**ISTANBUL TECHNICAL UNIVERSITY ★ EURASIA INSTITUTE OF EARTH SCIENCES**

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**M.Sc. THESIS**

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**Thesis Advisor: Prof. Dr. Alper ÜNAL**

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**İSTANBUL TEKNİK ÜNİVERSİTESİ★AVRASYA YER BİLİMLERİ ENSTİTÜSÜ**

# İZMİR'DEKİ HAVA KİRLİLİĞİNİN ATMOSFERİK MODELLEME YOLUYLA ANALİZİ

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**MAYIS 2016**

Duygu ÖZÇOMAK, a M.Sc. student of ITU Eurasia Institute of Earth Sciences 601131001 successfully defended the thesis entitled "ANALYSIS OF AIR POLLUTION OVER İZMİR VIA ATMOSPHERIC MODELING", which she prepared after fulfilling the requirements specified in the associated legislations, before the jury whose signatures are below.

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**To all my family,**

**FOREWORD**

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Istanbul, May 2016

Duygu ÖZÇOMAK
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**ABBREVIATIONS**

**NOx:** Nitrogen Oxides (Nitric oxide and Nitrogen dioxide)
**NMVOC:** Non-Methane Volatile Organic Compounds
**$CO_2$:** Carbon dioxide
**$CH_4$:** Methane
**$N_2O$:** Nitrous Oxide
**$NH_3$**: Ammonia
**$SO_2$:** Sulfur Dioxide
**$PM_{10}$ :** Particulate Matter (<10 μm diameter)
**$PM_{2.5}$ :** Particulate Matter (<2.5 μm diameter)
**CO:** Carbon Monoxide
**PAHs:** Polycyclic aromatic hydrocarbons
**POPs:** Persistent Organic Pollutants
**EPA:** Environmental Protection Agency
**COPERT 4:** COmputer Programme to Calculate Emissions From Road Transport
**EEA:** European Environment Agency
**WRF:** Weather Forecasting Model
**CMAQ:** Community Multiscale Air Quality Model
**TUVTURK:** Tuvturk Motor Vehicle Inspection Inc.
**EMEP:** European Monitoring and Evaluation Program
**TUIK:** Turkish Statistical Institute
**AQM:** Air Quality Models
**NCAR:** National Center for Atmospheric Research
**NCEP:** National Centers for Environmental Prediction
**FSL:** Forecast Systems Laboratory
**AFWA:** Air Force Weather Agency
**FAA:** The Federal Aviation Administration
**MoEU:** Ministry of Environment and Urbanization
**WHO:** World Health Organization
**TSMS**: Turkish State Meteorological Service
**VOC:** Volatile Organic Compound
**BVOC:** Biogenic Volatile Organic Compound
**IIASA GAINS:** International Institute for Applied Systems Analysis Greenhouse Gas and Air Pollution Interactions and Synergies
**SNAP:** Standard Nomenclatures for Air Pollution
**MB:** Mean Bias
**NMB:** Normalised Mean Bias
**RMSE:** Root Mean Square Error
**r:** Correlation Coefficient

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μg : microgram
$\mu gm^{-3}$ : microgram per cubicmeter
km : Kilometer
◦C : Celcius Degree
% : Percentage

## ANALYSIS OF AIR POLLUTION OVER IZMIR VIA ATMOSPHERIC MODELING


### SUMMARY

Besides being Turkey's third largest city with a population exceeding 4 million, İzmir is among the metropolitans that have major economic improvements. Economic growths of big cities inevitably bring some social and environmental issues as well. Among these, air pollution is the most serious and common one that both developed and developing countries are encountered. Air quality problem is affected from a lot of parameters especially in big cities. These include meteorology, topography, population, altitude, industrialization and social-economical developments. Exposure to pollution increases with the increasing human population living in developing urban areas. United Nations announced in 2000 that approximately half of the world population (48%) live in cities and every 3 years 2% growth is expected in the city populations. According to a research in 2013, twenty-three cities in the world have populations higher than 10 million.

Air pollution is the existence of the foreign substances suspended in different phases of the atmosphere in varying amount, density and duration that damage human health, living organisms, and ecological balance. Therefore being exposed to air pollution became one of the inevitable results of urban life due to intense anthropogenic activities. Different researches are done on air pollution, which is a significant problem for both developed and developing countries. Especially air pollutants can threaten human health in various ways and levels. While there are high amounts of air pollutants, especially in urban areas, increase in mortality and morbidity rates has been discovered. Particularly lung diseases, neurobehavioral disorders and the effects of cardiovascular diseases are the main adverse effects of air pollution.

Growing city population and industrialization level result in increasing energy demand. In densely populated areas, air pollution emission increases by rapid urbanization, transportation, energy production and industrial activities. Air quality management is one of the issues that need to be implemented urgently in the cities where strategical planning is limited or does not exist. Thus, developing emission inventories is one of the most important steps for air quality determination and improvement. These inventories are necessary tools for evaluating human and environmental risks, which are based on anthropogenic sources. Air quality control strategies are determined by air quality and emission standards defined by authorities in regional, national and global scales. Developing emission control strategies, determining applicability of control programs are required for creating reliable emission inventory. It is required to estimate the spatial and temporal density of emission sources in the best possible resolution for forming a healthy air quality control strategy and planning air pollution control reduction strategies. Having a reliable emission inventory is a primary

requirement for qualified air quality management system. An emission inventory system supports pollution evaluation activities by data collection and scanning, storing, data organization. Also it creates databases for emission scenarios that will be prepared in the future.

In this study, by improving existing emission inventory, activity data, which is more up-to-date and with reduced uncertainty, is compiled thus more reliable entries are provided for the air quality model. Via this model, which is run by the new inventory, temporal and spatial distribution of pollutants is investigated according to the sources. In the model, compiling of pollutants that are distributed according to the sources is set up based on sectoral distributions. Three types of source data is collected in the repository then are calculated depending on the calculation methods of source types. In the model, industry emissions are in SNAP-34 sector, traffic emissions exist in SNAP-7 sector. SNAP-7 also is divided into five based on source emissions. Regional sources named as domestic heating are calculated for SNAP-2 sector. While preparing emission inventory, for each sector required data is obtained from enterprises, calculations are done according to the related sector. Traffic emissions are calculated using COPERT 4 model, which is used in the transportation sector section of the İzmir's inventory. COPERT 4 traffic emission calculation model is commonly used for the calculation of vehicle emissions in several European countries. For industrial emissions, plants' direct emission measurements, which are provided by Izmir Provincial Directorate of Environment and Urban Planning, are calculated and used in the SNAP-34 sector of the study. For domestic heating emissions, which are provided by Izmır Provincial Directorate of Environment and Urban Planning by using the natural gas consumption and coal sales data, are calculated for SNAP-2 sector.

In this study, WRF/CMAQ models included in EPA Models-3 system are used together. Meteorological and chemical transport models are run as two domains. Main domain includes whole Europe, North Africa and Eastern Asia, second domain covers whole Turkey and the resolutions are 30 km and 10 km respectively. WRF model is with 3 days spin-up timing is run for January 2010. For the result of the model, temperature and wind speed/direction data that is provided by İzmir Turkish State Meteorological Service is used and Gaziemir station performance analysis is done. When the temperature and station data are evaluated together, it is found that at temperatures in 2 m, for the trend and temperature values partially in line with the model estimations. For the evaluations of the wind speed and direction, at lower levels of wind speed, model estimates are compatible with station observations, although there are some deviations at certain days. There are some uncertainties in the model estimates regarding the wind direction and which is an expected situation.

Following the evaluation of the changing model parameters' effects on emissions, air quality model is run to understand how these effects will be reflected into air quality. TNO/MACC-II inventory is used as a baseline scenario and run for 30 km and 10 km. Then CMAQ model is run once again for İzmir SNAP-2, SNAP-34 and SNAP-7 sectors with up-to-date emission data. For TNO inventory and new inventory that is created by new emission calculations, analyses are done by using different analysis methods and the affects of sectoral changes on the model results are investigated.

For the emissions as TNO-OUR, total emission maps are created separately for each, the differences from each others are drawn as maps. In OUR emissions, for all

pollutants changes are monitored according to the increases and decreases based on sectors. While $PM_{10}$ emissions are decreased in SNAP-2, increased in SNAP-34 and SNAP-7, as a result overall $PM_{10}$ emissions are increased. While CO is declined in SNAP-2 sector dramatically, it is increased sharply in SNAP-34 and SNAP-7 sectors. $NO_x$ is increased in the sectors except for SNAP-34. $SO_2$ from pollutants is increased in all sectors. As a result of all these changes in emissions, different results are observed in the concentrations for each pollutant. In this study, distributions based on sectors takes into account for the spatial distribution of TNO inventory. Thus, the differences are considered based on the TNO spatial distribution.

It is found that for all pollutant emissions and concentrations over İzmir, maximum changes are observed in city center. Through more detailed examinations, days and hours are determined where the maximum differences occur in concentrations and affects and results of these on emissions are investigated. Our findings indicate that the maximum impact of the CMAQ model's concentration results which are used by the newly developed emission inventory as an input, is observed in the İzmir city center where the most emission sources exist.

# İZMİR'DEKİ HAVA KİRLİLİĞİNİN ATMOSFERİK MODELLEME YOLUYLA ANALİZİ

## ÖZET

Türkiye'nin üçüncü en büyük kenti olmasının yanı sıra 4 milyonu aşan nüfusuyla İzmir, ekonomisinde büyük gelişmeler kaydeden metropoller arasındadır. Büyükşehirlerin ekonomilerindeki büyüme, kaçınılmaz olarak bazı sosyal ve çevresel sorunları da beraberinde getirmektedir. Bunların arasında en önemlisi olan hava kirliliği gelişmiş ve gelişmekte olan ülkelerde sıkça rastlanan problemlerdendir. Hava kalitesi problemi özellikle de büyükşehirlerde birçok parametreden etkilenmektedir. Bunlar arasında meteoroloji, topografya, nüfus, rakım, endüstrileşme ve sosyo-ekonomik gelişim bulunmaktadır. Dünyadaki gelişen kentsel alanlarda yaşayan insan nüfusunun artmasıyla birlikte kirliliğe maruziyet de artmaktadır. Birleşmiş Milletler 2000 yılında dünya nüfusunun (% 48) yaklaşık yarısı kentlerde yaşadığını ve kentlerin nüfuslarının önümüzdeki her üç yılda yılda % 2 oranında büyümesini beklediğini açıklamıştır. 2013 yılında yapılan bir çalışmaya göre dünyadaki 23 şehrin 10 milyonun üzerinde nüfusa sahip olduğu görülmüştür.

Hava kirliliği, farklı fazlarda bulunan yabancı maddelerin insan sağlığına, canlı hayatına ve ekolojik dengeye zarar verecek miktar, yoğunluk ve sürede atmosferde asılı kalmasıdır. Bu sebeple hava kirliliği maruziyeti yoğun antropojenik aktivitelerden dolayı kentsel yaşamın kaçınılmaz sonuçlarından biri haline gelmiştir. Gelişmekte olan ve gelişmiş ülkelerin en büyük problemi olan hava kirliliği üzerine farklı çalışmalar yapılmaktadır. Öncelikle hava kirleticileri insan sağlığını çok çeşitli şekillerde etkileyebilmektedir. Hava kirleticilerinin miktarlarının özellikle kentsel alanlarda yüksek olmasıyla beraber ölümlerin ve hastalık oranlarının arttığı tespit edilmiştir. Özellikle akciğer hastalıkları, nörodavranışsal hastalıklar ve kalp-damar hastalıkları başlıca görülen etkileridir.

Büyüyen kent populasyonu ve endüstrileşme seviyesi enerji talebini de arttırmaktadır. Yoğun nüfuslu bölgelerde hızlı kentleşme ile ulaşım, enerji üretimi ve sanayi aktiviteleri hava kirliliği emisyonlarının artmasına neden olmaktadır. Hava kalitesi yönetiminin stratejik planlaması zayıf olan ya da varolmayan şehirlerde acilen uygulanması gereken hususlardandır. Bu sebeple hava kalitesi seviyelerinin belirlenerek iyileştirilmesi için emisyon envanterlerinin oluşturulması önemli adımlardan biridir. Bu envanterler antropojenik kirletici kaynaklardan olan insan ve çevresel riskleri değerlendirmek için gerekli araçlardır. Hava kalitesi kontrol stratejileri yerel, ulusal ve global ölçekteki otoritelerin belirlediği hava kalitesi ve emisyon standartları ile belirlenir. Emisyon kontrol stratejileri geliştirmek, control programlarının uygulanabilirliğini belirlemek güvenilir emisyon envanterinin oluşturulması için gereklidir. Sağlıklı bir hava kalitesi control stratejisi oluştumak ve hava kirliliği kontrolü azaltma stratejileri planlamak amacıyla mümkün olan en iyi çözünürlükte

emisyon kaynaklarının mekansal ve zamansal yoğunluk miktarını tahmin etmek gerekir. Güvenilir emisyon envanterinin varlığı nitelikli hava kalite yönetim sistemi için temel bir gerekliliktir. Bir emisyon envanter sistemi, veri toplama ve tarama, depolama, veri düzenleyerek kirlilik değerlendirme faaliyetlerini desteklemektedir. Ayrıca gelecekte hazırlanacak emisyon semaryoları için veritabanı oluşturmaktadır.

Bu çalışmada, mevcut emisyon envanteri iyileştirilerek daha güncel ve belirsizliği indirgenmiş olan aktivite verileri derlenmiş böylece kullanılan hava kalitesi modeli için daha güvenilir girdiler hazırlanmıştır. Oluşturulan yeni envanter ile çalıştırılmış olan model yardımıyla kaynaklarına göre kirleticilerin zamansal ve mekansal dağılımları incelenmiştir. Kaynaklarına göre dağılımları yapılan kirleticilerin model içerisindeki derlenmesi modelin sektörel dağılımlarına göre oluşturulmuştur. Geliştirilen envanterin son haline gelmesinden önce hesaplanan ve düzenlenen veriler sektörel bazlı olarak modelin içerisinde dağıtılmıştır. Çalışmada üç tipte kaynağın verileri veri havuzunda toparlanmış ardından kaynak tiplerinin hesap yöntemlerine bağlı olarak hesaplanmıştır. Model içerisinde sanayi emisyonları SNAP-34 sektöründe bulunurken, trafik kaynaklı emisyonlar SNAP-7 sektöründe bulunmaktadır. SNAP-7 ayrıca kendi içerisinde kaynak emisyonlarına bağlı olarak 5'e ayrılmaktadır. Evsel ısınma olarak adlandırılan alansal kaynaklar ise SNAP-2 sektörü için hesaplanarak oluşturulmuştur. Emisyon envanteri hazırlanırken her sektor için gerekli olan veriler kurumlardan elde edilerek bağlı olduğu sektöre göre hesaplamalar yapılmıştır. COPERT 4 modeli ile trafik kaynaklı emisyonlar hesaplanarak İzmir'e ait envanterin ulaşım sektörü bölümünde kullanılmıştır. COPERT 4 trafik kaynaklı emisyon hesaplama modeli, Avrupa'da pek çok ülke tarafından araç emisyonların hesaplanması için kullanılan bir modeldir. Sanayi emisyonları için tesislerin direct ölçümlerden elde edilen veriler İzmir Çevre ve Şehircilik Müdürlüğü tarafından sağlanarak çalışmanın SNAP-34 sektörü için hesaplanarak kullanılmıştır. Evsel ısınma emisyonları İzmir Çevre Şehircilik Müdürlüğü tarafından sağlanan doğalgaz tüketim ve kömür satış verileri kullanılarak SNAP-2 sektörü için hesaplanmıştır.

Bu çalışmada, EPAs' models-3 sisteminin içerdiği WRF/CMAQ modelleri bir arada kullanılmıştır. Meteoroloji ve kimyasal taşınım modelleri 2 domain olarak çalıştırılmıştır. Ana domain tüm Avrupa'yı, Kuzey Afrika'yı ve Doğu Asya'nın bir kısmını, ikinci domain tüm Türkiye'yi kapsamaktadır ve çözünürlükleri sırasıyla 30 km ve 10 km'dir. WRF modeli 3 gün spin-up zamanı ile Ocak 2010 için çalıştırılmıştır. Modelin sonuçları için İzmir ili Meteoroloji Genel Müdürlüğü'den elde edilen sıcaklık ve rüzgar hızı/yönü verileri ile Gaziemir istasyonu için performans analizi yapılmıştır. Modelin sıcaklık verileri ile istasyon verileri beraber değerlendirildiğinde modelin 2mdeki sıcaklıklarda trend ve sıcaklık değerleri için kısmen doğru öngörü yaptığı tespit edilmiştir. Rüzgar hızı ve yönü verileri için yapılan değerlendirmelerde ise modelin rüzgar hızının düşük olduğu zamanlar için rüzgar hızı için doğru tahminlerde bulunduğu fakat bazı zamanlarda sapmalar olduğu gözlenmiştir. Rüzgar yönü için modelin tahmininde belirsizlikler söz konusudur, bu olası bir sonuçtur.

Model parametrelerindeki değişimin emisyonlar arasındaki etkisinin değerlendirilmesinin ardından bu etkinin hava kalitesine nasıl yansıyacağını belirlemek için hava kalitesi modeli çalıştırılmıştır. Baz senaryo olarak TNO/MACC-II envanteri kullanılarak 30 km ve 10 km için koşturulmuştur. Ardından CMAQ modeli İzmir ili için SNAP-2, SNAP-34 ve SNAP-7 sektörleri için hesaplanan güncel emisyon verileri ile tekrar çalıştırılmıştır. TNO envanteri ve yeni emisyon hesapları ile

oluşturulan yeni envanter için analizler farklı analiz yöntemleri kullanılarak sektörel değişimlerin model sonuçlarındaki etkileri incelenmiştir. Emisyonların TNO-OUR olarak ayrı ayrı toplam emisyon haritaları oluşturulmuş, birbirlerinden farkları da harita olarak çizdirilmiştir. OUR emisyonlarında her kirleticide sektörel bazlı arttırım ve azaltımlara göre değişimler gözlenmiştir. $PM_{10}$ emisyonları SNAP-2'de azaltılırken, SNAP-34 ve SNAP-7'de arttırılmıştır, sonuç olarak ise $PM_{10}$ emisyonları arttırılmıştır. CO SNAP-2 sektöründe büyük ölçüde düşürülürken, SNAP-34 ve SNAP-7 sektörlerinde büyük oranda arttırılmıştır. $NO_x$ ise çalışılan sektörlerde SNAP-34 hariç arttırılmıştır. Kirleticilerden $SO_2$ ise bütün sektörlerde arttırılmıştır. Tüm bu azaltım ve arttırımların sonucunda konsantrasyonlarda her kirletici için farklı sonuçlar gözlenmiştir. Çalışmada, sektörel dağılımlar TNO envanterinin mekansal dağılımını baz almaktadır. Dolayısıyla farklar TNO mekansal dağılımına bağlı olarak oluşmuştur.

İzmir tüm kirletici emisyonlarında ve konsantrasyonlarda maksimum değişimlerin şehir merkezinde olduğu görülmüştür. Daha detaylı inceleme yapılarak konsantrasyonlarda maksimum farkın olduğu gün ve saatler belirlenerek emisyonun etkisi ve sonuçları incelenmiştir. Tüm bu analizlerin sonucunda, geliştirilen yeni emisyon envanterinin input olarak kullanıldığı CMAQ modelinin konsantrasyon sonuçlarında görülen maksimum etki, emisyon kaynaklarının en fazla olduğu İzmir şehir merkezinde görülmüştür.

# 1. INTRODUCTION

More than 50 percent of the World's population is living in urban areas and there are twenty-three cities worldwide with a population of 10 million or greater (UN, 2013) hence, urban air pollution is listed among the most critical environmental problems in both the developed and developing countries. Besides, most of the highly populated urban areas are located in poor and developing regions and are identified by elevated air pollution levels (Baklanov et. al, 2016). Megacities cover under 0.2 percent of the Earth's surface, however represent around 10 percent of the world's population and have strong consequences for environmental conditions (Demographia, 2014). Consequently, people living in urban zones, especially megacities are subject to high risks associated with air pollution. Therefore, megacities residents are vulnerable to air pollution caused health impacts (Molina et. al, 2004; Gurjar et. al., 2008).

There is now substantial scientific evidence that link air pollution and health problems. In a study conducted by Poloniecki *et al.* (1997), over 370,000 emergency cardiovascular admissions in London hospitals were analyzed between April 1987 and March 1994. They have found positive correlations between acute myocardial infarction (AMI) and black smoke and air pollutant gases ($NO_2$, CO and $SO_2$)) and between angina and black smoke. The authors suggested that 1 in 50 heart attacks in London hospitals are triggered by air pollution. In another study, Ruidavets *et al.* (2005) found that short-term exposure to ozone (i.e., 1 to 2 days) is related to AMI events in middle-aged adults without heart disease. Nawrot and Nemery (2007), support these findings with their own study, which found that air pollution (especially pollution from traffic) ranks four in their list of environmental triggers.

APHEA-2 (Air Pollution and Health: a European Approach 2) (Atkinson *et al.*, 2001), study focused on the impact of increased particulate matter (PM) levels on daily mortality and hospital admissions for asthma and chronic obstructive pulmonary disease (COPD). APHEA-2 daily mortality studies were conducted in 29 European cities, covering over 43 million people for more than 5 years in the 1990s.

The results showed that all-cause daily mortality increased by 0.6 percent for 10μg/$m^3$ increase in $PM_{10}$. APHEA-2 hospital admission study was conducted in 8 European cities, covering 38 million people. Hospital admissions for asthma and COPD were observed to be increase by 1 percent per 10μg/$m^3$ increase in $PM_{10}$ among older people (65+) (Katsouyanni *et al.*, 2001). In other studies, the range for increase in all-cause daily mortality is between 0.6 and 1.2 percent per 10μg/$m^3$ increase in PM (Pope and Dockery, 2006).

Although long-term effect studies are not as numerous as the short-term effect studies, there are over 30 publications on this subject. As summarized by Pope and Dockery (2006), the range for all-cause mortality rates is between 1 and 17 percent per 10μg/$m^3$ increase in $PM_{2.5}$. For cardiopulmonary mortality rates this range is between 5 and 42 percent and for lung cancer it is between 0.8 and 81 percent. In a recent study conducted by Pascal et al. (2013), health burden of chronic exposure to PM2.5 was analyzed. The study revealed that complying with the WHO guideline of 10 μg/$m^3$ in annual mean, would make up of 22 months of life expectancy at age 30, which corresponds to a total of 19,000 deaths delayed. The monetary gain of this change is estimated to be €31 billion annually (including savings on health expenditures, absenteeism and intangible costs such as well-being, life expectancy and quality of life).

