

İSTANBUL TECHNICAL UNIVERSITY ★ GRADUATE SCHOOL OF SCIENCE
ENGINEERING AND TECHNOLOGY

**EVALUATION OF EMEP SO₂ EMISSIONS FOR TURKEY USING
WRF-CMAQ MODELING SYSTEM**



M.Sc. THESIS

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Environmental Science and Engineering Programme

JUNE 2016

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İSTANBUL TEKNİK ÜNİVERSİTESİ ★ FEN BİLİMLERİ ENSTİTÜSÜ

**EMEP SO₂ EMİSYONLARININ WRF-CMAQ MODEL SİSTEMİ
KULLANILARAK TÜRKİYE İÇİN DEĞERLENDİRİLMESİ**

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To my family,



FOREWORD

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ABBREVIATIONS

AERO6	: Aerosol Module 6
AFWA	: African Water Association
AGRMET	: Agricultural Meteorological Model
App	: Appendix
AQMEII	: Air Quality Model Evaluation International Initiative
AQS	: Air Quality System
ARW	: Advanced Research WRF
ASCII	: American Standard Code for Information Interchange
CAMx	: Comprehensive Air Quality Model with Extensions
CB05	: Carbon Bond 05
CEIP	: Centre on Emission Inventories and Projections
CMAQ	: Community Multi-scale Air Quality
CO	: Carbon monoxide
CSQY	: Cross-section and Quantum Yield
ECMWF	: European Centre for Medium-Range Weather Forecasts
EDGAR	: Emission Database for Global Atmospheric Research
EEA	: Environment European Agency
EMEP	: European Monitoring Evaluation Programme
EPA	: Environment Protection Agency
FNL	: Final Global Tropospheric Analyses
GEIA	: Global Emissions Initiative
GFS	: Global Forecast System
GMT	: Greenwich Mean Time
GNFR	: Nomenclature for Reporting
GOME	: Global Ozone Monitoring Experiment
GPS	: Global Positioning System
GRIB	: Gridded Information in Binary
ITU	: Istanbul Technical University
MNB	: Mean Normalized Bias
MEGAN	: Model of Emissions of Gases and Aerosols from Nature
MM5	: Mesoscale Model
N₂O	: Nitrous oxide
N₂O₃	: Dinitrogen trioxide
N₂O₄	: Dinitrogen tetroxide
N₂O₅	: Dinitrogen pentoxide
NAM	: North American Mesoscale Forecast System
NASA	: National Aeronautics and Space Administration
NCAR	: National Center for Atmospheric Research
NCEP	: National Centers for Environmental Prediction

NETCDF	: Network Common Data Form
NFR	: Nomenclature for Reporting
NH₃	: Ammonia
NO	: Nitrogen monoxide
NO₂	: Nitrogen dioxide
NO_x	: Nitrogen oxides
OMI	: Ozone Monitoring Instrument
PAN	: Peroxyacetyl nitrate
PBL	: Planetary Boundary Layer
PM	: Particulate Matter
PM₁₀	: Particulate Matter up to 10 micrometers in size
PM_{2.5}	: Particulate Matter up to 2.5 micrometers in size
RMSE	: Root Mean Square Error
RUC	: Rapid Update Cycle
SMOKE	: The Sparse Matrix Operator Kernel Emissions
SNAP	: Selected Nomenclature of Air Pollutants
SO₂	: Sulfur dioxide
TNO	: Netherlands Organization for Applied Scientific Research
UV	: Ultra Violet
VERDI	: Visualization Environment for Rich Data Interpretation
VOCs	: Volatile Organic Compounds
WPS	: WRF Preprocessing System
WRF	: Weather Research and Forecasting
WRF-Chem	: Weather Research and Forecasting- Chemistry

SYMBOLS

C₁, C₂, C'	: Concentration
T	: Temperature
P	: Pressure
R	: Gas Constant
MW	: Molecular Weight





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EVALUATION OF SO₂ EMISSIONS FOR TURKEY USING WRF-CMAQ MODELING SYSTEM

SUMMARY

Ambient atmospheric pollutants cause some unwanted odors that are known by their quality and magnitude. Particularly, humans have a low threshold to sense sulfur-containing components; therefore, they will be recognized easily. Some adverse effects on human health were found, especially on the respiratory system like bronchitis, lung cancers, and lung emphysema. A number of pollutants like ozone have probable mutagenic effects, while some others show carcinogenic effects. They also have synergistic effects; for instance, sulfur dioxide (SO₂) health effects can be intensified by the presence of particulate matters. In addition to health effects, pollutants impair the constructions and buildings by scratching, settling or removing, and electrochemical corrosion. It has significant importance in European countries because of several historical buildings and statues. Pollutants like ozone, sulfur dioxide, nitrogen dioxide, fluoride, peroxyacetyl nitrate (PAN) and ethylene can lead to some ecological issues due to damaging vegetation.

In a larger scale, pollutants can affect meteorological parameters like visibility due to solar radiation decrease and can have a significant impact on climate change. The other adverse effect is acid deposition in which acidic compounds such as sulfuric acid, nitric acid, and hydrochloric acid via wet and dry deposition on land and water bodies.

Acid deposition has various environmental effects such as soil acidification, fish deaths and health effects deteriorating human respiratory system with disorders such as asthma, bronchitis, and lung edema.

In air quality management, decision-makers need reliable information to first document and then control the emissions by the environmental policies. Reliable documentation are based on accurate data, up-to-date data processing, and modeling. Air quality models use pollutant emissions and some other crucial input parameters such as meteorology, chemical mechanism information, and land use to simulate the advection, dispersion and chemical transformation of the pollutants. It will result in ambient concentrations of different species in various locations at specific times. The quality of emission data, gathered as an inventory, is a key factor in the air quality modeling that can strongly affect the model results. Therefore, emission inventories should be evaluated extensively to decrease the uncertainty and to improve them not only in magnitude but also in their temporal and spatial distribution.

In this thesis, Community Multi-scale Air Quality (CMAQ) modeling system along with Weather Research and Forecasting (WRF) model were run for one winter (January) and for a summer (July) month for the year 2012 over Turkey using EMEP emission inventory. The CMAQ results were compared with satellite and ground observations of SO₂ for determining the probable issues in the SO₂ emission inventory. The satellite observations were extracted from Ozone Monitoring Instrument (OMI) on Aura satellite for the study period. Meanwhile, hourly ground measurements of 207

stations from the national ground-monitoring network in Turkey were used as well. There are uncertainties present in the emission inventories and meteorological inputs. In this thesis, the aim was to evaluate the SO₂ emission inventory used in the model and figuring out the discrepancies while the model results are compared with available observations.

WRF model simulated the meteorological processes while the nudging option was employed. The temperature, wind speed, and wind direction were the selected meteorological parameters to be compared with ground observations as well.

After disregarding the stations with lower than 30% measurements in simulation month, measurements of 44 and 46 stations were used for January and July respectively. The WRF temperature simulations for January and July showed a good agreement with the ground observations in the majority of the stations, except Igdir, and Kirikkale. Poor agreement between simulations and ground observations was observed in Kocaeli, Igdir, and Kirikkale for January. The comparison showed a low correlation in Igdir, Hakkari, Sinop, Kilis, Kirikkale, Icel. Overall, WRF simulations showed a good correlation for both January and July, considering coefficients of determination and trend line slopes. The simulations showed a better agreement for June than July.

The wind speed simulation was performed better in July than January, while the simulation of wind direction parameter was generally more correlated with the observations in January than July. By considering the evaluations that are performed, the quality of WRF outputs were acceptable to be used as input to CMAQ.

Several emission inventories were introduced which are different in terms of period coverage, sectors, temporal variability, and resolution. There are global and regional emission inventories such as TNO, HTAP, EDGAR, EMEP that cover Turkey. In this study, EMEP inventory was selected as emission data source because of spatial resolution, and year availability that includes the study period. The EMEP emissions were in 0.1°×0.1° resolution, pollutant-specific and associated with annual temporal variation. The first step in emission processing was the alternation of emissions to the gridded-hourly form by applying hourly and monthly factors that were dependent on the grid location and diurnal variations. The results were intersected with WRF daughter domain that covered Turkey with 10×10km resolution. At the final step, time zone arranging and speciation (consistent with CBO5 and AERO6 mechanisms) was performed on the anthropogenic emissions. Meanwhile, the biogenic emissions were simulated by MEGANv2.1 for the same period and domain. The simulated biogenic emission results were then integrated to the anthropogenic processed emissions including both anthropogenic and biogenic emissions for using as an input to the CMAQ.

In the next step, the CMAQ SO₂ simulations were assessed with satellite retrievals by comparing the OMI Planetary Boundary Layer (PBL) SO₂ column associated with the lowest part of the troposphere and anthropogenic SO₂ pollution. The comparison indicated similarities such as high concentrations around large point sources. However, there significant differences which indicated underestimations from CMAQ over Afşin Elbistan and Cayırhan power plants, and overestimations over power plants in Mugla and Iskenderun. In addition, over Marmara region, and specifically Istanbul, significant overestimations of CMAQ were observed, possibly indicating the SO₂ emissions should be lower than the reported values in EMEP.

The overall performance of CMAQ SO₂ predictions for the 2-month period (January–July 2012) is indicating a positive bias in the model. The performance in July is better than in January. The uncertainties in OMI retrievals in winter and issues in the estimation of the effect of the local use of coal for residential combustion could be the reason for this result. The scattered plot of CMAQ derived and OMI SO₂ columns indicated some significant overestimations for CMAQ. The correlation was very low for both months.

In addition, the comparison of CMAQ SO₂ simulations with ground observations was performed. The comparison was also performed for four other pollutants (NO, NO₂, PM₁₀, CO) in addition to SO₂. For PM₁₀, the comparison indicated better correlation in January than July. For the other pollutants, the comparison showed better agreement in July than January. Modeled SO₂ showed a reasonable positive bias (MNB=31.5%) for July and negative bias (MNB=-27.19%) for January. This means that model underestimated SO₂ for January and overestimated that in July. It could be because of residential combustions for Turkey in January did not correctly being estimated in EMEP.

The comparison of satellite retrievals and ground observations with model simulations helps to assess the emission inventory's reliability and helps to decrease the uncertainty of the inventories. The results indicated discrepancies in the emission inventories with OMI SO₂ columns and SO₂ ground measurements.

It should also be noted that the uncertainty in OMI SO₂ columns could be reduced by long-time averages i.e. yearly. In addition, one to one comparison of columns temporally would help to understand the reasons for these discrepancies.

By putting everything in a nutshell, the comparisons stated that the CMAQ evaluation with satellite retrievals resulted in an overall underestimation, while with ground-based observations it showed a reasonable SO₂ underestimation and overestimation for January and July, respectively.



EMEP SO₂ EMİSYONLARININ WRF-CMAQ MODEL SİSTEMİ KULLANILARAK TÜRKİYE İÇİN DEĞERLENDİRİLMESİ

ÖZET

Atmosferik kirleticiler tür ve miktarına bağlı olarak bazı istenmeyen kokulara sebep olurlar. Özellikle, insanlar sülfür içeren bileşiklere karşı yüksek hassasiyete sahiptir ve bu sebepten bu bileşikler kolaylıkla hissedilebilir. Bu bileşiklerin aynı zamanda insan sağlığına, özellikle, solunum sistemi üzerinde bronşit, akciğer kanseri ve amfizem hastalığı gibi yan etkileri bulunmaktadır. Ozon gibi bazı kirleticiler olası mutajenik etkilere sahipken diğerleri ise kanserojen etkilere sahiptir. Ayrıca bu kirleticiler sinerjik etkiler de gösterebilir, örneğin, kükürt dioksitin (SO₂) sağlık etkileri partikül madde varlığında şiddetlenerek artar. Sağlık etkilerinin yanında, kirleticiler yapı ve binaları da aşındırma, çökeltme ve elektrokimyasal korozyon vasıtasıyla harabiyet vermektedir. Bu durum, Avrupa'daki bazı tarihi bina ve heykeller için önemli bir problem olarak görülmektedir. Ozon, kükürt dioksit, azot dioksit, florür, peroksiasetil nitrat (PAN) ve etilen gibi kirleticiler bitki örtüsüne zarar vererek ekolojik sorunlara yol açmaktadır.

Daha geniş ölçekte bakıldığında, kirleticiler, solar radyasyonda düşüşe bağlı görüş mesafesigibi meteorolojik parametreleri etkileyebilmekte ve iklim değişikliğine kayda değer etkilere sebep olabilmektedir. Sülfürik asit, nitrik asit ve hidroklorik asit gibi kirleticilerin diğer bir yan etkisi de ıslak ve kuru çökeltme yoluyla toprak ve su alıcı ortamlarında asit birikimine yol açmalarıdır.

Asit birikimi çevre açısından toprağın asitlenmesi, balık ölümleri, gibi, ve insan sağlığı açısından insan solunum sisteminde astım, bronşit ve akciğer ödemi gibi etkilere sebep olmaktadır.

Hava kalitesi yönetiminde, karar verici mekanizmalar emisyonları öncelikle raporlamak ve sonrasında daçevre politikaları ile kontrol altına alabilmek için güvenilir bilgilere ihtiyaç duymaktadır. Güvenilir raporlama; tam ve doğru veri, güncel veri prosesi ve modellemeye bağlıdır. Hava kalite modelleri kirletici emisyonları ve meteoroloji, kimyasal mekanizma bilgisi ve arazi kullanımı gibi diğer önemli girdi parametrelerini kullanarak kirleticilerin öteleme, yayılım ve kimyasal dönüşümlerini simule ederler. Model simulasyonları çeşitli kirletici türlerinin belirli lokasyonlarda ve belirli zamanlarda ortam konsantrasyonu hesaplar. Envanter olarak toplanan emisyon verisinin kalitesi, hava kalite modellerinde önemli bir parametre olup, model sonuçlarını önemli ölçüde etkileyebilir. Bu sebepten, emisyon envanterleri, belirsizlikleri azaltmak için ayrıntılı olarak incelenmeli ve sadece miktar olarak değil, mekansal ve zamansal dağılımı da iyileştirilmelidir.

Bu tezde, Community Multi-scale Air Quality (CMAQ) modelleme sistemi Weather Research and Forecasting (WRF) modeli ile birlikte 2012 yılı için bir kış (Ocak) ve bir yaz (Temmuz) ayı için EMEP emisyon envanteri kullanılarak çalıştırılmıştır. CMAQ sonuçları, emisyon envanterindeki olası problemleri belirlemek için SO₂ uydu ve yer

ölçümleri ile karşılaştırılmıştır. Uydu verileri AURA uydusu üzerinde bulunan, Ozone Monitoring Instrument (OMI) enstrümanından elde edilmiştir. Aynı zamanda, Türkiye Ulusal Hava Kalite İzleme Ağındaki 207 istasyondan saatlik veriler elde edilmiştir. Meteorolojik girdiler ve emisyon envanterlerinde belirsizlikler mevcuttur. Bu tezdeki amaç, modelde kullanılan SO₂ emisyon envanterini değerlendirmek ve model sonuçlarını mevcut ölçümlerle karşılaştırarak uyumsuzlukları belirlemektir.

WRF modeli nudging özelliği kullanılarak meteorolojik simülasyonları gerçekleştirilmiştir. Bunun yanı sıra yer ölçümleriyle karşılaştırma yapmak için, sıcaklık, rüzgar hızı ve yönü gibi meteorolojik parametreler seçilmiştir.

Modellenen ay içerisinde %30'dan az ölçüme sahip istasyonlar çıkarıldıktan sonra, Ocak ve Temmuz ayı için sırasıyla 44 ve 46 istasyon değerlendirilmeye alınmıştır. WRF sıcaklık simülasyonları Ocak ve Temmuz ayları için yer ölçüm istasyonlarından Iğdır ve Kırıkkale hariç diğer istasyonlar için çoğunlukla iyi bir uyum göstermiştir. Ocak ayı için, Kocaeli, Iğdır ve Kırıkkale istasyonları ile model simülasyonları arasında uyumsuzluk gözlenmiştir. Aynı zamanda Iğdır, Hakkari, Sinop, Kilis, Kırıkkale ve İçel illerindeki için karşılaştırmalar düşük korelasyon göstermiştir. Genel olarak, korelasyon katsayısı ve eğri eğimi dikkate alındığında, WRF simülasyonları Ocak ve Temmuz ayları için yer ölçümleriyle benzerlik göstermiştir. Simülasyonlar, Haziran ayı için Temmuz'a göre ölçümler ile daha uyumlu görünmektedir.

Rüzgar hızı simülasyonları Temmuz için Ocak ayına göre daha iyi sonuçlar verirken, rüzgar yönü parametresi için yapılan simülasyonlar Ocak ayı için Temmuz ayına göre yer ölçümleriyle daha iyi uyum göstermiştir. Yapılan değerlendirmeler sonucunda, WRF modeli çıktı kalitesinin CMAQ modeli girdileri için kabul edilebilir düzeydedir.

Çözünürlük, zamansal değişiklik, sektör ve dönem kapsamı açısından değişik birçok emisyon envanteri bulunmaktadır. Türkiye'yi kapsayan TNO, HTAP, EDGAR ve EMEP gibi küresel ve bölgesel ölçekli emisyon envanterleri bulunmaktadır. Bu çalışmada, mekansal çözünürlük ve çalışma yılını kapsayan veri mevcudiyeti sebebiyle EMEP emisyon envanteri kullanılmıştır. EMEP emisyonları 0.1°×0.1° çözünürlükte, kirletici türlerine ve yıllık zamansal değişimlere göre raporlanmaktadır. Emisyon sürecindeki ilk adım grid lokasyonu ve günlük değişimlere bağlı saatlik ve aylık faktörler kullanarak emisyonların gridli-saatlik formlara dönüştürülmesidir. Sonuçlar Türkiye'yi kapsayan 10×10km² çözünürlükte WRF çalışma alanı ile kesiştirilmiştir. Son aşamada, zaman dilimi ayarlaması ve kirletici türlerin çeşitlendirilmesi (CBO5 ve AERO6 mekanizmaları ile uyumlu) antropojenik emisyonlar üzerinde uygulanmıştır. Biyojenik emisyonlar aynı zaman dilimi ve çalışma alanı için MEGANv2.1 kullanılarak simüle edilmiştir. Simüle edilen biyojenik emisyonlar antropojenik emisyonlar ile toplanarak antropojenik ve biyojenik emisyonlardan oluşan emisyonlar CMAQ modeli girdisi olarak kullanılmıştır.

Bir sonraki aşamada, CMAQ SO₂ simülasyonları troposferin en alt bölümüyle ve antropojenik SO₂ kirliliği ile ilişkili olan OMI Yüzeye Yakın Sınır Tabakası (PBL) SO₂ uydu verileri kullanılarak değerlendirilmiştir. Karşılaştırma, büyük nokta kaynaklar etrafında yüksek kirlilik konsantrasyonları görülmesi konusunda benzerlik göstermiştir. Fakat, yine de çalışma alanı içerisinde ciddi farklılıklar tespit edilmiştir. Afşin Elbistan ve Çayırhan termik santralleri etrafında CMAQ modeli, daha düşük kirlilik tahminde bulunurken, termik santrallerin bulunduğu Muğla ve İskenderun çevresi için de yüksektahminde bulunmuştur. Ayrıca, Marmara bölgesi ve özellikle İstanbul'da, CMAQ modelinin önemli derece yüksek kirlilik tahmin ettiği gözlenmiş,

bu sonuç EMEP envanterinde rapor edilen emisyonların daha düşük seviyede olması gerektiğine işaret etmiştir.

Ocak ve Temmuz 2012 ayları için CMAQ SO₂ tahminleri genel olarak değerlendirildiğinde modelde pozitif yanlılık olduğu görülmüştür. Modelin Temmuz ayı performansı Ocak ayına göre daha iyi bulunmuştur. Bunun sebebinin, OMI uydu verilerinin kış aylarındaki belirsizliği ve evsel ısınmada kullanılan linyit kömürünün yerel etkisinin tahminindeki sorunlar olabileceği düşünülmektedir. CMAQ modeli ve OMI SO₂ kolon konsantrasyonlarının kıyaslanması CMAQ modelinin önemli derecede fazla tahminde bulunduğunu göstermiştir. Ayrıca her iki ay için de korelasyon katsayısı oldukça düşüktür.

Bunun yanı sıra, CMAQ SO₂ simülasyonları ile yer ölçümleri karşılaştırılmış ve sonuçlar değerlendirilmiştir. SO₂ ve dört farklı kirletici (NO, NO₂, PM₁₀, CO) için bu karşılaştırma yapılmıştır. PM₁₀ için yer ölçümleriyle yapılan karşılaştırmada Ocak ayı için Temmuz'a göre daha iyi uyum görülmüştür. Diğer kirleticiler için ise Temmuz ayı, Ocak ayına göre daha iyi uyum göstermiştir. Model SO₂ konsantrasyonları Temmuz ayı için kabul edilebilir bir pozitif yanlılık (MNB=%31.5) ve Ocak ayı için negatif yanlılık (MNB=-%27.19) göstermiştir. Bu sonuç, Ocak ayı için modelin SO₂ konsantrasyonunu eksik tahminde bulunduğu, Temmuz ayı içinse fazla tahminde bulunduğunu göstermektedir. Bunun sebebinin Ocak ayında Türkiye genelinde evsel ısınma katkısının EMEP emisyon envanterinde yeteri kadar gösterilmemiş olması olabileceği düşünülmektedir.

Model simülasyonlarının uydu verileri ve yer ölçümleriyle karşılaştırılması emisyon envanterinin güvenilirliğini değerlendirmede ve envanterlerin belirsizliklerini azaltmakta yardımcı olmuştur. Sonuçlar emisyon envanterlerinin OMI SO₂ kolon ve SO₂ yer konsantrasyonları ile farklılıklar gösterdiğini işaret etmiştir.

Bilinmelidir ki, OMI SO₂ kolon konsantrasyonlarındaki belirsizlikler uzun zaman ortalama değerleri örneğin yıllık ortalamalar alınarak azaltılabilir. Ayrıca SO₂ kolon konsantrasyonlarının zamansal olarak birebir karşılaştırılması farklılıklardaki nedeni de anlamaya yardımcı olabilir.

Özet olarak, CMAQ modelinin değerlendirilmesinde, CMAQ SO₂ konsantrasyonlarının uydu verilerine göre az tahminde bulunduğunu, diğer yanda yer ölçümleriyle yapılan karşılaştırmada CMAQ modelinin Ocak ayı için düşük tahminde bulunurken, Temmuz ayı için yüksek tahminde bulunduğu gözlenmiştir.



1. INTRODUCTION

Air pollution is an important problem which affects more and more people and causes not only a lot of health issues (lung cancer, asthma, allergies, various breathing problems and skin, eye problems), but also it damages the ecological balance of 21st century seriously. It threatens the development sustainability and stability. At present, the Turkish economy is developing very fast. Air quality in megacities is of great concern due to migration towards urban areas and the health issues (Gurjar et al., 2008). The rise of energy demand and transportation, the urban population increase, and the quick development of large industrial zone, make the country's air pollution worse.

One of the efficacious methods of evaluation that can provide the opportunity for forecasting the drifts of air pollution, averting environmental catastrophes, as well as promoting individuals' environmental awareness, is Multi-Model of air quality prediction. By this system, we are able to reduce the inconsistency between weather and results of emission processing, besides to obtain factual evaluation results of various air quality modeling simulation.

1.1 Aim and Scope

The aim of this study is to assess and promote SO₂ emission inventories of Turkey using SO₂ satellite retrievals (tropospheric columns, molecules/cm²) and ground-based observations. Emission inventories are one of the main sources of uncertainty in regional air quality models. They impose a high discrepancy in model outputs. In this thesis, the share of other model inputs in uncertainty was decreased except the emission inventory.

