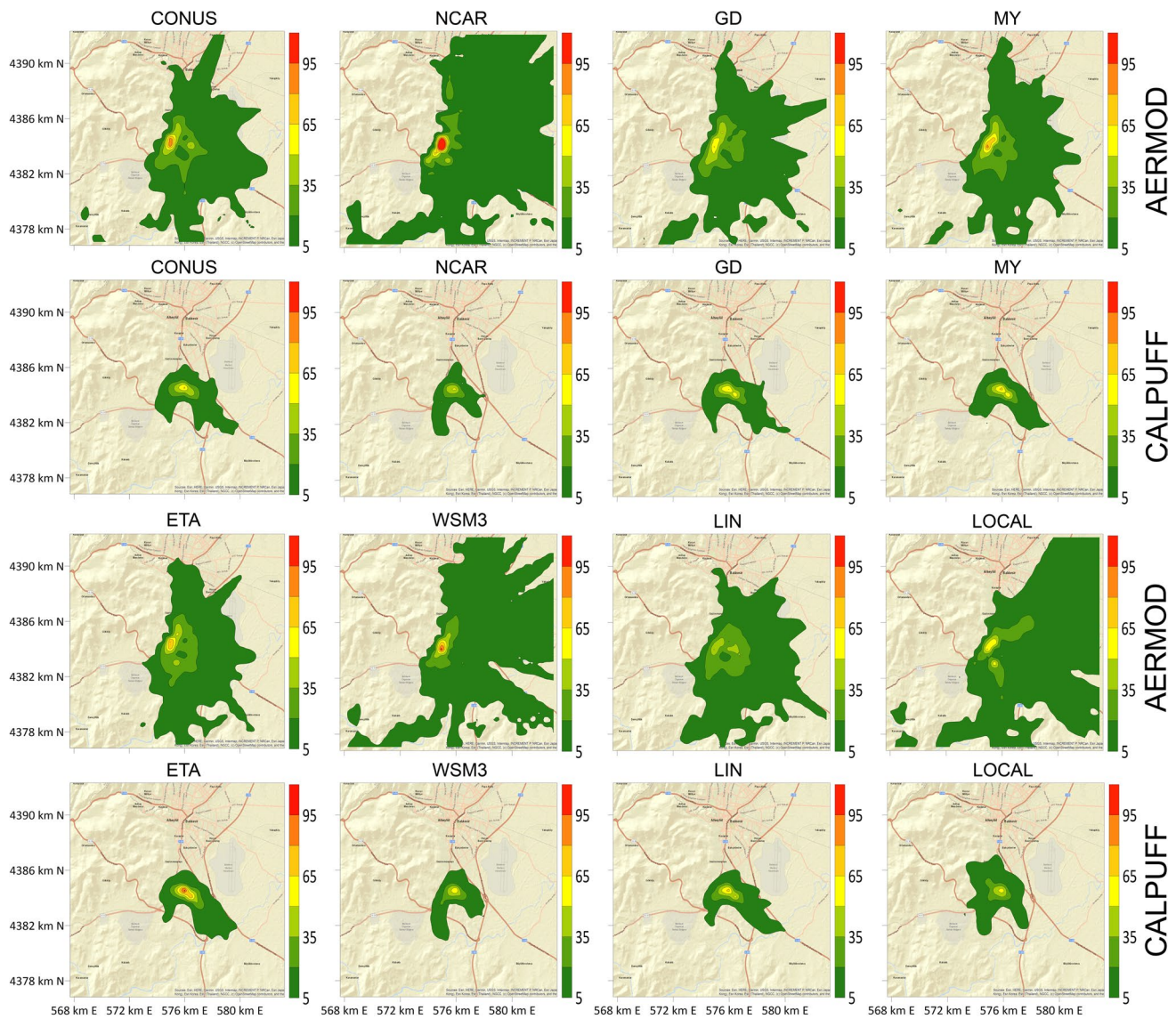


Fig. 6 Dispersion maps of daily maximum PM_{10} levels

2017). Based on the data, hotspot grids are expected to prove effective due to factors such as low wind speed, environmental variables, and model variations. NO_x and CO of the daily maximum and annual average dispersion maps are presented in Figs. 8, 9, 10, and 11.

The meteorological inputs were utilised with two different options. Satellite meteorological data GDAS and ERA are validated datasets used for large areas and many studies (Su et al. 2015; Haider et al. 2020; Gunwani et al. 2023). Moreover, these data sets have the advantages of being compatible with various meteorological simulation models, such as WRF and MM5. On the contrary, the distance of local stations to the study area and missing data cause uncertainties in the results. In this study, it is assumed that difficulties such as local station data being far

from the operation and missing data being replaced with previous-year data impact the model results. Another part is the effect of the physics used for WRF on the models. The physics models process many different meteorological data units, such as ds083.3 data, which has 35 different meteorological data sets. Air quality dispersion is affected by many variables, such as meteorology and topography, however, the primary causes of dispersion are generally (Verma and Desai 2008; Chen et al. 2015; Bozhkova et al. 2020). The WRF can estimate complicated weather phenomena such as rainfall, hurricanes, and climate change, which are difficult to anticipate. In summary, WRF physics options exhibited similar distribution and results, which may be read as the fact that the meteorological data outputs provided results close to each other.