In other studies, relation between air pollutants and reduced growth in children were analyzed. (Guaderman, et al., 2000) found that fourth graders who are exposed to PM, $NO_2$ and inorganic acid vapors, showed significant reduction in growth of lung function. Deficits were found to be higher for children spending more time outdoors. In a study conducted by Avol et. al (2001), children who relocated to areas of lower $PM_{10}$ showed increased growth in lung function whereas children who live in areas with high $PM_{10}$ show decreased growth in lung function. The authors concluded that changes in air pollution exposure during growth years have a significant impact on lung function growth and performance. In another study, Perera et al. (2009), monitored children from birth till 5 years of age and showed that children in high exposure group had full-scale and verbal IQ scores that were 4.31 and 4.67 points lower, respectively, than those of less-exposed children.

In a more recent study, Pujol et al. (2016) aimed at quantifying the impact of traffic-related pollution on school children. A total of 263 of school children (aged between

8 and 12) were diagnosed with MRI under different exposure levels. Although there was no indication of structural or anatomical change, higher levels of pollution was found to be slower brain functions and brain maturation.

In order to reduce the adverse impacts caused by air pollution there is a need for better implementation of the air quality management strategies. Setting and implementing air quality standards are the first steps of air quality management. In USA, Environmental Protection Agency (EPA), in Europe European Environmental Agency (EEA) and in Turkey, Ministry of Environment and Urbanization (Ministry of Environment and Urbanization, 2013) is tasked to set standards for air quality levels. The list of pollutants and their limited values for different temporal averages for these agencies along with World Health Organization's suggested levels are provided in Table 1.1.

**Table 1.1:** Air Quality Standards for WHO, US-EPA, EEA and Turkey

| Pollutant | WHO | EPA | EEA | MoEU |
|---|---|---|---|---|
| $SO_2$ | 500 µg/m3 (10 min) | 195 µg/m3 (hourly) | 350 µg/m3 (hourly) | 500 µg/m3 (hourly) |
| | 20 µg/m3 (24 hour) | 1300 µg/m3 (3 hourly) | 125 µg/m3 (24 hour) | 250 µg/m3 (24 hour) |
| $NO_2$ | 200 µg/m3 (hourly) | 188 µg/m3 (hourly) | 200 µg/m3 (hour) | 300 µg/m3 (24 hour) |
| | 40 µg/m3 (annual) | 100 µg/m3 (annual) | 40 µg/m3 (annual) | 60 µg/m3 (annual) |
| $PM_{10}$ | 50 µg/m3 (24 hour) | 150 µg/m3 (24 hour) | 50 µg/m3 (24 hour) | 100 µg/m3 (24 hour) |
| | 20 µg/m3 (annual) | - | 40 µg/m3 (annual) | 60 µg/m3 (annual) |
| $PM_{2.5}$ | 25 µg/m3 (24 hour) | 35 µg/m3 (24 hour) | 25 µg/m3 (annual) | - |
| | 10 µg/m3 (annual) | 12 µg/m3 (annual) | - | - |
| $O_3$ | 100 µg/m3 (8 hour) | 157 µg/m3 (8 hour) | 120 µg/m3 (8 hour) | (hourly) |
| | - | 235 µg/m3 (hourly) | - | 120 µg/m3 (8 hour) |
| CO | - | 40 mg/m3 (hourly) | 10 mg/m3 (8 hour) | - |
| | - | 10 mg/m3 (8 hour) | - | - |
| Pb | - | 0.15 µg/m3 (3 months) | 0.15 µg/m3 (annual) | 1 µg/m3 (annual) |

WHO: http://www.who.int/mediacentre/factsheets/fs313/en/
US-EPA: http://www.epa.gov/air/criteria.html
EEA: http://ec.europa.eu/environment/air/quality/standards.htm
Türkiye: http://www.ibb.gov.tr/sites/CevreKoruma/HavaKalitesi/Documents/LimitDegerler.pdf

As seen in Table 1.1, standards for Turkey are generally higher than EPA, EEA and WHO standards. For example, for $PM_{10}$, the standard for Turkey is 60 $\mu g/m^3$ (annual), whereas it is 40 $\mu g/m^3$ for EEA and 20 $\mu g/m^3$ for WHO. USEPA does not have annual standard for $PM_{10}$.

Particulate matter contain a complex mixture of a small and large particles of different origin and composition, involving fossil fuel emissions, industrial fugitive and dust, wind blown dust and secondary pollutants (Im, et al., 2010). In general, in terms of size particles are classified by their aerodynamic diameter and the size of particles determines the residence time in the air. Urban areas, where pretty high levels particulate matter (PM) is monitored, anthropogenic sources could considerably contribute to urban pollution. Therefore, PM was given priority to be examined in this study.

There are several studies in Turkey to determine air quality level locally and to make improvement plans. In a recent study conducted by (Baltacibasi, 2014) PM10 annual averages in Turkey is estimated to be 82.3, 76.5, 73.9 $\mu g/m^3$ for 2008, 2009 and 2010 respectively. All these values are above the WHO standards, but are under EEA and Turkey standards. Only 25 percent of the observations have $PM_{10}$ values lower than EU daily $PM_{10}$ standard of 50 $\mu g/m^3$, and 75 percent of the data are lower than 90 μg/m3. Baltacibasi (2014) estimated different clusters of $PM_{10}$ values for different regions Turkey. In general, air pollution level in the Eastern Anatolia Region is significantly higher than other regions in Turkey. However, some cities such as Afyon and Bolu also is categorized under highly-polluted cities.

$PM_{10}$ averages are below over all stations in Turkey (Figure 1.1). Ten percent of $PM_{10}$ averages have exceeded the limit value in Turkey in the last 6 years. On the other hand, while this percentage was 16% for 2009, this percentage decreased till 6% in 2015. This reduction can be seen as a result of the studies.

Developing a proper emission inventory is essential for generating air quality managing programs and mitigation strategies. Elbir and Müezzinoğlu (2004) worked on emission inventory that covers primary pollutants over Izmir. In this study, sources were classified as point, line and area sources. Activity data of industry, domestic and transportation sources were collected for year 2000 and emissions calculated by using proper emission factors. The results of study proved that different emission sources responsible from different type of pollutant emissions dominantly.

For example, for PM emissions the most pollutant sector is domestic heating, for $SO_2$ emissions industry sector has the highest portion and transportation sector contributes the highest emissions of $NO_x$ for Izmir city. Especially, emissions caused from industries, which are located outside the metropolitan city center, are much higher in amount for Izmir. Another study that indicates quantification of emissions from domestic heating from residential areas in Izmir studied by Sari and Bayram (2013). The study covers $PM_{10}$, $SO_2$, $NO_2$, VOC and CO that come from domestic heating and also greenhouse gases such as $CO_2$, $N_2O$ and $CH_4$ in Izmir for 2008-2009 winter season. In the study CALMET/CALPUFF dispersion model was used in order to quantify impact of new emissions over the city.

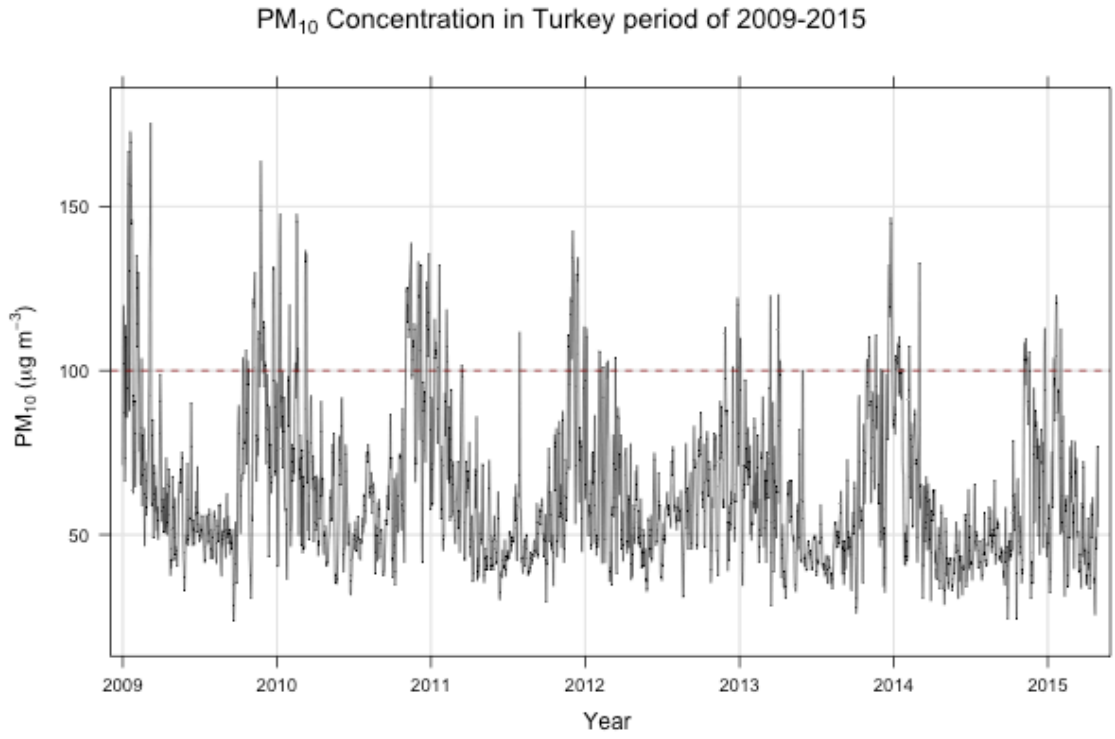


**Figure 1.1:** $PM_{10}$ average concentration (over all stations in Turkey) and red dashed line is Turkey limit value that is 100 μg/m3

Turkish Ministry of Environment and Urbanization has released circulars to combat with high air pollution levels in Turkey (Ministry of Environment and Urbanization, 2013). This circular includes adaptation and administration processes for limiting concentration of 13 different pollutants. (Sulfur dioxide, nitrogen dioxide, nitrogen oxides, particulate matter, lead, benzene, carbon monoxide, arsenic, cadmium, nickel and, benzopyrene). Regulation also takes aim at accurate, complete and reliable monitoring on air pollutant control and air quality. In an ongoing study of MOEU

(2013), provinces over Turkey consisting of 8 regions are classified as two parts. For evaluation, the cities that have population over than 750,000 in city center classified as major sub-regional and the cities, which have population between 250,000 and 750,000 in city center classified as minor sub-regional. According to this classification, there are 15 major sub-regional and 31 minor sub-regional cities over the all country. Metropolitan cities such as Istanbul, Ankara and Izmir are listed as major sub-regional cities and emissions inventory studies along with air quality modeling are required.

Air quality modeling is a mathematical tool that simulate atmospheric phenomenon (such as advection, diffusion, etc.) and provide opportunity to evaluate air quality for a specific region and time period. Eularian air quality models require emissions data along with meteorological data over a gridded domain. Scientific studies prove that input files are significantly important for obtaining better air quality model results (Russell & Dennis, 2000; Hanna et. al, 2001). The main inputs for the air quality chemical transfer models are meteorological data and emission inventory. Meteorological data is provided by weather forecast model outputs that clarify meteorological conditions for the selected study area and episode. Emission inventory preparation process is one of the most uncertain parts as input of the air quality model. Because of that, emission inventory is an essential issue to obtain high quality model outputs. Accurate emission inventory provides better air quality model results and by these results it is possible to identify impact of the emissions over the region better. For improving regulations and control technologies, modeling is the most preferred method that supports different scenario applications over selected region and condition.

In this study our objective is to analyze air pollution levels in İzmir, which is one of the major metropolitan areas of Turkey. According to Parilla et. al research, Izmir with 2% growth rate was determined as second fastest growing city in developing countries in the world (2014). Today, Izmir has a population of over 4 million and is the highest industrial region in the South-Western Turkey. In order to investigate air pollution levels in İzmir we have utilized the air quality data provided by Izmir Provincial Directorate of Environment and Urban Planning. Although air quality monitoring is a method to measure pollutant concentrations, the data, which is taken from point stations and belong to certain time and point locations, is not useful for

different areas, time or meteorological conditions. For that reason, air quality modeling is necessary for further scenario studies for a selected region and episode. The data provided by the Izmir Provincial Directorate of Environment and Urban Planning is utilized to estimate emissions inventory for Izmir. The generated emission inventory is used as input for CMAQ air quality model along with the prepared meteorology model, WRF, outputs to understand distribution of air pollution over the region. These data along with the air quality model runs conducted with TNO emissions inventory is used to understand the impact of change in different emissions estimation in Izmir.

# 2. METHODOLOGY

## 2.1. Study Area

Izmir is the third most populated metropolitan city in the western Turkey. According to Turkish Statistical Institute report which is based on Address Based Population Registration System (2015), it has 4 million population distributed over a land area of 12012 $km^2$ and population density is approximately 350 person/$km^2$. The city's land is between 26° 52' E and 27° 19' E longitudes and between 38° 19' N and 38° 32' N latitudes (Figure 2 .l). There are Aegean Sea and Aegean Islands on the west, Manisa on the east, Balıkesir on the north and Aydın on the south of the city. Izmir is composed of the following districts: Aliaga, Balcova, Bayındır, Bergama, Beydag, Bornova, Buca, Ceşme, Cigli, Dikili, Foca, Gaziemir, Guzelbahce, Karaburun, Karsiyaka, Kemalpasa, Kınık, Kiraz, Konak, Menderes, Menemen, Narlidere, Odemis, Seferihisar, Selcuk, Tire, Torbali and Urla. It is described as the cultural and industrial center of Aegean Region and Turkey. The northern part of the city has been mostly developed as industrial zones, and the eastern district has been mostly determined by agriculture, and the western and the southern district have tourism and residential areas. The country's only shipbreaking area is located in the province. The elevation of city center is 35 m, but the altitude of city changes up to 1000 meters height in the east side. The distribution of city population depends on employment distribution as well as topographic conditions. Therefore, the population decreases from west to east and it is higher in the coastal zone due to mild climatic conditions and growing employment opportunities in Izmir. The number of motor vehicles has expanded essentially due to rapid increase in population and economic development (Increased from 300,000 in 1990 to 1,150,817 in 2015) (Turkish Statistical Institute, 2015).

**Figure 2.1:** The satellite view of İzmir.

Izmir has a Mediterranean climate that is characterized by long, hot and dry summers and mild to cool, rainy winters. July and August are the hottest and January and February are the coldest months in İzmir. In İzmir, snowfall does not occur; the maximum snow cover was 8 cm in 1979 (Turkish State Meteorological Service, 2015). Sea breeze is seen in hot summer and this wind type occurs difference of heating and cooling of sea and land in day and night (Izmır Provincial Directorate of Environment and Urban Planning, 2015). Dominant wind direction is north-northeast for Gaziemir station as can be seen in the Figure 2.2 in İzmir (Distribution stayed almost the same between 2008 and 2015).

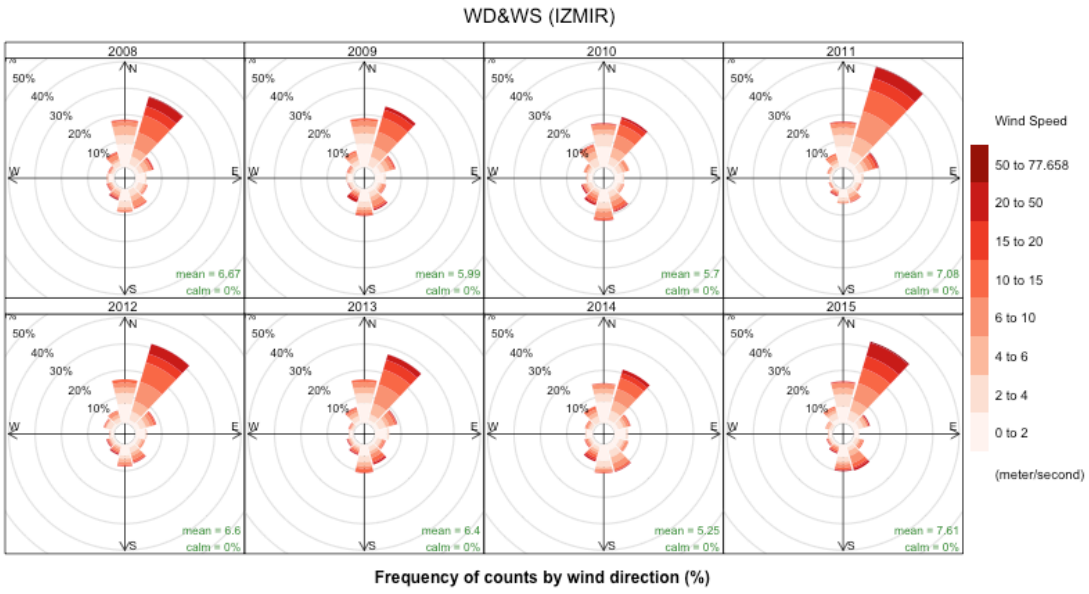


**Figure 2.2:** The wind speed and direction in İzmir.

## 2.2. Air Quality and Meteorology Observations

### 2.2.1. Air quality monitoring stations

The monitoring network contains 8 stations, which are operated by the Turkish Ministry of Environment and Urbanization. These stations are located at Alsancak, Bayrakli, Bornova, Çigli, Gaziemir, Guzelyali, Karsiyaka and Sirinyer. Pollutants measured at each station is provided in Table 2.1 and their locations are given in Figure 2.3.

**Table 2.1:** The measured pollutant at air quality stations in Izmir.

| Pol./Sta. | Alsancak | Bayraklı | Bornova | Çiğli | Gaziemir | Güzelyalı | Karşıyaka | Şirinyer |
|---|---|---|---|---|---|---|---|---|
| $PM_{10}$ | + | + | + | + | + | + | + | + |
| $SO_2$ | + | + | + | + | + | + | + | + |
| CO | + | - | + | - | - | + | + | + |
| NO | + | - | + | - | - | + | + | + |
| $NO_X$ | + | - | + | - | - | + | + | + |
| $NO_2$ | + | - | + | - | - | + | + | + |


**Figure 2.3:** Locations of air quality stations in Izmir.

### 2.2.2. Meteorological monitoring stations

There are 5 meteorological stations in İzmir, which belong to the Turkish State Meteorological Service (Figure 2.4). These are Izmir (Center), Çigli, Gaziemir (Adnan Menderes), Cesme and Dikili stations. These stations are synoptic weather observation stations. Synoptic observation stations that have all meteorological parameter measurements every three hours is a basic type used for weather observation (Karakas, 2015). The soil temperature, wind, temperature, humidity, precipitation and pressure parameters are measured at these stations. Temperature, wind speed and direction data were used in this study.


**Figure 2.4:** Locations of meteorological stations in Izmir.

## 2.3. Model Domain & Modeling

### 2.3.1. Model domain

In this study, EPA's Models3 framework was used to quantify the impact of different emission sectors on air quality over Izmir. 2-nested WRF simulations were performed and meteorological model domains were given Figure 2.5. Mother domain contains Europe, a major part of Asia and a minor part of North Africa (30km x 30 km resolution), second domain covers Balkans and Turkey (10 km x 10 km resolution). The first and main domain (d01) covering Europe of 191 x 159 grid

cells, the second domain covering the Balkan region and Turkey (d02) contain 241 x 154 horizontal grid cells, and 35 vertical layers. The vertical resolution is stretched from approximately 93 m above the surface and increased to 16 km.

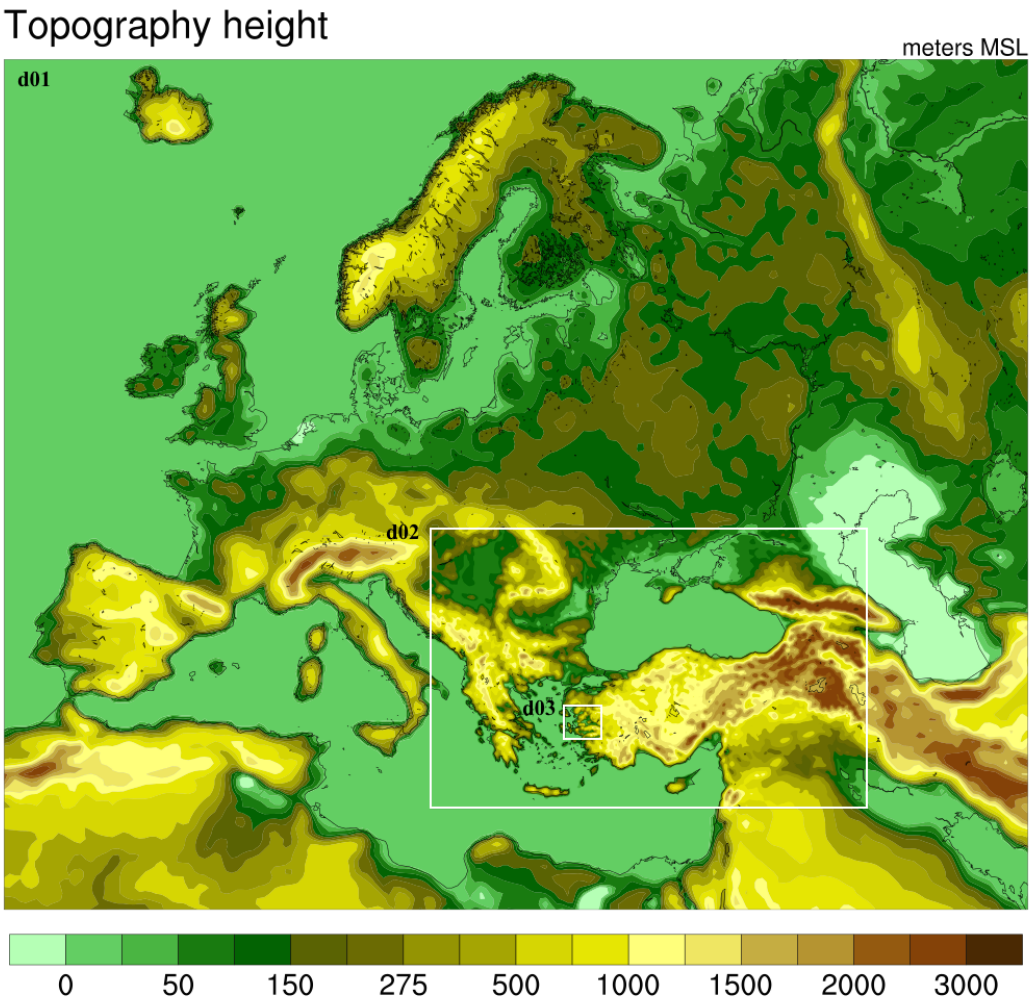


**Figure 2.5:** The 2-nested Models-3 domains.

### 2.3.2. Models3 air quality modeling framework

The EPA Community Multiscale Air Quality (CMAQ) modeling framework is a third-generation air quality modeling system. This framework includes meteorological modeling, air quality modeling, initial and boundary data processing, photolysis rate estimation, and emissions processing (Figure 2.6). Details of this figure are given below for different processes.