For this purpose, WRF-CMAQ modeling system was run by use of EMEP SO₂ emission inventory as well as WRFv3.7 as Metrological model. For assuring that the models were working properly, we applied some assessment methods to evaluate them. At the first step, the outputs of WRF model were compared to ground station measurements. In the case of high variation, some initial parameters had to be changed

in the model. Moreover, the nudging option was enabled for improving the model results. These are the primary tasks that have to be done to reduce uncertainty. Otherwise, the role of emission inventory will not be bold enough in either underestimation or overestimation of pollutant concentrations.

To evaluate air quality models some observations are used to find the correlation between model outputs and reality. In this study, two different kinds of observations were used: satellite retrievals and ground observations.

In this study, OMI Level2 (L2) SO₂ Planetary Boundary Layer (PBL) column data for 2012 (<http://mirador.gsfc.nasa.gov>) with following qualifications was used to ensure data quality: Solar Zenith Angle (SZA) < 70°, Radiative Cloud Fraction (RCF) < 0.3, Ozone Column Amount (O₃) < 1500 DU (OMI, 2014).

Annual SO₂ retrievals for 10×10 km² gridded domain were averaged around 12 km of each grid center and assigned to the grids for 2012. By this smoothing method (Fioletov et al., 2011; Lu et al., 2013), noise in the SO₂ pollution maps was reduced. The average monthly SO₂ columns were also calculated for one summer and one winter month; July and January 2012 for comparison with modeling results.

In addition, 117 different air quality monitoring stations were selected as ground data sources in Turkey. After performing statistical calculations, They compared with CMAQ results to find discrepancies and variations of model outputs.

1.2 Literature Review

During recent years, quite a few studies were carried out for evaluation of community multiscale air quality (CMAQ) modeling system over mostly United States, Europe, and Asia, respectively; with satellite or ground observations. The number of studies has been carried out over some regions and in particular countries like Turkey are very low with respect to the Northern America and Europe. The conclusions of those studies manifested a good correlation between the simulations and reality.

Trends in air quality across the Northern Hemisphere from 1990 to 2010 have been simulated by the WRF-CMAQ model driven with a representation of historical emission inventories derived from the EDGAR (Xing et al., 2015). The model results were compared with several ground observation networks mostly in Europe and North America. CMAQ was generally able to capture the trends of ground observations and

also the statistical indices were compared with the other studies which were performed over Northern Hemisphere. The results showed that the model still suffered from different uncertainties in emission inventory (especially due to temporal variation and speciation), the low resolution of emission inventory (EDGAR was used as emission inventory) and also the impacts of those on nonlinear atmospheric chemistry. The biogenic emissions did not take into account in that study. Hence, it could also affect the discrepancies in the conclusions. The lack of long-term ground observations in Asia, particularly over China and India, limits a robust model performance evaluation and O₃ and PM chemistry assessment in these polluted areas. CMAQ-simulated air quality trends over the past 2 decades largely agree with those derived from observations (Xing et al., 2015).

In another study, ozone predictions which were carried out by CMAQ were evaluated by observations (Eder et al., 2006) over the northeastern United States. Examination of the overall, 4-month performance, from a discrete perspective, revealed a systematic tendency to overestimation of concentrations resulting in an NMB of 22.8%, an NME = 28.1%, and a correlation of 0.59. The evaluation results showed that the CMAQ performance was reasonably well in that study.

Zhang et al. (2014) studied the performance of WRF-CMAQ modeling system over eastern part of United States. They observed an overestimation in temperature and well-simulated water vapor but with significant biases in the winter. Although the wind speed predicted well, wind direction results did not have a good agreement with surface observations. In this study, the prediction of O₃, PM₁₀ and PM_{2.5} was satisfactory (Zhang et al., 2014).

Satellite retrievals are an important observation source for evaluation of the air quality models. Some instruments like Aura's OMI, EUMETSAT's GOME, ENVISAT's SCIAMACHY are widely used in air quality monitoring from the space. In some studies, researchers used satellite data alone and in some others, it was used along with surface and aircraft observations.

In this study, long-term analysis of tropospheric nitrogen dioxide (NO₂) columns retrieved from GOME, SCIAMACHY, OMI and GOME-2 satellites, carbon monoxide (CO) columns from MOPITT satellite, and aerosol optical depths (AODs) from MODIS satellite was performed for Southeast Asian countries including Japan

and China during 1996–2012. The results show that satellite observations are able to capture the trend and seasonal variability of the emissions and ground concentrations. The model simulations were conducted using CMAQ model. Generally, simulated model results agree well with those retrieved from satellite measurements for spatial distribution and seasonal pattern. However, the modeled results underestimate satellite data probably due to the inaccuracy in emission inventories, the inaccuracy of spatial and temporal allocations, and the uncertainties in the satellite retrievals (Lalitaporn et al., 2013).

Kaynak et al. (2013) were performed an analysis of NO, NO₂, and O₃ between model simulations and ground-based, aircraft, and satellite observations. Low biases between NO₂ predictions and both ground-based and satellite observations were observed. Although the aircraft-based observations showed a higher positive bias and error, the overall NO₂ vertical profile was well-simulated. The results indicated a similar satellite and model spatial gradient for NO₂. The comparison showed underestimation between model and both ground and aircraft observations. Simulated O₃ captured the aircraft- and ground-based observations. The results showed overestimation in OH by CMAQ (Kaynak et al., 2013).

By considering the studies that were discussed, WRF-CMAQ modeling system has a reasonable well performance and it can be used to predict the pollutant concentrations in the condition of lacking practical pollutant data. Hence, CMAQ is appropriate to be applied in the case studies such as China, Turkey, and so on.

2. MATERIALS AND METHODS

2.1 Meteorological Modelling

Weather Research and Forecasting (WRF-ARW) model, version 3.7 was used in this study as a meteorological model (Skamarock and Klemp, 2008; Borge et al., 2008), which was developed based on the Fifth-Generation Penn State/NCAR Mesoscale Model (MM5) (Grell et al., 1994). Two domains have been set up for the meteorological modeling system on Lambert Conformal projection: a mother domain covering Europe of 191 by 159 grid cells on 30 km spatial resolution, and the daughter domain covering the Turkey and part of eastern European countries of 244 by 157 grid cells on 10 km resolution (Figure 2.1). To provide the initial and boundary conditions which are needed by the WRF model, The National Centers for Environmental Prediction (NCEP) Final Analyses (FNL) data of $1^\circ \times 1^\circ$ was used as meteorological input. Besides 15 sigma layers were used for the vertical resolution of the model. The vertical resolution was stretched from the surface and gradually decreased up to the model top (1 kPa). Additionally, the nudging analysis was performed on temperature, wind and humidity parameters for the mother domain.

The WRF ARW model can be compressed completely, also it is a nonhydrostatic model (with a hydrostatic option). The vertical coordinate in WRF model follows terrain for hydrostatic pressure coordinate. The Arakawa C-grid is applied as grid staggering. The numerical methods used WRF ARW are higher-order. This includes the Runge-Kutta 2nd- and 3rd-order time integration schemes, and 2nd- to 6th-order advection schemes in both horizontal and vertical directions. The dynamics conserve scalar variables (<http://www2.mmm.ucar.edu>).

In WRF ARW model consists of some modules such as initialization programs (ideal.exe and real.exe), numerical integration program (wrf.exe), and a program to perform one-way nesting (ndown.exe). The WRF ARW model Version 3 has many capabilities such as:

- Wide range of applications from meters to thousands of kilometers

- Simulations for Real-data and idealized cases
- Flexible to select different lateral boundary condition options for both real-data and idealized cases
- Full physics options
- Non-hydrostatic and hydrostatic (runtime option)
- One-way, two-way nesting, and a moving nest
- Regional climate research
- Forecast research
- Real-time NWP
- Hurricane research

Figure 2.1 shows the mother and daughter domain in this study.

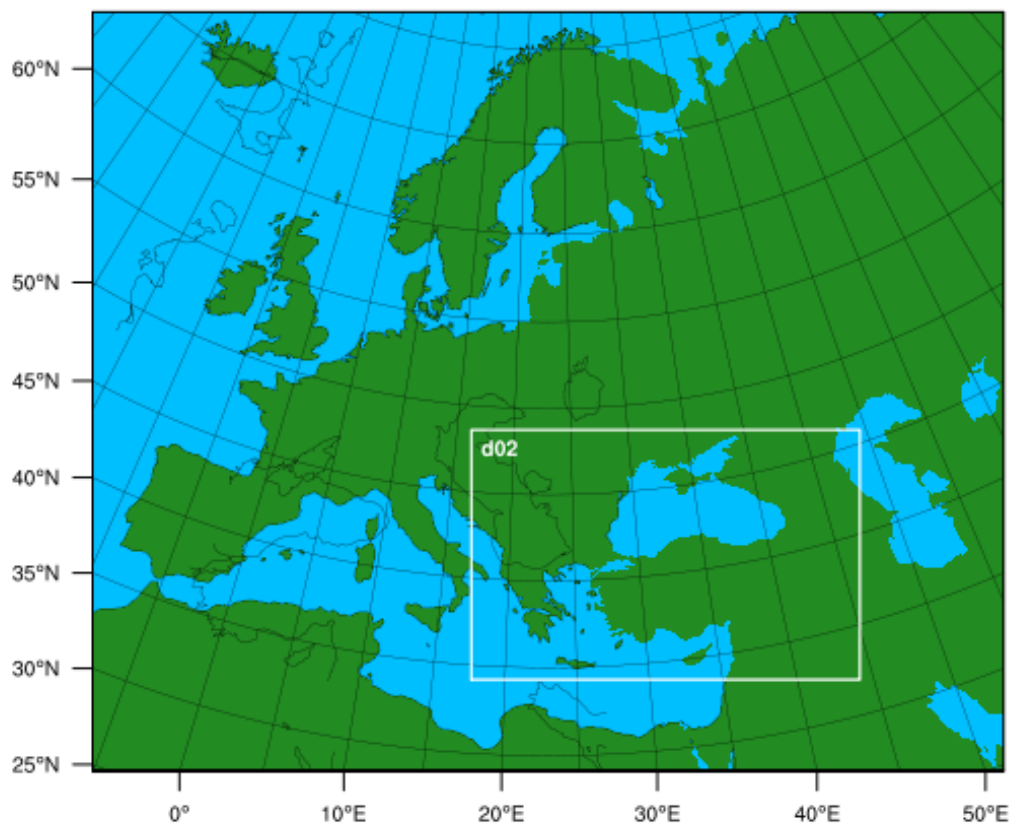


Figure 2.1 : Domains definition and coordination (adapted from WRFv3.7 User Guide).

2.1.1.1. The WRF modeling system program modules

The WRF program components and processes are shown in the following figure.

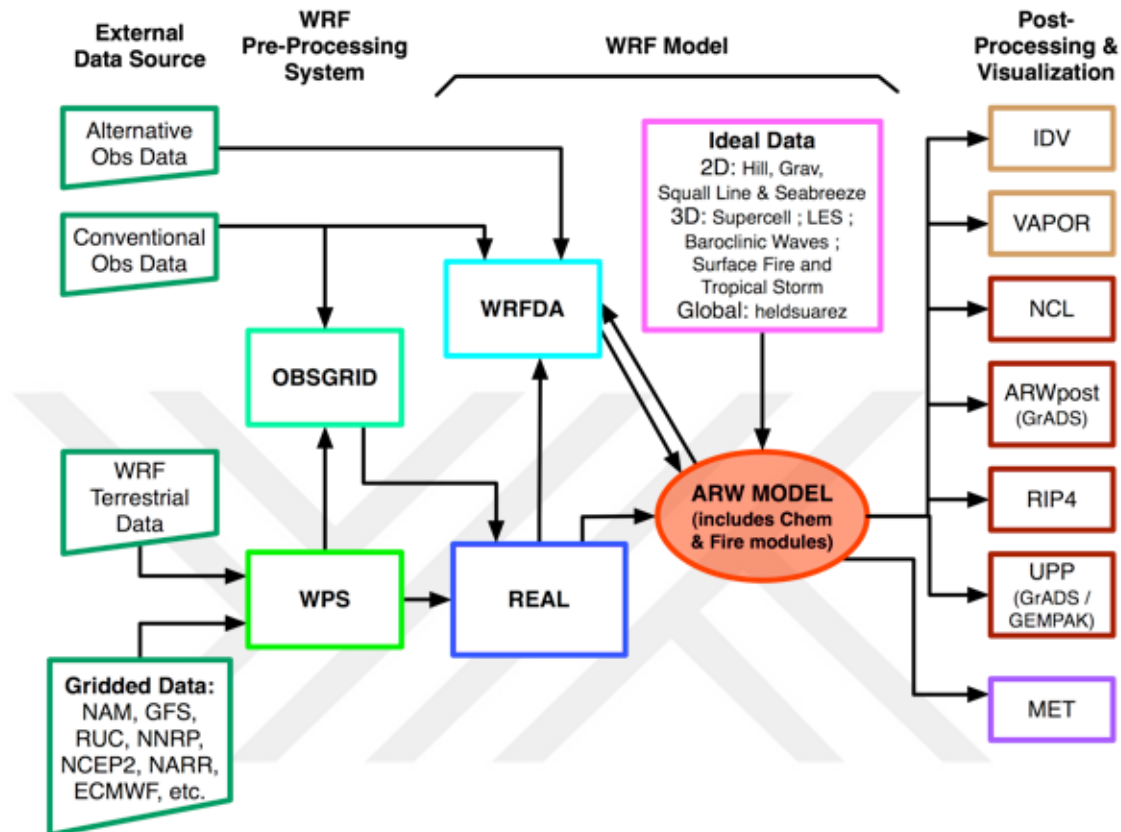


Figure 2.2 : WRF modeling system flow chart (adapted from WRFv3.7 User Guide)

As presented in Figure 2.2, the structure of WRF modeling system is based on these main programs:

- The WRF Preprocessing System (WPS)
- WRF-DA
- ARW solver
- Post-processing & Visualization tools

2.1.1.1 WPS

For real-data cases, this program has to be used primarily. These tasks are done by its functions:

- I. Defining and determining of model domains.

- II. Interpolating terrestrial data (such as types, land use, and terrain) to the simulation domain.
- III. Degribbing and interpolating meteorological data from another model to this simulation domain.

2.1.1.2 WRF-DA

Using this component is optional. Its feature is to ingest observations into the interpolated analyses produced by WPS. It can also be used to update WRF model's initial conditions when the WRF model is run in cycling mode.

2.1.1.3 ARW solver

This is the major module of the modeling system, which consists of so many initialization programs for real-data, and idealized simulations, and the numerical integration program.

2.1.1.4 Graphics and verification tools

There are many programs which are supported, including RIP4 (based on NCAR Graphics), NCAR Graphics Command Language (NCL), and conversion programs for other readily available graphics packages like GrADS.

Program VAPOR, Visualization and Analysis Platform for Ocean, Atmosphere, and Solar Researchers (<http://www.vapor.ucar.edu>) is a 3-dimensional data visualization tool, and it is developed by the VAPOR team at NCAR.

Program MET, Model Evaluation Tools (<http://www.dtcenter.org/met/users/>), is developed and supported by the Developmental Testbed Center at NCAR.

Figure 2.3 shows the order of the data processing and data flow between the programs of WPS. The static geographical data is processed by “geogrid” module. Besides, “ungrib” module processes the gridded weather data and the results of them will interpolate by “metgrid”. The output of “metgrid” is used by WRF.

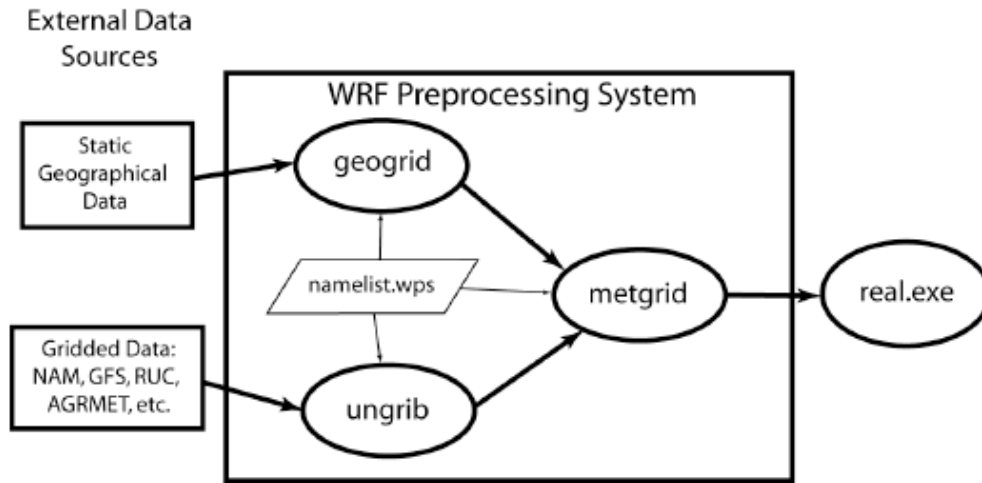


Figure 2.3 : Data flow between the programs of WPS (adapted from WRFv3.7 User Guide).

2.1.2 WRF preprocessing system (WPS)

The WRF Preprocessing System (WPS) includes three programs which prepare input to the real program for real-data cases. Each of the programs does one part of the preparation stages: “geogrid” defines model domains and interpolates static geographical data to the grids; “ungrib” extracts meteorological fields from GRIB formatted files; and “metgrid” horizontally interpolates the meteorological fields extracted by “ungrib” to the model grids defined by “geogrid”. The work of vertically interpolating meteorological fields to WRF eta levels is performed within the real program.

As shown in the Figure 2.2., parameters are read from a common namelist file by WPS programs. This namelist file has two types of records. Separate records which is read by each of the programs and a shared namelist record, which contains parameters that are needed by more than one WPS program.

2.1.2.1 Function of each WPS program

The WPS includes three independent programs: “geogrid”, “ungrib”, and “metgrid”.

Program “geogrid”

The aim of “geogrid” is to define the simulation domains, and interpolate various terrestrial data sets to the model grids.

Output from “geogrid” is written in the WRF I/O API format, and thus, by selecting the NetCDF I/O format, “geogrid” can be made to write its output in NetCDF for easy visualization using external software packages, including NCVIEW, NCL, and RIP4.

Program “ungrib”

The function of “ungrib” program is to read GRIB files. In other words, it “degrib” the data, and writes them in a so-called intermediate format which is a simple format. The GRIB files consist of time-varying meteorological fields and are typically from another regional or global model, such as NCEP's NAM or GFS models. The “ungrib” program supports GRIB Edition 1 and, if compiled with a “GRIB2” option, GRIB Edition 2 files as the input file.

There are some fields in GRIB files that are not used to initialize WRF. The codes which are used to identify the variables and levels in the GRIB file are diverse. For a creating intermediate file, “ungrib” needs to define which fields to extract from the GRIB file. For this purpose, it uses tables of these codes which are called Vtables for “variable tables”. “ungrib” program is used to provide Vtables for common GRIB model output files.

The common Vtables are available for the NCEP/NCAR Reanalysis archived at NCAR, ECMWF, NAM 104 and 212 grids, the NAM AWIP format, GFS, RUC (pressure level data and hybrid coordinate data), AFWA's AGRMET land surface model output, and other data sets. It is also possible for users to create a custom Vtable for other model output using any of the Vtables as a template.

Program “metgrid”

The aim of “metgrid” program is to interpolate horizontally the intermediate-format meteorological data that are extracted by the “ungrib” program onto the model domains defined by the “geogrid” program. These outputs can be ingested by the WRF real program. For this process, The range of dates are defined in the “share” namelist record of the WPS namelist file, and date ranges must be specified individually in the namelist for each simulation domain. Due to that, this program is a time-dependent system as “ungrib” program so “metgrid” is run coincide with each new initialized simulation.

Control over how each meteorological field is interpolated is provided by the “METGRID.TBL” file. The “METGRID.TBL” file provides one section for each

field, and within a section, it is possible to specify options such as the interpolation methods to be used for the field, the field that acts as the mask for masked interpolations, and the grid staggering (e.g., U, V in ARW; H, V in NMM) to which a field is interpolated.

“METGRID.TIB” file is used for controlling the interpolation procedure for every meteorological field, besides that it provides a specific section for each field which makes it possible to particularize options for interpolated fields like the utilized interpolation methods.

The format of final “metgrid” output is WRF I/O API; consequently by selecting NetCDF I/O format, the outputs of this program are in NetCDF.

2.1.2.2 Running WRF preprocessing system (WPS)

After installation required libraries, compilers, and scripting languages, the following procedure has to be done sequentially:

- I. Domain definition has to be performed by “geogrid”. A couple of domains can be determined as mother domain and nested domains.
- II. Meteorological data should be extracted from GRIB data for model time episode by “ungrib”.
- III. Interpolation between meteorological fields and simulation domain has to be done horizontally by “metgrid”.

“geogrid” and “ungrib” programs are independent of each other. That is to say, for running WPS for one particular domain and different time periods, it is necessary to run “geogrid” once. In other words, the time-dependent data has to be processed for each run using tasks 2,3. Likewise, for diverse simulation domains that are being run for the same time episode, it does not need to run “ungrib” a couple of times. It is possible to use intermediate files that were obtained from first “ungrib” run.

In this case, “geogrid” program needs to be run for each domain separately and then, running “metgrid” by using the “ungrib” outputs will create the final WPS results. In the following sections, WPS running steps will be expressed in detail.

Step 1: Domain definition with “geogrid”

After installation of WPS, “geogrid.exe”, “ungrib.exe” and “metgrid.exe” have to be created and linked in the WPS main path. Otherwise, the programs was not installed completely or they were corrupted.

Domain sizes and locations are defined in “namelist.wps” under ““geogrid”” section. Moreover, the parameters that are under “share” have to be set as well. They determined the maximum number of domains and model core type. Besides, the grid size and parent grid ratio should be defined separately in “namelist.wps” for different domains. There are four map projection methods included in the model. For selecting each of them, specific parameters should be set (Figure 2.4).

Map projection / value of map_proj	Projection parameters
Lambert Conformal / 'lambert'	truelat1
	truelat2 (optional)
	stand_lon
Mercator / 'mercator'	truelat1
Polar stereographic / 'polar'	truelat1
	stand_lon
Regular latitude-longitude, or cylindrical equidistant / 'lat-lon'	pole_lat
	pole_lon
	stand_lon

Figure 2.4 : Map projection options and their parameters in WPS (adapted from WRFv3.7 User Guide).

There is a significant matter that should be considered in selecting map projection and it is minimization distortion. This means that for a specific domain which is enclosed in between two latitudes, the best map projection has to be applied.

Generally, the polar stereographic projection is suitable for high latitude domains. For domains with middle and low latitude, lambert conformal and mercator projection are well-suited respectively. Another map projection option in WPS is cylindrical equidistant that is appropriate for global ARW models. However, it can be applied in regional scales by modification of some parameters.