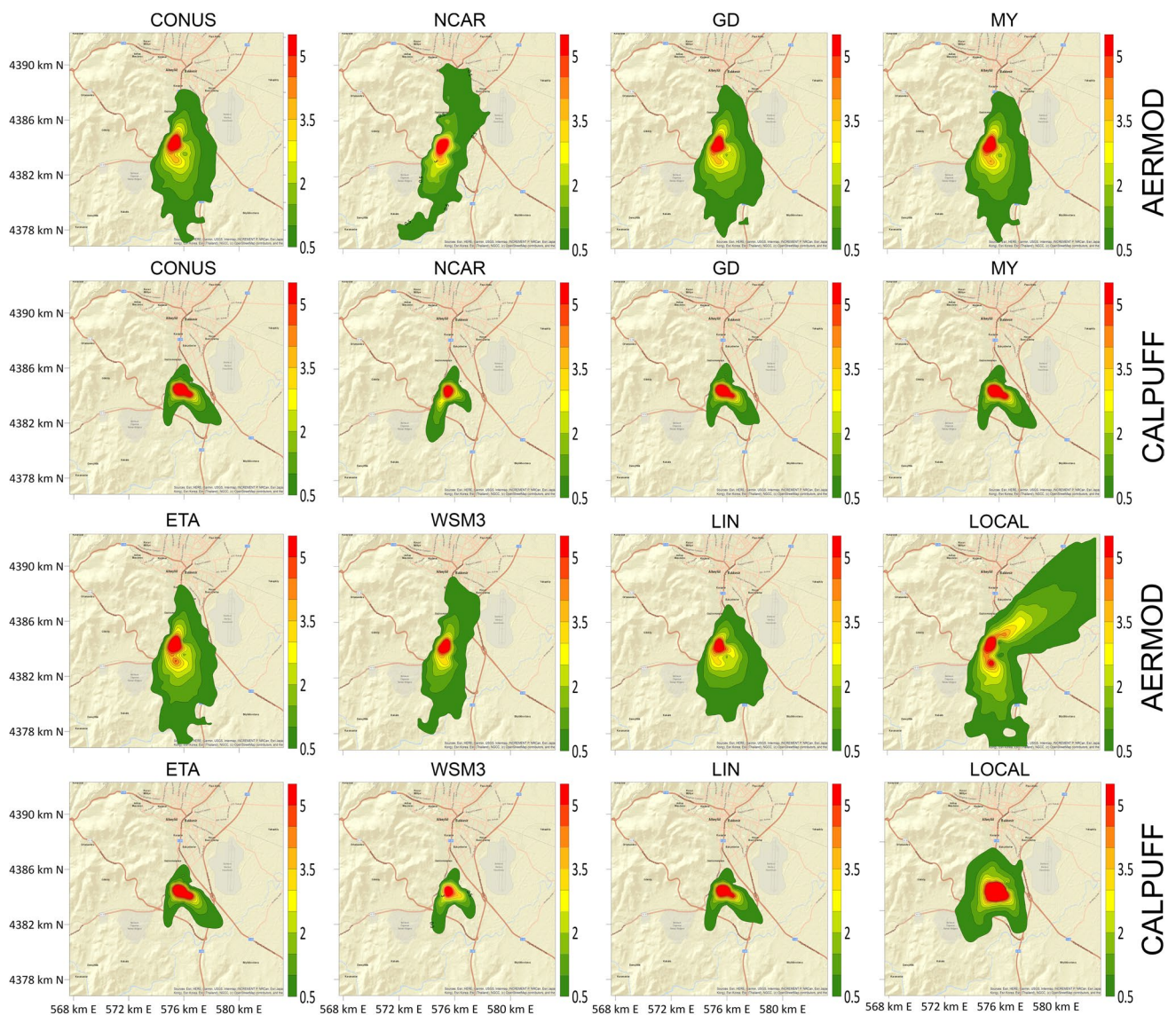


Fig. 7 Dispersion maps of annual average PM_{10} levels

Health risk

In this study, in addition to PM_{10} , NO_x , and CO emissions used for air quality dispersion models, along with heavy metal pollutants released from the source, there are 962 receiver points in total, including the receiver points created in 500 m squares in a total area of 15 x 15 km and Balikesir Central Hospital in Fig. 1. For health risk analysis, acute and chronic risk of respiratory cancer was estimated using only PM_{10} data outputs along with heavy metal data from four chimneys in Table 1. The health risk models were only used for exposure to cement factory and did not use background pollutants or other external sources. The model analysis was designed with the respiratory risk scenario defined as lifetime (70 years) by the EPA. The EPA has determined the

minimum expected risk for respiratory cancer as one person per million (1×10^{-6}) (US EPA 2009; OEHHA 2015).

In this study, while the limit risk specified by the EPA was exceeded at 49 receiver points in the total of all model results, the highest risk value was 3.08×10^{-6} people and the limit value was most frequently exceeded in the results estimated using the CALPUFF-LIN model. At the same time, the "NCAR" physics model showed that the maximum cancer risk ratio for AERMOD was 1.77×10^{-6} . It was stated that exceeding the noncarcinogen acute and chronic risk limit values determined by the EPA as 1 would pose a risk (US EPA 2009; OEHHA 2015). On examination of the model results, while there was no receiver point exceeding the limit value of acute risk, the maximum risk value of the receiver point was 0.211. The results with the highest