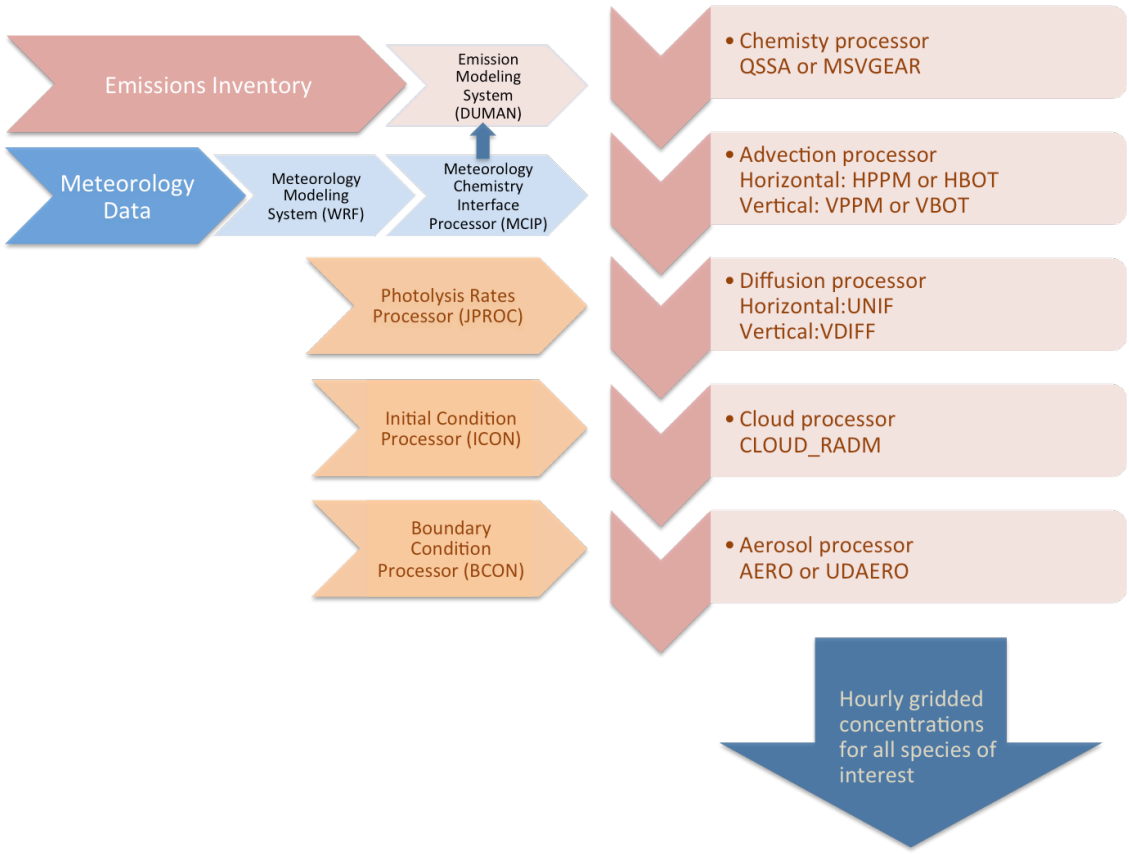


**Figure 2.6:** CMAQ modeling system flow chart.

### 2.3.2.1. The community multi scale air quality model (CMAQ)

CMAQ is intended for applications running from administrative and arrangement examination to comprehension the complex communications of atmospheric chemistry and physic. It is a three-dimensional Eulerian (i.e.,gridded) atmospheric chemistry and transport modeling framework that reproduces ozone, particulate matter (PM), toxic airborne pollutants, visibility, and acidic and nutrient pollutant species all through the troposphere that compute a mass equalization inside of every grid cell by solving the transport across each cell boundary and chemical transformations within each cell throughout a given time period. As a structure for simulation interactions of several complex atmospheric procedures, in this way; CMAQ requires two essential sorts of inputs: meteorological data, and emission rates from sources of emissions that influence air quality (CMAQv4.7.1 Operational Guidance, 2010). CMAQ is comprised of chemistry, advection, diffusion, aerosol and cloud processors. All these modules are linked to each other and solved numerically. CMAQ model requires hourly three-dimensional gridded

meteorological data. Meteorological models are created to research climatic occasions and generate input data for chemical transport models.

To obtain inputs on emissions, CMAQ relies on an emissions model to estimate the magnitude, location, and temporal variability of pollution sources, so DUMAN was used for this process. Before the DUMAN processing, there are five essential parts and these are:

- The initial condition processor (ICON)
- The boundary condition processor (BCON)
- The clear-sky photolysis rate calculator (JPROC)
- The Meteorology-Chemistry Interface Processor (MCIP)
- The CMAQ Chemistry-Transport Model (CCTM)

Firstly, the specific chemical mechanism clear sky photolysis rates were calculated according to fixed altitudes, solar hour angles and latitude bands from absorption cross section and quantum yield data at JPROC section. The main design alternative required for JPROC is the choice of the chemical mechanism to use in the modeling. The output from JPROC is an ASCII look-up table of photolysis rates that CCTM uses to compute gas-phase chemical changes and pollutant concentration. Second process of CMAQ modeling system is Initial Condition Processor (ICON) part. A gridded binary netCDF file of the chemical conditions in the modeling domain was generated for the first hour of simulation. ICON configuration selections contain chosen the chemical mechanism to model. Carbon bond chemical mechanism (CB-V) and aerosol mechanism (AERO5) were used in this study. The calculation of sea-salt emissions were used AERO5 (Im et al., 2010). In addition to that, ACM modules were used for cloud simulation option, respectively. Chemical kinetics was solved by Euler backward approximation (EBI) that depends on nonlinear differential mathematical statements (Hertel et.al, 1993). Third part of the model system is Boundary Condition Processor and it creates a gridded binary file of chemical conditions throughout the horizontal boundaries of the model domain. BCON create time-varying boundary conditions differently from ICON. The output files from the WRF model were used for create netCDF-formatted input meteorology data that are used by DUMAN and by CMAQ in MCIP. This part plans and determinations every single meteorological field that are needed for DUMAN and CCTM. Structure of MCIP contains the time periods that extract data from the meteorological model

outputs, horizontal and vertical grid description, options for calculation of dry deposition velocities and integrating satellite cloud observations into MCIP output. CCTM is the last part of CMAQ, it incorporates the output from other programs (JPROC, BCON, ICON and MCIP) and additionally CMAQ emissions inputs (e.g. output from DUMAN) to simulate continuous atmospheric chemical conditions. In this study, CMAQ version 4.7.1 was used to figure out regional air quality. 35 vertical layers used in WRF simulation were reduced to 24 layers for the CMAQ simulation.

#### 2.3.2.2. The weather research & forecasting model (WRF)

Meteorological models are created to research climatic occasions and generate input data for chemical transport models. In this study Weather Research and Forecast (WRF) was used as the meteorological model. The WRF model is a next-generation mesoscale numerical weather prediction framework intended for both atmospheric research and operational forecasting needs. WRF can create atmospheric simulations utilizing real data (observations, analysis) or ideal case. The WRF system involves two dynamical solvers, and these are ARW (Advanced Research WRF) core that was developed and maintained by the MMM Laboratory, and the NMM (Nonhydrostatic Mesoscale Model) core that was developed by the National Centers for Environmental Prediction. National Center for Atmospheric Research (NCAR), the National Oceanic and Atmospheric Administration (represented by the National Centers for Environmental Prediction (NCEP) and the Forecast Systems Laboratory (FSL)), the Air Force Weather Agency (AFWA), the Naval Research Laboratory, the University of Oklahoma, and the Federal Aviation Administration (FAA) collabration improved WRF.

In Figure 2.7 was shown steps of WRF running. “geogrid.exe” part of WRF is to characterize the simulation domains and interpolate different terrestrial data set to the model grids. The motivation behind “ungrib.exe” is to open GRIB file (GRIB1&GRIB2) meteorological information data and pack it into an intermediate file format. The next step of modeling is “metgrid.exe” that is to horizontally interpolate the meteorological data onto model domain; the output from this part is used as input to WRF. “real.exe” step vertically interpolates the met_em* files, produce boundary and initial condition files, and then “wrf.exe” produces the model forecast. First three steps are preprocessing system of WRF and they are WPS,

while the others are WRF. WRF model version 3.6 was set up for days between 00:00 UTC January 1, 2010 and 00:00 UTC January 31, 2010.

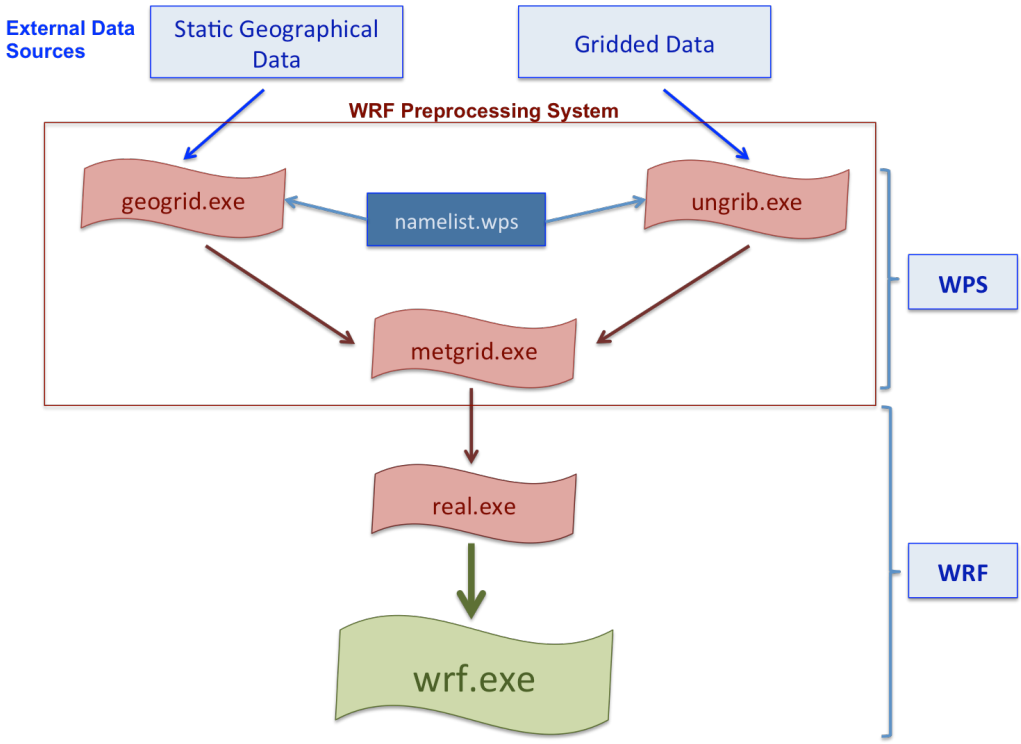


**Figure 2.7:** WRF modeling system flow chart.

### 2.3.2.3. Emission inventory

The emissions are any sort of substance discharged into the air from natural or anthropogenic sources such as flows of gases; liquid droplets or solid particles and these particles cause important wellbeing and natural problems. All these natural problems are specifically identified with the emissions of substances to air. Dependable emission inventories are an essential to comprehend these environmental problems and to create effective moderation alternatives (Kuenen et al., 2014). The measure of air pollutants in a region relies on upon the number and size of emission sources, alongside the weather condition and topography of area. The spatially dispersed emissions need to cover the entire area, and identify the emissions in a consistent way, i.e. in all nations the same sources ought to be contained, and these sources ought to be surveyed as precisely and reliably as would be possible (Kuenen et. al, 2014). Emission inventories are regularly created by utilizing a base up methodology, i.e. consolidating accessible measurements on fuel combustion,

industrial creation, transportation etc. with the most suitable emission factors (Seinfield & Pandis, 1998). As it is seen Figure 2.8, the most important part of model is presence of reliable emission inventory and it required for good air quality management system.

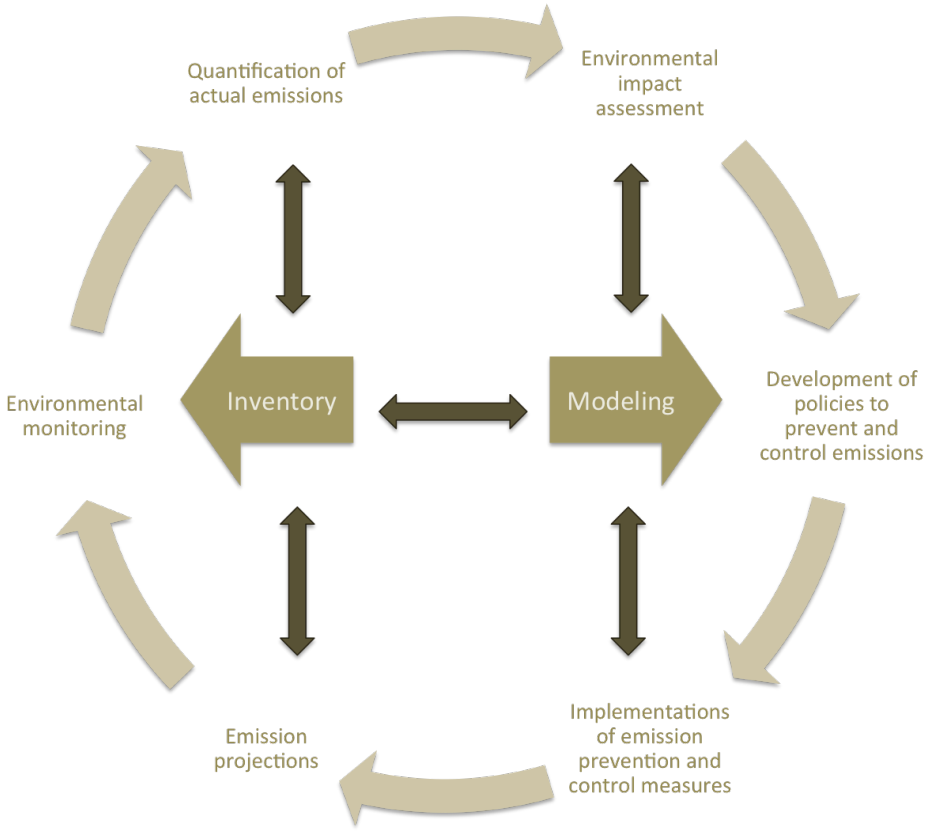


**Figure 2.8:** Roles of the emission inventory for air quality management.

Emissions generally classify in two groups as anthropogenic and biogenic. Anthropogenic emission sources are separated into for the most part four groups by looking emitting attributes: Point sources, area sources, mobile sources are the main anthropogenic sources. Point sources are stable and discrete sources of emissions that can be identified by name and area. Power plants, modern boilers, petroleum refineries, mechanical surface coatings and substance fabricating commercial enterprises are defined as point sources. The emissions of point sources are released from stacks. The major emitters of nitrogen oxides ($NO_x$) and certain part of VOCs were originated from point sources.

Area sources contain prescribed burning, residential wood use, light industry, and other residential, commercial and institutional sources. Despite the fact that emissions from individual zone sources are moderately small, collectively their

emissions can be of concern-particularly where large numbers of sources are located in heavily populated areas (Im, 2009). Area sources are important contributors of particulate matter and volatile organic compound (VOC) emissions.

Mobile sources are classed as highway and off-highway sources. The automobile, bus, truck and other vehicles are included in mobile sources. CO, HC, $NO_x$ and PM emissions were obtained from highway vehicles especially in cities (Unal et. al, 2004). The emission from highway vehicles represents one third of the overall national (VOC) and 40 percent of the overall ($NO_x$) emissions. Mobile sources are responsible around 75 percent of carbon monoxide emissions and more oxides of nitrogen pollution than area or point sources. Motor vehicle commitment to carbon monoxide emission can surpass 90 percent in urban areas. In a common urban region, in any event half of the hydrocarbon and nitrogen oxide emissions were originate from vehicle sources (Im, 2009). Biogenic emissions were come from natural sources, such as plants and trees. Biogenic emissions are identified biogenic volatile organic compounds and biogenic volatile organic compounds (BVOCs) originate from vegetation for natural areas, crops, and urban vegetation. BVOC emissions are functions of the species leaf mass, emission factors, temperature, and light conditions. Generally, only the emissions from vegetation and soils are incorporated, but other related sources contain volcanic emissions, lightning, and sea salt. The reason being BVOC emission important for the air quality model is input for their formation because of they are source for secondary pollutants such as ozone and secondary organic aerosols. Therefore, Guenther, et al., 1995 developed Global-Model of Natural Volatile Organic-Compound Emissions in 1995.

Emission factors and emissions producing activity data are used to develop inventory. An emission factor is the amount of pollutant produced per unit activity. TNO/MACC-II emission inventory was developed for AQ requirement and users' specific needs. The TNO/MACC-II inventory was developed using the official reported emissions (EMEP-CEIP), before quality of report data is checked. This control system contains errors, incompleteness, unknown values, countries' resubmission, modifications of reports, methods change, etc. Alternative data from the **I**nternational **I**nstitute for **A**pplied **S**ystems **A**nalysis **G**reenhouse Gas and **A**ir Pollution **In**teractions and **S**ynergies model (IIASA GAINS) (http://www.gains.iiasa.ac.at/models/) or TNO defaults were used to fill the blanks.

Anthropogenic emission sources have been classified into ten various Standard Nomenclatures for Air Pollution (SNAP) categories. The available data include annual total emissions of CO, $NH_3$, NMVOC, $NO_X$, $PM_{10}$, $PM_{2.5}$, and $SO_2$ for area and point sources and they were categorized ten SNAP categories. In addition to these, SNAP7 separates five categories in it and these are:

- **SNAP1:** Energy industry
- **SNAP2:** Residential-commercial and other combustion
- **SNAP34:** Industrial combustion
- **SNAP5:** Extraction distribution of fossil fuels
- **SNAP6:** Product use
- **SNAP7:** Road transport
    - **SNAP71:** Road transport exhaust emissions, gasoline
    - **SNAP72:** Road transport exhaust emissions, diesel
    - **SNAP73:** Road transport exhaust emissions, other fuels
    - **SNAP74:** Road transport non-exhaust emissions, evaporation of gasoline
    - **SNAP75:** Road transport non-exhaust emissions, road, brake and tyre wear
- **SNAP8:** Other mobile sources
- **SNAP9:** Waste treatment and disposal
- **SNAP10:** Agriculture

In this study, TNO/MACC-II emission inventory was used with a high-resolution (~ 7 km x 7 km) stable distribution patterns for road transport, industry and non-industrial combustion. To decide a consistent inventory, a new inventory was created with compiling current data and compare with of TNO/MACC-II inventory. Emission inventory was created with calculated and collected emission data for Izmir. SNAP 7, SNAP 2 and SNAP 34 were focused for sensitivity analysis throughout this study.

There are three different ways for the calculation of emission such as the direct measurement method, material balance method and emission factors method. Emission factors, which were used in this study, were given in Table 2.2.

E = A x EF x (1-ER/100) (Equation 1)

E = emissions

A = activity rate

EF = emission factor

ER = overall emission reduction efficiency, %

Three types of emission factors can be used to prepare emission inventory,

a) Mass of emissions per mass of fuel burned (g / kg dry fuel or g/m3 gas- liquid fuel)

b) Mass of emissions per unit of heat delivered (g/mJ)

c) Mass of emissions per unit time of activity (g/hr)

**Table 2.2:** Emission factor of the study as natural gas ($g/m^3$), import coal (kg/ton), domestic coal (kg/ton) (EPA, 2008; Durmaz et. Al, 1993).

| Fuel Type | Natural gas | Import coal | Domestic coal |
|---|---|---|---|
| **PM** | 0.12 | 5.00 | 40.00 |
| **$SO_2$** | 0.01 | 25.93 | 24.37 |
| **CO** | 0.64 | 0.30 | 137.50 |
| **VOC** | 0.13 | 4.00 | 0.02 |
| **NOX** | 1.51 | 1.50 | 2.90 |

In this study, the emission data of point sources obtained from Izmır Provincial Directorate of Environment and Urban Planning. There are the measurement of stack height, pollutants and emission values each pollutant (with different units) for all industrial plants in acquired dataset. After all different formal correction of data, all units were converted from various units to ton per year a by working days/hours of industry. This unit conversion process has led to analyze the dataset easily. In addition to that, there is no need for any further changes of data given as input to the model.

Emissions of area sources, residential heating, are calculated by using activity data for that is obtained from Izmir Provincial Directorate of Environment and Urban Planning. Common fuels for residential heating are natural gas, domestic and import fuel in the city. District based monthly natural gas consumption and yearly coal (import and domestic) selling amount is used for emission calculations. Methodology method for emission calculations requires activity data that include fuel consumption and emission factors for each pollutant and fuel. For the calculations, the activity data is multiplied with emission factors of the pollutants for each fuel after unit conversions.

The mobile source emissions were calculated with **Co**mputer **P**rogramme to Calculate **E**missions from **R**oad **T**ransport (COPERT 4), which was developed by the Laboratory of

Applied Thermodynamics of the Aristotle University of Thessaloniki (EMISIA, 2006). COPERT 4 is a software tool commonly used to calculate air pollutant and greenhouse gas emissions from road transport. COPERT 4 predict emissions of all major air pollutants (CO, $NO_x$, VOC, PM, $NH_3$, $SO_2$, heavy metals) generated by various vehicle types (passenger cars, light commercial vehicles, heavy duty trucks, busses, motorcycles, and mopeds) as well as greenhouse gas emissions ($CO_2$, $N_2O$, $CH_4$). Also, this program provides speciation for $NO/NO_2$, elemental carbon and organic matter of PM and non-methane VOCs, containing PAHs and POPs. COPERT 4 model needs input parameters and these are:

- Mean fleet mileage
- Mileage per year
- Population
- Urban road speed per hour
- Rural road speed per hour
- Highway road speed per hour
- Urban road share percentage
- Residential road share percentage
- Urban road share percentage
- Fuel tank size
- Canister size
- Fuel injection percentage
- Evaporation control percentage
- Distribution of evaporation emissions to different driving modes percentage
- Monthly minimum and maximum temperatures
- Reid Vapor Pressure (RVP)
- Annual fuel consumption
- Fuel type (content)

As a result, the obtained data from TUVTURK and TSI for Izmir was processed in COPERT4. The output of COPERT was given as input file of traffic emissions to the model. SNAP7 category (SNAP71, SNAP72, SNAP73, SNAP74 and SNAP75) was created with the values by calculated COPERT4. After calculation of all emission, TNO inventory was modified using as calculated emission values dependent source type and updated inventory was generated for Izmir.