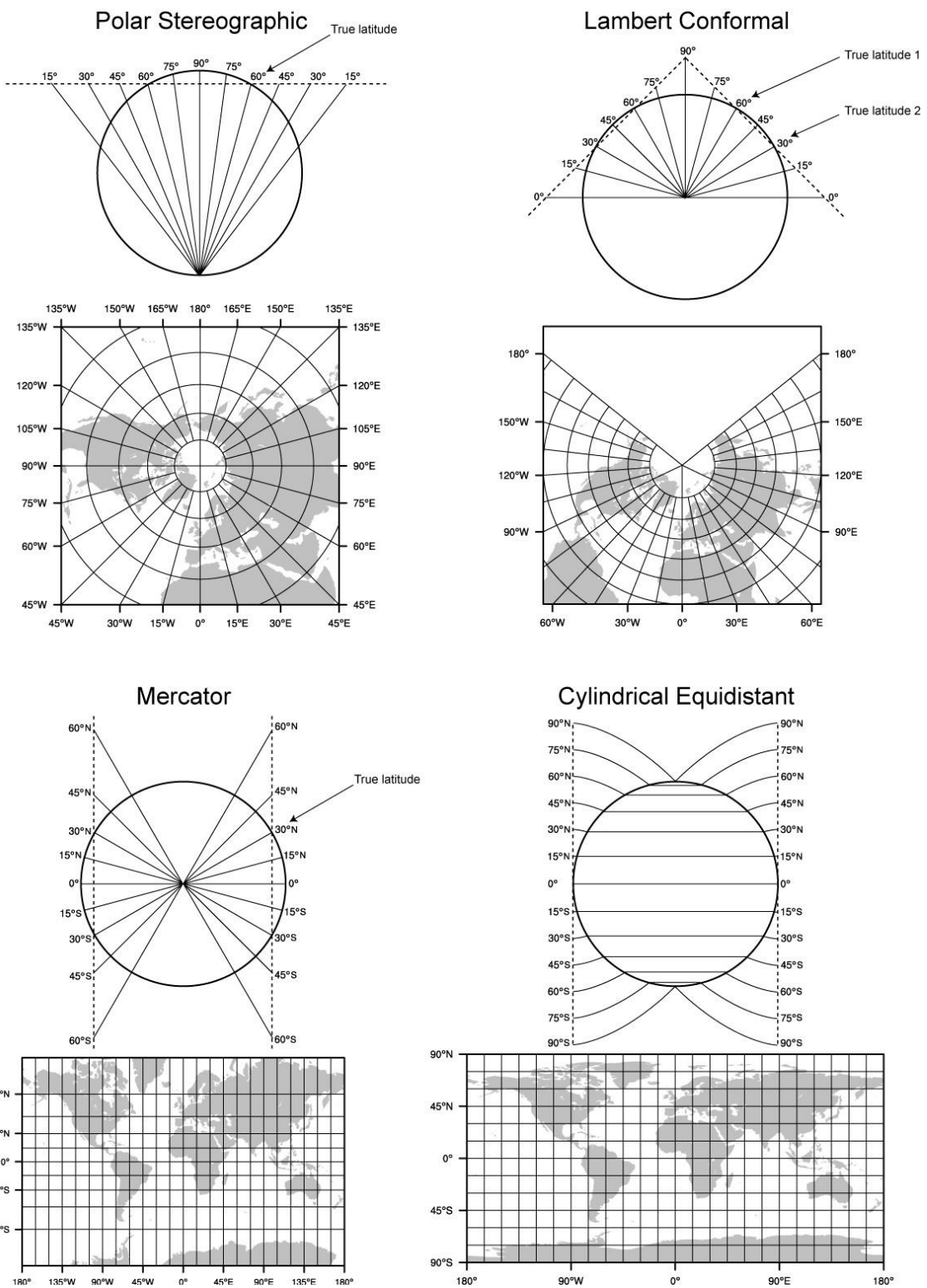


Figure 2.5 : True latitude(s) for different map projection options in WPS (UCAR, 2014).

At the end of this step, one or some netcdf files are created. The number of netcdf files is equal to the number of domains.

Step 2: Reading GRIB files to extract meteorological fields with “ungrib”

At this step, the parameters that define the starting and ending time of the coarse domain should be modified. Also, the interval between meteorological data should be set in “namelist.wps” file. Thereafter, following tasks should be performed:

- I. Downloading GRIB file(s) as meteorological data file(s)
- II. Finding and linking the consistent Vtable with GRIB file(s)
- III. Creating intermediate files

Step 3: Interpolation of meteorological fields and simulation domain with “metgrid”

The “fg_name” parameter in “namelist.wps” file, should be the same as the prefix of the intermediate files name. after setting that, “metgrid.exe” should be executed to produce final WPS files which will ingest with “real.exe”.

2.1.3 Running WRF

WRF can be run for both ideal and real cases. After running codes in ideal case mode to check if WPS and WRF worked properly, the model was run by real case configurations.

There are some variables in “namelist.input” file which is in the WRF run folder that needs to be set according to the model conditions. e.g. the start and the end of the simulation time period, grid size, model time step, the number of vertical layers, domain dimensions in different horizontal directions and soil levels which can be extracted from “metgrid” output files. We can also find other options in “namelist.input” file that is used to improve calculations in upright direction. Below, a set of variables in “namelist.input” are shown that they have to be modified according to the arbitrary case (Figure 2.6).

a)

start_*, end_*	start and end times for data processing and model integration
interval_seconds	input data interval for boundary conditions
time_step	model time step, and can be set as large as 6*DX (in km)
e_ws, e_sn, e_vert	domain dimensions in west-east, south-north and vertical
dx, dy	model grid distance in meters
num_metgrid_levels:	number of incoming data levels (can be found by using the ncdump command on the met_em.* file)
num_metgrid_soil_levels:	number of incoming soil data levels
eta_levels:	model eta levels from 1 to 0, if you choose to do so. If not, real will compute a nice set of eta levels. The computed eta levels have 7 half levels in the lowest 1 km or so, and stretches to constant δz .

b)

use_surface:	whether to use surface input data
extrap_type:	vertical extrapolation of non-temperature fields
t_extrap_type	vertical extrapolation for potential temperature
use_levels_below_ground	use levels below the input surface level
force_sfc_in_vinterp	force vertical interpolation to use surface data
lowest_lev_from_sfc	place surface data in the lowest model level
p_top_requested	pressure top used in the model, default is 5000 Pa
interp_type	vertical interpolation method: linear in p or log(p) (default)
lagrange_order	vertical interpolation order, linear or quadratic (default)
sap_close_levels	allow surface data to be used if it is close to a constant pressure level
smooth_cg_topo	smooth topography on the outer rows and columns in domain 1
use_tavg_for_tsk	whether to use diurnally-averaged surface temp as skin temp. The diurnally-averaged surface temp can be computed using the WPS utility avg_tsfc.exe. This option can be used when SKINTEMP is not present.

Figure 2.6 : WRF “namelist.input” file parameters: a) General parameters b) interpolation variables (adapted from WRFv3.7 User Guide).

After editing those variables “real.exe” should be run to create files that would be ingested by ARW solver. In all of the steps of WRF running, the outputs of each program should be domain specific except “ungrib” program. As an example, for two domains there should be different output files in which the domain identification number is included in the file name.

The last stage is to execute “wrf.exe” for obtaining the final results. The results can be visualized by a variety of post-processing software such as NETCDF, VERDI, NCL, MATLAB and so on.

These results have to be prepared by MCIP program to input CMAQ and emission processing unit.

2.2 Emission Processing

To process emissions by air quality models, they have to be in the specific format and frame which is applicable to those programs. For this aim, emission processing is performed by considering AQM species name list, WRF domain dimensions, and temporal profiles. Emission processing is a crucial section in running CMAQ is able to strongly increase or decrease the variation of simulation results in some cases. In this study, it was performed by the codes, which were written in İTÜ using MATLAB program.

The steps that accomplished are as follows:

- I. Selecting the well-suited emission inventory.
- II. Temporal allocation.
- III. Vertical distribution.
- IV. Spatial allocation
- V. Speciation
- VI. Biogenic emission processing by MEGANv2.1
- VII. Combination of the results of the anthropogenic and biogenic processed emissions

In the following sections, each of the processing steps will be explained.

2.2.1 Emission inventory

There are several emission inventories that are distinguished by the coverage period, grid size, type of emissions such as anthropogenic and biogenic, temporal variability and covered region. There are some key points that have to be regarded when an emission inventory is being selected.

First, the resolution of the inventory; lower grid size can provide more details and consecutively better inputs for air quality models (AQM). Second, the temporal variability; the narrower emission time episode can contain more reliable data for a AQM. It is not necessarily true but it can often be.

Third, the episode is also an important point to use an emission inventory. It is better that an emission inventory, which is selected, covers the simulation period, otherwise emission projection might be necessary to account for the changes.

The emission data are reported by the parties to LRTAP Convention through EMEP program annually. The reports are processed at the national level. Before 1990, the emission reports were based on “Selected Nomenclature for Air Pollutants (SNAP)” categories. SNAP included eleven sectors and it did not have enough details. In the 1990s, “Nomenclature For Reporting (NFR)” became the dominant template of emission data reports. It had 102 categories, hence it could provide the more detailed data more reliable database. The national inventories are based on national statistics and country specific, and technology dependent emission factors (ECCAD, 2013). For some area, there are either low quality or lack of data. In these cases, filling the gaps or modifying the data are done by using independent estimates and either interpolation or extrapolation.

In this study, EMEP emissions for the year 2012 with $0.1^{\circ} \times 0.1^{\circ}$ longitude-latitude spatial resolution for GNFR14 sectors was used. Pollutants that include in EMEP are SO_x , NO_x , CO, PM_{10} , $\text{PM}_{\text{coarse}}$, $\text{PM}_{2.5}$, NMVOC, NH_3 . It covers an area which is between 30°N - 82°N latitude and 30°W - 90°E longitude (Figure 2.7).

Global emissions					
inventory	period covered	categories	temporal variability	grid size	
ACCMIP	1850 -2000	anthropogenic	-annual	0.5 x 0.5	
		biomass burning	-annual		
RCPs (scenarios)	2000 -2100	anthropogenic	-annual	0.5 x 0.5	
		biomass burning	-annual		
EDGAR 3.2FT2000 (2005)	2000	anthropogenic	-annual	1 x 1	
		biomass burning	-annual		
RETRO	1960 -2000	anthropogenic	-monthly	0.5 x 0.5	
		biomass burning	-monthly		
EDGAR-HYDE 1.3	1890 -1990	anthropogenic	decadal	1 x 1	
Junker&Liousse - BC/OC	1860 -2003	anthropogenic	decadal (1860-1946) annual (1946-2003)	1 x 1	
GFED3	1997 - 2009	biomass burning	monthly	0.5 x 0.5	
GFEDv2	1997 - 2005	biomass burning	monthly 8 day (on GFEDv2 page)	1 x 1	
GICC	1900 -2000 (decadal) 1997 -2005	biomass burning	monthly	1 x 1	
MEGANv2 -biogenic	2000 decade	biogenic	monthly	0.5 x 0.5	
MEGANv2.1-CH3OH	2003-2009	biogenic	monthly	0.5 x 0.5	
GEIA v1	species dependent	anthropogenic	species dependent	1 x 1	
		biomass burning			
		natural			
Regional emissions					
inventory	period covered	categories	temporal variability	grid size	
TNO	2003 -2007	anthropogenic	annual	0.5 x 0.5	
EMEP (Europe)	1970 -2020	anthropogenic	annual	0.5 x 0.5	
REAS (Asia)	1980 -2020	anthropogenic	annual	0.5 x 0.5	
ABBI (Asia)	March-May 2000, March-May 2001	biomass burning	daily	1 x 1	

Figure 2.7 : Examples of global and regional emission inventories available (ECCAD, 2013).

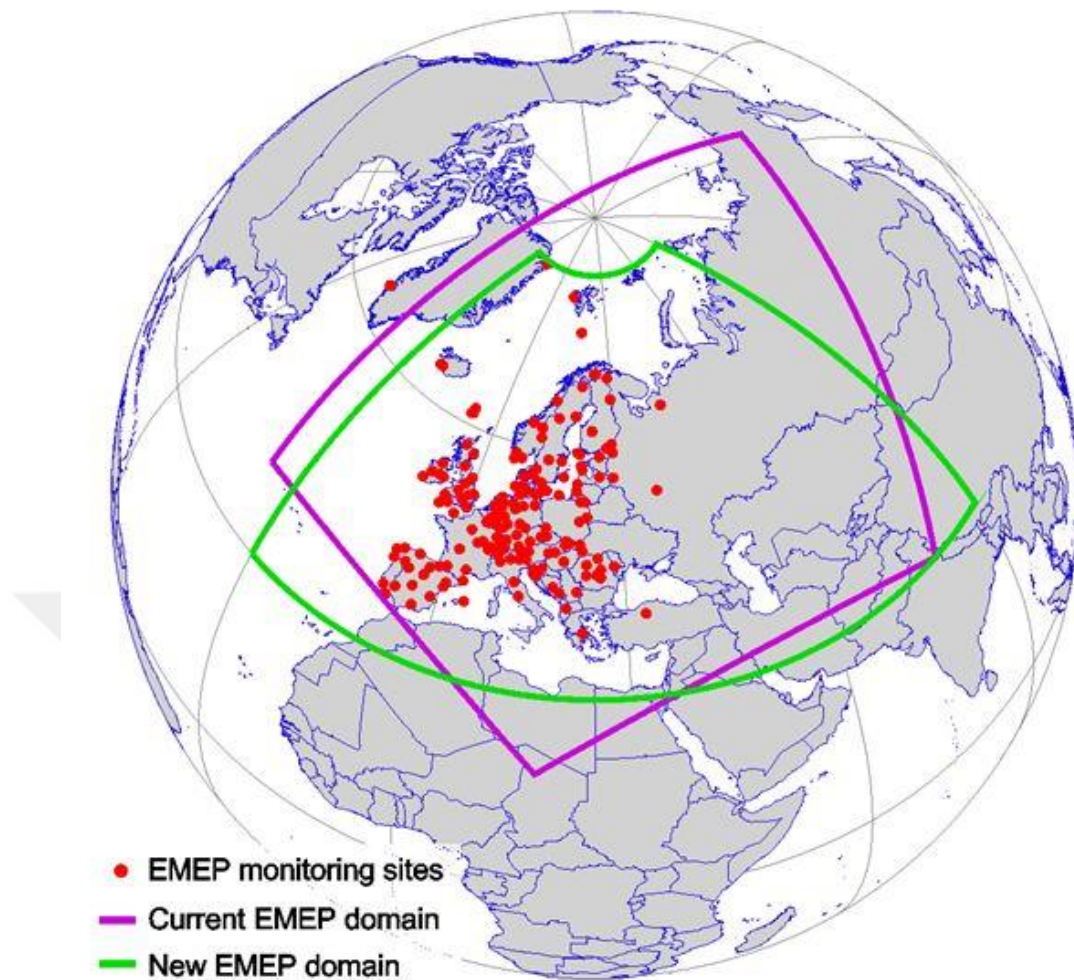


Figure 2.8 : EMEP current and new domains as well as EMEP monitoring sites (CEIP, 2014).

Sulfur dioxide (SO_2) is an atmospheric pollutant with anthropogenic sources such as coal combustion at power plants and industrial facilities, industrial processes, and high sulfur containing fuel use by locomotives, large ships, and non-road equipment. Satellite retrievals indicated high SO_x concentrations in Turkey, especially regions with coal power plants in the recent years. EMEP emission inventory for three years showed a significant decrease (Table 2.1) with largest contribution from public power sector.

Table 2.1 : Annual reported total SO_x emissions of Turkey for 2011-2013 (EMEP, 2012).

GNFR SECTORS	2011		2012		2013	
	(SO ₂ , Gg)	(%)	(SO ₂ , Gg)	(%)	(SO ₂ , Gg)	(%)
A Public Power	1475.72	55.1	1362.11	50.16	1152.03	59.41
B Industry	587.79	21.95	682.43	25.13	459.19	23.68
C Other Stationary Combustion	573.44	21.41	657.05	24.2	319.87	16.5
D Fugitive	-	-	-	-	-	-
F Road Transport	20.56	0.77	-	-	-	-
G Shipping	13.88	0.52	13.88	0.51	8	0.41
H Aviation	0.8	0.03	-	-	-	-
I Offroad	-	-	-	-	-	-
J Waste	0.01	0	0.01	0	0.01	0
L Agricultural-Other	6.17	0.23	-	-	-	-
National Total	2678.36		2715.49		1939.1	

2.2.2 Temporal allocation

The time variability in the emission data that are available in different emission inventories is typically annual. In air quality models like CMAQ, input emission rate should be in terms of moles/second. Hence, some conversion factors must be applied on emission inventories to obtain the proper input emissions for AQM. Temporal factors depend on the population of country, city, and even neighborhoods as well as the year, month, day, and hour of emissions. For instance, the temporal profile distribution for NO_x emission in Istanbul in the city center can be different with other places in this city. In addition, it can differ from the day and night time because of factors such as traffic volume, and other human activities.

The temporal factors that were used in this study are available in the Appendix. After implementation of temporal factors, sector specific gridded-hourly files were created for each pollutant separately. Since CMAQ is a three-dimensional model, vertical distribution was also performed.

2.2.3 Vertical distribution

The number of layers has to be consistent with the meteorological modeling stage. The reason of dissimilarity is related to different plume rises, stack heights, and emission sources. As an example, the emission vertical profile of the power plant sector is different than the industrial sector.

In this study, fifteen sigma-pressure layers were defined the same as vertical layers in WRF (Appendix C). Besides, the emissions of each sector are distributed to those layers according to the coefficients of the vertical profile. The vertical coefficients were calculated by interpolation between the defined emission layers and those that studied in other articles (Bieser et al., 2011; Simpson et al., 2012) . As a case in point, the road transport emissions are dispersed just in the first layer while the power plant emissions are distributed from layer six up to fifteen.

2.2.4 Spatial allocation

The emission processing outputs have to be gridded-hourly. In addition, domain dimensions of the emissions must be the same as WRF domain. For this purpose, WRF results were processed by MCIP to be prepared for CMAQ and used in spatial allocation step to define the emission spatial distribution.

To prepare the final emission spatial distribution, WRF domain of 10km×10 km and EMEP gridded emissions of 0.1°×0.1° resolution had to be intersected.

Hence, EMEP gridded emissions had to be projected to WRF domain. Since the projection type in WRF was selected as Lambert Conformal Conic - which was suitable for our case study due to the latitude range of domain - the same projection (true latitudes) were applied to the EMEP gridded emissions.

The calculation of emissions for each grid was performed as explained. First, the ratio of intersected area between each EMEP and WRF grid to the WRF grid was calculated. Then the emission for a particular pollutant in one WRF grid was calculated from the multiplication of intersected area ratio and the emission of that pollutant for that specific grid in EMEP. At the last step, emissions had to be summed up to result in the total emissions for that WRF grid.

At the end of this stage, the emissions were projected to WRF grid size and dimensions.

2.2.5 Speciation

Emission inventories were composed of a variety of pollutants. To input the processed emissions to the air quality model, which includes a streamlined set of equations, they have to be speciated according to the model chemical mechanism (e.g., CBO5). For this aim, a conversion matrix was prepared to result in the species that are consistent

with the photochemical mechanism selected in CMAQ. These species include organics, PM species, and toxics species (SMOKE v3.5 User's Manual, 2013).

The speciation matrix comprises rows that own specific values for each of the pollutants to convert them to the species that will be used in CMAQ. Those values represent the fraction of species to the main pollutant given in the emission inventory and also it shows that the pollutant is speciated to which species.

During performing this stage, arranging the time zones for the domain was performed as well. For this purpose, time zone differences were assigned for each grid based on Greenwich Mean Time (GMT).

In this study, Carbon Bond 05 (CB05) along with Aerosol Module 6 (AERO6) were used as chemical mechanisms. In addition, "cloud_acm_ae6" was selected as cloud module for modeling the impacts of clouds on deposition, mixing, photolysis, and aqueous chemistry (CMAQ WIKI, 2015).

2.2.6 Biogenic emission processing

To decrease uncertainty from the emission processing stage, emissions with a variety of sources have to be included in the final emissions. Some biogenic pollutants such as isoprene and terpenes are being released from natural sources. They are classified as biogenic emissions. EMEP emission inventory only reports anthropogenic emissions and does not contain any biogenic emissions. Therefore, a complementary biogenic emission inventory and emission processing are needed.

Model of Emissions of Gasses and Aerosols from Nature (MEGAN) is a modeling system for estimating the emission of gasses and aerosols from terrestrial ecosystems into the atmosphere (UCAR, 2016). It uses land cover, weather, and atmospheric chemical composition. MEGAN covers all regions and its base resolution is about 1 km. It can be run as a stand-alone model for generating emission inventories, but is also being incorporated as an on-line component of chemistry-transport and earth system models (UCAR, 2016).

Biogenic emissions resulted from MEGAN v2.1 were vertically located on the lowest ground level. Besides, the emissions from MEGAN was hourly results with diurnal temporal variation.

Layer 1 ISOP

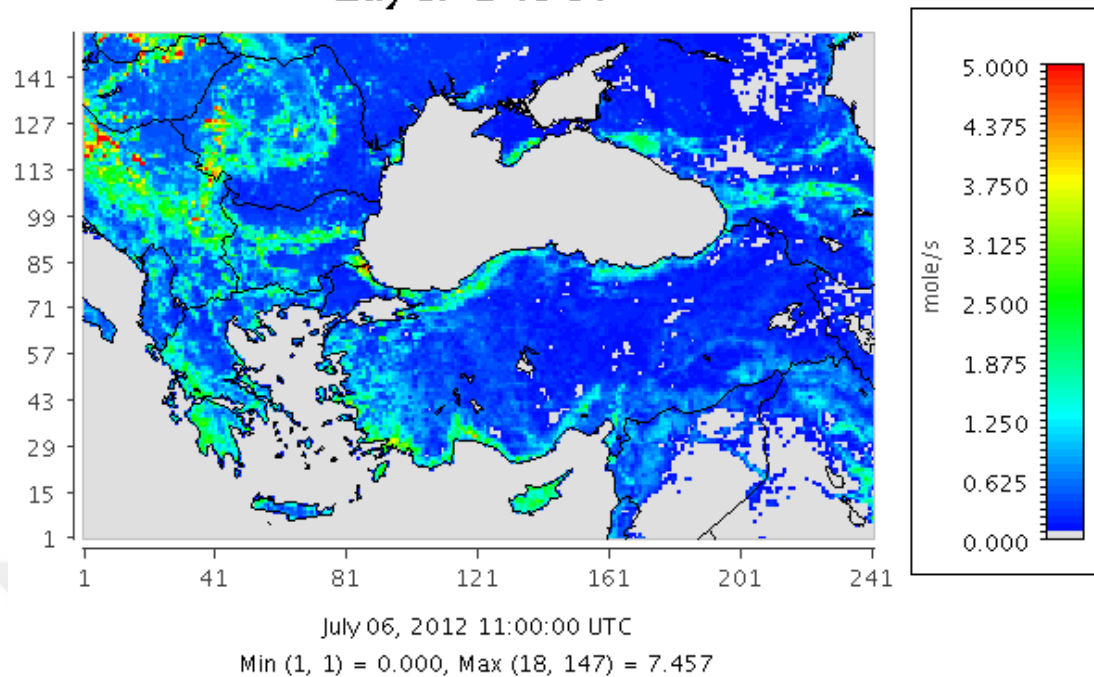


Figure 2.9 : Isoprene emissions for July 06, 2012.

2.2.7 Combining the prepared anthropogenic and biogenic emissions

Biogenic emissions obtained from MEGANv2.1 were integrated with EMEP anthropogenic emissions. The final gridded hourly emission files were a netcdf format which included both anthropogenic and biogenic pollutants.