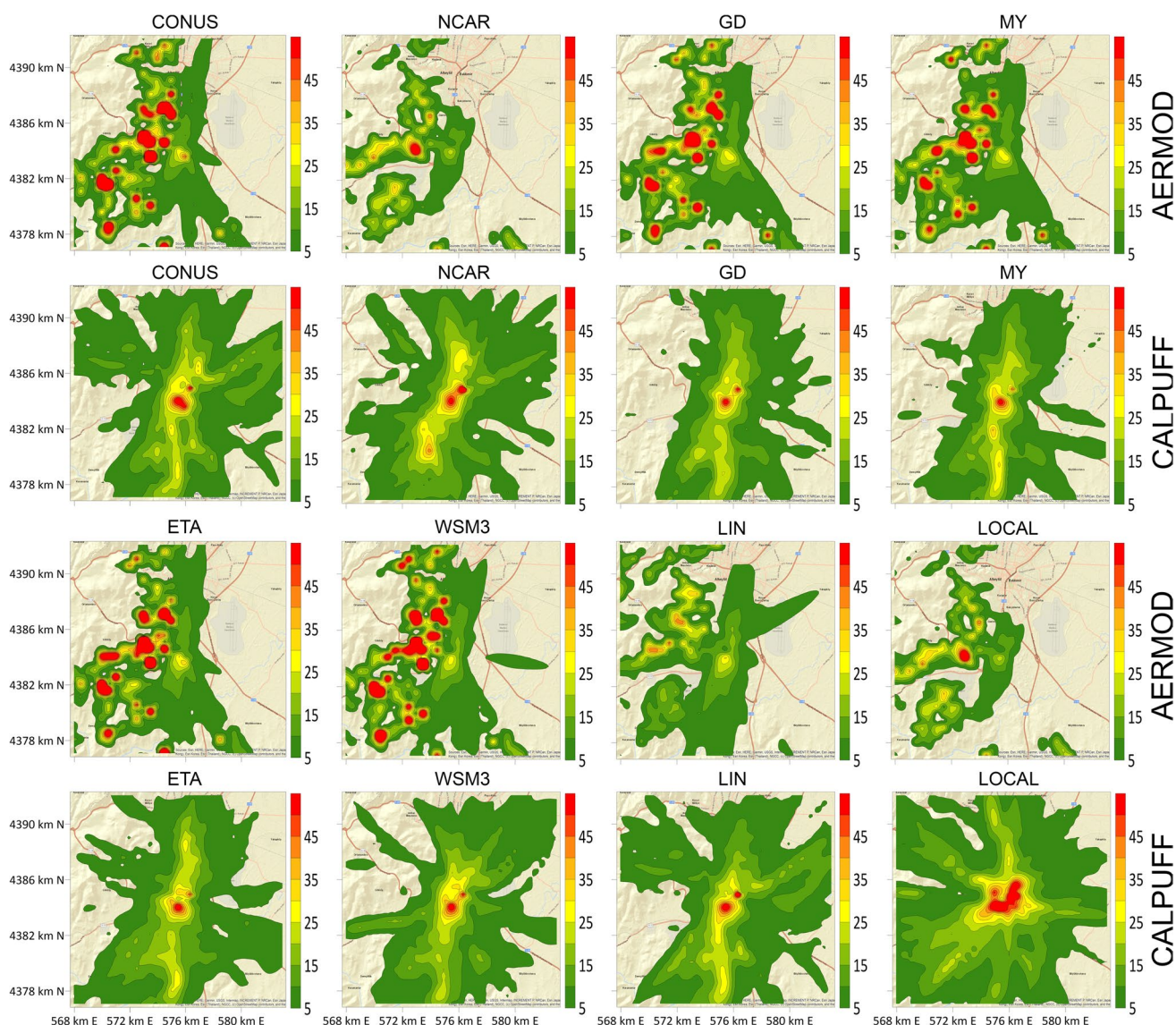


Fig. 8 Dispersion maps of daily maximum NO_x levels

acute risk were obtained with the AERMOD model. While the chronic risk limit values were observed to be exceeded at only 5 receiver points in the model results, the highest value of the receiver point was 1.22 with the CALPUFF-LIN model also, which was 500 meters to the south of the central point from the facility. AERMOD-LIN results also have a lower risk rate value of 0.51, which has the highest value in the same position for both models. On examination of the cancer, chronic, and acute risk results in Balikesir Central Hospital which is the closest sensitive point to the facility, only the cancer risk value exceedance was seen with a value of 1.84×10^{-6} in the CALPUFF-Local model using the local meteorological data set, while there was no limit exceedance in the acute and chronic risk model results shown on Fig. 12. The cancer value excess of the hospital is highly

near to the facility, and local meteorological data also has low wind speed and calm conditions. Therefore, the annual PM₁₀ concentration is substantially higher than the other model values.

On the evaluation of the point sources, which compared differences among each other, the highest risk rates were observed predominantly in Stack 1 sources, followed by those discovered in Stack 3, Stack 4, and Stack 2. The findings are believed to be linked to the input sources and influenced by the risk rates derived from the "HARP database" used in this model. When accounting for variations in physics, all dispersion models produce results that closely resemble each other. This connection is particularly evident in assessing PM₁₀ concentrations in air quality, which encompass daily and annual measures. Upon