# 3. RESULTS

The first step in analysis is the determination of air quality levels in Izmir. Hourly $PM_{10}$ and $SO_2$ measurements of eight stations are investigated for Izmir. When the air quality station data examined, the exploratory data analysis method that is time series analysis, hierarchical cluster analysis and box plot analysis are applied to dataset. In this step meteorological analysis is conducted for temperature, pressure, wind speed and wind direction. The following step of analysis is emission evaluation section. This section includes examination about using emission inventory and calculated emission inventory. The comparison of TNO inventory and our inventory is done in this part of the study. The last analysis of the study is model evaluation. After that, the performance analysis of WRF-model and CMAQ model is examined. Finally, in order to determine maximum response to our modification the day, which has the maximum $PM_{10}$ difference concentration between our CMAQ output and TNO CMAQ output, was selected. For this day, detailed analysis was done and concentration difference map was presented. Moreover, hourly concentration differences during the selected day were analyzed. The hour that has maximum concentration differences was determined and map for this hour was presented at the end of this analysis. In addition to that, the same analysis was done for all pollutants ($SO_2$, $NO_2$ and CO) in appendix of the study.

## 3.1. Air Quality Evaluation

In Izmir, $PM_{10}$ concentrations were measured at eight-air quality station. All air quality observation data was investigated from 2009 to 2015. The boxplot analysis was done using averages of all station between the years of 2009-2015 and episode period was chosen as 2010 (Figure 3.1). These boxplot analyses explain distribution of $PM_{10}$ concentration data by years. The colored points on graph show outlier value of data. Each different color shows years in the data. Top of the boxes show upper quartile, bottom of the boxes is lower quartile of data. The middle line of boxes is median; the highest median was seen in 2010. Besides, the mean of measurement

data from 2010 is higher than other years. Average of these data is 63 µg/m$^3$, spread of quartile is small according to other year. Winter period is important part of this study due to domestic heating. Therefore, January 2010 was selected to see the effects of domestic heating.

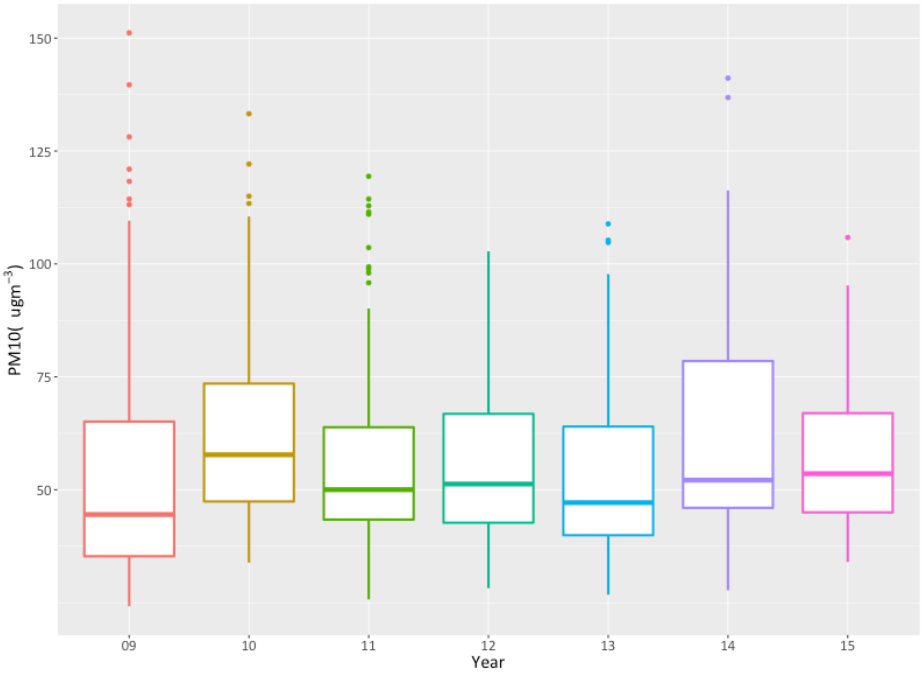


**Figure 3.1:** $PM_{10}$ concentration yearly box plot between the years of 2009-2015.

The following graphs were created to examine the period. The dates that are the maximum $PM_{10}$ values of the station are shown with colored boxes. (Figure 3.2). In the measurements, the maximum values for $PM_{10}$ were seen many stations in the same time period. Cigli station has high values during the January 2010. The maximum hourly $PM_{10}$ level was observed in Bayrakli station with 368 µg/m$^3$ on date of January 29, but Bayrakli station (and Guzelyali station, too) has many missing data, so it is not included in the chart. Following station, which has the highest hourly $PM_{10}$ level, is Sirinyer with 367 µg/m$^3$ on 27$^{th}$ January. On 27$^{th}$ January, Gaziemir is third station that has high $PM_{10}$ concentration values with 324 µg/m$^3$, too. The maximum daily $PM_{10}$ level was seen in Sirinyer and Cigli and these values were 60 µg/m$^3$ and 58 µg/m$^3$. However, the concentration of most of stations is approximately similar. The monthly mean and daily mean of $PM_{10}$ is close each other.

The dates that are the maximum $SO_2$ values of the station are shown with colored boxes. (Figure 3.3). When $SO_2$ concentrations of all stations were examining,

Karsiyaka and Bornova separated from other stations because of maximum $SO_2$ values. These maximum values are 47 µg/m$^3$ and 37 µg/m$^3$, respectively. Although; the annual averages suggest approximate values for the $SO_2$ concentrations.

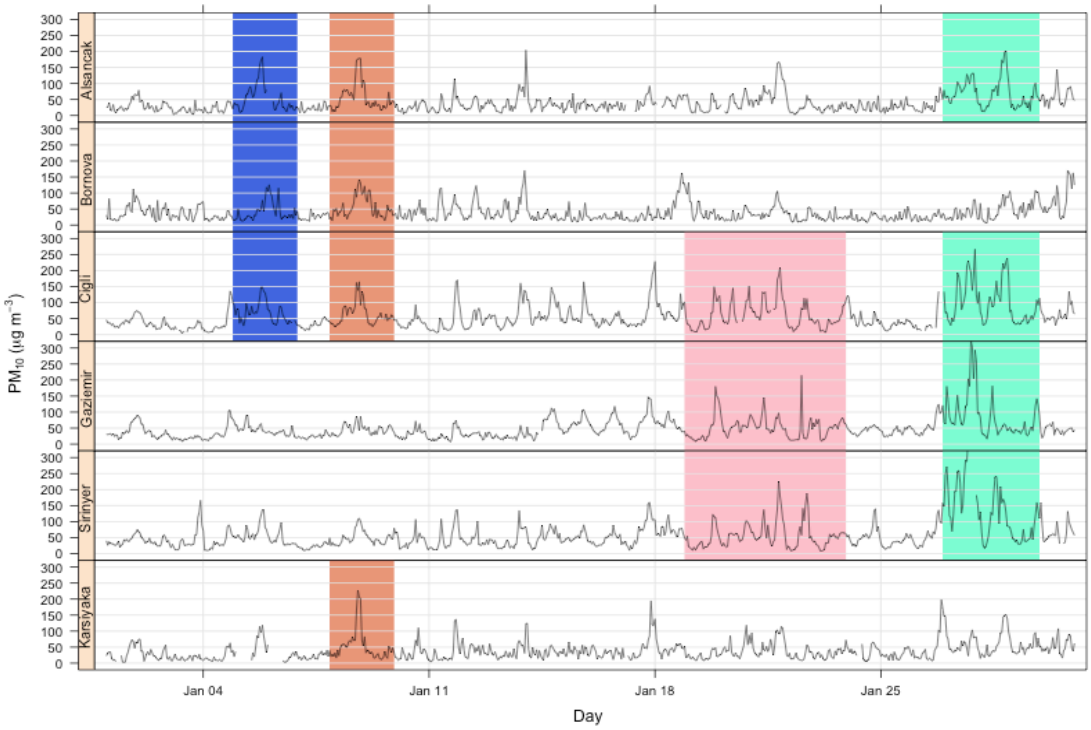


**Figure 3.2:** $PM_{10}$ concentration time series for determined episode in this study.

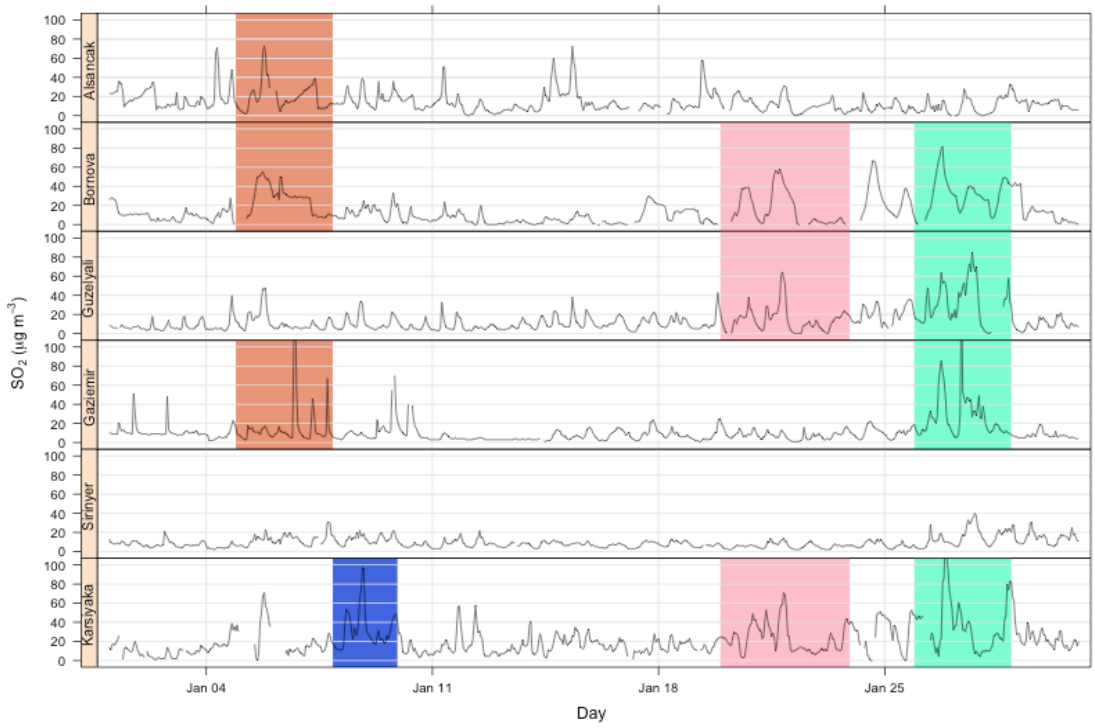


**Figure 3.3:** $SO_2$ concentration time series for determined episode in this study.

Hierarchical cluster analysis method is used to build a binary tree of the data that successively merges similar groups of points (Blei, 2007). This analysis results support previous analysis about $PM_{10}$ level in Izmir (Figure 3.4 & Figure 3.5). Bayrakli, Sirinyer, Cigli and Gaziemir separated from the other stations because of high $PM_{10}$ level. Cigli and Gaziemir (Adnan Menderes Airport) appear similar in this analysis, but Şirinyer have higher value than Gaziemir and Cigli stations. Bayrakli has the highest $PM_{10}$ values in all stations. Karsiyaka, Alsancak and Bornova are the same cluster, but Bornova station is higher than the others at results of cluster analysis. Guzelyali and Sirinyer air quality stations have the lowest measurements in all stations. This situation may be caused by locations of the stations. For example, Bayraklı where is in the center of the city has higher $PM_{10}$ and $SO_2$ concentrations due to high population. On the other hand, Gaziemir and Cigli where are in sub-urban areas of city have lower pollutant concentrations with respect to center of Izmir.

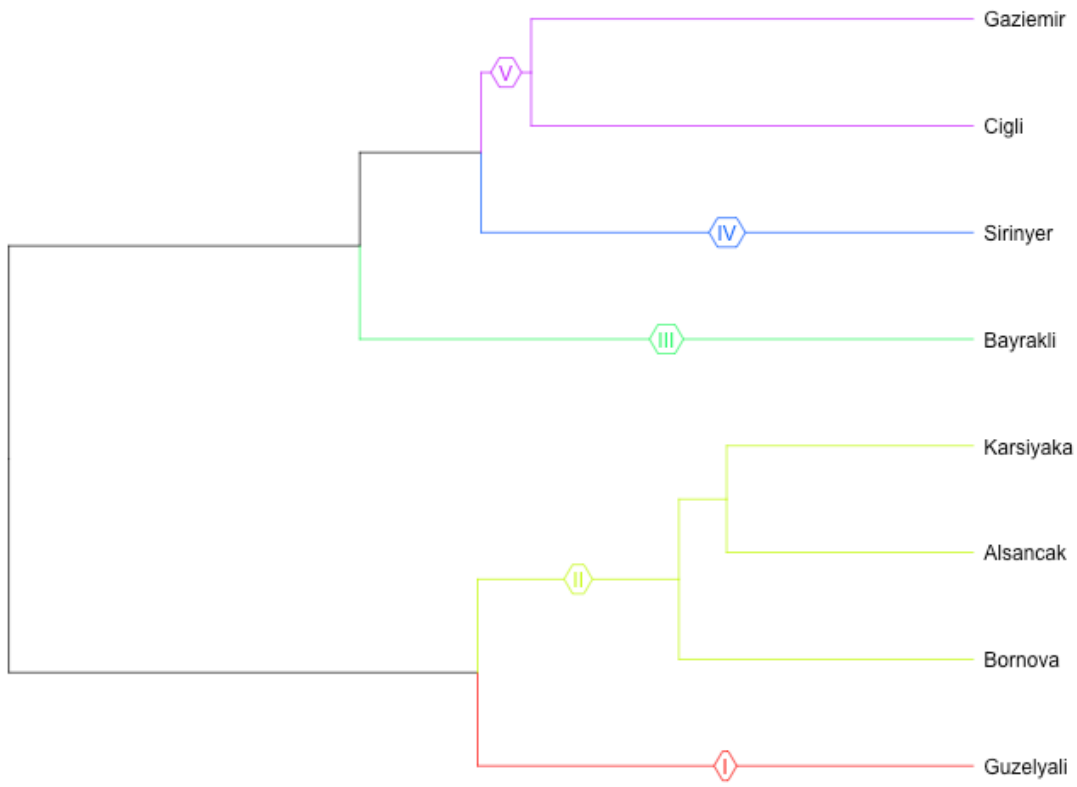


**Figure 3.4:** Hierarchical cluster analysis for $PM_{10}$ concentration in 2010.

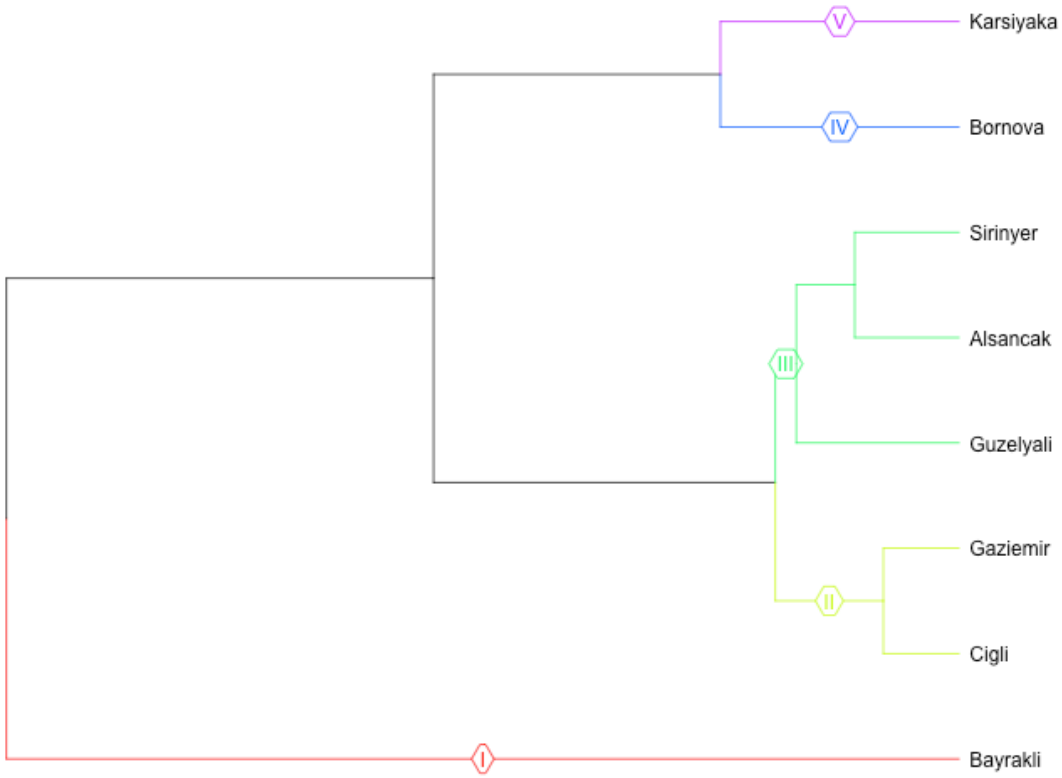


**Figure 3.5:** Hierarchical cluster analysis for $SO_2$ concentration in 2010.

### 3.2. Meteorological Evaluation

Wind speed, wind direction, pressure and temperature as meteorological parameters were investigated in meteorological evaluation section. Meteorological stations and their coordinates are shown in Table 3.1. Wind speed and wind direction are the most important meteorological parameters for the air quality. Wind speed effects the dilution level while wind direction determines the areas that the pollutants will be transported. Wind roses were plotted for Izmir and the dominant wind direction was found for period of January 2010. The dominant wind directions are seen clearly in (Figure 3.6). More than 15 percent of wind direction is south (S) and near 20 percent of wind is north-east (NE) of January episode of 2010. In this Figure 14, when wind speed is higher than 10 m/s, wind direction is NE in general, its mean that wind is breeze in region. The 60 percent of wind speed measurements are calm as scale.

**Table 3.1:** Compared meteorological stations and their coordinates.

| Station | Longitude | Latitude |
|---|---|---|
| CİGLİ | 27.0603 | 38.4961 |
| AIRPORT | 27.1483 | 38.2944 |
| IZMIR(CENTRE) | 27.0603 | 38.3944 |
| CESME | 26.3147 | 38.3297 |
| DIKILI | 26.8981 | 39.0739 |

The air pressure is the most significant parameter for the air quality. Throughout high pressure systems, in general the air is still which allows pollution levels to get strong but during low pressure systems the weather is often wet and windy, causing pollutants to be dispersed or washed out of the atmosphere by rain. The mean sea level pressure is low during the January period except 26$^{th}$ January, mean sea level pressure is 1030 hPA on 26$^{th}$ January (Figure 3.7). The inversion can be seen in the region. This situation prevents the dispersion of air pollutants, because of the wind speed is low, it is not blow, air pollutant is not move away from source. If there is a high air pollutant values in the circumstances, it shows presence of local sources in the region. The explanation of this situation will be detailed based on episode in other sections.

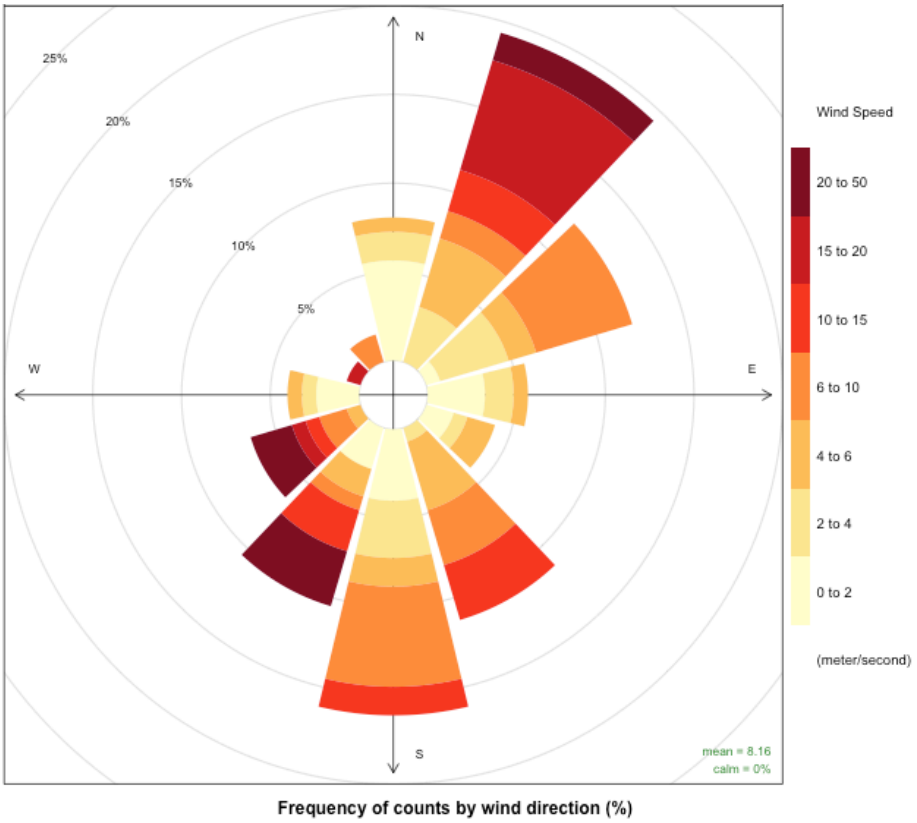


**Figure 3.6:** Wind direction frequency belongs to January 2010 period.

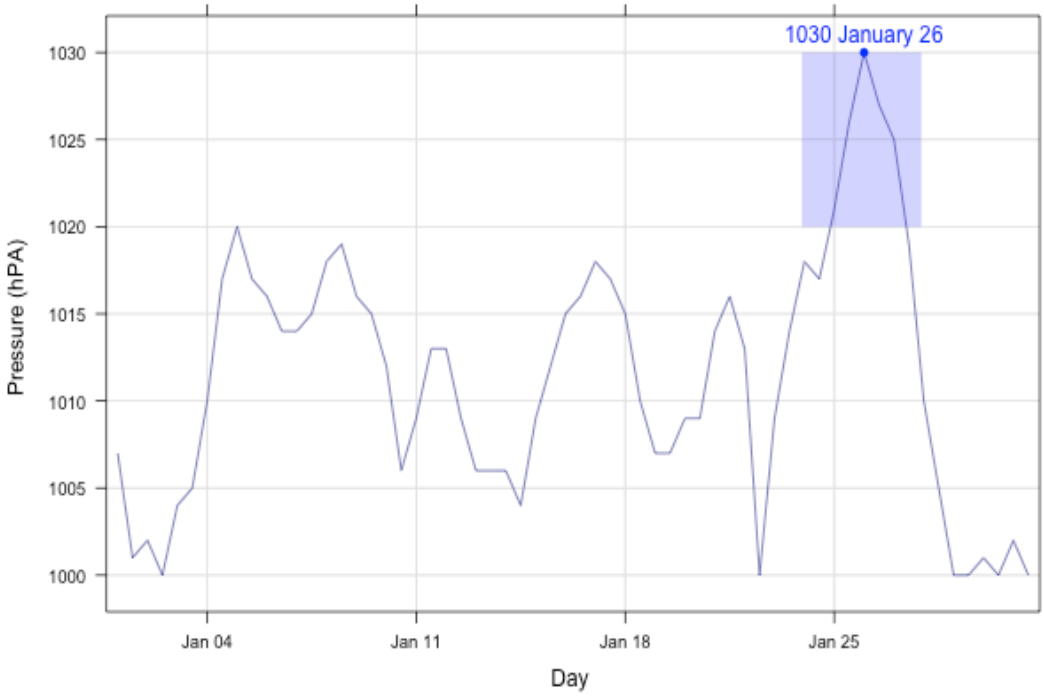


**Figure 3.7:** Mean sea level pressure belongs to January 2010 period.

### 3.3. Emission Evaluation

The annual emission calculation was made for pollutant groups of CO, $NO_x$, $SO_2$, NMVOC, $NH_3$, PM coarse (particulates between $PM_{10}$ and $PM_{2.5}$) and $PM_{2.5}$ for each source category are presented for TNO and our in Figure 3.8, respectively. Firstly, TNO emission inventory values will be explained, after that new created inventory will be introduced (Figure 3.8). Domestic heating (SNAP2) play a significant role for CO emissions, this source is responsible of 70.01% CO. The 12 percent of CO emission comes from SNAP71 in this inventory. SNAP34 is other important source for CO and it is at the rate of 10 percent. The most contribution of $NH_3$ emission comes from agricultural production considerably. 88.72% of $NH_3$ emissions originate from agricultural activities. In addition to that, $NH_3$ emission rate is 8% in SNAP34. NMVOC emissions emitted from industrial combustion in ratio of 39.28. Other sources of NMVOC are product use and road transport (especially gasoline and other fuels). NOx that is air pollutant emit from energy industry at the rate of 37%. The 28 percent of NOx emissions originate from industrial activities and third important source is road transport (SNAP72) according to TNO inventory. Finally, SNAP8 (non-road) is other important source (6%). Industrial activities (SNAP34),

domestic heating (SNAP2) and energy industry (SNAP1) play significant roles for $PM_{2.5}$ emissions and they are responsible of 50%, 24% and 19%, respectively. The similar results are true for PM course emissions. Energy industry and other industrial activities are most important rate, which is 45% and 46% for PM emissions. Combustion in manufacturing industry plays the major role in $SO_2$ emissions (70.31%). On the other hand, domestic heating is another major source for $SO_2$ emissions with 27.21 percent.