2.3 Regional Air Quality Modelling

2.3.1 Overview

Under the authority of the Clean Air Act, the U.S. Environmental Protection Agency (EPA) has established National Ambient Air Quality Standards (NAAQS) (U.S. EPA, 2008). These standards are designed to protect human health and the environment from high levels of criteria pollutants, such as ozone and particulate matter. Meeting the NAAQS often requires the use of controls on sources of air pollutants. The complex nature of air pollution scenarios requires control strategies to be effective for a variety of air pollutants, geographic regions, and scales. As part of the effort to decrease ambient concentrations of criteria pollutants, the EPA has approved air quality simulation models for use at regional, state, and local scales within the United States.

The models have been applied to estimate the ability of various control strategies to improve air quality and ensure cost-effective results.

So-called first-generation air quality models simulated air quality using simple chemistry at local scales, and Gaussian plume formulation was the basis for prediction. Second-generation models covered a broader range of scales (local, urban, regional) and pollutants, addressing each scale with a separate model that often focused on a single pollutant or issue (e.g., ozone, acid deposition). It became apparent, however, that single-pollutant models were not sufficient. Depending on the release characteristics, the pollutants in question, and the surrounding meteorological conditions at the time of pollutant release, modeling scenarios can range from a localized, short-term phenomenon to a long-term regional event. Because some emission sources contribute to the ambient levels of more than one pollutant and can affect an entire region on various time scales, an integrated modeling approach capable of handling multiple air pollutants and spatiotemporal scales was needed to isolate control strategies that improve overall air quality in a cost-effective manner. New air quality issues identified by the Clean Air Act Amendments of 1990 (such as visibility, fine and coarse particles, and indirect exposure to toxic pollutants) made an integrated modeling approach that could address multiple pollutants even more essential. Third-generation models were needed that could treat multiple pollutants simultaneously and at scales up to continental or larger.

The EPA Community Multi-scale Air Quality (CMAQ) modeling system is a third-generation air quality model. It is available online at <http://www.cmaq-model.org> and is designed for applications ranging from regulatory and policy analysis to understanding the complex interactions of atmospheric chemistry and physics. It is a three-dimensional Eulerian (i.e., gridded) atmospheric chemistry and transport modeling system that simulates various pollutant species throughout the troposphere. Designed as a “one-atmosphere” model, CMAQ can address the complex couplings among several air quality issues simultaneously across spatial scales ranging from local to hemispheric. The CMAQ source code is open and modular to facilitate the model’s extensibility through community development by all members of the air quality modeling community.

Air quality models integrate our understanding of the complex processes that affect the concentrations of pollutants in the atmosphere. Establishing the relationships

among meteorology, chemical transformations, emissions of chemical species, and removal processes in the context of atmospheric pollutants is the fundamental goal of an air quality model (Seinfeld and Pandis, 2012). In contrast to statistical air quality models that use historical trends in observed atmospheric conditions to predict air pollution, CMAQ uses coupled mathematical representations of actual chemical and physical processes to simulate air quality. The model is based upon the underlying concept of preserving mass through a series of contiguous three-dimensional (3-D) grid cells covering a fixed model grid (i.e., an x-y-z array that is fixed in space and covers a particular domain, i.e., the geographic area of interest). CMAQ, therefore, belongs to the Eulerian class of mathematical models that calculate a mass balance within each grid cell by solving the transport across each cell boundary and chemical transformations within each cell during a given time period. As a framework for simulating the interactions of multiple complex atmospheric processes, CMAQ thus requires two main inputs: meteorological information, and emission rates from sources of emissions that affect air quality.

With weather conditions contributing the primary physical driving forces in the atmosphere (such as the changes in temperature, winds, cloud formation, and precipitation rates), representative gridded meteorology forms the basis of all 3-D air quality model simulations. The Fifth-Generation Pennsylvania State University/National Center for Atmospheric Research (PSU/NCAR) Mesoscale Model (MM5) (Grell et al., 1994) and the Weather Research and Forecasting (WRF) model – Advanced Research WRF (WRF-ARW) (Skamarock et al., 2005) are two meteorological models that are compatible with CMAQ. The meteorology inputs dictate the following CMAQ configuration parameters:

- Horizontal grid coordinate system (e.g., latitude-longitude) and map projection (e.g., Lambert Conformal Conic).
- Horizontal grid resolution (i.e., the size of the cells composing the grid).
- Maximum spatial coverage (horizontal geographic extent, i.e., *the domain*) of the grid.
- Maximum vertical grid extent (model top).
- Temporal extent (the starting and ending dates and times and the meteorology update frequency).

To obtain inputs on emissions, CMAQ relies on an emission model to estimate the magnitude, location, and temporal variability of pollution sources. Open-source models such as the Sparse Matrix Operator Kernel Emissions (SMOKE) model (Environment, 2008) and the Consolidated Community Emissions Processing Tool (CONCEPT) are available for computing emissions inputs to CMAQ from annual, county-level emissions inventories for the United States. These emissions inputs must be on the same horizontal and vertical spatial scales and cover the same time period as are used in the air quality model simulation. The emissions inputs to CMAQ must also contain volatile organic compound (VOC) emissions using a chemical parameterization supported by CMAQ; currently supported photochemical mechanisms are the 2005 update to the Carbon Bond mechanism (CB05) (Yarwood et al., 2005), and the Statewide Air Pollution Research Center, Version 1999 (SAPRC-07) mechanism (Carter, 1990, 2000). It is possible to add new emissions species to CMAQ that are not supported in the distributed version of the software by using the chemical mechanism compiler (CHEMMECH) that is one of the CMAQ utility programs.

CMAQ was designed from the start as a community model. “Community modeling” is the concept that air quality model development should be a collective effort by a broad community of developers. By adopting a standardized modeling architecture, the air quality modeling community can focus its efforts on creating software enhancements and new science modules. CMAQ’s modular structure facilitates customization and open-source development by the community. Using the Input/Output Applications Programming Interface (I/O API) library (<https://www.cmascenter.org/ioapi/documentation/3.1/html/AA.html>) to control the internal and external data flows to the model, and the network Common Data Form (netCDF) library (<http://www.unidata.ucar.edu/software/netcdf>) to control the input and output file formats, CMAQ is based on a transparent and platform-independent code infrastructure that promotes extensibility. The modularity of CMAQ also leads to multiple science configuration options (i.e., how various processes are represented) that model users can choose from when setting up new simulations. The trade-off for this flexibility is complexity in the model configuration; the model user is faced with hundreds of different configuration combinations when designing new simulations.

CMAQ is designed to meet the needs of the multiple groups contained within the air quality modeling community: research and regulatory modelers, algorithm and science module developers, air quality forecasters, and planners and policy makers. While each of these groups has distinct individual requirements of CMAQ, they also share a common need for an efficient, transparent, and scientifically credible tool to simulate air pollution formation and transport (CMAQ WIKI, 2015). To address these individual and common needs, CMAQ development and maintenance have the following goals:

- Scientific Integrity – Ensure that the model remains state-of-the-science through use of regular peer reviews.
- Community Development – Utilize a design that encourages innovations and enhancements by all members of the air quality modeling community.
- Multi-scale Modeling – Provide adequate technical formulations to address air quality issues on multiple spatial scales, from urban to hemispheric.
- One-Atmosphere Design – Provide robust and integrated science for modeling multiple, coupled air quality issues in a single simulation.
- Modularity – Maintain flexibility to add new or select from existing science modules to optimize model performance for specific applications.
- Transparency – Utilize programming practices that promote understanding of the model formulation at the source-code level.
- Computational Efficiency – Provide scientifically acceptable results without compromising the speed at which the results are generated.
- Open-Source Design – Enable no-cost distribution and application by the modeling community.

CMAQ is a suite of Fortran 90 programs that work in concert to estimate ozone, PM, toxic compounds, and acid deposition throughout the troposphere. The five main CMAQ modules are as follows:

- The initial conditions processor (ICON).
- The boundary conditions processor (BCON)
- The clear-sky photolysis rate calculator (JPROC)

- The Meteorology-Chemistry Interface Processor (MCIP)
- The CMAQ Chemistry-Transport Model (CCTM)

2.3.2 The meteorology-chemistry interface processor (MCIP)

MCIP uses output files from the MM5 meteorological model to create netCDF-formatted input meteorology data that are used by CMAQ. MCIP prepares and diagnoses all meteorological fields that are required for CCTM. In addition, MCIP is currently used to calculate the time-varying, species-dependent dry deposition velocities that are used in CCTM. MCIP can be used to uniformly trim cells off the horizontal boundary of the domain defined by the meteorological model, or to window in on a subset of that domain. MCIP can also decrease the vertical resolution of the meteorological data by “layer collapsing.” Configuration options for MCIP include the time periods over which to extract data from the meteorological model output files, horizontal and vertical grid definitions, and selections for calculating dry deposition velocities and integrating satellite cloud observations into MCIP output.

2.3.3 The initial conditions processor (ICON)

ICON generates a gridded binary netCDF file of the chemical conditions in the modeling domain for the first hour of a simulation. It can generate these initial conditions from either an ASCII file of vertically resolved concentration profiles (distributed with CMAQ) or from an existing CCTM output file. If the profiles in an ASCII file do not have the same vertical structure as the CCTM configuration to be used, ICON will interpolate the data to a vertical structure consistent with CCTM’s. Using an existing CCTM output file to generate initial conditions is applicable when extrapolating initial conditions from a coarse to a fine grid simulation, as may occur when setting up nested simulations (simulations with finer-resolution grids that cover part of coarser-resolution grids). The configuration options for ICON include selecting the chemical mechanism to model, defining the horizontal and vertical grids, and choosing whether the initial conditions are generated from an ASCII profile or from an existing CCTM output file.

2.3.4 The boundary conditions processor (BCON)

BCON generates a gridded binary netCDF file of the chemical conditions along the horizontal boundaries of the modeling domain. These boundary conditions can be either static or time-varying, and (as with ICON) can be generated from either an ASCII file of vertically resolved concentration profiles or from an existing CCTM output file. Also as with ICON, BCON will interpolate the data in ASCII profiles to a vertical resolution that is consistent with the CCTM configuration. BCON differs from ICON, however, in that it can generate time-varying (i.e., dynamic) boundary conditions. Dynamic boundary conditions are typically extracted either from CCTM outputs from a coarse-grid simulation for nested simulations or from a CCTM simulation using a global-scale model. The file structure of the ASCII input profiles can also support the creation of dynamic boundary conditions, but generally these files are used only for creating static data. The configuration options for BCON include selecting the chemical mechanism to model, defining the horizontal and vertical grids, and choosing whether the boundary conditions are generated from an ASCII profile or from an existing CCTM output file.

2.3.5 The clear-sky photolysis rate calculator (JPROC)

JPROC calculates chemical-mechanism-specific clear-sky photolysis rates at fixed altitudes, solar hour angles, and latitude bands from tabulated absorption cross-section and quantum yield (CSQY) data. While CMAQ is distributed with CSQY data that support the default chemical mechanisms, updating or adding new CSQY data is straightforward. The only configuration option required for JPROC is the selection 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 calculate gas-phase chemical transformations and pollutant concentrations.

2.3.6 The CMAQ chemistry-transport model (CCTM)

CCTM integrates the output from the preprocessing programs described above (JPROC, BCON, ICON, and MCIP), as well as CMAQ-ready emissions inputs (e.g., output from SMOKE), to simulate continuous atmospheric chemical conditions. The modeled concentrations of relevant species can be captured for output at a user-definable time-frequency (typically hourly). The CCTM output files are all binary

netCDF files of gridded and temporally resolved air pollutant information, such as gas- and aerosol-phase species mixing ratios, hourly wet and dry deposition values, visibility metrics, and integral-averaged concentrations. The spatial and temporal coverages of CCTM are dictated by the input meteorology information. The science configuration is specific to each application of the model and can be adjusted to optimize model performance both computationally and in the numerical reproduction of observed air quality trends. Configuration options for CCTM include the temporal coverage of the simulation, the chemical mechanism to use in the modeling, the physics scheme to use for modeling pollutant transport, heterogeneous and aqueous chemistry options, and diagnostic options. CCTM has the largest number of configuration options of all the CMAQ programs.

In this study, Before running CMAQ, for the integral average concentration of species (ACON) and hourly instantaneous concentration of species (CONC), different components and vertical layers were defined. For CONC, nine species including CO, HNO₃, NO, NO₂, NO₃, O₃, PAN, SO₂, and Sulfuric acid gas with 15 vertical layers were selected. For ACON, 39 different pollutants along with one vertical layer were considered to be reported by CMAQ.

2.4 Observations

To determine the quality of model outputs, the model results have to be evaluated and compared with some observations. In this investigation, satellite retrievals and ground observations were applied to assess the model results. The differences between CMAQ outputs and observations were mainly due to EMEP uncertainty, wind speed, and wind direction.

2.4.1 Satellite retrievals

OMI (Ozone Monitoring Instrument) on Aura satellite provides continuous SO₂ column data with global daily coverage and 13×24 km² spatial resolution at nadir. OMI Level2 (L2) SO₂ Planetary Boundary Layer (PBL) column data for 2012 (<http://mirador.gsfc.nasa.gov>) with following specifications was used to ensure data quality: Solar Zenith Angle (SZA) < 70°, Radiative Cloud Fraction (RCF) < 0.3, Ozone Column Amount (O₃) < 1500 DU (OMI, 2014) in this study.

Annual SO₂ retrievals for 10×10 km² gridded domain were averaged around 12 km of each grid center and assigned to the grids for 2012 (Figure 2.10). The detailed methodology can be seen elsewhere (Firatli, 2016). By this smoothing method (Fioletov et al., 2011; Lu et al., 2013), noise in the SO₂ pollution maps was reduced. The average monthly SO₂ columns were also calculated for one summer and one winter month; July and January 2012 (Figure 2.11) for comparison with modeling results.

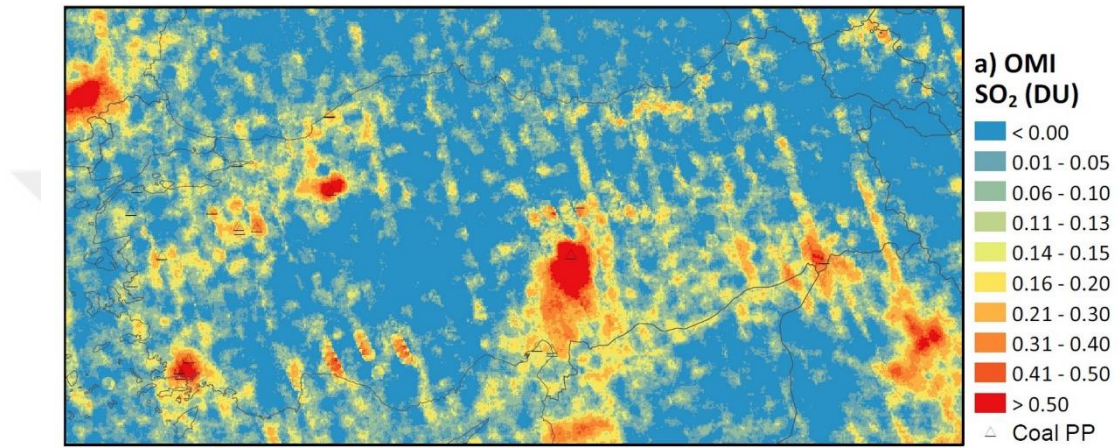
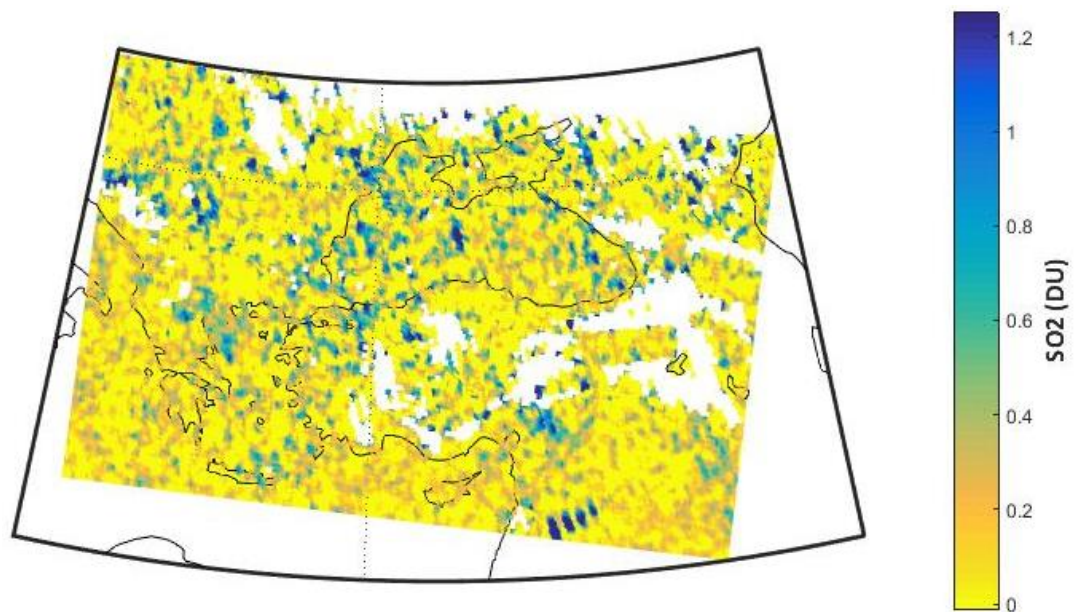


Figure 2.10 : Average yearly OMI SO₂ PBL column (DU) around Turkey for 2012.

a)



b)

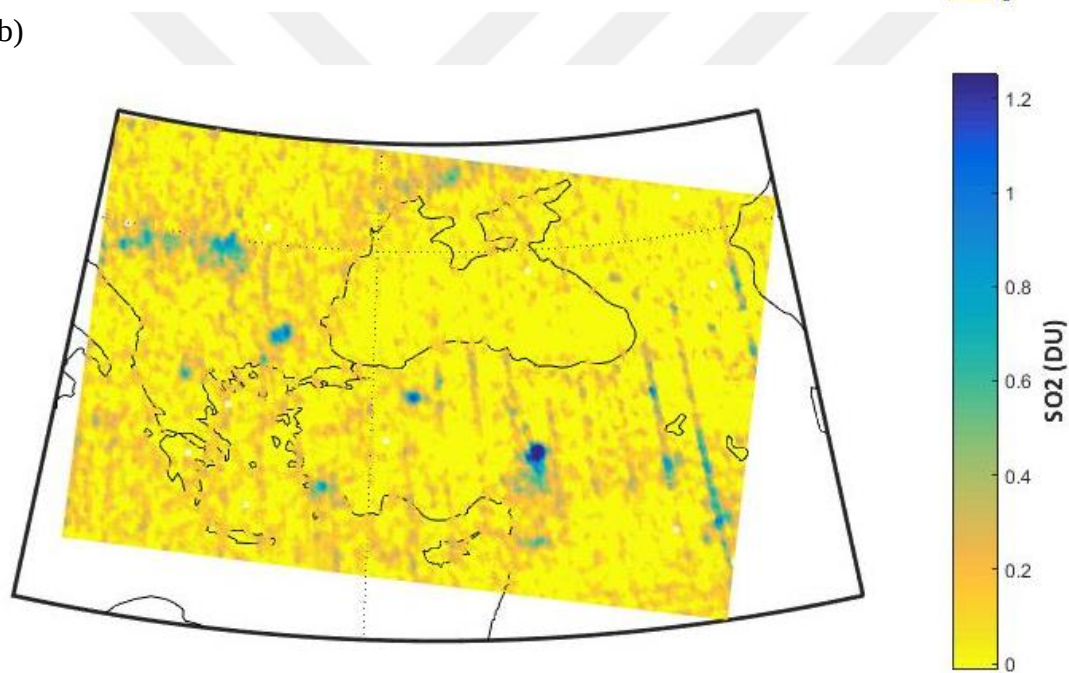


Figure 2.11 : Average monthly OMI SO₂ columns for a) January and b) July.

2.4.2 Ground-based observations

There is a total of 207 ground stations over the study region (Turkey). The location of the stations is located in the Figure 2.12. Hourly data from stations were averaged for January and July 2012. In some days, there was not enough data. Data filtration was performed accordingly; The stations that contained more than 70% missing values for the month were excluded in the calculations.

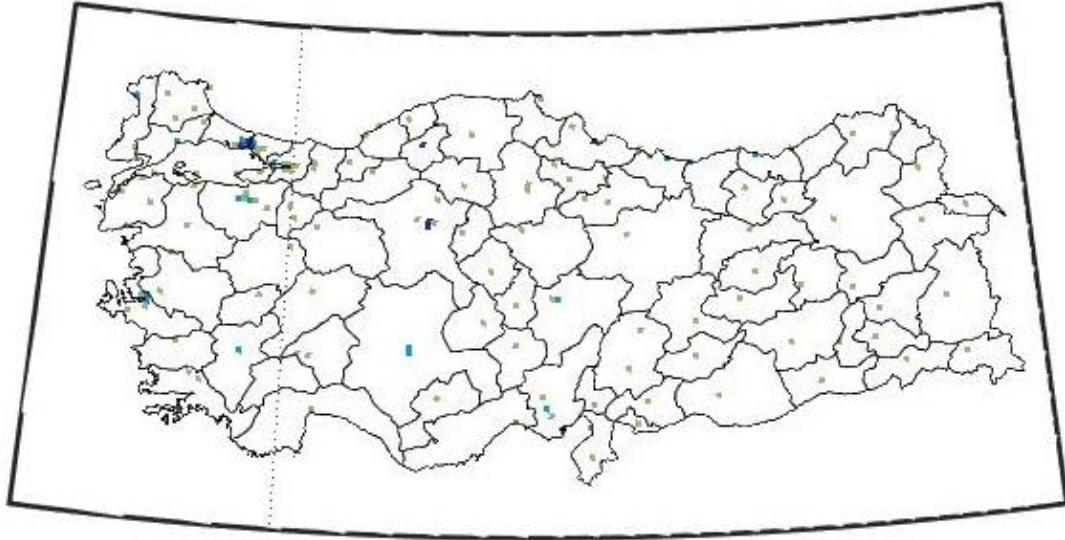


Figure 2.12 : The location of the monitoring stations over Turkey.

To evaluate meteorological results that were obtained from WRF, the hourly measurements of 45 ground monitoring stations were used for January and July 2012. The temperature was selected as one of the significant meteorological variables to be compared with model results. The data were fitted by linear regression. The statistical parameters were calculated for each station separately.



3. RESULTS AND DISCUSSIONS

3.1 Meteorological Results Evaluation

Hourly measured temperature from 43 monitoring stations over Turkey in January and July 2012 were selected for comparison with the simulation results using WRF. The results show a good agreement between the model results and ground observations in most of the stations in the cities such as Canakkale, Ankara, Bitlis, Kayseri, Karaman, Tokat, Giresun, and so on. In a few stations such as Igdir, Sinop, Kilis, and Hakkari low correlation was observed for both January and July. It could be because of some issues in the device or calibration of the measuring instruments. The maximum of correlation coefficient was 0.92 for Nevsehir in January and the minimum value was 0.00 for Igdir in January (Figure 3.2). The time series of temperature at the stations and the relative statistics showed that, overall, the model reproduced the magnitudes and variations of temperature during the period. In Figure 3.3, the time series of six selected stations for January and July presented separately. Although in some stations underestimations were observed in January, the simulation followed the extremums of ground observations. For instance, the time series of “Canakkale – Biga Icdas” showed that the maximum and minimum points of temperature simulation trend was mostly coincided with the ground monitoring measurement variations. Despite there was a gap between simulation and observations graphs for Ankara, the WRF outputs followed the ground observations especially in the maximum and minimum hours. In July, there was a distance between the model results and ground observations in some stations, but the overall performance was acceptable. By comparing the time series of Ankara for January and July, It could be concluded that the space between those was because of the inversion phenomena and consequently, raising the temperature in the urban areas.