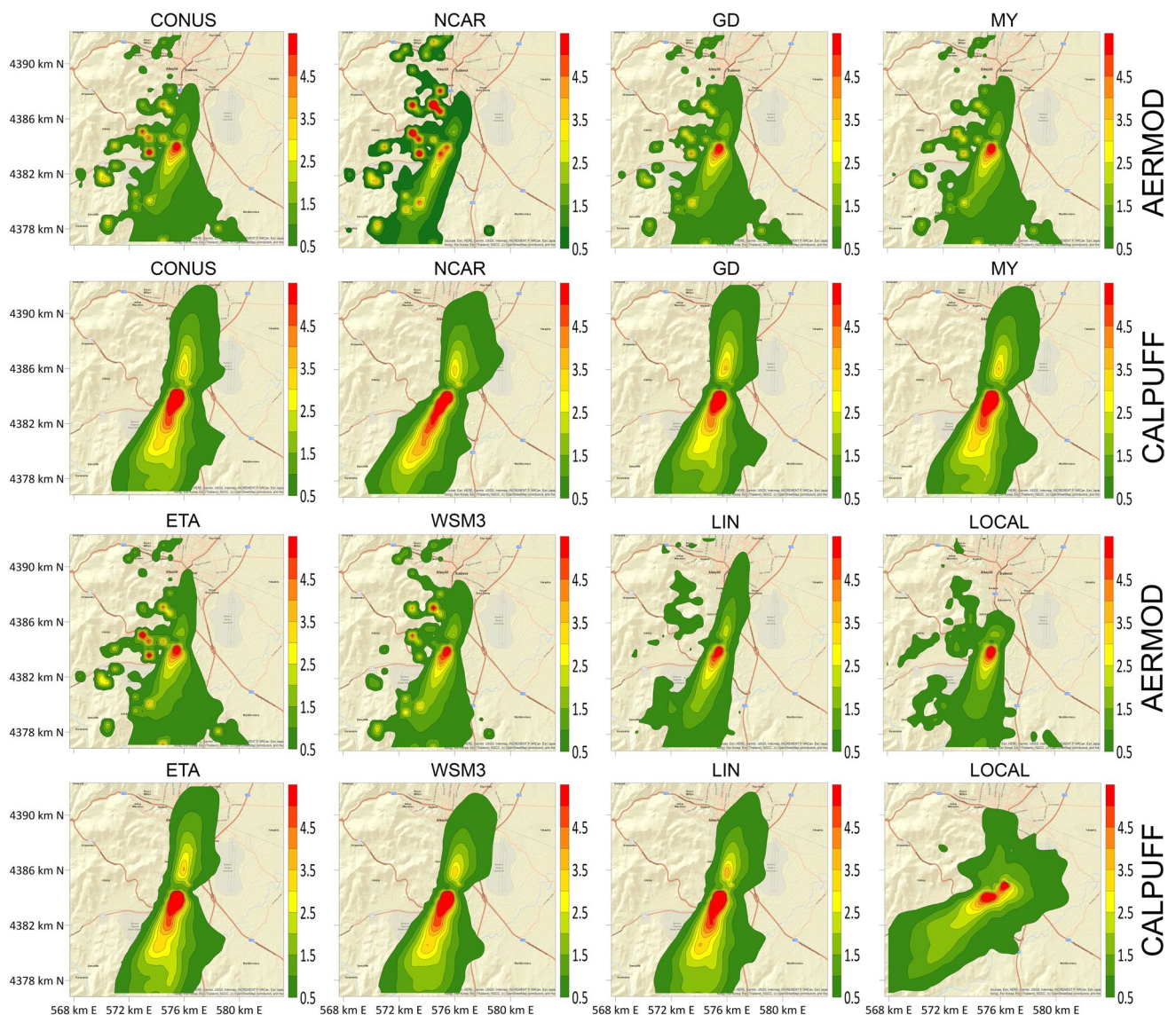


Fig. 9 Dispersion maps of annual average NO_x levels

analyzing locations with the highest cancer risk, it was observed that the distributions across the models were consistent. The highest peaks of health risks were identified as 500–1000 meters south of the facility.

In this study, the health risk results for each point measured by the grid points were displayed in a box plot. The line dividing the framed box into two parts is the median value. The top and bottom lines of the framed box plot represent the interquartile range value. The lower and upper lines of the framed box indicate the minimum and maximum health risk values. The outlier data in the box plot has been represented by points. Health risk models are presented in Figs. 13, 14, and 15. In this study, only cancer and acute risks were observed to be exceeded as a result of the evaluations of PM₁₀ and heavy metal inputs for emission inputs,

respiratory risks, cancer, and acute and chronic lifetime risks.

According to the previous literature, Donoghue and Coffey (2014) examined health risks associated with an aluminium refinery that used a harp model to assess the lifetime exposure level. Also, the risk analysis was conducted at a distance range of 3–5 km. As a consequence, cancer risks were above the limit values. However, acute and chronic risks did not exceed the limit values, and the research also indicated that the PM₁₀ pollutant was dominating the acute health risk (Environ Australia 2008). Schuhmacher et al. (2004) estimated the inhalation risk implications of heavy metals from a cement factory, which was the lifetime exposure level. It was found that although cancer risk levels surpassed the limited mean values, the non-cancer risk was within the limit. Parlak et al. (2023) observed that Cr