Figure 3.8 shows sources of CO, $NO_x$, $SO_2$, NMVOC, $PM_{10}$ and $PM_{2.5}$ emissions according to sectors for our inventory. Road transport (all categories for SNAP7) plays a major role in CO (28%), $NO_x$ (47%) and NMVOC (26%) emissions. The most important source of CO is industrial facilities at the rate of 67%. Energy industry (SNAP1) is important source for $SO_2$ emissions in Izmir. 80.1 percent of $SO_2$ emissions represent energy industry. Other major source of $SO_2$ is combustion in manufacturing and it is responsible of 17%. On the other hand, NOx emissions mostly come from energy industry (34%) and total road transport (47%). SNAP1 and SNAP34 is significant source for $PM_{2.5}$ emissions at the rate of 13.3% and 80%. Also, PMco is emitted from same source and the ratio is 45% and 46%.

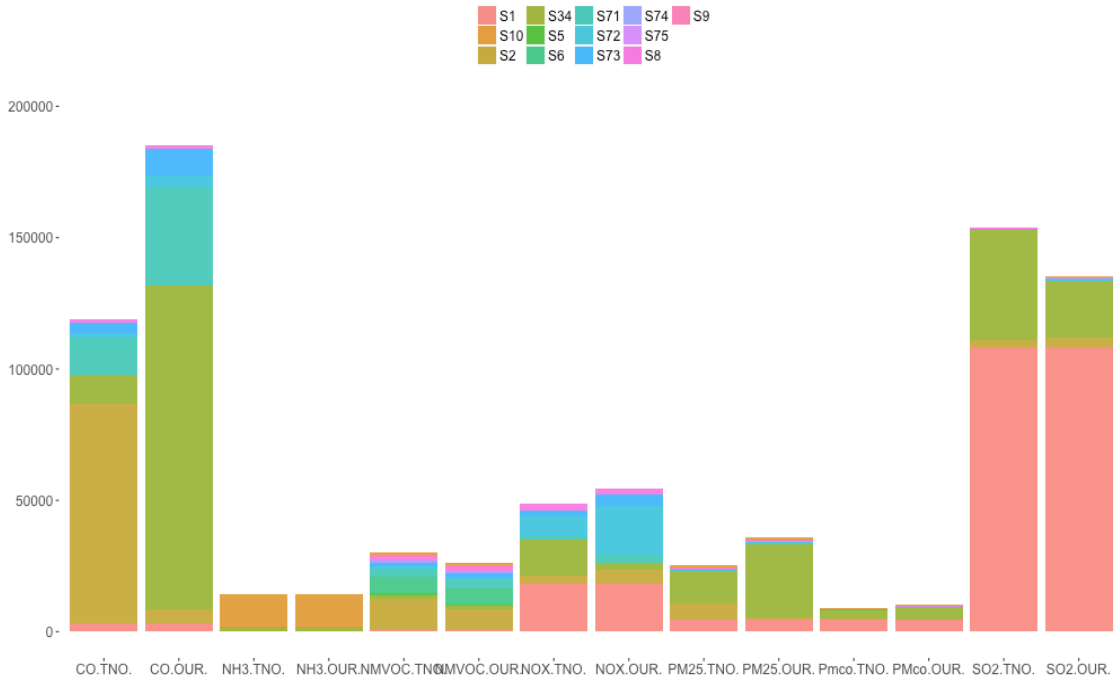


**Figure 3.8:** TNO&OUR emission inventory sectorial distribution each pollutant.

Table 3.2 shows that TNO emission amount belongs to 2009 data. Our emission values that are calculated with updated data represents in Table 3.3. Total emission amount of CO is 118,991 ton/year for TNO emission, but it is 185,224 ton/year in our inventory. Domestic heating has the maximum value for CO in TNO, however combustion process of production that is industrial activities emission is higher than domestic heating emission in our inventory. There is not $NH_3$ activity data, so TNO emission data was used when emissions calculated in the study. Total NMVOC emission is 30,235 ton/year in Table 3.3, but in our inventory this value is 24,731 ton/year. $NO_x$ emissions of TNO are 48,688 ton/year when it is 54,678 ton/year in our inventory. Total $PM_{2.5}$ and PMco emissions were increased in our inventory; when both of emissions were reduced in SNAP2, they were increased in SNAP34. When there is increasing $SO_2$ emissions in SNAP2, it is decreased for industry sector, which is SNAP34.

**Table 3.2:** TNO/MACC-II emission inventory in this study (ton/year).

| | **CO** | **$NH_3$** | **NMVOC** | **$NO_X$** | **$PM_{25}$** | **PMco** | **$SO_2$** |
|---|---|---|---|---|---|---|---|
| *SNAP-1* | 3353.18 | 35.26 | 716.53 | 18424.16 | 4714.61 | 4519.78 | 108180.33 |
| *SNAP-2* | 83301.13 | 138.39 | 11877.19 | 2854.91 | 5985.54 | 323.95 | 2767.36 |
| *SNAP-34* | 11251.78 | 1157.86 | 1330.39 | 13672.34 | 12429.00 | 3371.50 | 41867.10 |
| *SNAP-5* | 0.00 | 0.00 | 756.22 | 0.00 | 29.22 | 185.06 | 0.00 |
| *SNAP-6* | 0.00 | 0.00 | 6181.84 | 0.00 | 0.00 | 0.00 | 0.00 |
| *SNAP71* | 14183.82 | 77.94 | 3166.58 | 1390.30 | 60.94 | 3.54 | 27.48 |
| *SNAP72* | 1731.76 | 6.25 | 801.55 | 7883.09 | 391.16 | 10.58 | 332.04 |
| *SNAP73* | 3897.97 | 8.80 | 1572.33 | 1922.40 | 5.31 | 0.46 | 0.00 |
| *SNAP74* | 0.00 | 0.00 | 771.10 | 0.00 | 0.00 | 0.00 | 0.00 |
| *SNAP75* | 0.00 | 0.00 | 0.00 | 0.00 | 86.28 | 158.46 | 0.00 |
| *SNAP-8* | 1271.78 | 0.76 | 1259.98 | 2521.66 | 226.55 | 12.70 | 664.92 |
| *SNAP-9* | 0.00 | 173.01 | 998.59 | 0.00 | 477.01 | 0.00 | 0.00 |
| *SNAP-10* | 0.00 | 12574.81 | 803.47 | 19.94 | 722.30 | 509.82 | 21.35 |
| ***TOTAL*** | **118991.44** | **14173.08** | **30235.78** | **48688.80** | **25127.91** | **9095.85** | **153860.59** |

The calculated PMco emission is higher than TNO emission and their values are 9095 ton/year and 10,091 ton/year, respectively. In our inventory, $PM_{2.5}$ emissions are 35,458 ton/year, but it is calculated 25,127 ton/year by TNO inventory. Total $SO_2$ emission was decreased from 153,860 ton/year to 135,075 ton/year. The emission values belong to SNAP34, SNAP2, SNAP71, SNAP72, SNAP73, SNAP74 and SNAP75 were modified with re-calculated emission values. TNO emission values were used for other sectors and pollutants, which have missing data.

**Table 3.3:** The calculation of our emission inventory in this study (ton/year).

| | CO | $NH_3$ | NMVOC | $NO_X$ | $PM_{25}$ | PMco | $SO_2$ |
|---|---|---|---|---|---|---|---|
| *SNAP-1* | 3353.18 | 35.26 | 716.53 | 18424.16 | 4714.61 | 4519.78 | 108180.33 |
| *SNAP-2* | 5153.92 | 138.39 | 7702.89 | 5261.76 | 542.13 | 29.34 | 3613.17 |
| *SNAP-34* | 123247.71 | 1157.86 | 0.00 | 2599.41 | 28203.41 | 4661.05 | 21843.98 |
| *SNAP-5* | 0.00 | 0.00 | 756.22 | 0.00 | 29.22 | 185.06 | 0.00 |
| *SNAP-6* | 0.00 | 0.00 | 6181.84 | 0.00 | 0.00 | 0.00 | 0.00 |
| *SNAP71* | 37366.31 | 77.94 | 3166.58 | 3210.31 | 100.62 | 5.84 | 57.49 |
| *SNAP72* | 4562.21 | 6.25 | 801.55 | 18202.69 | 645.92 | 17.47 | 694.65 |
| *SNAP73* | 10268.94 | 8.80 | 1572.33 | 4438.98 | 8.77 | 0.75 | 0.00 |
| *SNAP74* | 0.00 | 0.00 | 771.10 | 0.00 | 0.00 | 0.00 | 0.00 |
| *SNAP75* | 0.00 | 0.00 | 0.00 | 0.00 | 142.46 | 261.67 | 0.00 |
| *SNAP-8* | 1271.78 | 0.76 | 1259.98 | 2521.66 | 226.55 | 12.70 | 664.92 |
| *SNAP-9* | 0.00 | 173.01 | 998.59 | 0.00 | 477.01 | 0.00 | 0.00 |
| *SNAP-10* | 0.00 | 12574.81 | 803.47 | 19.94 | 722.30 | 509.82 | 21.35 |
| ***TOTAL*** | **185224.06** | **14173.08** | **24731.09** | **54678.90** | **35813.0** | **10203.49** | **135075.90** |

Table 3.4 represents rate of emission change for TNO and OUR inventory (OUR-TNO). There are only 7 sectors in table. They are the most important sectors due to amount of emission and major emission source type, so they were calculated in this study especially. When these values were calculated, our inventory used as a base. For example, CO emissions were increased at the rate of 36%, totally. In SNAP2, CO emission reduction is high, but increasing CO emission is 91 percent and 61 percent in other sectors. SNAP 71, SNAP72 and SNAP73 were increased for all pollutant type such as CO (62%), $NO_x$ (57%), PMco (11%) and $SO_2$ (52%). NMVOC was decreased 16 percent in total. Increasing of $PM_{2.5}$ is 56% for SNAP34, change of $PM_{2.5}$ emissions is 29% and $PM_{2.5}$ emission was increased in value. PMco emission has been changed ten percent, positively. The 11 percent of NOx emission changed in SNAP34. In addition to them, change of $SO_2$ emission is 14 percent reduction. Other sector values were not given because of having same values with TNO inventory.

Table 3.5 represents change of emission and concentration by percentage. When $PM_{10}$ emission change was 25.62 %, $PM_{10}$ concentration decreased 5.19 %. On the other hand, when $SO_2$ emission was reduced at the rate of 14 %, concentration of this pollutant increased 3.48 percent in total. CO emission was increased percent of 35.76, but CO concentration decreased 6.83 %. When $NO_2$ emission was changed 10.96%, positively, concentration of $NO_2$ increased percent of 16.44. All results can

relate to different sectoral emission changes in this study. This changes effected results of pollutant concentration. As mentioned in Table 3.5 below, emissions of pollutants were given by percentage.

**Table 3.4:** Rates of emission change for TNO vs OUR inventory.

| | **CO** | **$NH_3$** | **NMVOC** | **$NO_X$** | **$PM_{25}$** | **PMco** | **$SO_2$** |
|---|---|---|---|---|---|---|---|
| *SNAP-2* | -1516% | 0% | -54% | 46% | -1004% | -1004% | 23% |
| *SNAP-34* | 91% | 0% | 0% | -426% | 56% | 28% | -92% |
| *SNAP71* | 62% | 0% | 0% | 57% | 39% | 39% | 52% |
| *SNAP72* | 62% | 0% | 0% | 57% | 39% | 39% | 52% |
| *SNAP73* | 62% | 0% | 0% | 57% | 39% | 39% | 0% |
| *SNAP74* | 0% | 0% | 0% | 0% | 0% | 0% | 0% |
| *SNAP75* | 0% | 0% | 0% | 0% | 39% | 39% | 0% |
| ***TOTAL*** | **36%** | **0%** | **-16%** | **11%** | **30%** | **11%** | **-14%** |

**Table 3.5:** Changes in concentration as a result of emissions changes (%).

| | **Change of emission (%)** | **Change of concentration (%)** |
|---|---|---|
| **$PM_{10}$** | 25.62 | -5.19 |
| **$SO_2$** | -13.91 | 3.48 |
| **CO** | 35.76 | -6.83 |
| **$NO_2$** | 10.96 | 16.44 |

Figure 3.9 shows emissions of TNO and our inventory. These maps were prepared with DUMAN outputs as an input to the CMAQ. On the left side total emission of $PM_{10}$, $SO_2$, CO and $NO_x$ as unit of ton/hour were given. The distribution of emission amount changes spatially. The maximum total $PM_{10}$ emission is 100 ton/hour in one grid city center. In addition to that, $SO_2$ emission is 900 ton/hour as maximum value on the maps. Total maximum CO emission is up to 1000 ton/hour. Total maximum $NO_x$ emission is 800 ton/hour in TNO inventory, but in our inventory, total maximum $NO_x$ emission is up to 1200 ton/hour in the city center, especially. Figure 3.10 shows emission amount differences of TNO and our emission inventory. CO and $SO_2$ only increased for this period, but $PM_{10}$ both increased and decreased with range of 40 and -10 ton/hour. CO emissions redoubled as noted earlier, so this situation appears in the figure clearly. $NO_x$ emission was increased 400 ton/hour by our inventory.

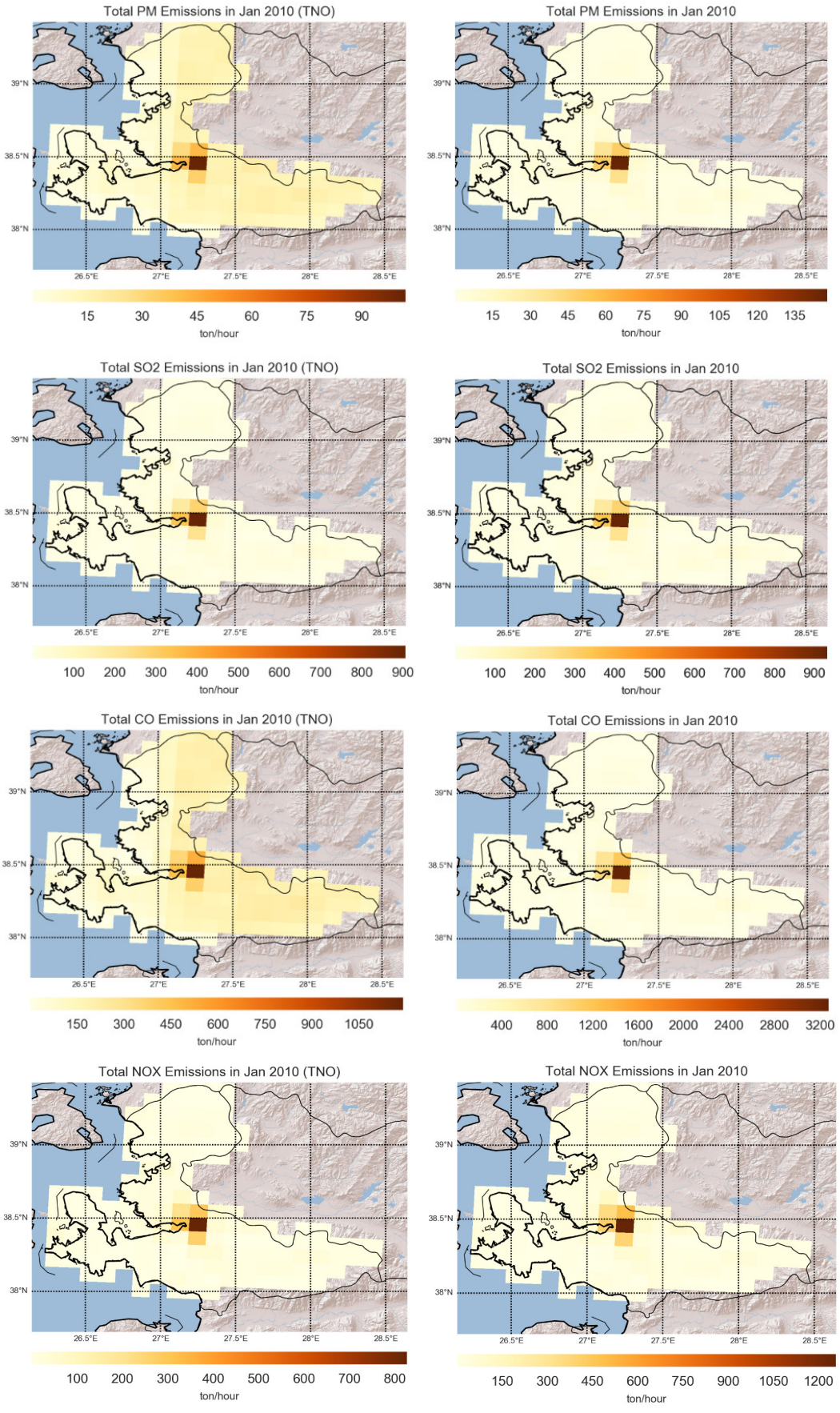


**Figure 3.9**: TNO vs OUR emission inventory for all pollutants in January 2010.

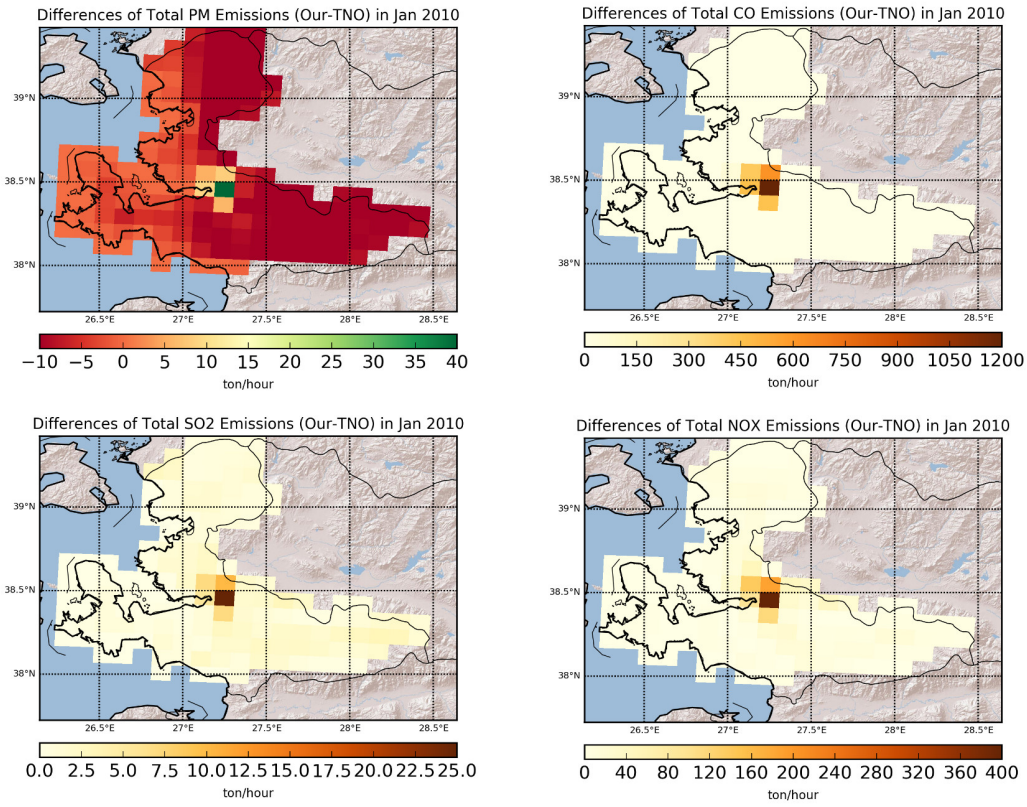


**Figure 3.10**: Emission differences between inventories (OUR-TNO) for all pollutants in January 2010.

## 3.4. Model Evaluation

### 3.4.1. WRF performance analysis

Temperature, wind speed and direction, which are meteorological parameters, selected for WRF model performance and the performance analysis were done for these parameters. Figure 3.11 shows monthly average of temperature, wind speed and prevailing wind direction in İzmir for January 2010. Monthly temperature results change between approximately 5°C and 13°C in January 2010. The temperature of coastal are is higher than the temperature of inner area in İzmir. This situation is normal due to mountain region in İzmir. At the same time city center temperature is lower than city surrounding. The city center temperature values change between the range of 7.5°C and 9°C. This is risk for air pollution because of domestic heating emission. If air temperature is lower in city, domestic heating increased and pollutant concentrations will increase coming from emission source. On the other hand, the maximum wind speed is 10 meter/second according to WRF (Figure 3.10). Wind rose taking by WRF output shows south-south east as prevailing wind direction.