A comprehensive statistical comparison was performed on the temperature data. The results were shown in Appendix B.

An investigation on wind speed and wind direction data showed that the correlation between WRF results and observations was much lower in comparison with temperature. It could be because of the seasonal meteorology or instrumental errors. The simulation of wind speed was better in July than January while the better agreement was observed for the wind direction simulation in January. The following plots show the spatial distribution of temperature for two specific days in winter (January) and summer (July) (Figure 3.1).

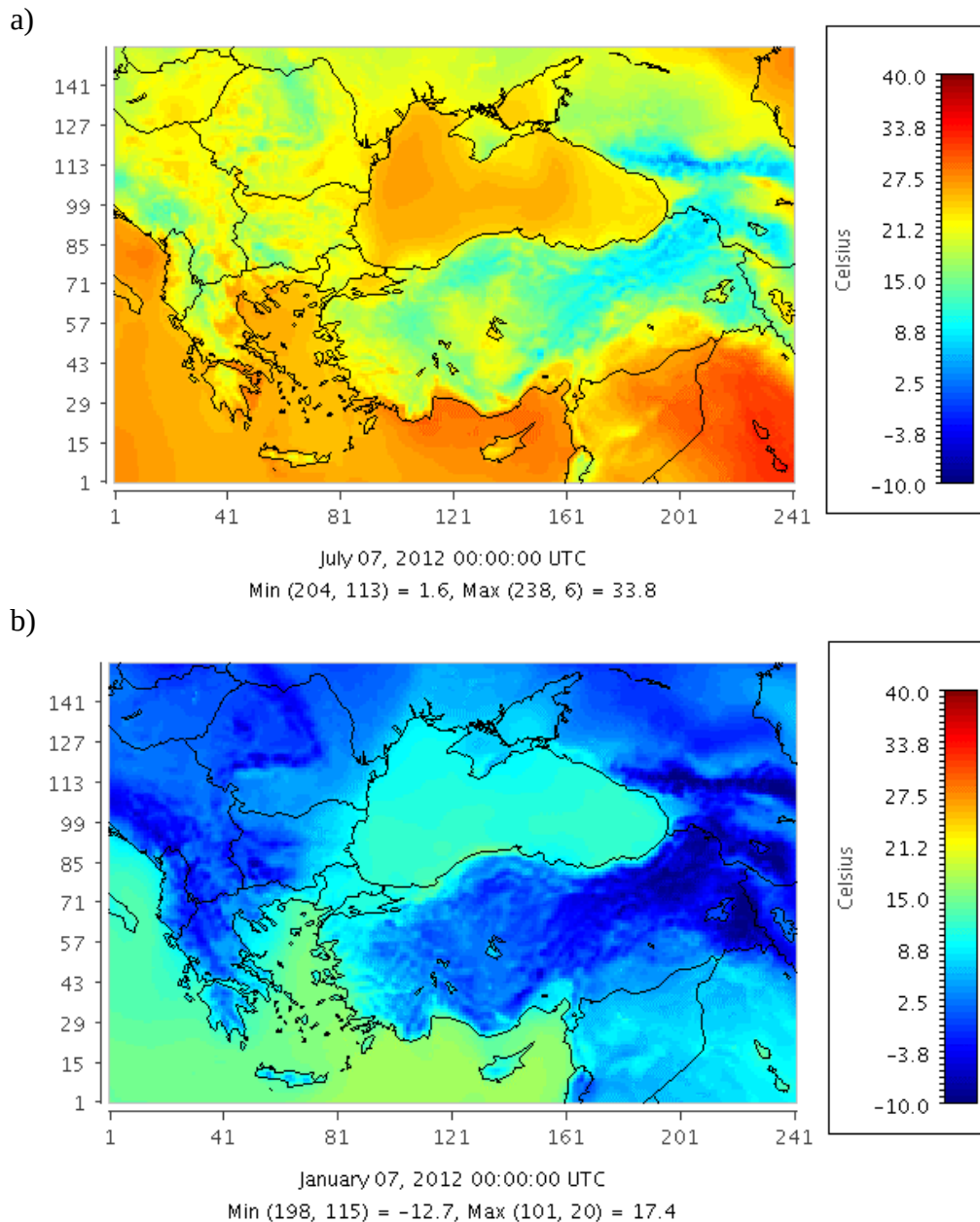


Figure 3.1 : WRF temperature simulation for a) January 07, 2012 at 11:00, b) July 07, 2012 at 11:00.

The maximum of the coefficient of determination was 0.37 for “Balikesir” station in July. The table of statistical calculations is in Appendix C.

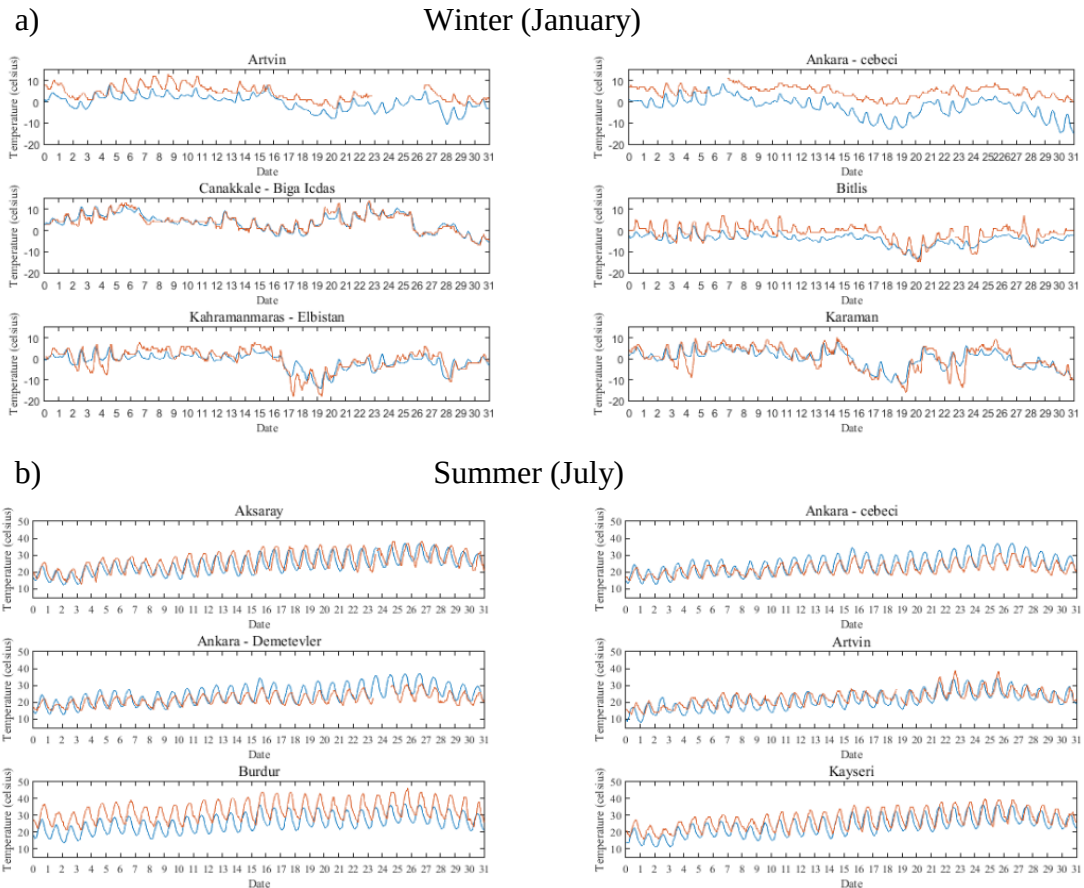


Figure 3.2 : The Time series of observed (red) and simulated temperature by WRF (blue) in the selected cities for a) January b) July 2012.

The temperature simulation results showed that WRF had better performance in July than January according to the statistical calculations (MNB= -9.46% for July and MNB= -50.04% for January). The results showed a lower bias for July than January and for January the results were quite satisfactory (Table 3.1).

Table 3.1 : Performance evaluation of WRF simulations with temperature ground observations for summer (July) and winter (January).

Parameter	July		January	
	Aver	St Dev	Aver	St Dev
WRF-derived Temperature (°C)	24.7	4.36	0.91	5.21
Ground Monitoring Stations (°C)	26.1	9.31	3.28	6.06
MNB (%)	-9.46		-50.04	
MNE (%)	14.91		26.92	
RMSE (DU)	10.18		7.08	

The R-square of model results and ground-based observations for temperature measurements from 43 stations for January and July 2012 is shown in Figure 3.3.

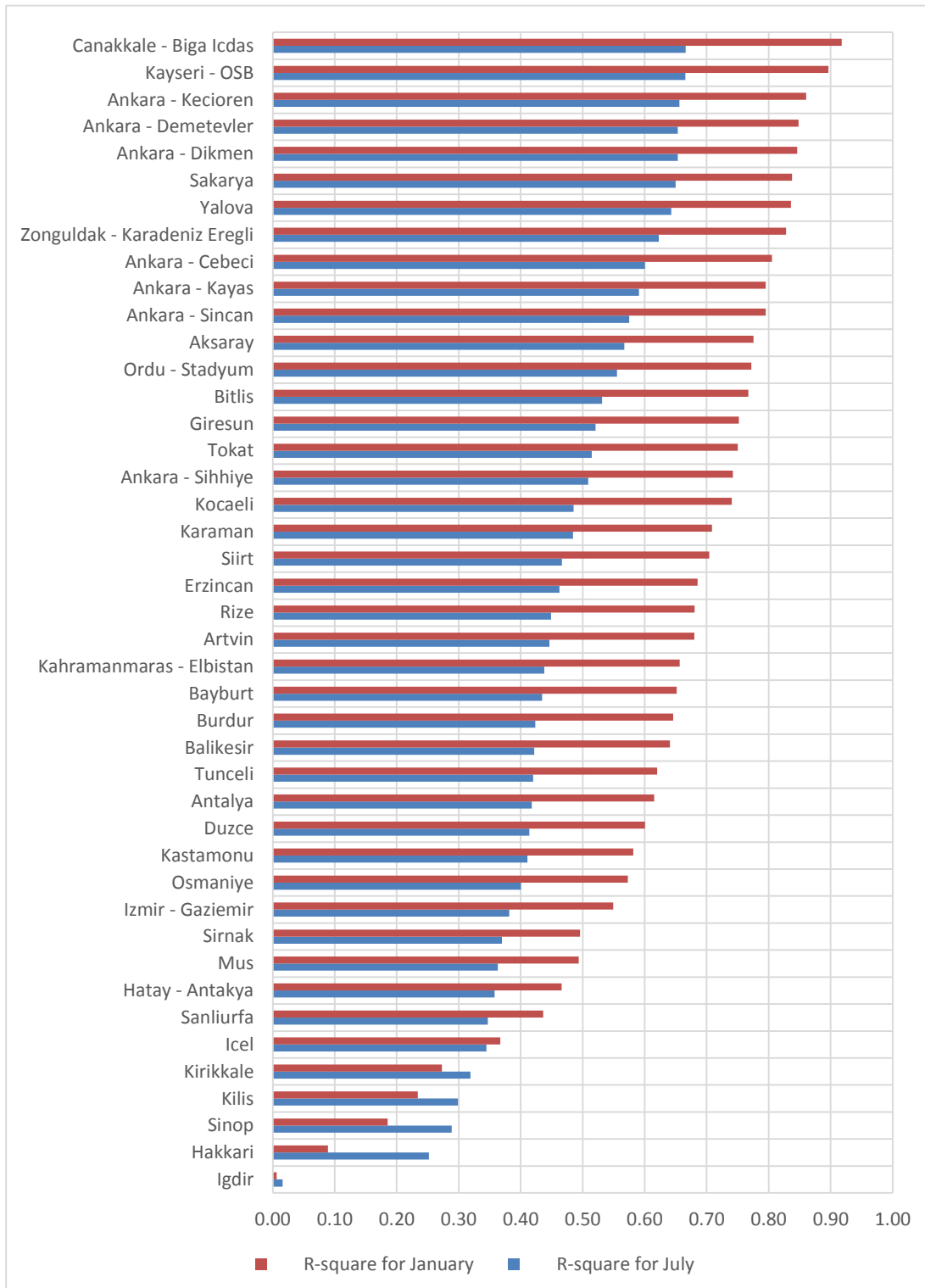


Figure 3.3 : The coefficient of determination of WRF and ground observations for temperature measurements from 43 stations in January and July 2012.

The R-square of model results and ground-based observations for wind speed measurements from 19 stations for January and July 2012 is shown in Figure 3.4.

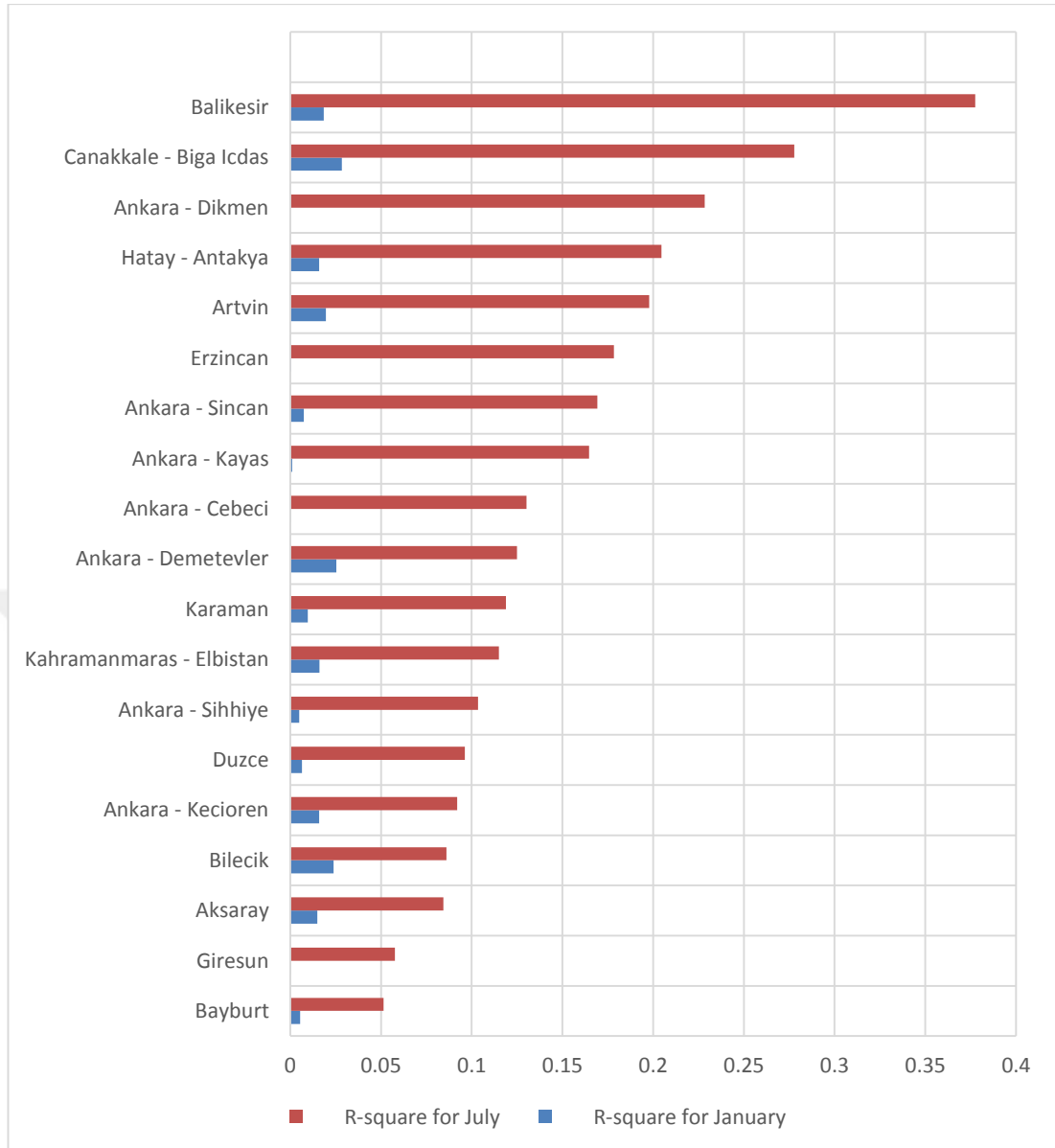


Figure 3.4 : The coefficient of determination of WRF and ground observations for wind speed measurements from 19 stations in January and July 2012.

The R-square of model results and ground-based observations for wind direction measurements from 24 stations for January and July 2012 is shown in Figure 3.5.

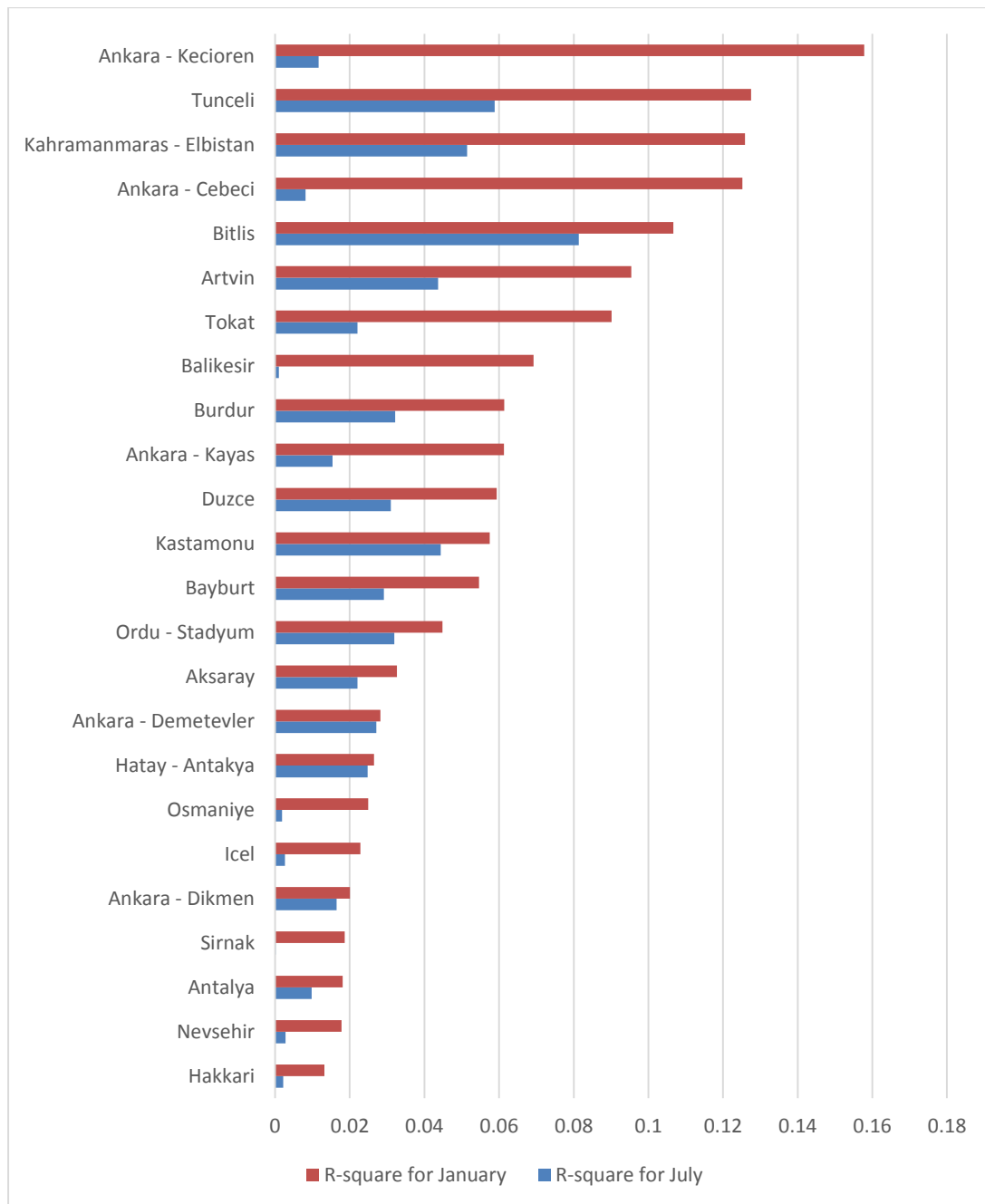


Figure 3.5 : The coefficient of determination of WRF and ground observations for wind direction measurements from 24 stations in January and July 2012.

3.2 CMAQ Comparison with OMI SO₂ Retrievals

SO₂ concentrations for one winter and one summer month in 2012 were simulated using a regional air quality modeling system for investigating the effect of different sources on SO₂ concentrations. WRFv3.7.1 was used for simulating the meteorology. EMEP 2012 emission inventory with a spatial resolution of 0.1°×0.1° were used with MEGANv2.10 to estimate biogenic emissions. CMAQv5.0.2 was used to obtain atmospheric concentrations over modeling domain that covers Turkey with a spatial resolution of 10 km.

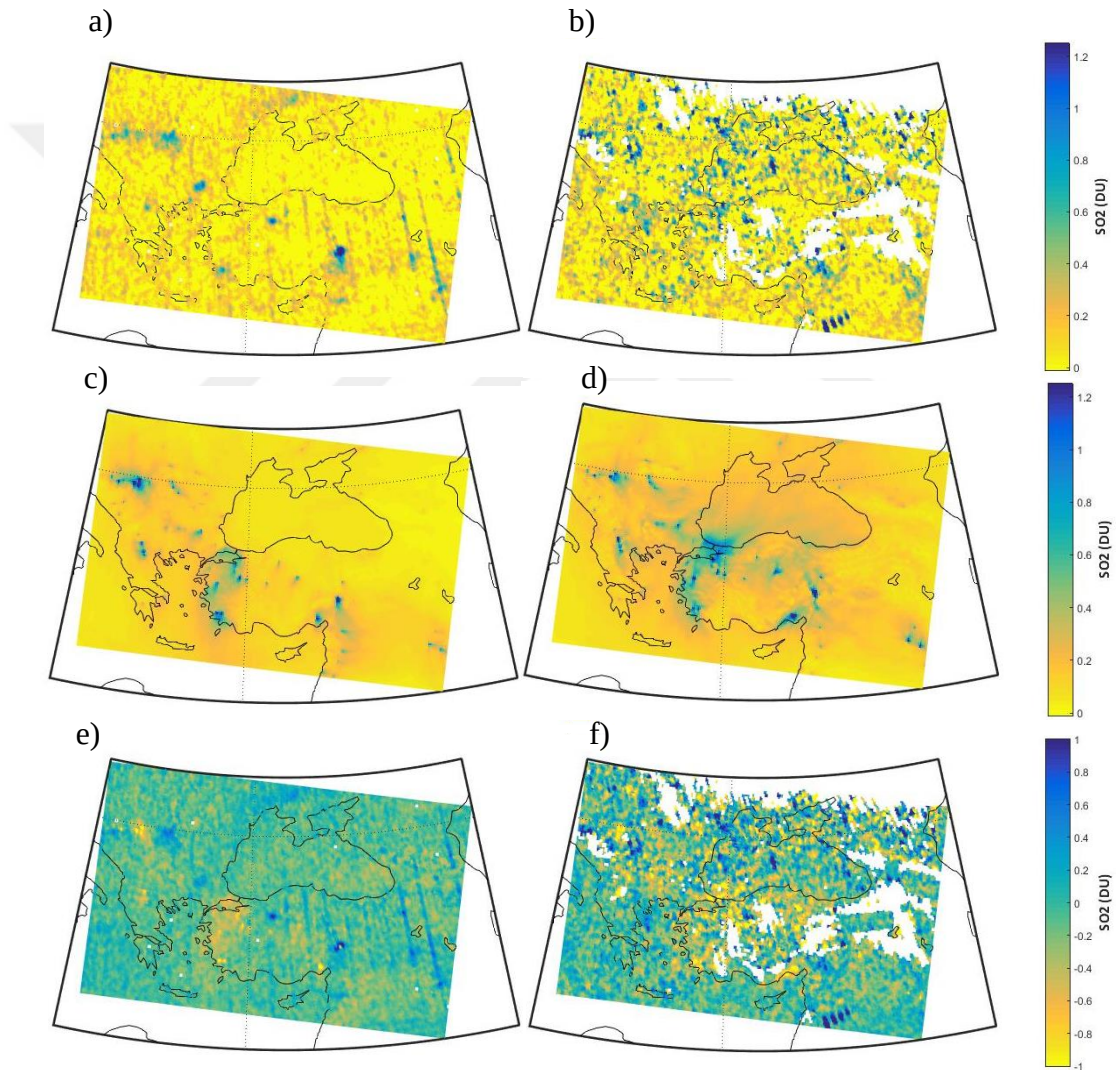


Figure 3.6 : Average monthly OMI (a-b) and CMAQ derived (c-d) SO₂ columns for July (left) and January (right) and differences (OMI-CMAQ) (e-f) for July and January.