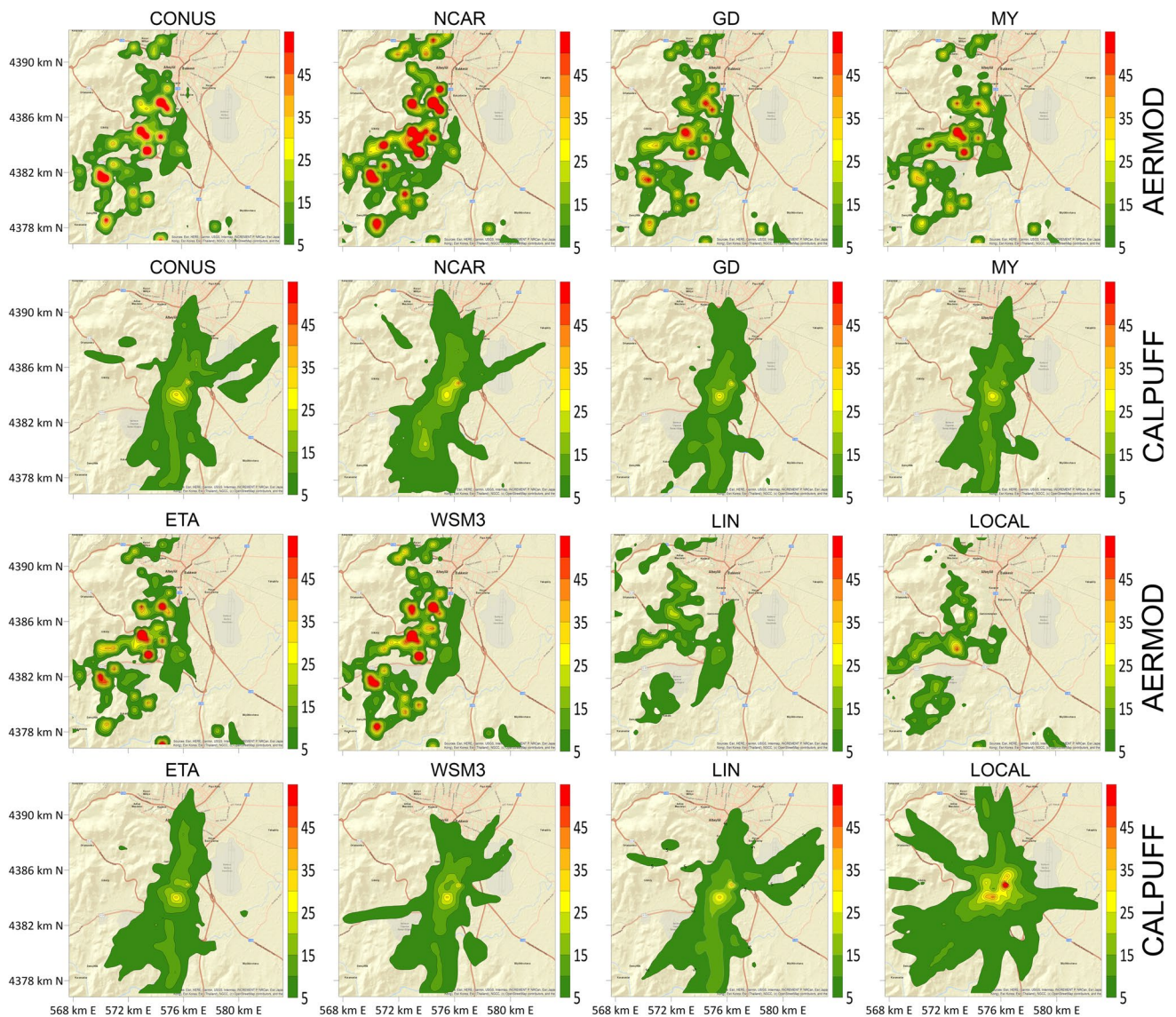


Fig. 10 Dispersion maps of daily maximum CO levels

and Pb pollution from a cement mill in the Canakkale Ezine area, which was close to the Balikesir region, exceeded the acceptable adult limit. Kamaludin et al. (2020) and (Jafari et al. 2023) examined the risks of heavy metal inhalation from the cement industry on workers such that Cr pollutants exceeded the acceptable cancer risk limit values, and the ventilation system, masks, and dust filters were unable to reduce them down to acceptable limit levels.

Summary and conclusions

This study was carried out to analyze the pollution emitted by a cement factory operating in the central region of Balikesir province and to analyze the performance of the models as well as to foresee possible long-term health risks.