According to observations, it was not more accurate result for wind direction. The model has done better prediction for high wind speed, but wind speed was lower than observation. However, when wind speed was high, wind direction prediction of this was true generally, this is important for pollutant dispersion for model system.

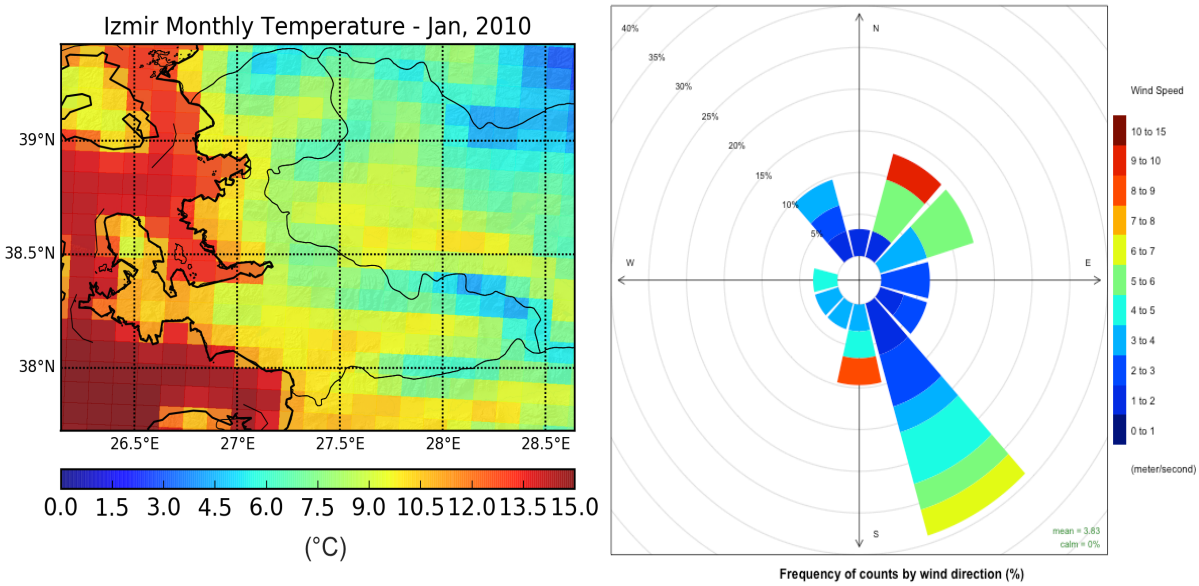


**Figure 3.11:** Monthly average of temperature and wind rose for İzmir, January 2010.

The time series of model output temperature were compared with daily observations provided by Turkish State Meteorological Service in Izmir. Adnan Menderes Airport was selected as a sample station. The comparison between WRF results and 2-meter temperature observations was presented in Figure 3.12. When the temperature and station data is evaluated together, it is identified that in the temperatures in 2 m, for the trend and temperature values the model does partially correct simulations. In the evaluations for the wind speed and direction, model results are not reliable when the wind speed is low but there are some deviations in some situations. There are some uncertainties in model for the wind direction and this is a possible result. WRF model underestimated parameters with observation results. The performance analysis shows trends between model and observation for wind speed values are under the station values. A trend is not significant parameter for wind direction because of each value describes each different wind direction, so model is similar with observations in some days.

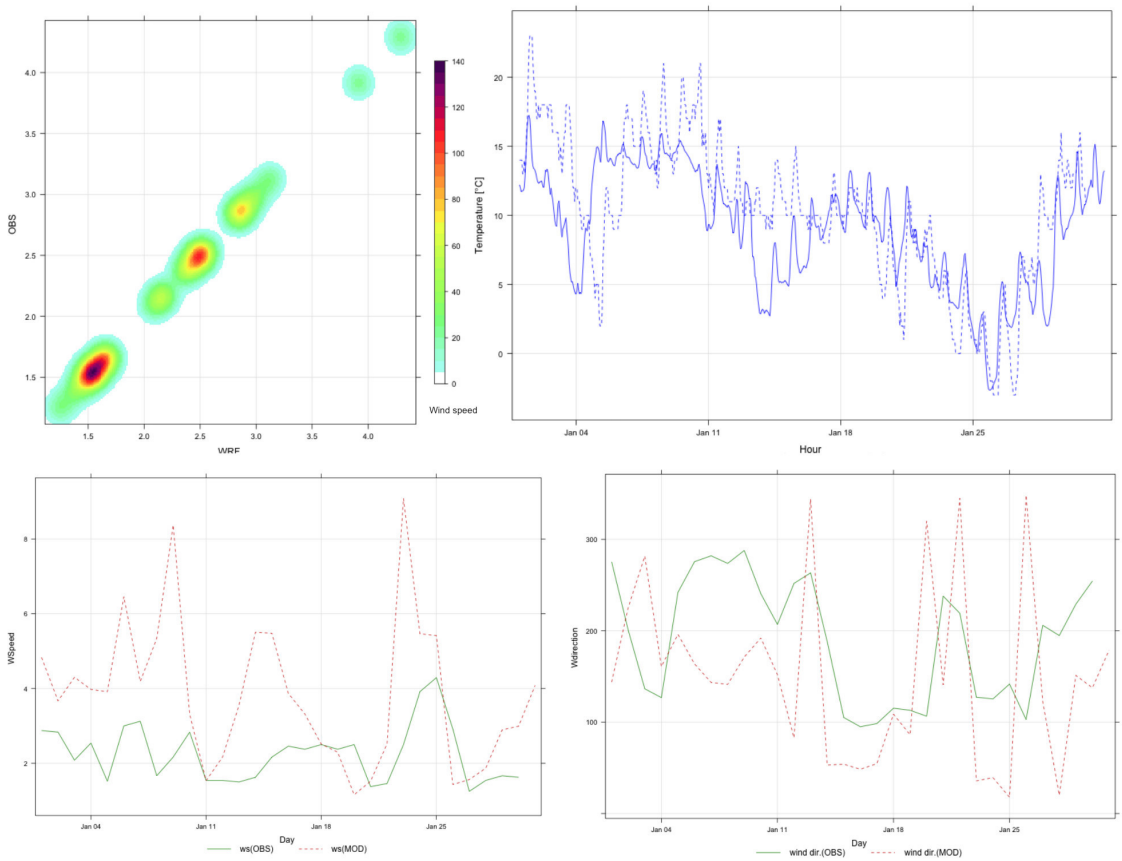


**Figure 3.12:** Wind speed and wind direction comparison (time series, scatter plot analyses) between model and observation, temperature performance analysis for January 2010.

In addition to analysis, difference between observations and our simulated WRF model outputs, statistical analysis was performed. These analyses contain MB, NMB, RMSE and r. Table 3.6 explains statistical relation between observation and WRF output with the help of different statistical parameters. The mean bias provides a good indication of the mean over or under estimate of predictions, (Patryla & Galeriua, 2011). Firstly, MB has negative value for each three parameters, this means model is under-predicted, especially wind direction, but results of this analysis can be significant parameter for wind speed and temperature, but it is not suitable analysis for wind direction. As mentioned before, each wind direction value describes each different wind direction**.** NMB means normalized mean bias that is useful for comparing values that covers different concentration scales. In addition to that, the mean bias is normalized by divided observations. NMB values are negative and small, it means that model is underestimated and observations have higher values for all scales. The RMSE is a commonly used statistic that provides a good

overall measure of how close modeled values are to predicted values (Carslaw, 2014). According to this information, wind direction, which was predicted by model, has not good results; it has the biggest one in all values. Correlation coefficient (r) changes in between -1 and 1. If r is 0 means that there is no linear relationship between the variables. Correlation coefficient of temperature is 0.71 and it is acceptable values in all results. r is 0.35 and 0.19 for wind speed and wind direction, it is bad result for model. Model run for 10x10 $km^2$ area, the reason of that, the model resolution is low. The differences between observations and the model results are high because of model gives average value for 10x10 $km^2$ area and model results quality decreases.

**Table 3.6:** Statistical relation between observation and WRF simulated results for wind speed, wind direction and temperature.

| OBS&WRF | MB | NMB | RMSE | r |
|---|---|---|---|---|
| **W. Speed** | -1.56 | -0.41 | 2.39 | 0.35 |
| **W. Direction** | -41.39 | -0.22 | 114.09 | 0.19 |
| **Temperature** | -1.27 | -0.12 | 4.02 | 0.71 |

### 3.4.2. CMAQ performance analysis

In this section, CMAQ air quality model outputs were investigated with different analysis methods. Firstly, pollutant concentrations were analyzed using spatially. Figure 3.13 shows TNO concentrations and difference concentration values between our and TNO outputs. The maximum concentration values of all pollutants appear in city center. $PM_{10}$ differences increased in the city center, but it is reduced out of city center. This is related to the spatial distribution of sectors such as road transport, industrial facilities and domestic heating. In this study, these three sectors' emission values were changed and this variation effects concentrations of spatial distribution. For example, the difference is high in industrial area because of increasing of SNAP34. On the other hand, $PM_{10}$ emissions were reduced in SNAP2 that is domestic heating emission. When the spatial distribution of concentrations is examined, concentrations are reduced in these areas, which has domestic heating source. Besides, there is the same situation for CO concentrations. $NO_2$ concentrations increased 6 $mg/m^3$ totally. Maximum $NO_2$ concentrations observed in city center and close to city center according to TNO inventory output as pollutants.

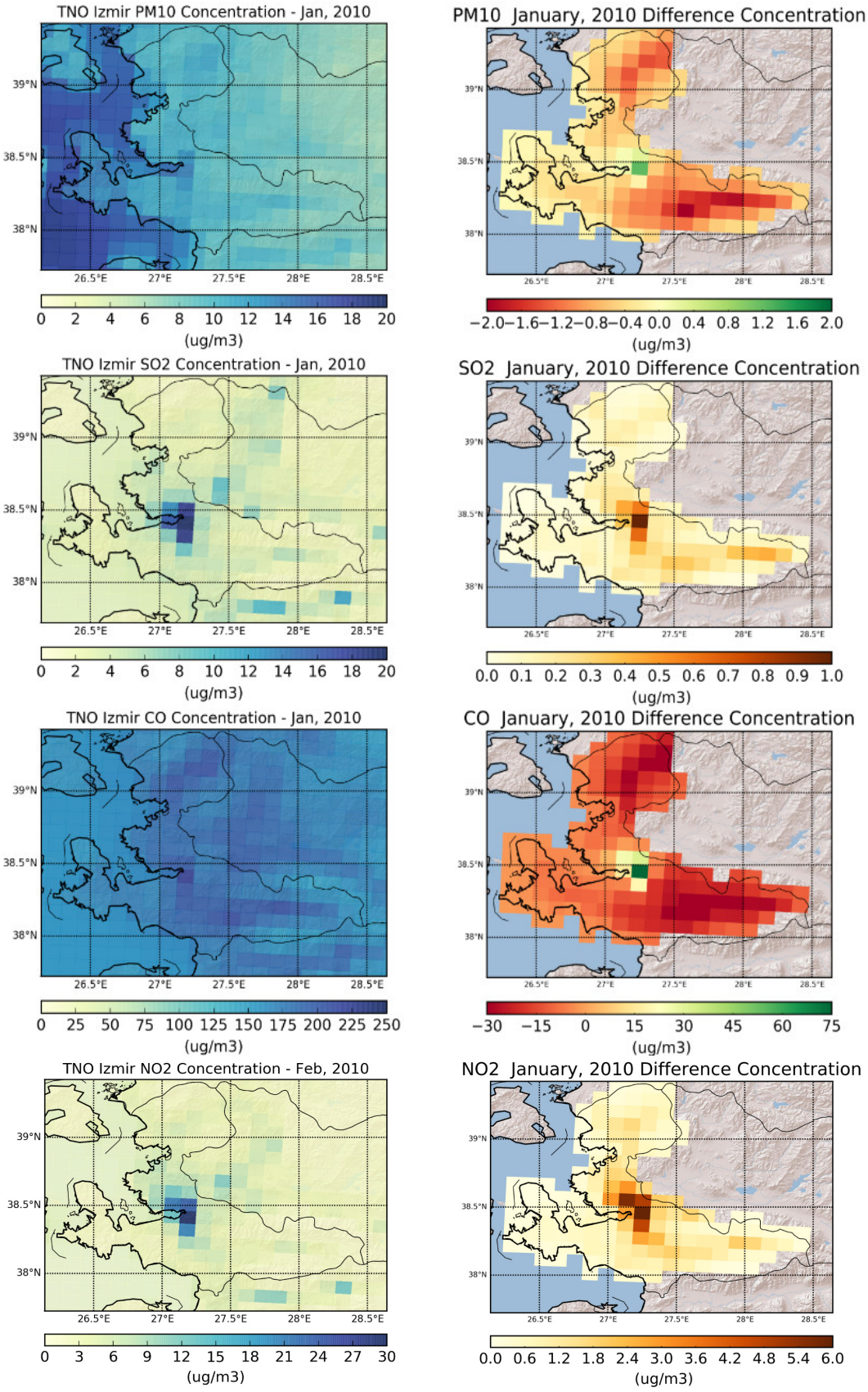


**Figure 3.13:** TNO concentration and OUR-TNO difference concentration for January 2010.

Table 3.7 explains comparisons between simulated CMAQ model and observation station results with statistical parameters such as MB, NMB, RMSE and r. As stated in WRF performance analysis part of this study, the statistical relation between model outputs and observation values for $PM_{10}$ is low because of low resolution. The model is under-predicted according to statistical parameters. This situation was explained by NMB method, it is negative. For example, r is close to 0 for TNO and our model simulations. This mean, relation between our model simulation and observations is low, their values are approximately 36. The differences between observations and the model results are high because of model gives average value for 10x10 $km^2$ area and model results quality decreases.

**Table 3.7:** Statistical relation between simulated CMAQ model outputs and observation station values for $PM_{10}$ concentrations.

| | MB | NMB | RMSE | r |
|---|---|---|---|---|
| **TNO** | -30.180 | -0.717 | 35.145 | 0.005 |
| **OUR** | -30.769 | -0.731 | 35.746 | -0.012 |

In Figure 3.14 is showed comparison of daily $PM_{10}$ concentrations of Izmir all observation stations average, our and TNO CMAQ outputs in January 2010. There is a slightly different between TNO and our concentration value. There is an increasing trend in model for some days the calculated concentrations were underestimated in some days according to observations.

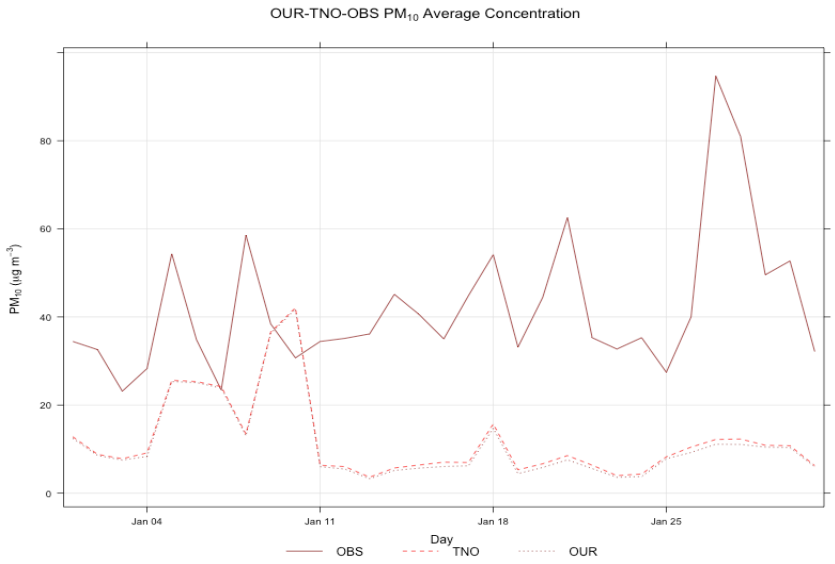


**Figure 3.14:** Comparison of daily $PM_{10}$ concentrations of Izmir all observation stations, OUR and TNO CMAQ outputs January 2010.

Our simulated CMAQ output for hourly $PM_{10}$ concentrations were compared with observation station values in Gaziemir Adnan Menderes Airport (Figure 3.15). The red line represents limit value (50 µg/m$^3$) that is determined by European Union. Observation values were shown as green line and model outputs were shown as blue line. As it is seen in Figure 3.14, while observation values generally higher than limit value, model output values for $PM_{10}$ concentrations were low during this episode. It means that model under predicted $PM_{10}$ values.

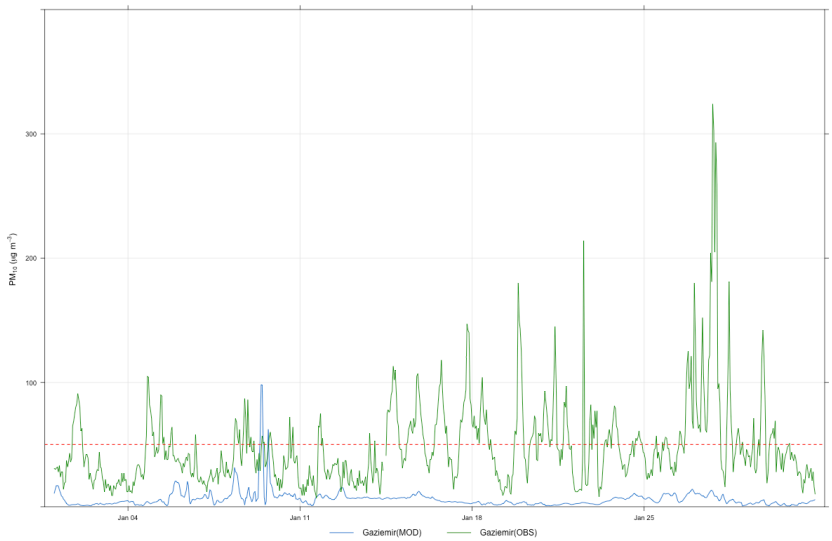


**Figure 3.15:** Our CMAQ and observation comparison for $PM_{10}$ concentrations in episodic period as January 2010 for Gaziemir (Adnan Menderes Airport).

Figure 3.16 shows the days and the hours when the maximum, minimum and average $PM_{10}$ differences. The maps show selected days as based on maximum differences value of graphs. On 26$^{th}$ January, the difference between TNO concentration and our concentration is maximum magnitude. The difference value is quite low on 8$^{th}$ January.

Then, the value belongs to 26$^{th}$ January was examined in detailed (Figure 3.16). In these analysis, different sectors impacts overall was seen because of reduction and increasing of sectors. This is the most affected by the changes of the city center because of high $PM_{10}$ levels. Also, results of concentration distribution related to spatial distribution of emissions.

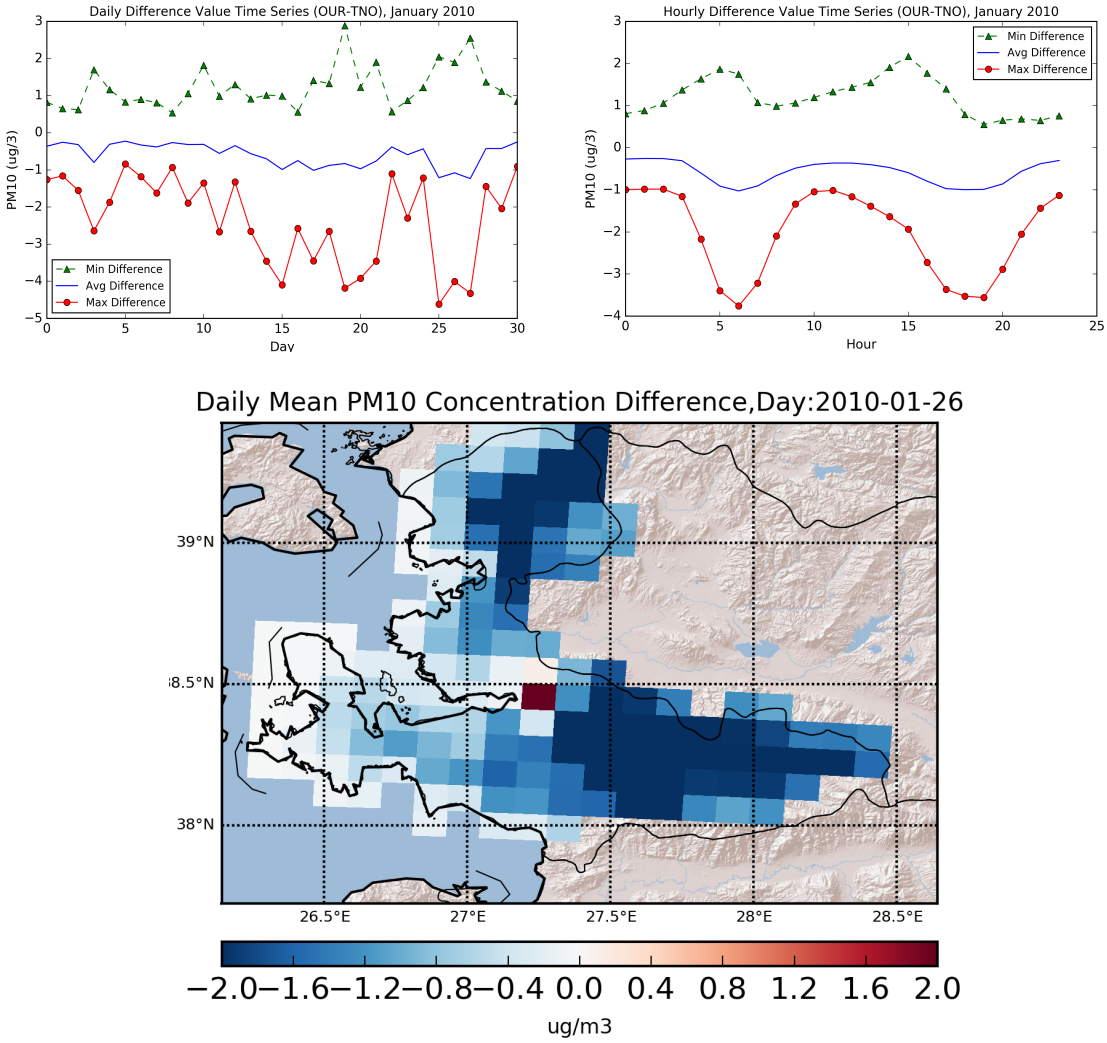


**Figure 3.16:** Daily and hourly $PM_{10}$ max-average-min differences time series, the map that is maximum difference day.