SO₂ concentrations simulated using CMAQ for hours 13:00-14:00 were integrated over 10 layers to obtain column amounts and then compared with OMI SO₂ retrievals.

$$C' = C \times \frac{P}{T \times R} \times H \times A_{\text{avg}} \times 0.371 \times 10^8$$

Where C' is the concentration of pollutant in terms of DU (molecule/cm²) for a specific layer, C is the concentration of species in terms of ppmv, T is the temperature of the particular vertical layer for the specific grid in terms of Kelvin, P is the pressure of the particular vertical layer for the specific grid in terms of Pascal, R is the gas constant and H is the thickness of the corresponding layer. In this case, C' values for 10 layers were integrated to obtain the SO₂ column.

This comparison indicated similarities such as high concentrations around large point sources. However, there were significant differences which indicated underestimations from CMAQ over two power plants; Cayirhan and Afşin Elbistan and overestimations over power plants in Mugla and Iskenderun. In addition, over Marmara region, and Istanbul, significant overestimations of CMAQ were observed (Figure 3.6).

The overall performance of CMAQ SO₂ predictions for the 2-month period (January–July 2012) is indicating (Table 3.1) a negative bias in the model.

Table 3.2 : Performance evaluation of CMAQ simulations with OMI satellite retrievals for summer (July) and winter (January).

Parameter	July		January	
	Aver	St Dev	Aver	St Dev
CMAQ-derived SO ₂ column (DU)	0.114	0.107	0.181	0.139
OMI SO ₂ column (DU)	0.032	0.172	0.091	0.455
MNB (%)	-93.7		-83.6	
MNE (%)	-67.5		-45.1	
RMSE (DU)	0.191		0.452	

The performance in July is better than in January with respect to RMSE. The uncertainties in OMI retrievals in winter and the effect of the local use of coal for residential combustion could be the reason for this result.

The scattered plot of CMAQ derived and OMI SO₂ columns indicated discrepancies in between. The correlation was very low for July ($R^2=0.1$) and no correlation was observed for January (Figure 3.7).

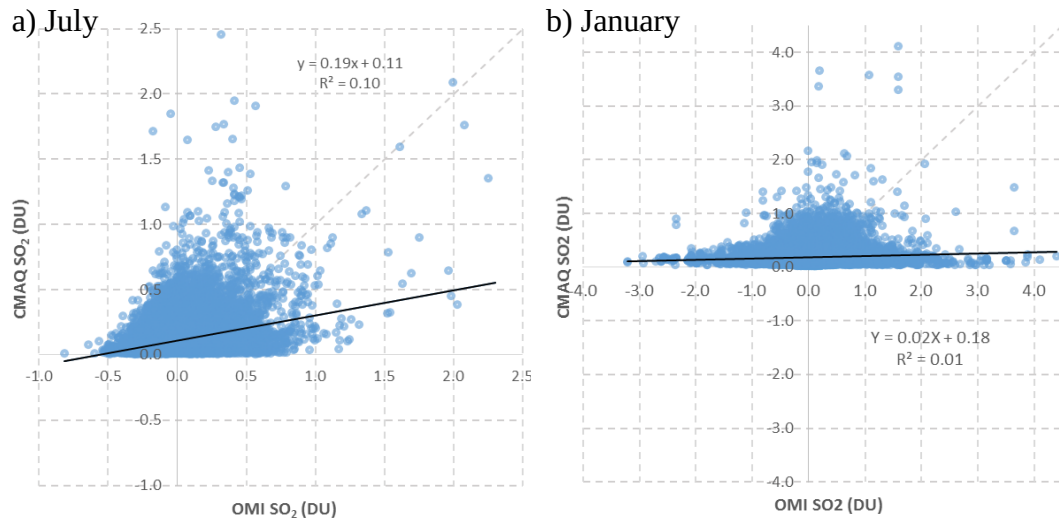


Figure 3.7 : Average monthly OMI SO₂ versus CMAQ derived SO₂ columns for July and January 2012.

In addition, geographically weighted regression (GWR) was applied to indicate detailed local variations in the data adequately (Figure 3.8). GWR is an exploratory technique mainly intended to indicate where non-stationarity is taking place on the map, that is where locally weighted regression coefficients move away from their global values (Bivand, 2013).

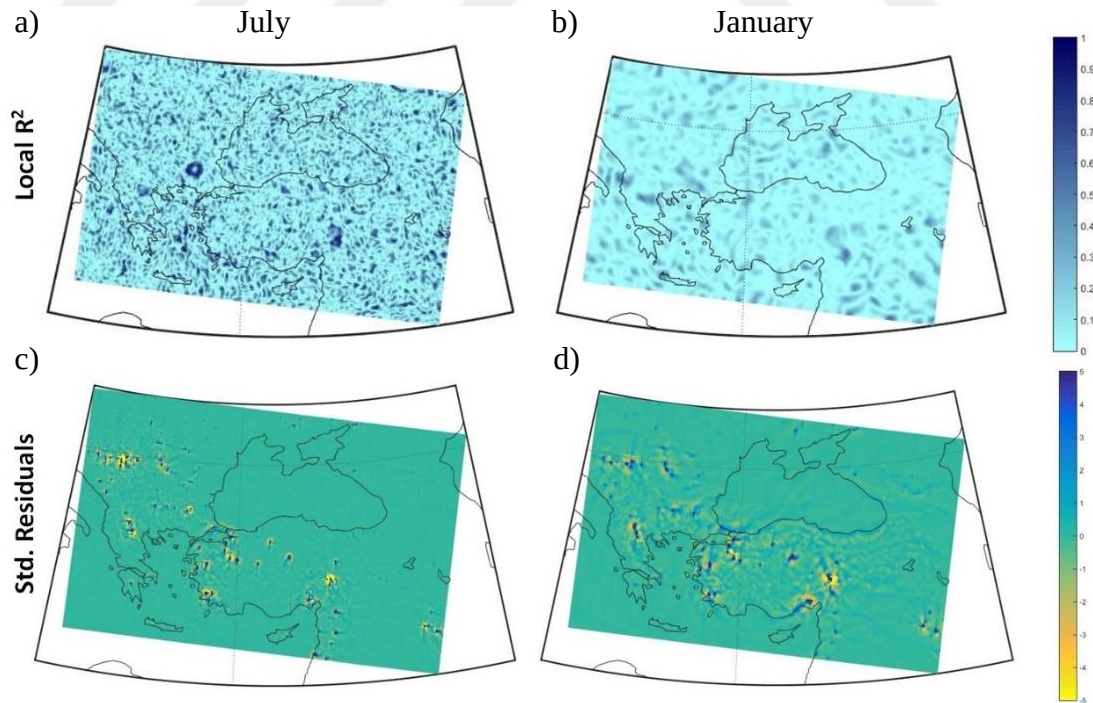


Figure 3.8 : Local R^2 (a-b) and standardized residuals (c-d) obtained using Geographically Weighted Regression (GWR) for OMI and CMAQ SO₂ columns for July (left) and January (right) 2012.

The comparison of satellite retrievals with model simulations helps to assess the emission inventory's reliability and helps to decrease the uncertainty of these inventories. The results indicated discrepancies in the emission inventories with OMI SO₂ columns.

It should also be noted that the uncertainty in OMI SO₂ columns can be reduced by long-time averages i.e. yearly. In addition, one to one comparison of columns temporally would help to understand the reasons for these discrepancies.

3.3 CMAQ Comparison with Ground SO₂ Observations

After obtaining the results from CMAQ, the hourly integral average concentration of CO, NO, NO₂, O₃, SO₂, and PM₁₀ were extracted. Since the unit of CMAQ outputs (ppmv) was not the same as observations (µg/m³), the pressure and temperature data was needed for each grid for converting the unit. For this purpose, the values were read from MCIP files for each grid separately. The unit was converted using the idea gas law as following:

$$C_2 = C_1 \times 10^{-6} \times \frac{T}{P \times R} \times MW$$

Where C₂ is the concentration of pollutant in terms of (µg/m³), C₁ is the concentration of species in terms of ppmv, T is the temperature at the bottom vertical layer for the specific grid in terms of Kelvin, P is the pressure at the bottom vertical layer for the specific grid in terms of Pascal, R is the gas constant and MW is the molecular weight of that pollutant.

After performing those calculations for January and July, ground monitoring stations data was processed. The station which had lower than 30% of data for a month, were excluded from the comparison. Moreover, for the hours that no data was recorded, those points were omitted as well.

Modeled SO₂ showed a good correlation relatively. The SO₂ simulation indicated reasonable positive bias (MNB=31.5%) for July. Also, a negative bias (MNB= - 27.19%) was observed for January. This underestimation could be due to residential combustion that released a considerable amount of emissions (especially SO₂).

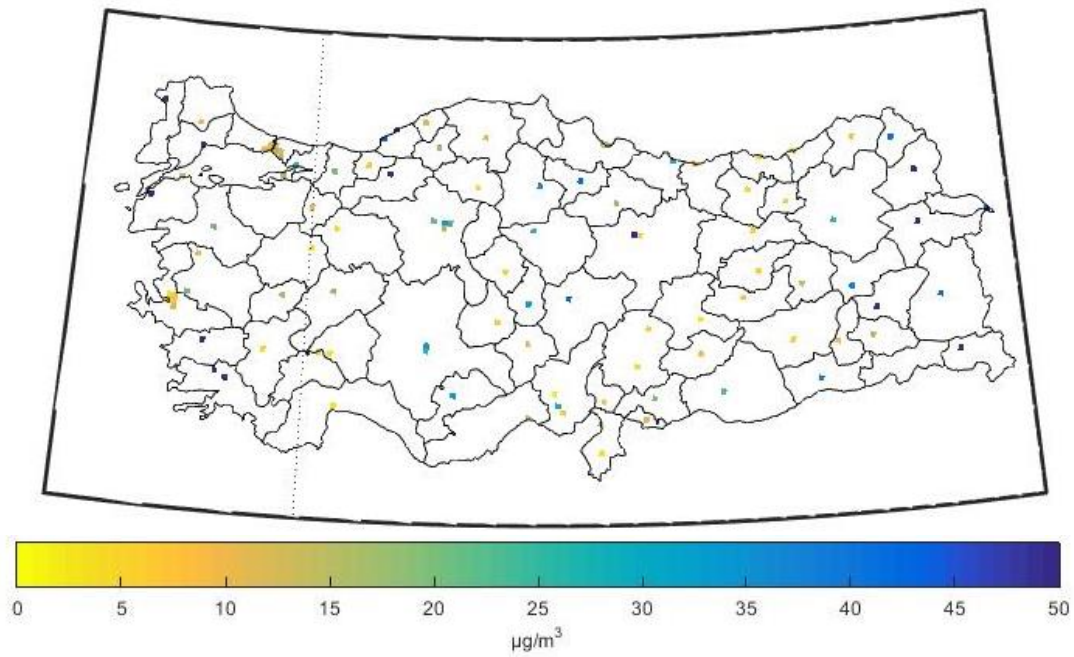
Table 3.3 : Performance evaluation of CMAQ simulations with SO₂ ground observations for summer (July) and winter (January).

Parameter	July		January	
	Aver	St. Dev.	Aver	St. Dev.
CMAQ-derived SO ₂ concentration (µg/m ³)	4.94	5.94	6.83	6.05
Ground Observations (µg/m ³)	7.39	7.38	27.7	49.7
MNB (%)	31.5		-27.19	
MNE (%)	126.07		77.26	
RMSE (µg/m ³)	10.33		55.22	

Statistical analysis was performed on the ground-based observations for all of the stations and pollutants separately. By considering, the coefficients of determination and trend line slopes, the predictions in Istanbul–Alibeykoy station were better than other stations. Generally, in the cities which included power plants like Mugla, Kahramanmaras, Zonguldak, Ankara, and so on, there was a large difference between the measurements and CMAQ results. SO₂ concentration in those regions is significantly higher than CMAQ predictions. For instance, the ground measurements of SO₂ in January were 48.35 (µg/m³) while CMAQ prediction was 1.85 (µg/m³).

Average monthly ground-based observations and CMAQ derived SO₂ concentrations for January and July are shown in Figure 3.9 and Figure 3.10 respectively.

a)



b)

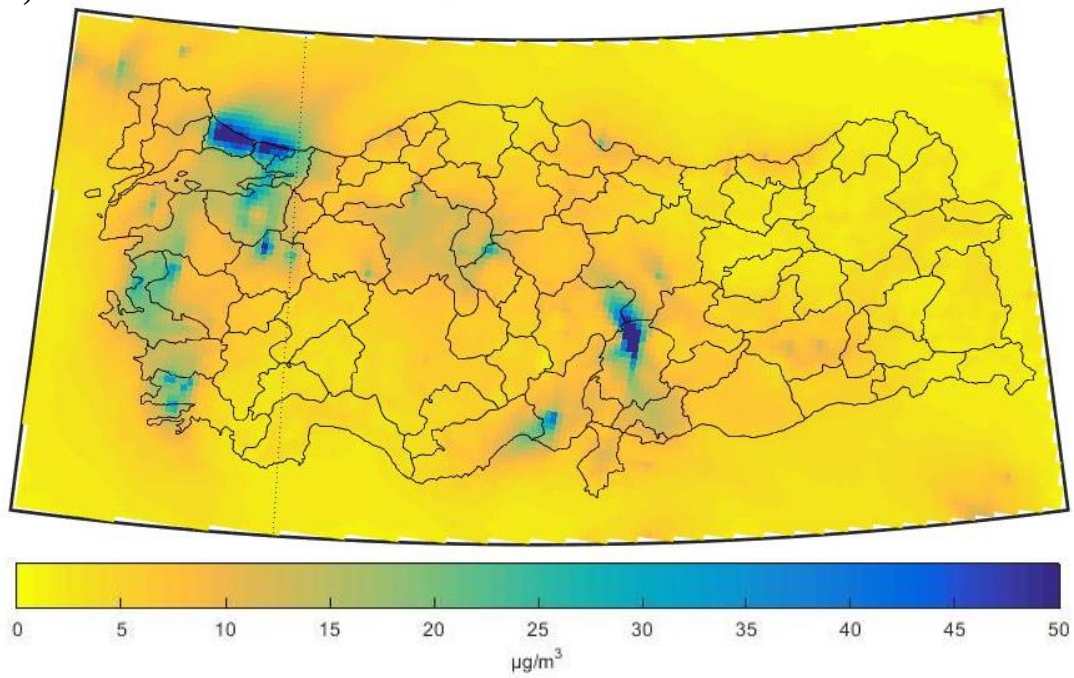
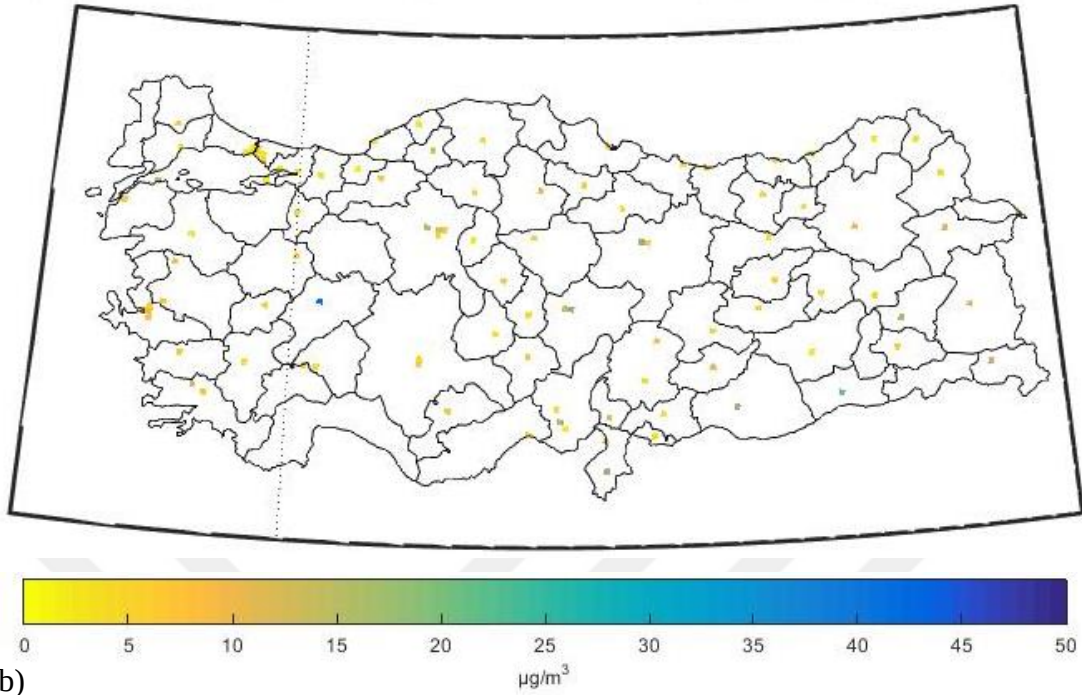


Figure 3.9 : a) Average monthly ground-based observations and b) CMAQ derived SO_2 concentrations for January.

a)



b)

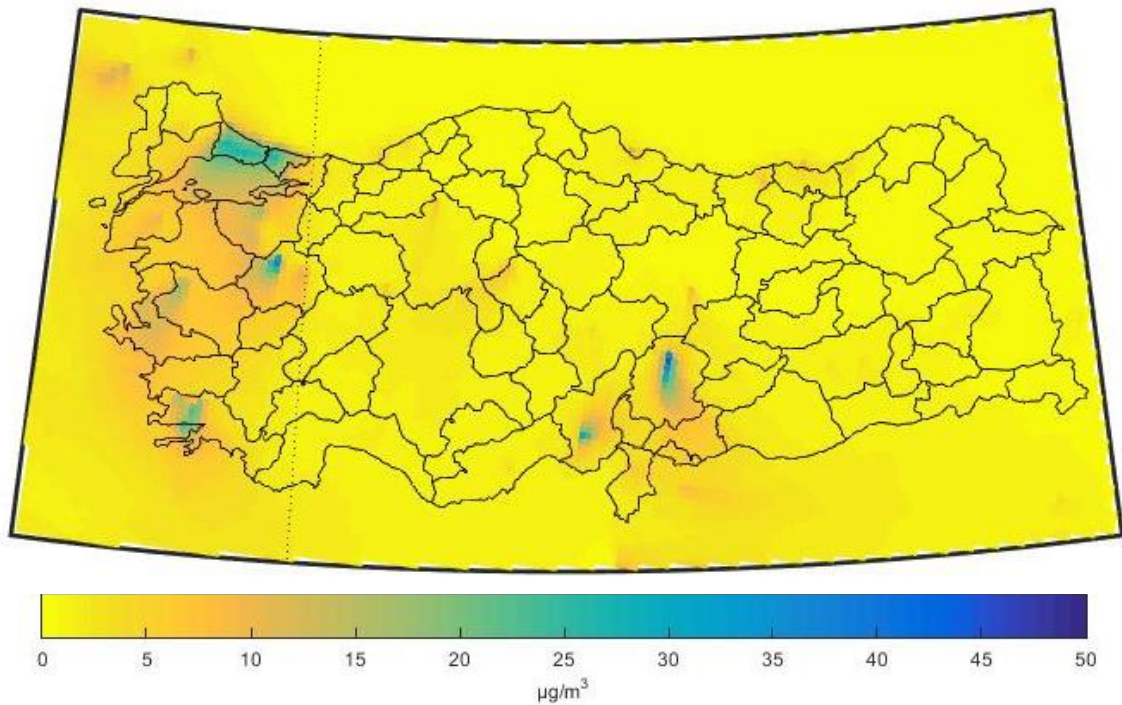


Figure 3.10 : a) Average monthly ground-based observations and b) CMAQ derived SO_2 concentrations for July.

The first reason that could be caused to the low correspondency of the measurements and CMAQ results, was the quality, accuracy, and maintenance of the measuring devices. Damaged and old instruments are not able to have good measurements. The second reason could be the uncertainty in emission inventory and meteorological data. By considering the methods that were applied to reduce the uncertainty of

meteorological data and the comparisons, the uncertainty could be more referred to emission inventory.

The R-square of model results and ground-based observations for SO₂ measurements for July 2012 is shown in Figure 3.11.

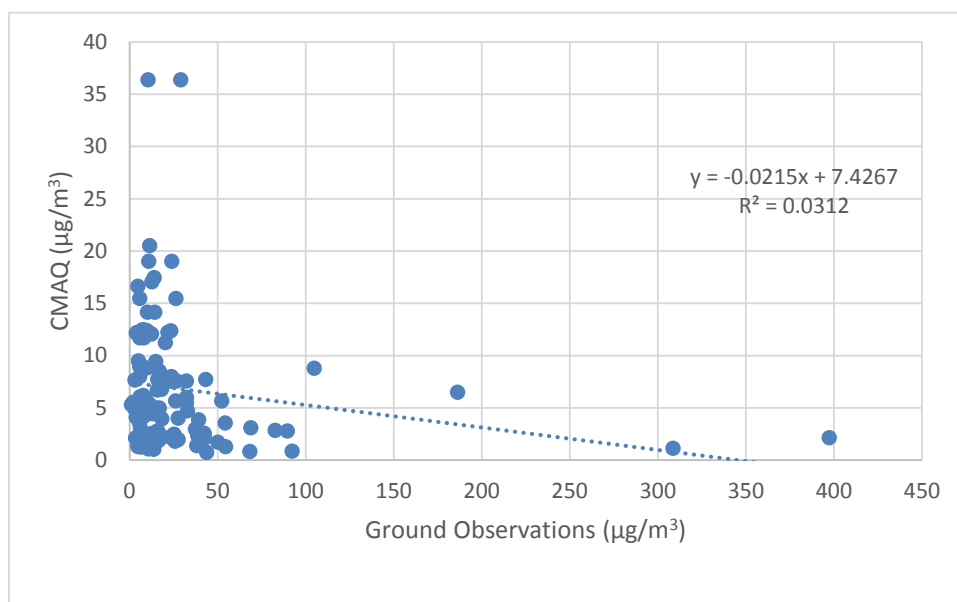


Figure 3.11 : Model Results vs. Ground Observations for SO₂.