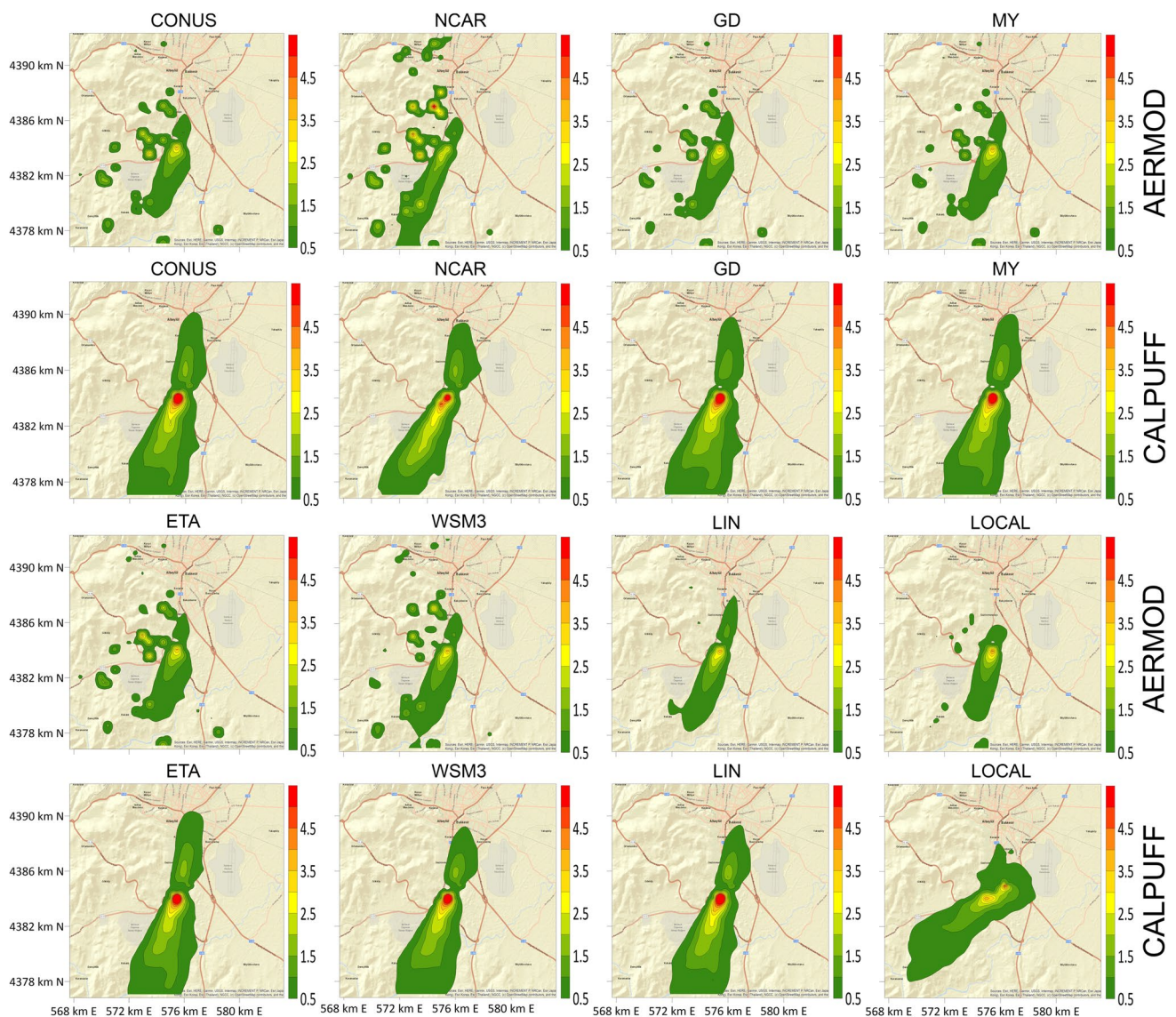


Fig. 11 Dispersion maps of annual average CO levels

Correlation of daily models and AQMS results were accomplished more adequately than the hourly correlation results of both models. The WRF data set utilising GDAS/ERA5 is more suited and dependable for evaluating meteorological simulations than meteorological stations. Among the physics models used for WRF, the best results were achieved with daily No. 3 (GD) and No. 4 (MY) and hourly No. 5 (ETA). Additionally, validation parameters compared to physical models suggest that daily results were more valid than the hourly AQMS results. In this study, it is hard to claim that there is a

considerable difference between all physical models. On the other hand, the WRF default physics parameter of No. 1 (CONUS) is compatible and also the other suggested physics No. 2 (NCAR) is suitable for this study. When the air quality dispersion models were compared, while the correlation value of the CALPUFF model was higher, the AERMOD model produced good results as well. Furthermore, the model validation findings of each model are consistent with daily time intervals in pollutant distributions, hence the AERMOD and CALPUFF models are appropriate for this study.