Figure 3.17 shows hourly average concentration changes of 26$^{th}$ January. The maps explain status of hourly maximum differences of the selected day. The maximum differences hour was at 07:00 am and 06:00 pm. It can be depended on road transport emissions because of increasing of SNAP71 etc. It can be analyzed with time series of observation values and model output concentration values on the same graph for Gaziemir station (Adnan Menderes) (Figure 3.18). The graph explains daily trend of $PM_{10}$ concentration in 26$^{th}$ January, 2010 according to observation stations and model results. While the concentration values are different, trends are generally similar between model results and observation.

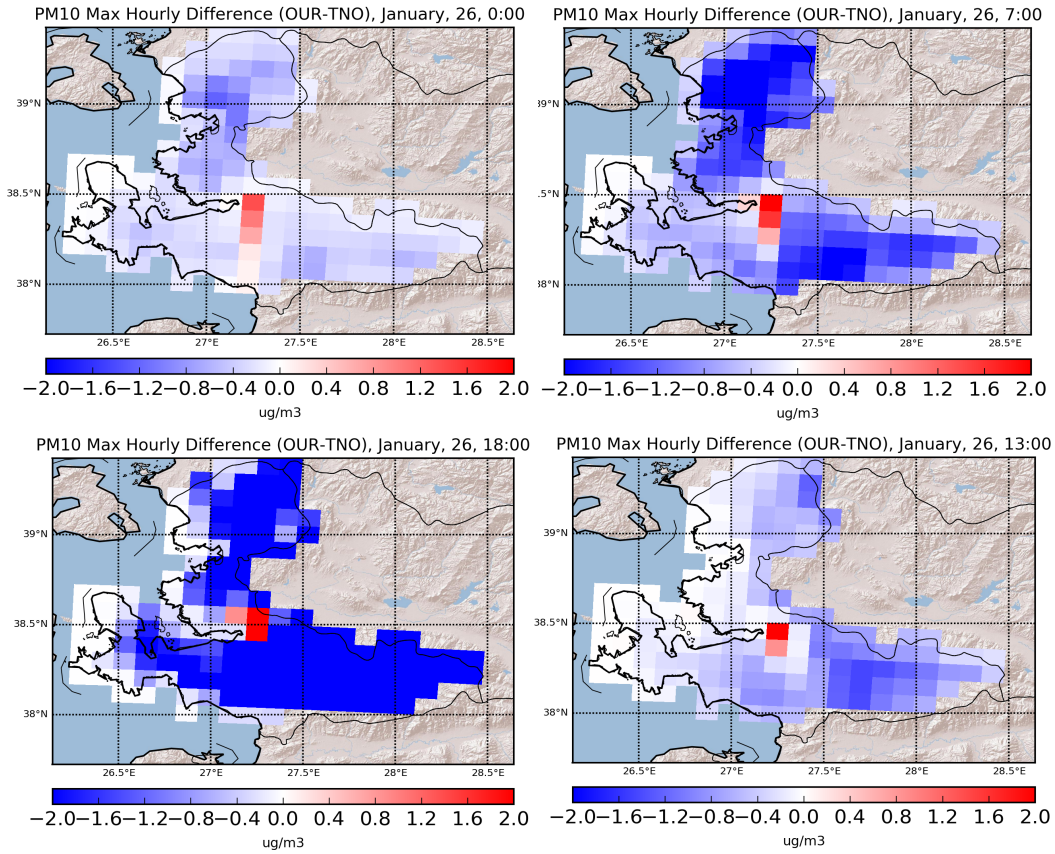


**Figure 3.17:** The maximum difference hours of the day.

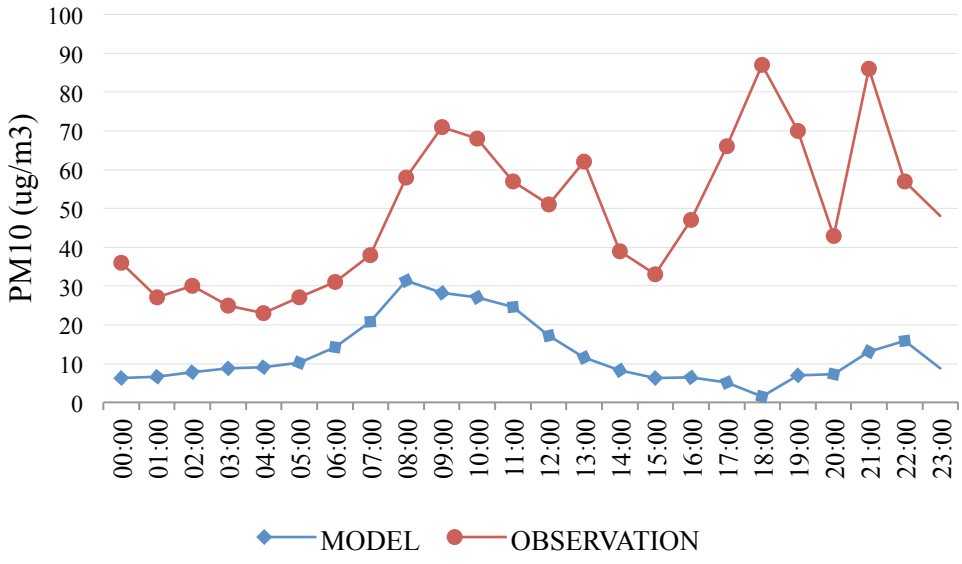


**Figure 3.18:** 2010, January 26, hourly $PM_{10}$ concentration level comparison between model and observation for Gaziemir (Adnan Menderes).

Moreover, these analyses were done for other pollutants as $PM_{10}$ analysis. Figure C.1 in Appendix C shows the maximum, average and minimum differences time series of other main pollutants, which are $SO_2$, CO and $NO_x$. The maximum difference days were determined for these pollutants, and maps belong to these days were generated (see also Appendix C). For $SO_2$ pollutants, the day that has the maximum differences between our and TNO simulations was at 05:00 pm 28$^{th}$ January, and range of daily concentrations changed between 0 and 3.2 $\mu g/m^3$, hourly concentration was between 0 and 2.0 $\mu g/m^3$. The maximum differences for CO concentration was in 28$^{th}$ January as $SO_2$ and the maximum differences hour was 03:00 pm. While daily maximum concentration difference was approximately 200 $\mu g/m^3$, hourly maximum concentration difference was 180 $\mu g/m^3$. On the other hand, daily and hourly minimum concentration differences were 100 $\mu g/m^3$ and 80 $\mu g/m^3$, respectively. The maximum changes were seen in CO concentrations, it is about maximum change of emissions were done for CO pollutant. Daily and hourly maximum differences of $NO_2$ concentration were 13 $\mu g/m^3$ (16$^{th}$ January) and 35 $\mu g/m^3$ (15.00 pm), respectively. While hourly concentration differences examined, there was reduction of concentration after 12:00 am. Consequently, all pollutants differences changed positively generally because of emission changes.

# 4. CONCLUSION

The purpose of this study is to analyze air pollution levels in İzmir, which is one of the major metropolitan areas of Turkey. In order to generate more dependable emission inventory for İzmir, TNO inventory was used as base case. The TNO inventory was modified for SNAP2, SNAP34 and SNAP7, which are domestic heating, industry and road transport sectors, respectively. Although for the other sectors emissions were not changed, the impact of improving on these main sectors evaluated for İzmir in January 2010 study episode. The reason of selecting January was to prefer a winter month in order to handle domestic heating emission sources in the inventory. Moreover, year 2010 has the maximum PM10 concentrations in the last 5-year average.

Firstly, CMAQ air quality model was run with TNO gridded emission inventory as base case and the inventory improved with calculated and more accurate emissions with current activity data for selected sources for İzmir. TNO emissions, which were residential heating, industry and road transport, were generally increased in new emission inventory. SO2 and NMVOC were decreased approximately 20 percent. PMco, PM2.5, $NO_x$ and CO were increased 11, 30, 11 and 36 percent, respectively. As a result of these changes, concentration values come from CMAQ simulations was analyzed and the changes especially affected city center in Izmir. It is about TNO spatial distribution.

The difference of $PM_{10}$ concentrations from model outputs was examined in order to evaluate response over the city. The days and hours that include maximum, minimum impacts on $PM_{10}$ concentrations was determined.

As mentioned in the beginning parts of the thesis, high-pressure system was observed on 26$^{th}$ January. That day is also coincidence with the same day where the maximum difference on $PM_{10}$ concentrations was observed. This situation points a local pollution in the city. The maximum response to modifying TNO emission

inventory is determined on this date with almost 5 $\mu g/m^3$ increasing on $PM_{10}$ concentrations.

It is seen that all İzmir pollutant emissions and concentrations, maximum changes are in city center. By a more detailed study, days and hours are determined that maximum differences occur in concentrations and affects of emissions and the results are analyzed. At the result of all these analysis, the maximum affect in the CMAQ model's concentration results, which used the new developed emission inventory as an input, is seen in the İzmir city center where the most emission sources exist.

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**APPENDIX**

**APPENDIX A:** List of Industrial Facility
**APPENDIX B:** R Programing Codes
**APPENDIX C:** Pollutant Concentration Analysis (CO, $SO_2$, $NO_x$)
**APPENDIX D:** Model Evaluation Method Formulas

**APPENDIX A:** List of Industrial Facility

| FACILITY NAME | CO | PM | NOX | NO2 | NO | SO2 | VOC |
|---|---|---|---|---|---|---|---|
| FACILITY 1 | 163506.85 | 7194.26 | 5165.91 | NA | NA | NA | 14708.66 |
| FACILITY 2 | 300.00 | 9146.00 | 2581.00 | NA | NA | 194.65 | 5321.11 |
| FACILITY 3 | 15516.00 | 490.02 | 7554.00 | NA | NA | 504.00 | 8748.00 |
| FACILITY 4 | 0.08 | 0.16 | NA | 0.72 | NA | 0.01 | 0.18 |
| FACILITY 5 | 0.20 | 0.14 | NA | 3.12 | NA | NA | 0.06 |
| FACILITY 5 | 0.29 | 0.16 | NA | 2.55 | NA | 0.00 | 0.68 |
| FACILITY 6 | 2.17 | 0.20 | NA | 1.26 | NA | NA | 0.63 |
| FACILITY 6 | 0.03 | 0.05 | NA | 0.54 | NA | NA | 0.03 |
| FACILITY 7 | 644.31 | 596.06 | 1752.74 | NA | NA | 0.00 | NA |
| FACILITY 8 | 302.40 | 1983.60 | 345.60 | NA | NA | 43.20 | 1267.20 |
| FACILITY 9 | 259966.25 | NA | 86516.04 | NA | NA | 0.00 | NA |
| FACILITY 9 | 151885.85 | NA | 72447.48 | NA | NA | 0.00 | NA |
| FACILITY 10 | 929.20 | 3769.38 | 34494.21 | NA | NA | 376.94 | NA |
| FACILITY 11 | 1104.52 | 3260.95 | NA | 59100.37 | 38526.57 | 0.00 | NA |
| FACILITY 11 | 7459.87 | 7959.53 | NA | 103210.88 | 67340.41 | 0.00 | 8318.93 |
| FACILITY 11 | 3681.72 | 36115.92 | NA | 80279.03 | 52333.02 | 0.00 | 4461.89 |
| FACILITY 11 | 3287.25 | 4198.91 | NA | 97039.62 | 63264.22 | 0.00 | 4917.73 |
| FACILITY 11 | 350.64 | 2173.97 | NA | 10124.73 | 6600.80 | 0.00 | NA |
| FACILITY 11 | 5250.83 | 4453.13 | NA | 43996.55 | 28717.42 | 0.00 | NA |
| FACILITY 12 | 12.59 | 0.67 | 7.09 | NA | NA | 4.28 | 0.01 |
| FACILITY 13 | 0.00 | 0.00 | 1.09 | NA | NA | 0.08 | 29.39 |
| FACILITY 14 | 0.02 | 0.01 | 1.56 | NA | NA | 0.08 | 18.01 |
| FACILITY 15 | 1.198.012 | 33.23 | NA | 1.074.169 | 689.19 | NA | NA |
| FACILITY 15 | 1.662.345 | 44.79 | NA | 1.403.830 | 901.12 | 8.94 | NA |
| FACILITY 15 | 78.43 | 1.03 | NA | 133.37 | 86.85 | NA | NA |
| FACILITY 16 | 275072.29 | 2495.31 | NA | 315522.24 | 20557.98 | 0.00 | 31247.90 |
| FACILITY 16 | 0.00 | 1065.70 | NA | 136848.78 | 88582.62 | 0.00 | NA |
| FACILITY 17 | 747338.38 | 38745.48 | 852990.98 | NA | NA | NA | NA |
| FACILITY 17 | 856469.58 | 109342.32 | 2685713.51 | NA | NA | NA | NA |
| FACILITY 18 | 115.75 | 975.42 | NA | 1806.99 | 1159.85 | NA | NA |
| FACILITY 19 | NA | 66.85 | NA | NA | NA | NA | NA |
| FACILITY 20 | 135735.00 | NA | 215.5 | NA | NA | NA | 77907.00 |
| FACILITY 21 | NA | NA | 10941.00 | NA | NA | 23337.00 | NA |
| FACILITY 22 | 490111.20 | 27885.00 | NA | NA | 94091.40 | 1414099.20 | NA |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| FACILITY 23 | 265025.92 | 35953.67 | 117032.72 | NA | NA | 255972.46 | 45160.43 |
| FACILITY 23 | 372080.12 | 35372.88 | 60871.49 | NA | NA | 127587.65 | 49251.35 |
| FACILITY 23 | 1459.42 | 106.87 | 2854.01 | NA | NA | 666.64 | 1775.65 |
| FACILITY 23 | 0.00 | 224.26 | 13478.14 | NA | NA | 0.00 | 357.41 |
| FACILITY 23 | 17637.38 | 545.75 | 5085.18 | NA | NA | 0.00 | NA |
| FACILITY 23 | 10532.15 | 476.54 | 13742.69 | NA | NA | 0.00 | NA |
| FACILITY 23 | 11728.76 | 400.33 | 6916.02 | NA | NA | 0.00 | NA |
| FACILITY 23 | 8208.12 | 423.11 | 7637.84 | NA | NA | 0.00 | NA |
| FACILITY 23 | 7299.71 | 181.33 | 2786.56 | NA | NA | 4860.92 | NA |
| FACILITY 23 | 2046.34 | 113.88 | 2557.04 | NA | NA | 317.99 | 1843.10 |
| FACILITY 23 | 1672.28 | 125.27 | 5527.56 | NA | NA | 0.00 | 2065.61 |
| FACILITY 23 | 7949.70 | 897.02 | 751.61 | NA | NA | 626.34 | NA |
| FACILITY 23 | 265025.92 | 35953.67 | 117032.72 | NA | NA | 255972.46 | 45160.43 |
| FACILITY 23 | 372080.12 | 35372.88 | 60871.49 | NA | NA | 127587.65 | 49251.35 |
| FACILITY 23 | 1459.42 | 106.87 | 2854.01 | NA | NA | 666.64 | 1775.65 |
| FACILITY 23 | 0.00 | 224.26 | 13478.14 | NA | NA | 0.00 | 357.41 |
| FACILITY 23 | 17637.38 | 545.75 | 5085.18 | NA | NA | 0.00 | NA |
| FACILITY 23 | 10532.15 | 476.54 | 13742.69 | NA | NA | 0.00 | NA |
| FACILITY 23 | 11728.76 | 400.33 | 6916.02 | NA | NA | 0.00 | NA |
| FACILITY 23 | 8208.12 | 423.11 | 7637.84 | NA | NA | 0.00 | NA |
| FACILITY 23 | 7299.71 | 181.33 | 2786.56 | NA | NA | 4860.92 | NA |
| FACILITY 23 | 2046.34 | 113.88 | 2557.04 | NA | NA | 317.99 | 1843.10 |
| FACILITY 23 | 1672.28 | 125.27 | 5527.56 | NA | NA | 0.00 | 2065.61 |
| FACILITY 23 | 7949.70 | 897.02 | 751.61 | NA | NA | 626.34 | NA |
| FACILITY 24 | 77061.00 | 12762.00 | 176.00 | NA | NA | 0.00 | NA |
| FACILITY 24 | 37318.00 | 11.88 | 87.12 | NA | NA | 0.00 | NA |
| FACILITY 24 | 84733.00 | 28.51 | 160.77 | NA | NA | 0.00 | NA |
| FACILITY 24 | NA | 30.09 | NA | NA | NA | 0.00 | NA |
| FACILITY 24 | NA | 7.12 | NA | NA | NA | 0.00 | NA |
| FACILITY 25 | 0.00 | 8186.38 | 135794.92 | NA | NA | 0.00 | NA |
| FACILITY 25 | 4757.13 | 10920.79 | 147257.57 | NA | NA | 21598.56 | NA |
| FACILITY 25 | 0.00 | 7843.76 | 139189.97 | NA | NA | 42486.39 | NA |
| FACILITY 25 | 9711.10 | 10628.56 | 222756.62 | NA | NA | 59992.67 | NA |
| FACILITY 26 | 1046.88 | 2543.04 | NA | 5173.92 | 3201.84 | 144.00 | 18493.20 |
| FACILITY 26 | NA | NA | NA | NA | NA | NA | 21038.40 |
| FACILITY 27 | 114340.78 | 6637.45 | NA | 10761.66 | 6945.80 | NA | NA |
| FACILITY 27 | 112741.20 | 5328.71 | NA | 15255.54 | 9948.73 | 1909.68 | NA |
| FACILITY 28 | 1.55 | 0.41 | NA | 9.40 | 6.11 | NA | NA |
| FACILITY 28 | 2.36 | 0.13 | NA | 3.73 | 2.43 | NA | NA |
| FACILITY 29 | 328.41 | 261.52 | NA | 566.84 | 351.19 | NA | NA |
| FACILITY 30 | 0.00 | 6132.00 | NA | 440628.00 | NA | 28032.00 | 1637.24 |
| FACILITY 30 | 0.00 | 7008.00 | NA | 470412.00 | NA | 25404.00 | 1525.12 |
| FACILITY 30 | 0.00 | 5256.00 | NA | 319740.00 | NA | 55188.00 | 1941.22 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| FACILITY 30 | 7884.00 | 6132.00 | NA | 333756.00 | NA | 39420.00 | 1453.28 |
| FACILITY 30 | 20498.40 | - | NA | 53874.00 | NA | 68678.40 | NA |
| FACILITY 30 | 0.00 | 398.00 | NA | 31044.00 | NA | 7164.00 | 285.57 |
| FACILITY 31 | NA | NA | NA | NA | NA | NA | 397.66 |
| FACILITY 31 | NA | NA | NA | NA | NA | NA | 63.68 |
| FACILITY 32 | NA | 161.04 | NA | 468.00 | 307.20 | 26.40 | 20190.00 |
| FACILITY 33 | 36273.84 | 850.08 | NA | 87701.76 | 56048.16 | 0.00 | NA |
| FACILITY 34 | NA | 270.48 | NA | 36.00 | NA | NA | NA |
| FACILITY 34 | 52.80 | 210.00 | NA | 40.80 | NA | NA | NA |
| FACILITY 34 | 477.60 | 50.40 | NA | 890.40 | NA | NA | NA |
| FACILITY 34 | NA | NA | NA | NA | NA | NA | 330.24 |
| FACILITY 34 | NA | NA | NA | NA | NA | NA | 67.52 |
| FACILITY 34 | NA | NA | NA | NA | NA | NA | 400.57 |
| FACILITY 34 | NA | NA | NA | NA | NA | NA | 579.15 |
| FACILITY 34 | NA | NA | NA | NA | NA | NA | 882.59 |
| FACILITY 34 | NA | NA | NA | NA | NA | NA | 588.45 |
| FACILITY 34 | NA | NA | NA | NA | NA | NA | 775.63 |
| FACILITY 34 | NA | NA | NA | NA | NA | NA | 116.22 |
| FACILITY 34 | NA | NA | NA | NA | NA | NA | 63.24 |
| FACILITY 34 | NA | NA | NA | NA | NA | NA | 398.14 |
| FACILITY 35 | 9150.00 | 11300.00 | 94750.00 | NA | NA | 550160.00 | NA |
| FACILITY 35 | 11100.00 | 2120.00 | 27390.00 | NA | NA | 23910.00 | NA |
| FACILITY 35 | 3770.00 | 530.00 | 4880.00 | NA | NA | 3770.00 | NA |
| FACILITY 35 | 4030.00 | 2930.00 | 53980.00 | NA | NA | 26980.00 | NA |
| FACILITY 35 | 2730.00 | 1050.00 | 21060.00 | NA | NA | 11390.00 | NA |
| FACILITY 35 | 6500.00 | 10800.00 | 130450.00 | NA | NA | 120760.00 | NA |
| FACILITY 35 | 31660.00 | 9470.00 | 31760.00 | NA | NA | 1900.00 | NA |
| FACILITY 35 | 10180.00 | 25080.00 | 13070.00 | NA | NA | 1650.00 | NA |

**APPENDIX B:** R Programing Codes

IZMIR WRF MODEL TEMPERATURE PERFORMANCE ANALYSIS

```
rm(list=ls())
library(ggplot2)
library(ggdendro)
library("dendroextras")
library(dplyr)
library(cluster)
library(openair)
library(latticeExtra)
setwd("/Users/duygu/Documents/izmir/TEZ/")
izm=import(file="gaziemir_temp.csv",file.type="csv",sep=",",header.at=1,date="dat
e",date.format="%d/%m/%y %H:%M")
png(filename="WRF_perf_izm.png",width =800, height =600)
timePlot(izm, pollutant = c("MOD","OBS"),main="ADNAN MENDERES
AIRPORT WRF PERFORMANCE (TEMPERATURE) ",xlab="Hour",ylab =
expression(paste("Temperature [",degree,"C]")),cols="blue",group=TRUE)
dev.off()
```