3.4 CMAQ Comparison for Other Ground Observations

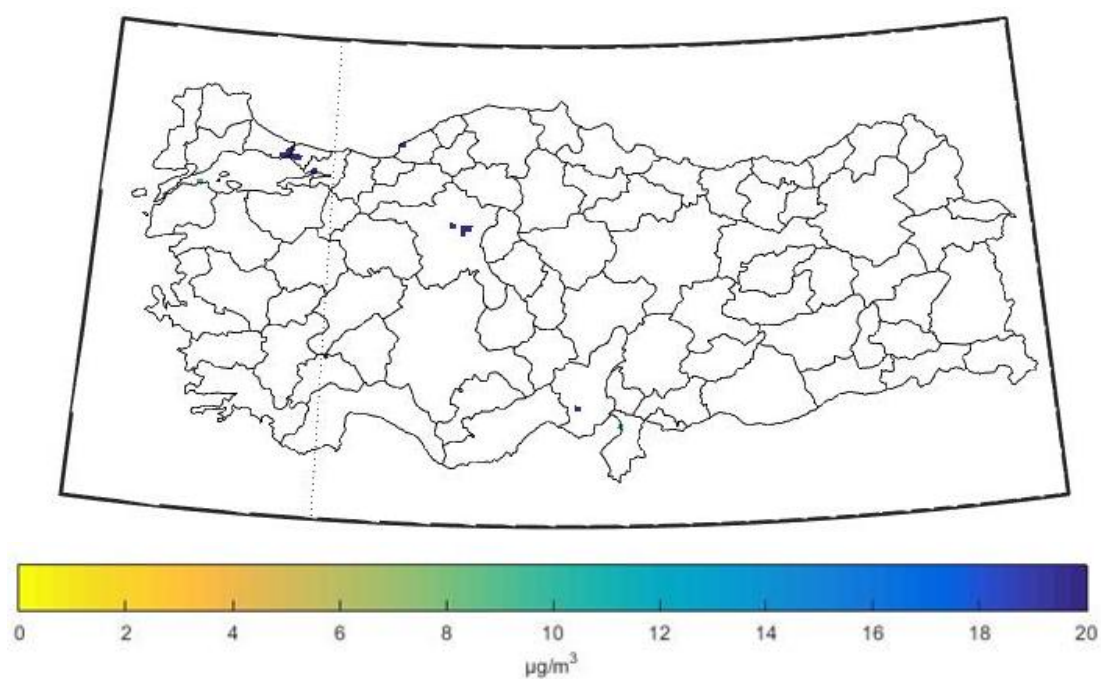
To investigate the performance of the modeling system, statistical calculations were performed for NO, NO₂, CO, and PM₁₀ as well (Table 3.3 and 3.4). The comparison between simulations and ground-based observations showed a relatively high negative bias for NO₂, NO, and PM₁₀ for both January and July. That should be noted that the bias of those species was at the same range. For instance, the MNB for PM₁₀ simulations were -85.98% and -84.84% for January and July, respectively; while for NO₂, those were -83.31% and -73.29% during January and July, respectively. Also, the negative bias for NO was -97.89% and -97.27% during January and July, respectively. The results showed that underestimations for NO, NO₂ and PM₁₀ were approximate to the same extent. The underestimation of PM₁₀ agreed with results from other studies (Im et al., 2014). The comparison of MNB and MNE revealed that model underestimated NO in all of the stations during the episodes. Similarly, NO₂ and PM₁₀ were underestimated in all of the monitoring stations during January. For July, the difference between MNE and MNB showed that model in some stations had overestimations.

Although modeled CO indicated a negative bias during the time episodes, it was lower in comparison with NO, NO₂, PM₁₀. This means that the simulated CO was generally more close to the ground-based observations than NO, NO₂, and PM₁₀. Modeled CO captured the observations very well in January (MNB -18.02%). Although simulated CO had a negative bias in July (MNB -37.06%), the underestimations for July were lower comparing with NO, NO₂, and PM₁₀. The comparison of MNB and MNE for CO showed a remarkable difference due to overestimations in some stations (Table 3.4). However, MNB showed the overall underestimation for CO.

The spatial distribution of NO₂, NO, CO, and PM₁₀ for January and July are shown in Figure 3.12 to 3.20 respectively.



a)



b)

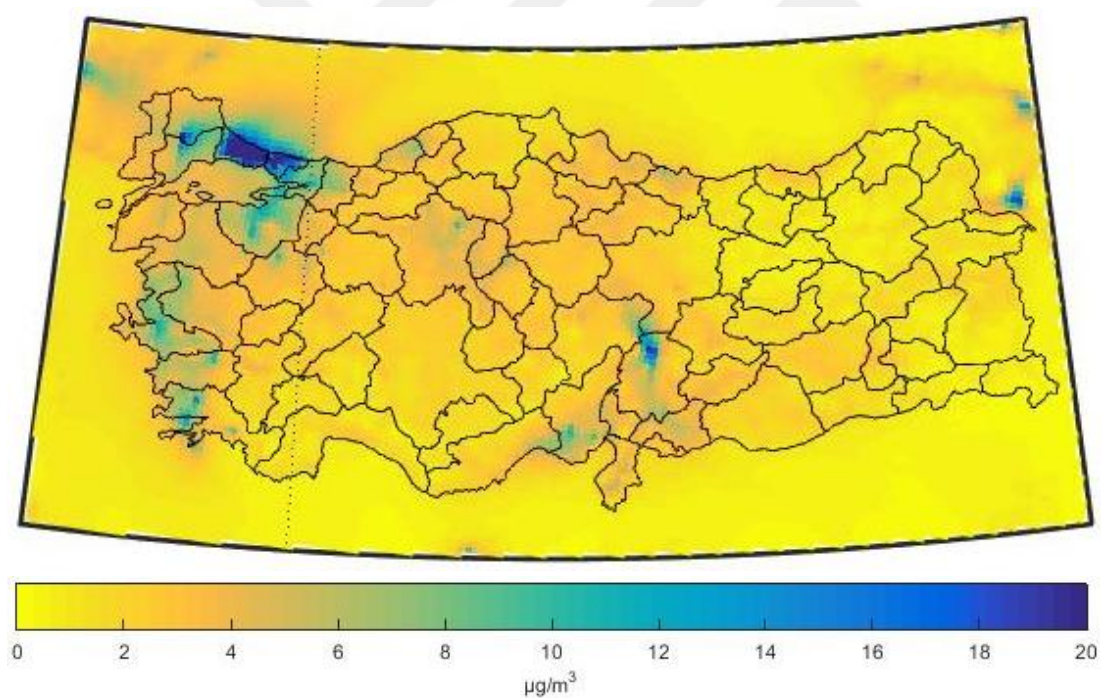
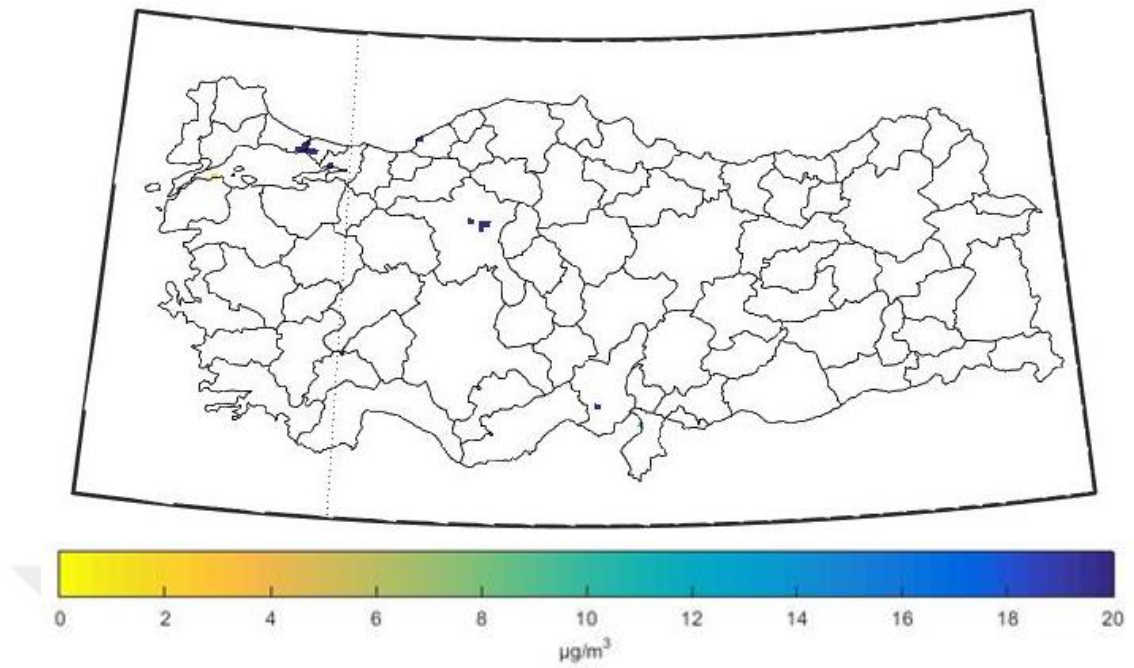


Figure 3.12 : a) Average monthly ground-based observations and b) CMAQ derived NO₂ concentrations for January.

a)



b)

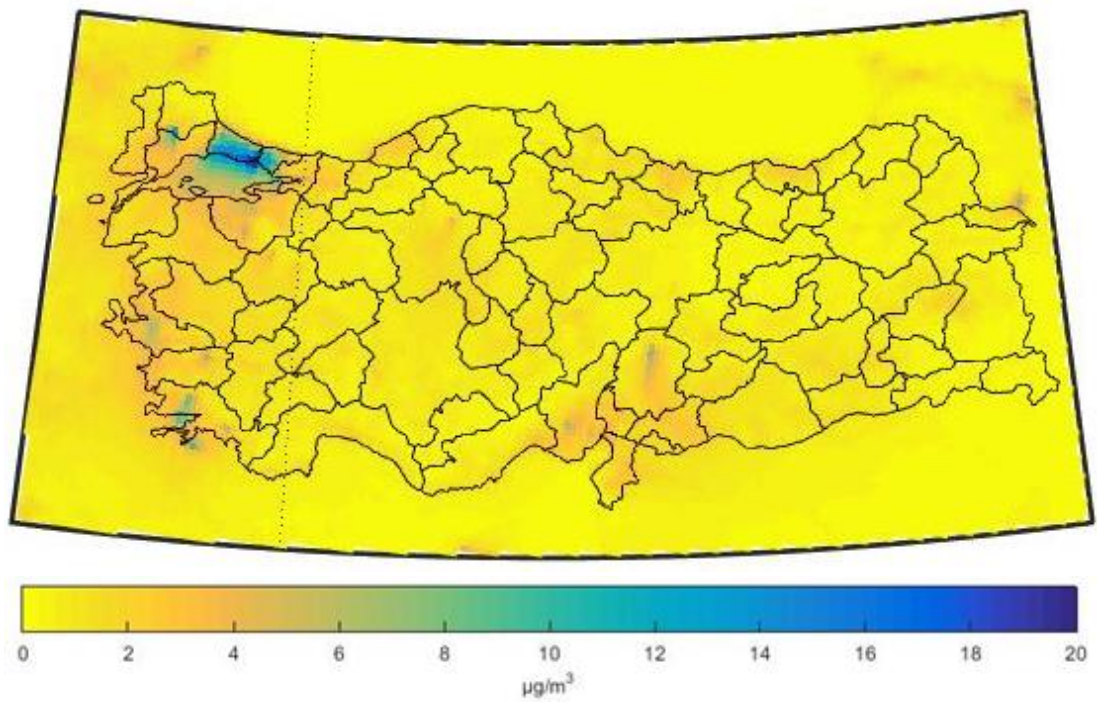
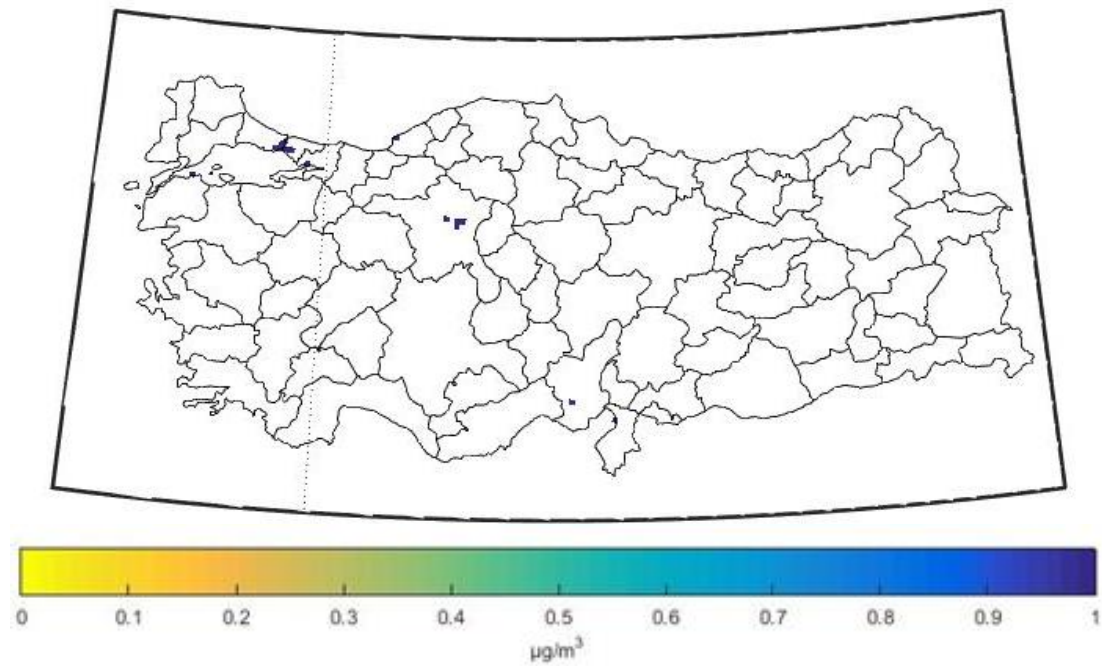


Figure 3.13 : a) Average monthly ground-based observations and b) CMAQ derived NO₂ concentrations for July.

a)



b)

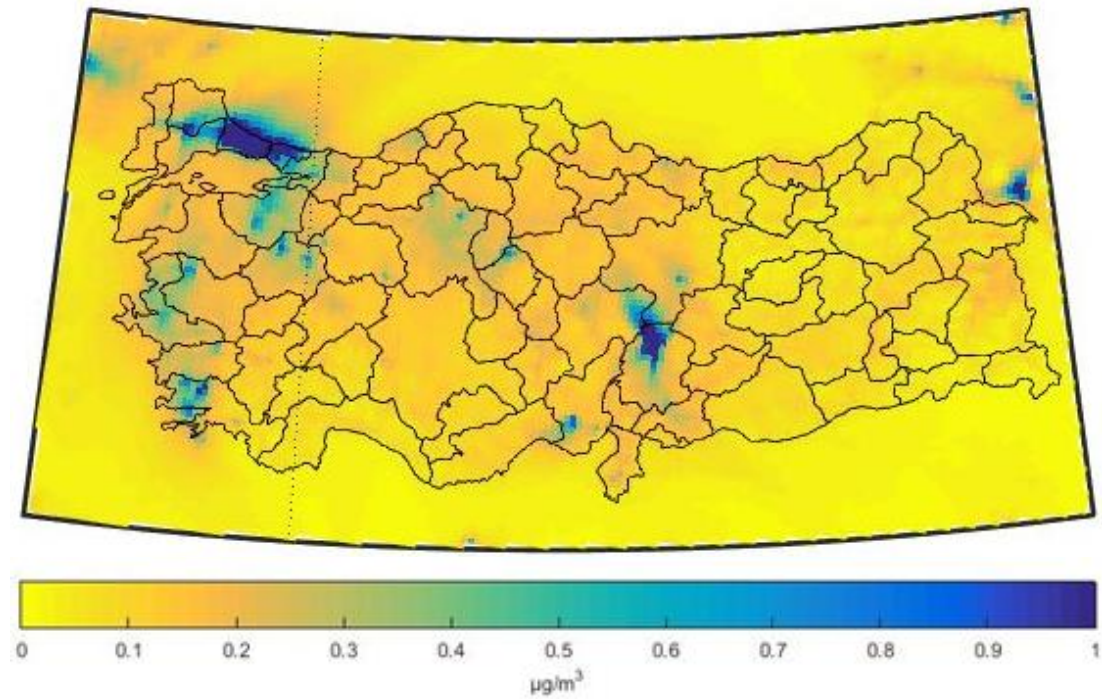
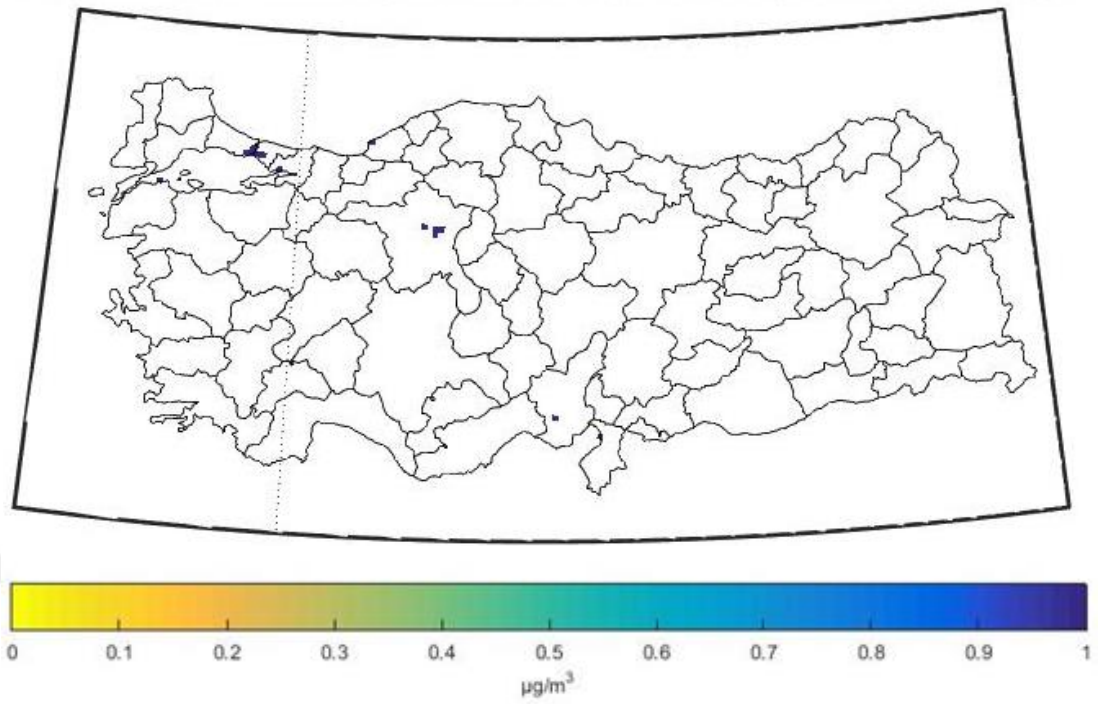


Figure 3.14 : a) Average monthly ground-based observations and b) CMAQ derived NO concentrations for January.

a)



b)

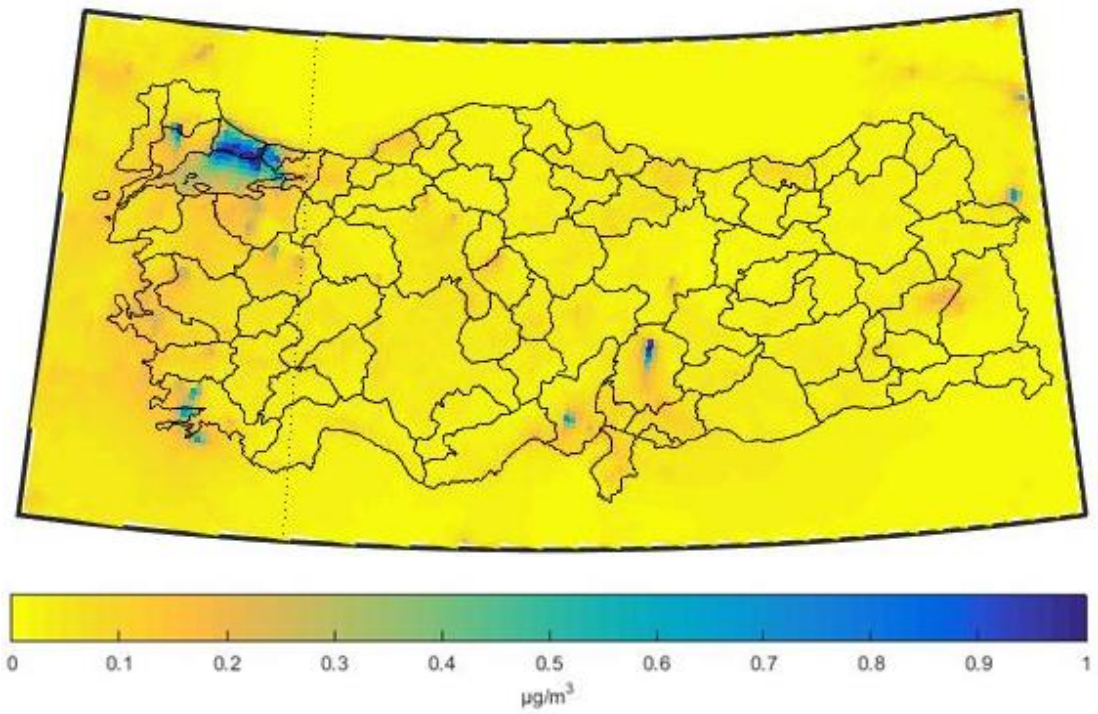
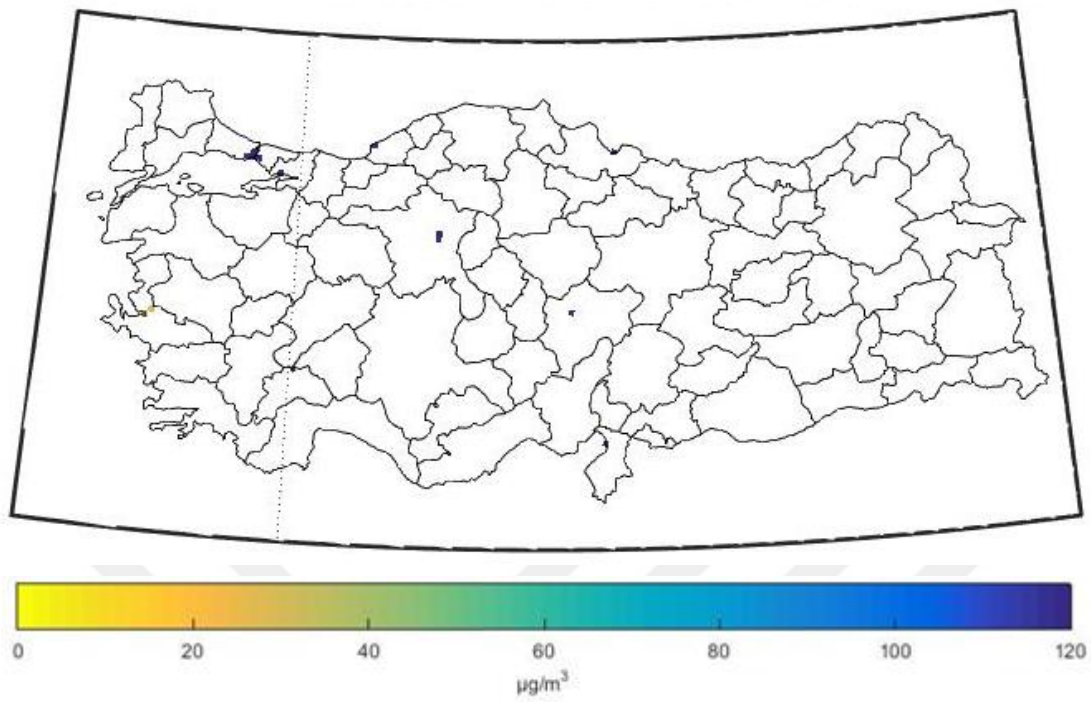