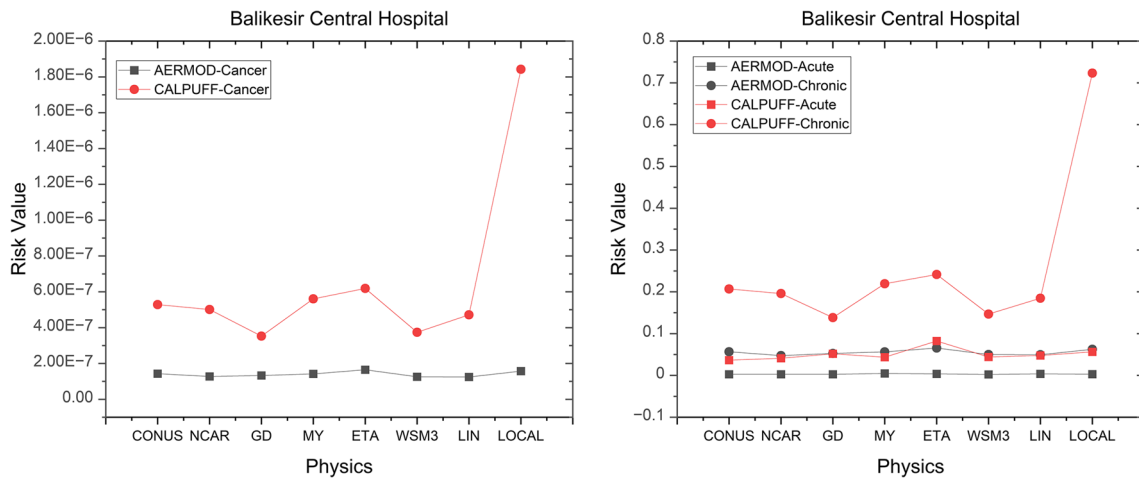


Fig. 12 Risk results of Balikesir Central Hospital

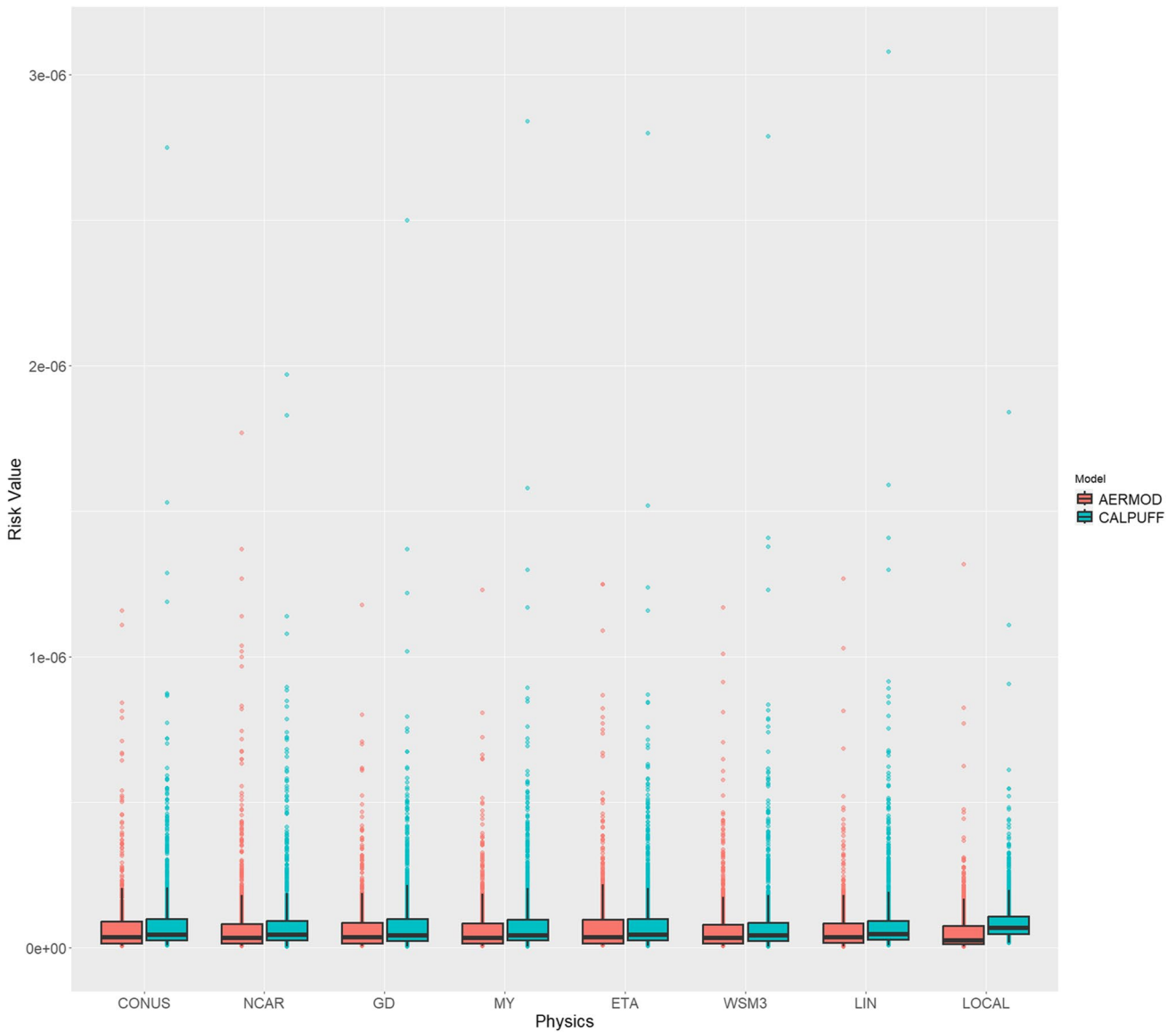


Fig. 13 Cancer risk implications

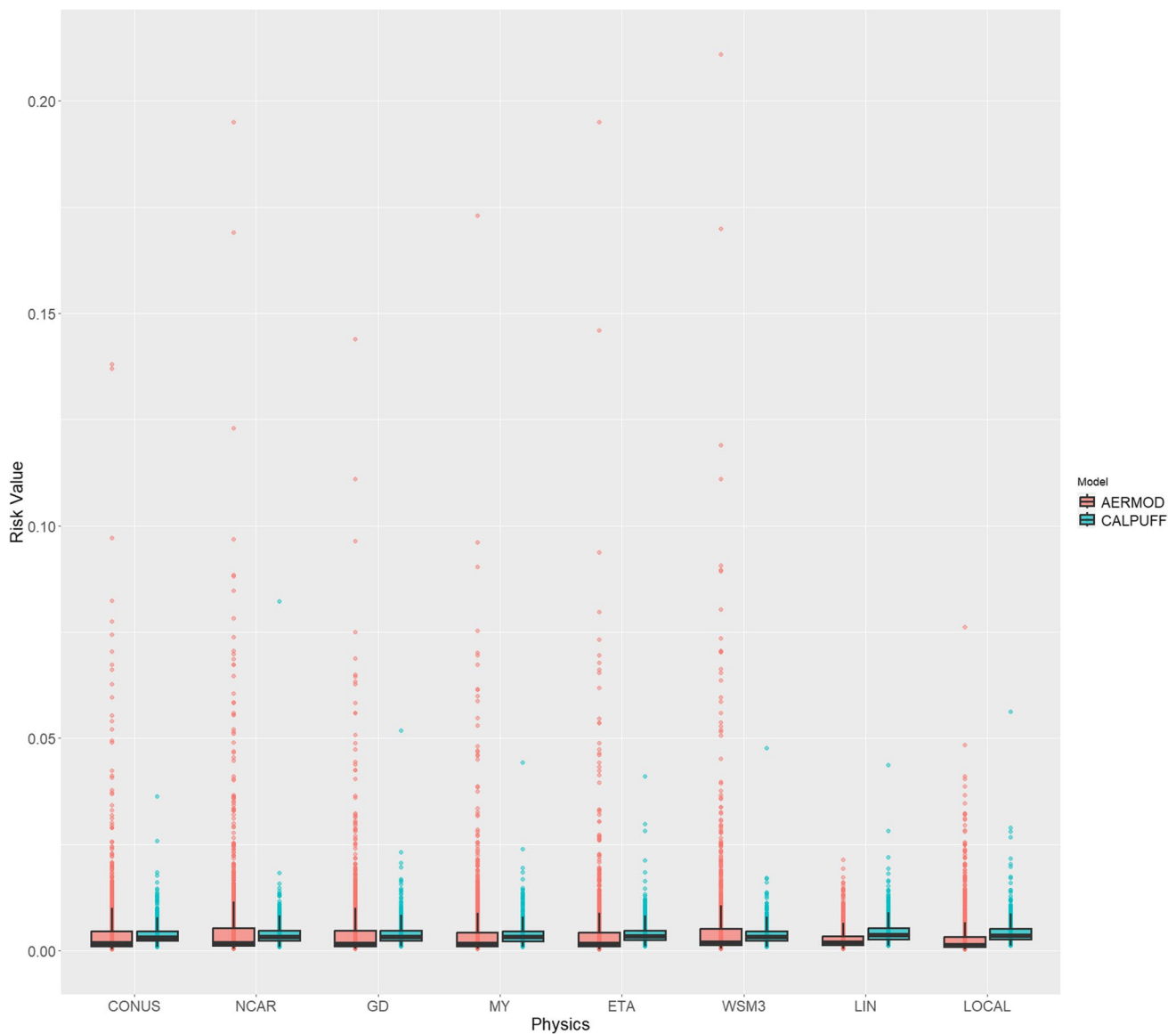


Fig. 14 Acute risk implications

Dispersion model results for PM_{10} , NO_x , and CO concentrations reveal that low wind speeds and model features produced differences daily and annually. Further, differences in emission source types exhibited variances in PM_{10} , NO_x , and CO distribution maps. While the dispersion was more distributed in the environmental area in the maps created in the hourly period, line and area sources in the near ground had an effect on PM_{10} pollutant distributions. The facility is located in the upwind region. As a result, the distributions for each model showed a southward distribution in long-term. Although the highest concentration values vary depending on the model, pollutant, and period, these were mostly No. 2 (NCAR), No. 6 (WSM3), and local data sets, while the lowest concentration was