IZMIR WRF MODEL WIND PERFORMANCE ANALYSIS

```
ANALİZİsetwd("/Users/duygu/Desktop/IZM_THESIS/WRF_output/WRF_wind/")
u=import(file="izm_U10_Daily.csv",file.type="csv",sep=",",header.at=1,date="Date
",date.format="%d/%m/%y")
v=import(file="izm_V10_Daily.csv",file.type="csv",sep=",",header.at=1,date="Date
",date.format="%d/%m/%y")
u=u$U10        # as numeric
v=v$V10      # as numeric
#wind speed calculation
ws=(u^2+v^2)^0.5
#wind direction calculation
windDir <- function(u, v) {
  (180 / pi) * atan(u/v) + ifelse(v>0,180,ifelse(u>0,360,0))
}
wd=windDir(u,v);
ws <- data.frame(ws)
wd <- data.frame(wd)
izm_wd_ws=cbind(ws,wd)
izm_wd_ws=data.frame(izm_wd_ws,date=seq(from=as.Date("2009-12-
01"),to=as.Date("2010-02-28"),by="day"))
#wind data file is used in this section
png(filename="WRF_perf_izm.png",width =800, height =600)
timePlot(izm_wd_ws, pollutant =
c("wd(OBS)","wd(MOD)","ws(OBS)","ws(MOD)"),main="WRF PERFORMANCE
(Adnan Menderes Airport) ",xlab="Day",ylab =
"WSpeed&Wdirection",cols=c("green4","red3","green4","red3"),group=FALSE)
dev.off()
png(filename="WRF_perf_izm_ws.png",width =600, height =600)
```

```
scatterPlot(izm, x = "ws", y = "ws", method = "density", col = "increment",xlab="WRF",ylab="OBS",main="Wind Speed Perf. Analysis (Adnan Menderes)" )
dev.off()

IZMIR WRF MODEL WIND STATISTICAL ANALYSIS
setwd("/Users/duygu/Desktop/IZM_THESIS/WRF_output/WRF_wind/")
total=import(file="obs_mod_wd_izm.csv",file.type="csv",sep=",",header.at=1,date="Date",date.format="%d/%m/%y")
wind<-data.frame(obs=total$wd,mod=total$wdOBS,model="wind")
modStats(wind, obs = "obs", mod = "mod", type = "model")

COMPARISON OF OBS&TNO&OUR CONCENTRATION
setwd('/Users/duygu/Desktop/')
PM10_all=import(file="PM_izmir.csv",file.type="csv",sep=",",header.at=1,date="Date",date.format="%d/%m/%y")
png(filename="OBS_TNO_OUR.png",width =800, height =600)
timePlot(PM10_all, pollutant = c("OBS","TNO","OUR"),main="OUR-TNO-OBS PM10 Average Concentration",xlab="Day",ylab = "PM10 (ug/m3)",cols=c("red4","red","red4"),group=TRUE)
dev.off

STATISTICAL ANALYSIS BETWEEN OBS&TNO&OUR
setwd('/Users/duygu/Desktop/')
PM10_all=import(file="PM_izmir.csv",file.type="csv",sep=",",header.at=1,date="Date",date.format="%d/%m/%y")
PM10_all<-
data.frame(obs=PM10_all$OBS,mod=PM10_all$OUR,model="model1")
modStats(PM10_all, obs = "obs", mod = "mod", type = "model")

PIE CHART FOR EACH POLLUTANT BY SECTORS
library(ggplot2)
setwd('/Users/duygu/Desktop/IZM_THESIS/')

browsers <- structure(list(browser = structure(c(1L, 2L, 3L, 4L,
                                5L,6L), .Label = c("SNAP1", "SNAP2", "SNAP34","SNAP7","SNAP9","SNAP10"), class = "factor"), version = structure(c(1L,2L, 3L, 4L, 5L, 6L), .Label = c("SNAP1","SNAP2", "SNAP34", "SNAP71",

"SNAP9","SNAP10"),

class = "factor"), share = c(0.25,0.98,8.17,0.55,1.72,88.72), ymax = c(35,138,1158,78,173,12575)), .Names = c("browser", "version", "share", "ymax"), row.names = c(NA, -6L), class = "data.frame")

#browsers$total <- with(browsers, ave(share, browser, FUN = sum))
givemedonuts <- function(file, width = 15, height = 11) {
  ## house keeping
  if (missing(file)) file <- getwd()
```

```
  plot.new(); op <- par(no.readonly = TRUE); on.exit(par(op))

  pdf(file, width = width, height = height)
  nr <- nrow(browsers)
  width <- max(sqrt(browsers$share)) / 0.8
  tbl <- with(browsers, table(browser)[order(unique(browser))])
  cols <- c('cyan3','red3','darkorange','green3','dodgerblue','pink','tomato','navy')
  #'cyan2','red','orange','green','dodgerblue2'
cols <- unlist(Map(rep, cols, tbl))
# loop creates pie slices
  plot.new()
  par(omi = c(0.5,0.5,0.75,0.5), mai = c(0.1,0.1,0.1,0.1), las = 1)
  for (i in 1:nr) {
    par(new = TRUE)
    ## create color/shades
    rgb <- col2rgb(cols[i])
    f0 <- rep(NA, nr)
    f0[i] <- rgb(rgb[1], rgb[2], rgb[3], 190 / sequence(tbl)[i], maxColorValue = 255)
    lab <- with(browsers, sprintf('%s: %s',version,share))
    lab<- paste(lab,sep = " ","%")
    if (with(browsers, share[i] == max(share))) {
      lab0 <- lab
    } else lab0 <- NA
    pie(browsers$share, border = NA, radius = 5 / width, col = f0,
        labels = lab0, cex = 1.8)
    par(new = TRUE)
    rgb <- col2rgb(cols[i])
    f0[i] <- rgb(rgb[1], rgb[2], rgb[3], maxColorValue = 255)
    pie(browsers$share, border = NA, radius = 4 / width, col = f0, labels = NA)
  }
  ## center labels, guess and check?
  text(x = c(-.05), y = c(.05),
     labels = "NH3", col = 'white', cex = 3.0)

 # mtext('CO SNAP SECTOR', side = 3, line = -2, adj = 1.0,
  #      cex = 2, outer = TRUE)
#  mtext('TNO',
 #       side = 1, line = 0, adj = 1.0, cex = 1.2, outer = TRUE, font = 3)
  dev.off()
}
givemedonuts('/Users/duygu/Desktop/IZM_THESIS/NH3.pdf')
SO2 TIME SERIES WITH EPISODE PERIOD JANUARY
setwd("/Users/duygu/Documents/Alka_izmir_erzurum/TEZ/")
SO2_hourly=import(file="SO2_Saatlik.csv",file.type="csv",sep=",",header.at=1,date
="Date",date.format="%d.%m.%Y",time="Hour",time.format="%H:%M")
png(filename="SO2_episode.png",width =800, height =600)
timePlot(SO2_hourly,                    pollutant                    =
c("Alsancak","Bornova","Cigli","Gaziemir","Sirinyer","Karsiyaka"),main="PM10
January 2010 Concentration (ug/m3)",xlab="Day",ylab = "PM10
(ug/m3)",key=FALSE,cols="black",lwd=0.75,ylim = c(0, 300))
```

```
trellis.last.object() +
  layer(lpolygon(x = c(as.POSIXct("2010-01-26"),
                       as.POSIXct("2010-01-26"),                    as.POSIXct("2010-01-29"),
as.POSIXct("2010-01-29")), y = c(-20, 600, 600, -20), col = "aquamarine", border =
NA), under = TRUE, rows = c("3","5","6","8"))
trellis.last.object() +
  layer(lpolygon(x = c(as.POSIXct("2010-01-06"),
                       as.POSIXct("2010-01-06"),                    as.POSIXct("2010-01-08"),
as.POSIXct("2010-01-08")), y = c(-20, 600, 600, -20), col = "darksalmon", border =
NA), under = TRUE, rows = c("5"))
trellis.last.object() +
  layer(lpolygon(x = c(as.POSIXct("2010-01-08"),
                       as.POSIXct("2010-01-08"),                    as.POSIXct("2010-01-10"),
as.POSIXct("2010-01-10")), y = c(-20, 600, 600, -20), col = "royalblue", border =
NA), under = TRUE, rows = c("8"))
dev.off()
```

PM10 TIME SERIES WITH EPISODE PERIOD JANUARY

```
PM10_hourly=import(file="PM10_Saatlik.csv",file.type="csv",sep=",",header.at=1,
date="Date",date.format="%d.%m.%Y",time="Hour",time.format="%H:%M")
png(filename="PM10_episode.png",width =800, height =600)
timePlot(PM10_hourly,                                pollutant                                =
c("Alsancak","Bornova","Cigli","Gaziemir","Sirinyer","Karsiyaka"),main="PM10
January 2010 Concentration (ug/m3)",xlab="Day",ylab = "PM10
(ug/m3)",key=FALSE,cols="black",lwd=0.75,ylim = c(0, 300))
#trellis.last.object() +
# layer(ltext(x = as.POSIXct("2010-01-28 12:00"), y = 250,
#           labels = "episode", col = "red",
#         font = 3, cex = 1.25), rows = 2)
trellis.last.object() +
  layer(lpolygon(x = c(as.POSIXct("2010-01-26"),
                       as.POSIXct("2010-01-26"),                    as.POSIXct("2010-01-29"),
as.POSIXct("2010-01-29")), y = c(-20, 600, 600, -20), col = "aquamarine", border =
NA), under = TRUE, rows = c("3","5","6","8"))
trellis.last.object() +
  layer(lpolygon(x = c(as.POSIXct("2010-01-06"),
                       as.POSIXct("2010-01-06"),                    as.POSIXct("2010-01-08"),
as.POSIXct("2010-01-08")), y = c(-20, 600, 600, -20), col = "darksalmon", border =
NA), under = TRUE, rows = c("5"))
trellis.last.object() +
  layer(lpolygon(x = c(as.POSIXct("2010-01-08"),
                       as.POSIXct("2010-01-08"),                    as.POSIXct("2010-01-10"),
as.POSIXct("2010-01-10")), y = c(-20, 600, 600, -20), col = "royalblue", border =
NA), under = TRUE, rows = c("8"))
dev.off()
```

PM10 TIME SERIES WITH ALL DATA OF TURKEY

```
setwd("/Users/duygu/Documents/Alka_izmir_erzurum/TEZ/")
ave_tr=import(file="Average_Turkey_PM10.csv",file.type="csv",sep=",",header.at=
1,date="Date",date.format="%d/%m/%y")
```

```
timePlot(ave_tr, pollutant = c("Average"),main="PM10 Concentration in Turkey period of 2009-2015",xlab="Year",ylab = "PM10 (ug/m3)",key=FALSE,cols="black",lwd=0.75,ref.y=(list(h=100,lty=2,col="red4")))
dev.off()

PRESSURE ANALYSIS FOR EPISODE PERIOD
png(filename="pressure_ts.png",width =600, height =400)
timePlot(metopar, pollutant = c("Pressure"),xlab="Day",ylab = "Pressure (hPA)",key=FALSE,cols="navy",lwd=0.75,ylim = c(1000, 1030),group=FALSE)
trellis.last.object() +
  layer(lpolygon(x = c(as.POSIXct("2010-01-24"), as.POSIXct("2010-01-24"),
                       as.POSIXct("2010-01-28"), as.POSIXct("2010-01-28")), y = c(1020, 1030, 1030, 1020), col = "blue", border = NA,
              alpha = 0.2))
trellis.last.object() + layer({maxy <- which.max(y);
                        lpoints(x[maxy], y[maxy], col = "blue", pch = 16)})
trellis.last.object() + layer({maxy <- which.max(y);
                        ltext(x[maxy], y[maxy], paste(y[maxy], "January 26"), col = "blue",pos = 3)})
dev.off()

WIND SPEED AND DIRECTION ANALYSIS FOR EPISODE DATE
temp=import(file="izm_ocak2010_wswd.csv",file.type="csv",sep=";",header.at=1, date="date",date.format="%d/%m/%Y %H:%M")
png(filename="IZMIR_polrose.png",width =800, height =600)
pollutionRose(temp,pollutant = "ws",type="year",breaks=c(0,2,4,6,10,15,20,50),cols="heat",key.header = "Wind Speed",main="IZMIR WIND SPEED&DIRECTION",key.footer = "(meter/second)")
dev.off()



OUR SECTORS BARPLOT
setwd('/Users/duygu/Desktop/IZM_THESIS/TNO_Emission/')
sectors=read.csv(file="new_inventory_duygu.csv", header=TRUE, sep=",")
sec = melt(sectors,id=c("Sectors"),preserve.na = TRUE)
png(filename="izm_sectors_our.png",width =800, height =600)
aggplot(sec, aes(x = variable, y = value,fill = Sectors))+labs(x = NULL, y = NULL,fill = NULL)+ geom_bar(stat = "identity", position = "stack",alpha = 0.8)+scale_colour_hue(l=70, c=150)+theme(panel.background = element_rect(fill = 'white', colour = 'white'))+theme(legend.position = "top")
dev.off()

TNO SECTORS BARPLOT
setwd('/Users/duygu/Desktop/IZM_THESIS/TNO_Emission/')
sectors=read.csv(file="TNO_inventory.csv", header=TRUE, sep=",")
sec = melt(sectors,id=c("Sectors"),preserve.na = TRUE)
png(filename="izm_sectors_tno.png",width =800, height =600)
ggplot(sec, aes(x = variable, y = value,fill = Sectors))+
```

```
  labs(x = NULL, y = NULL,fill = NULL)+ geom_bar(stat = "identity", position = "stack",alpha = 0.8)+scale_colour_hue(l=70, c=150)+theme(panel.background = element_rect(fill = 'white', colour = 'white'))+theme(legend.position = "top")
dev.off()

OUR&TNO SECTORS BARPLOT
setwd('/Users/duygu/Desktop/IZM_THESIS/TNO_Emission/')
sectors=read.csv(file="combine_inventory.csv", header=TRUE, sep=",")
sec = melt(sectors,id=c("Sectors"),preserve.na = TRUE)
png(filename="izm_sectors_combine.png",width =1000, height =600)
c <- ggplot(sec, aes(x = variable, y = value,fill = Sectors))+
  labs(x = NULL, y = NULL,fill = NULL)
d <- c + geom_bar(stat = "identity", position = "stack",alpha = 0.8)+scale_y_continuous(limits = c(0, 200000))+scale_colour_hue(l=70, c=150)+theme(panel.background = element_rect(fill = 'white', colour = 'white'))+theme(legend.position = "top")+theme(text = element_text(size=15))
d
dev.off()
```

**APPENDIX C:** Pollutant Concentration Analysis ($CO$, $SO_2$, $NO_x$)

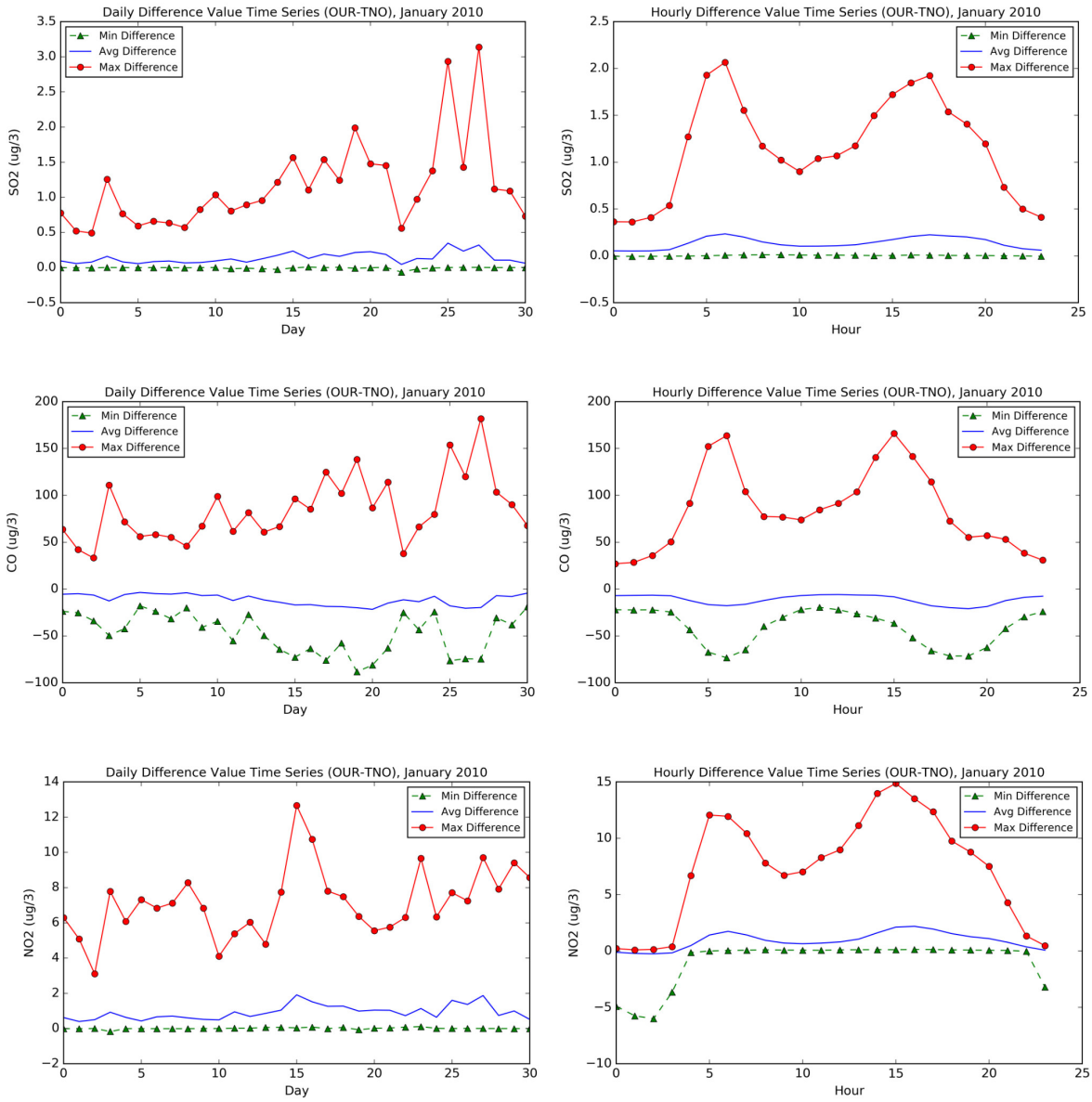


**Figure C.1:** Daily and hourly $SO_2$ ,$CO$ and $NO_x$ maximum-average-minimum differences time series.

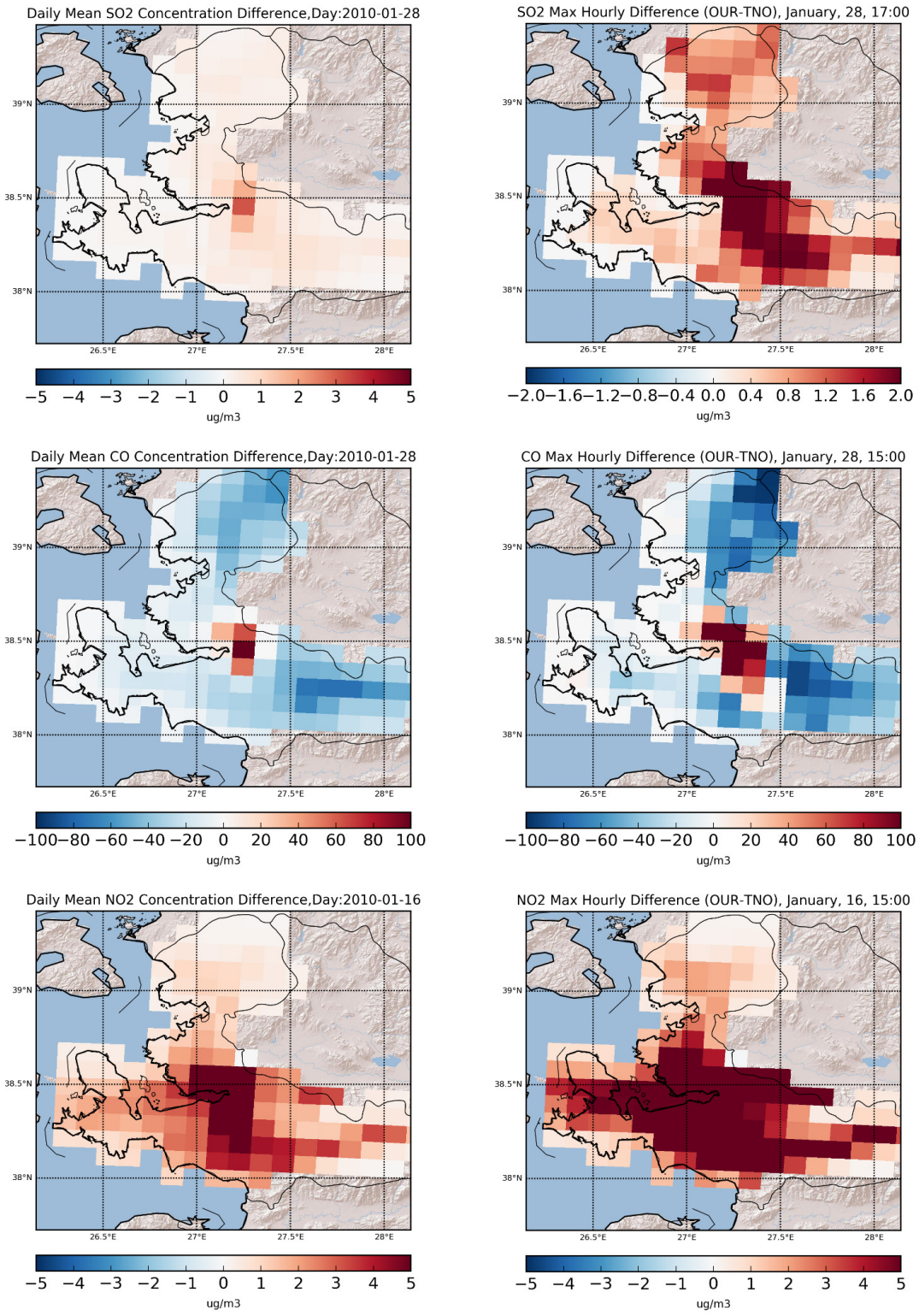


**Figure C.2:** The map that is maximum difference day on the left side and the maximum difference hours of the day on right side.

**APPENDIX D:** Model Evaluation Method Formulas

**Table D.1:** Formulas of model evaluation methods (See also p. 38-39).

| MB | NMB | RMSE | r |
|---|---|---|---|
| $\frac{1}{n}\sum_{i=1}^{N} M - O$ | $\frac{\sum_{i=1}^{N} M - O}{\sum_{i=1}^{N} O}$ | $\left(\frac{\sum_{i=1}^{n}(M_i - O_i)^2}{n}\right)^{1/2}$ | $\frac{1}{(n-1)}\sum_{i=1}^{n}\left(\frac{M_i - \overline{M}}{\sigma_M}\right)\left(\frac{O_i - \overline{O}}{\sigma_O}\right)$ |

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***Conference Proceedings***

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