found particularly in the AERMOD-LIN physic model. While AERMOD obtained the highest concentration levels in daily results, CALPUFF reached higher concentrations in the annual time. The days when the pollutants reached peak concentration were mostly during the winter season.

When the models for health risk analysis were examined, AERMOD and CALPUFF model in health risk results were near to each other. Furthermore, the variation in air quality model findings did not result in a substantial rise in health risk levels. In this study, health risks are negligible for the neighboring settlements in the facility area. Similarly, the Balikesir Central Hospital health risks are negligible for long-term respiratory. Risk exceedances were mostly observed in the southern part of the facility.

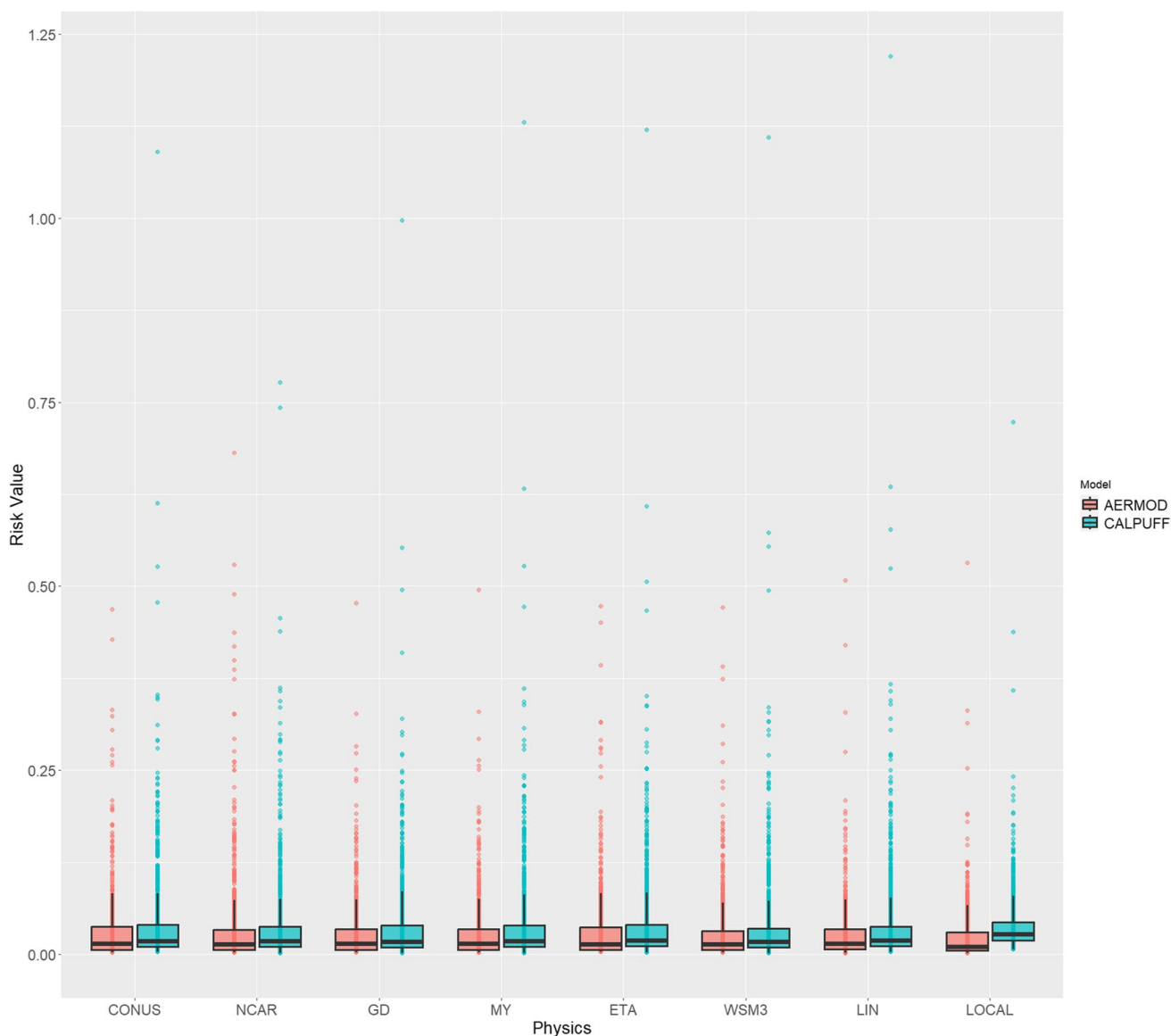


Fig. 15 Chronic risk implications

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Data availability We, as authors, confirm that data will be available on reasonable request.

Declarations

Consent to publish We, as authors, approved the manuscript for publication.

Competing interests We, as authors, declare no competing interests

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