Figure 3.15 : a) Average monthly ground-based observations and b) CMAQ derived NO concentrations for July.

a)



b)

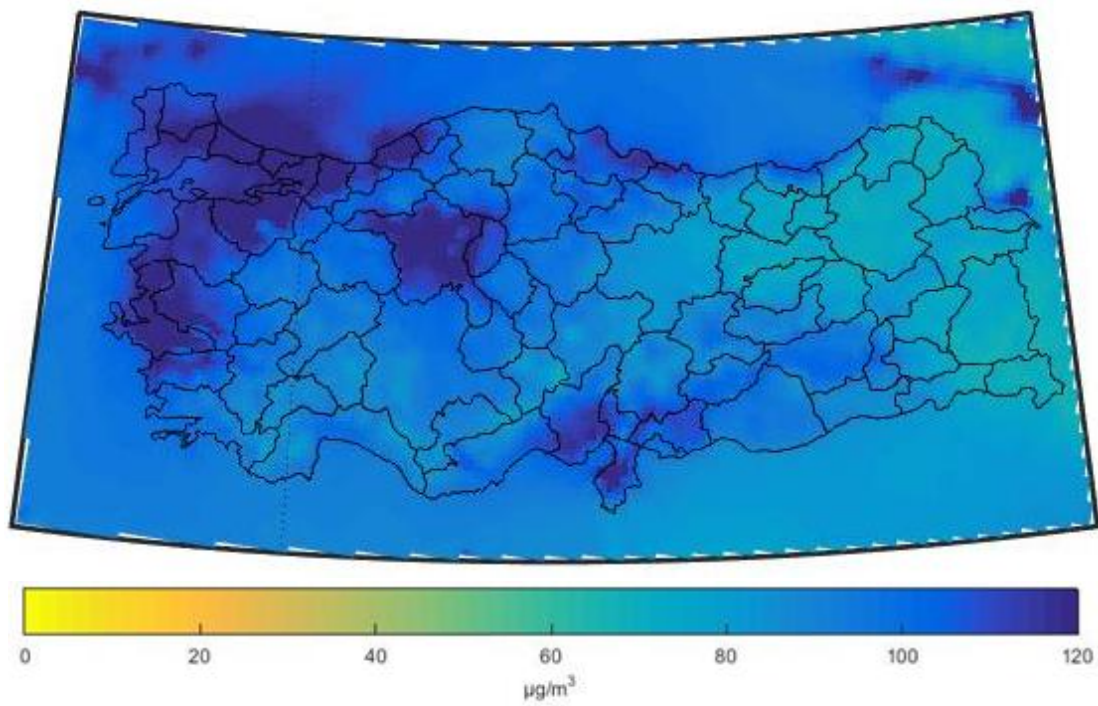
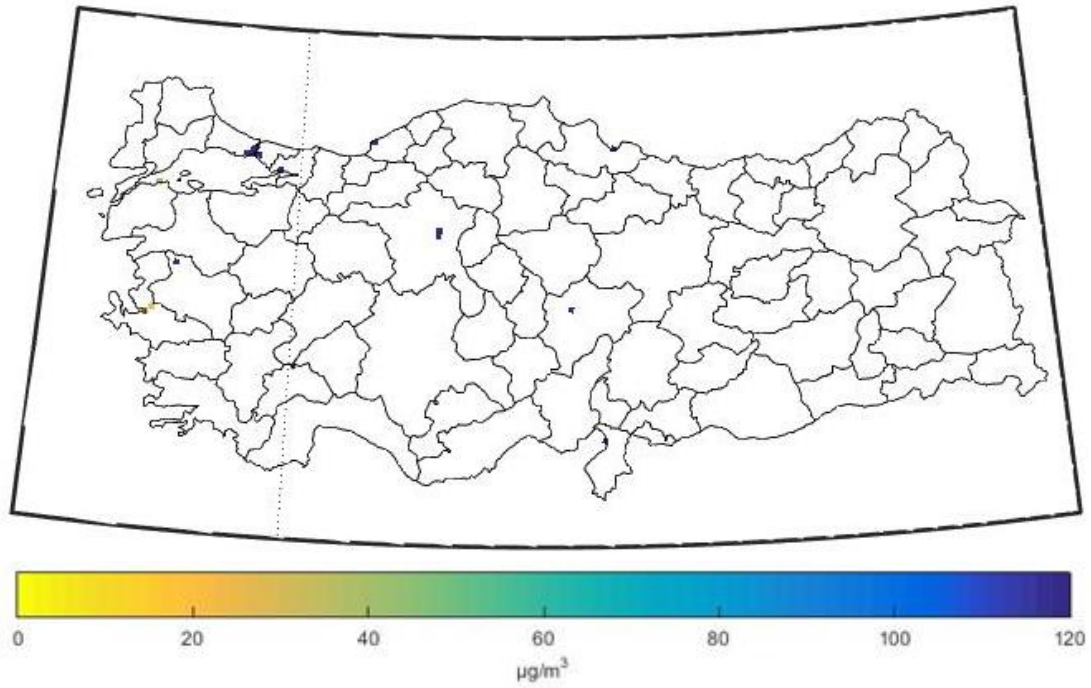


Figure 3.16 : a) Average monthly ground-based observations and b) CMAQ derived CO concentrations for January.

a)



b)

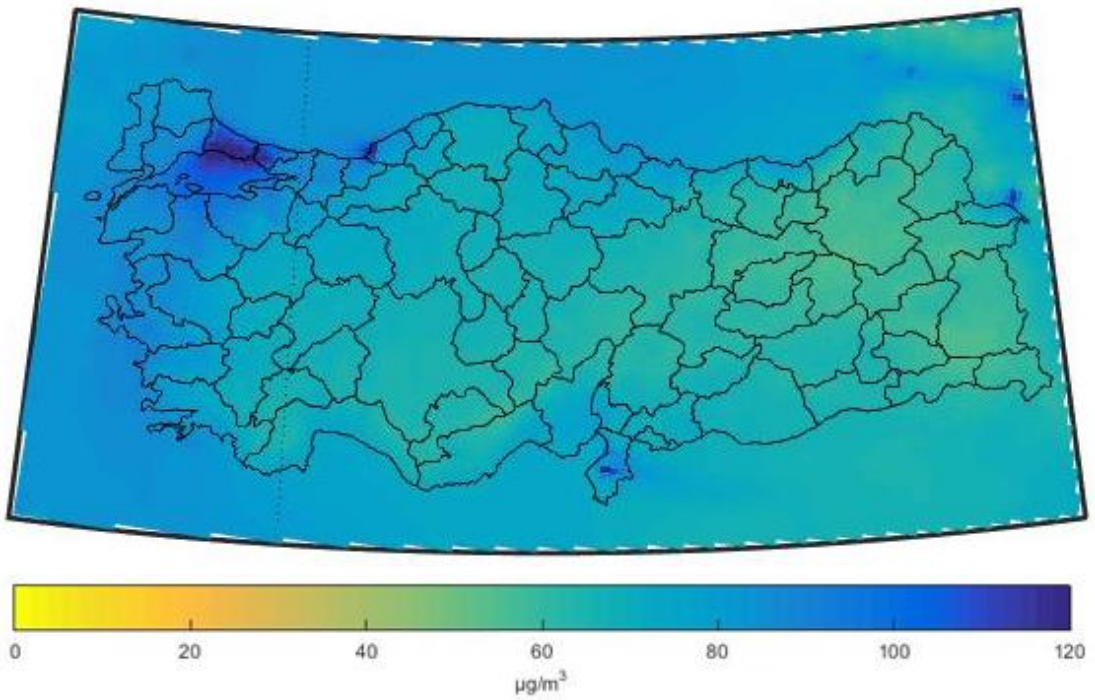
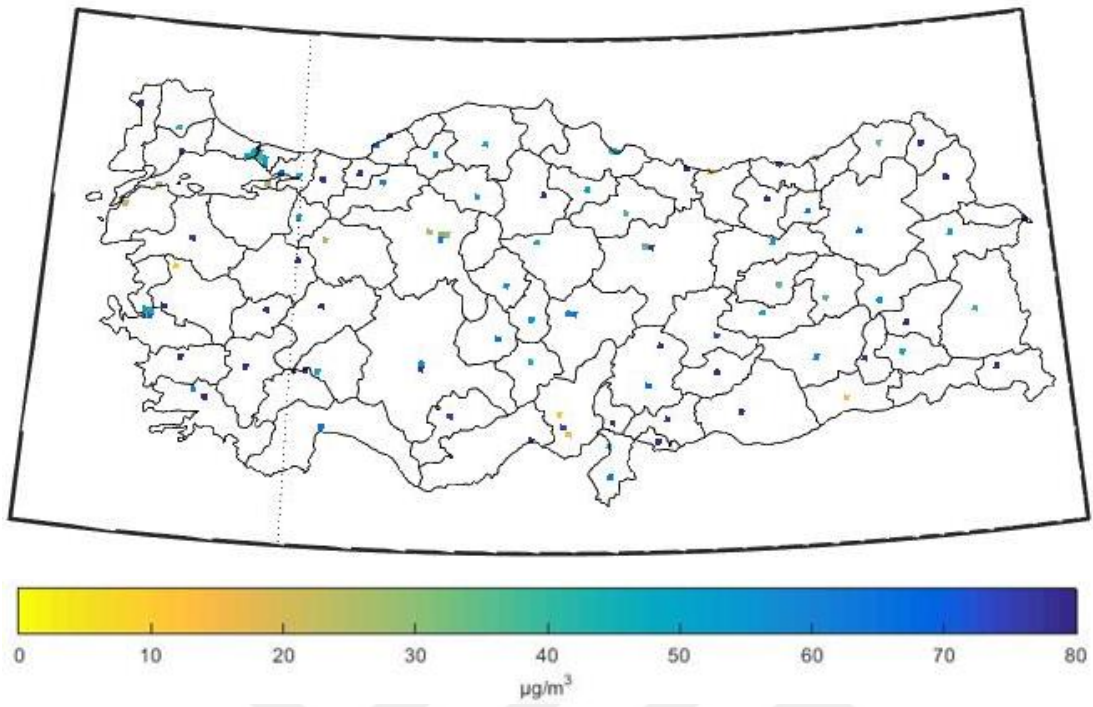


Figure 3.17 : a) Average monthly ground-based observations and b) CMAQ derived CO concentrations for July.

a)



b)

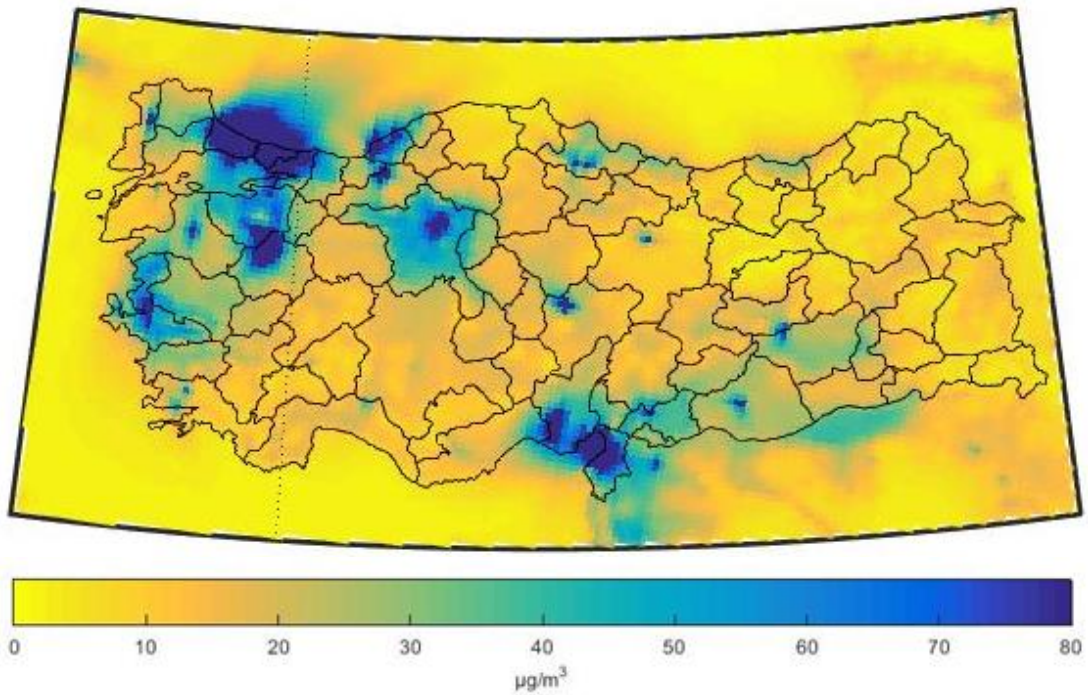
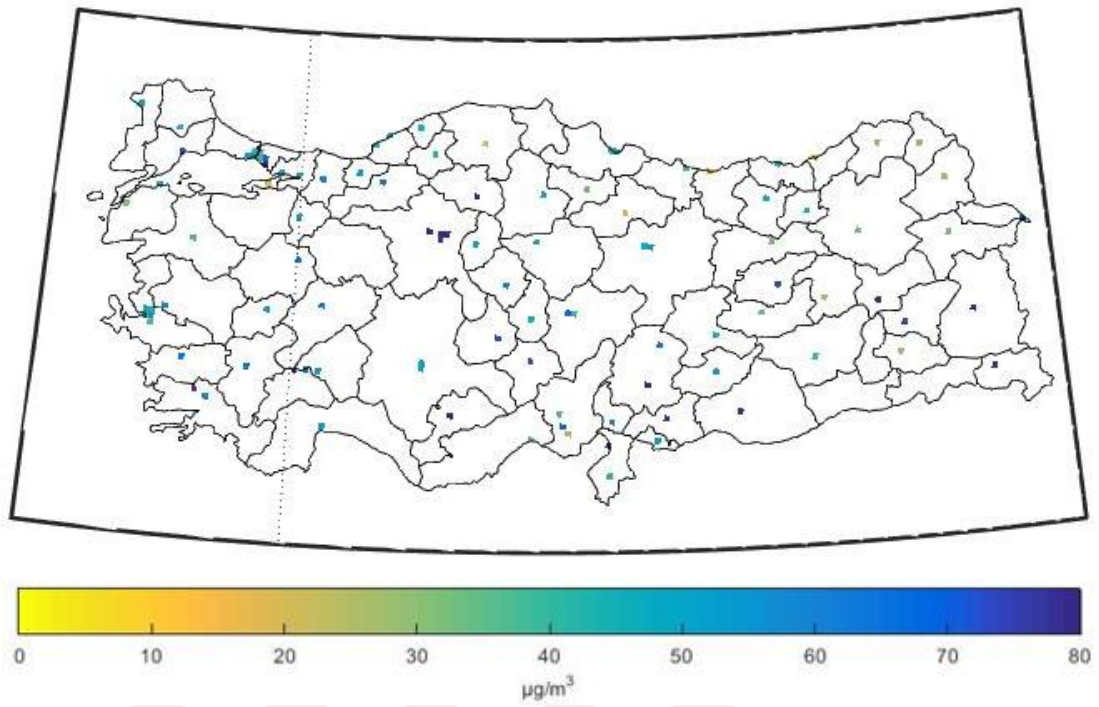


Figure 3.18 : a) Average monthly ground-based observations and b) CMAQ derived PM₁₀ concentrations for January.

a)



b)

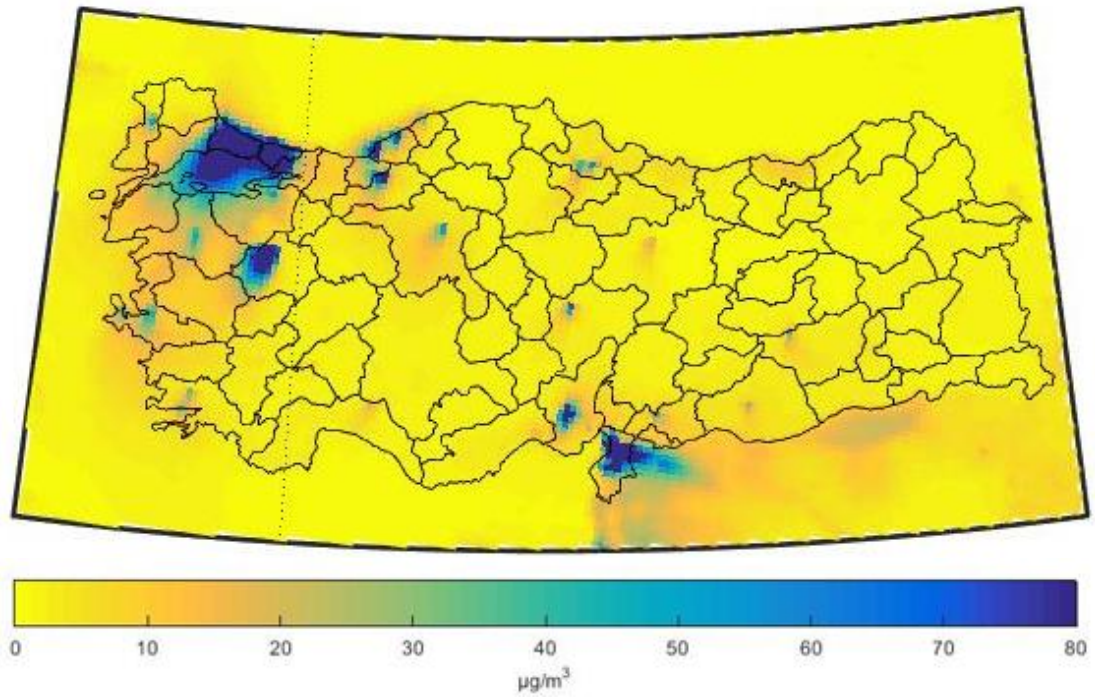


Figure 3.19 : a) Average monthly ground-based observations and b) CMAQ derived PM₁₀ concentrations for July.

Table 3.4 : Statistics of selected ground-based NO, NO₂, CO, and PM₁₀ observations with model simulations during the episodes.

Species	Mean(observations) (µg/m ³)		Observations Std. Dev.		Mean (model) (µg/m ³)		Model Std. Dev.	
	January	July	January	July	January	July	January	July
NO ₂	43.64	43.31	21.76	25.17	5.73	6.50	3.04	7.80
NO	34.38	22.61	22.26	26.76	0.54	0.45	0.34	0.78
CO	837.38	710.96	511.95	462.98	119.77	91.08	16.25	19.94
PM ₁₀	63.52	56.57	30.76	27.07	6.82	4.95	6.09	5.93

Table 3.5 : Statistics of selected ground-based NO, NO₂, CO, and PM₁₀ observations with model simulations during the episodes.

Species	MNB (%)		RMSE (µg/m ³)		MNE (%)	
	January	July	January	July	January	July
NO ₂	-83.31	-73.29	42.85	43.48	83.31	87.13
NO	-97.89	-97.27	40.16	34.09	97.89	97.27
CO	-18.02	-37.06	872.64	770.40	124.43	107.47
PM ₁₀	-85.98	-84.84	65.09	58.41	85.98	94.09

The coefficients of determination of CMAQ and ground observations for PM₁₀, NO₂, NO, and CO measurements in January and July 2012 are shown in Figure 3.20, 3.21, 3.22, and 3.23.

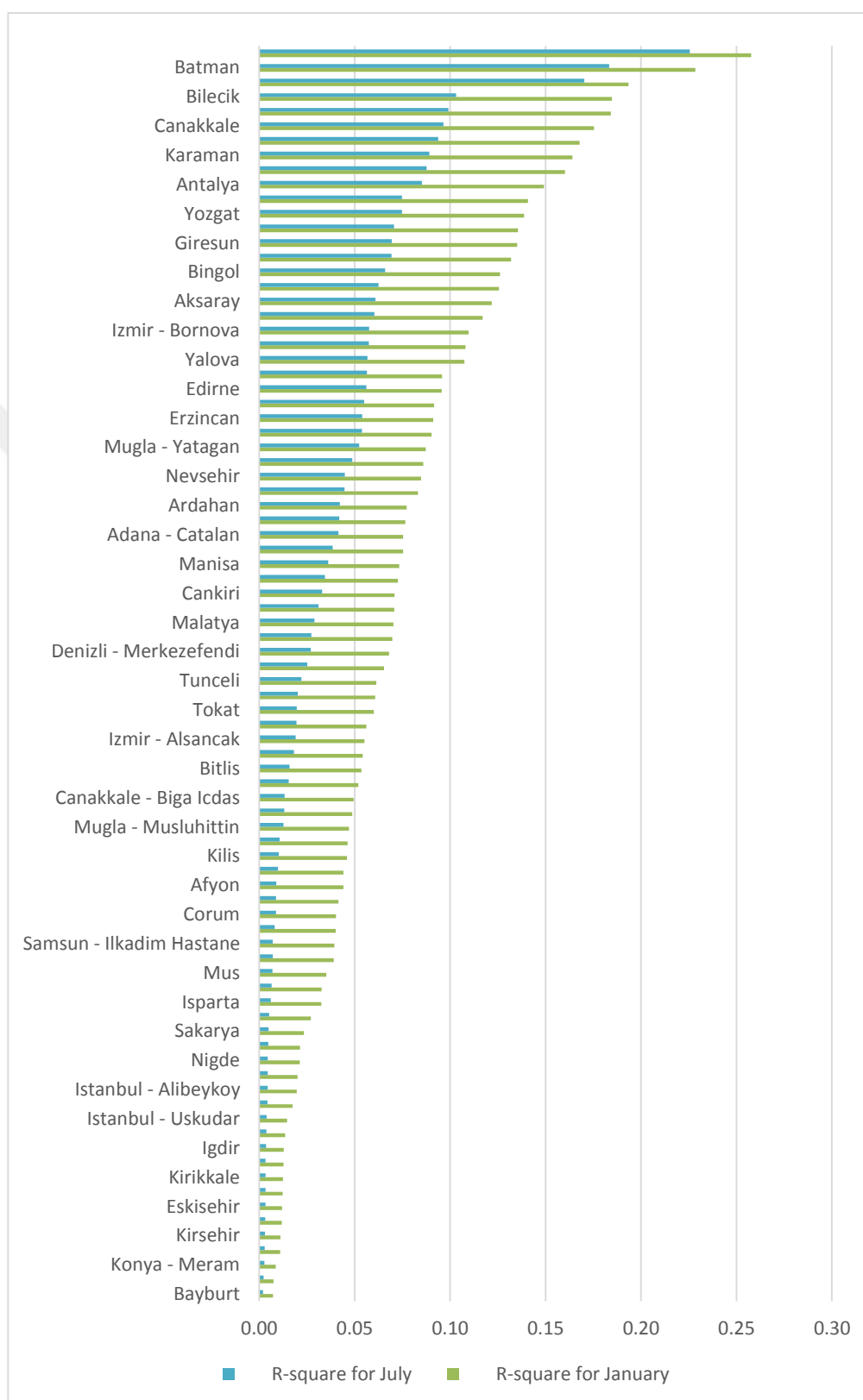


Figure 3.20 : The coefficients of determination of CMAQ and ground observations for PM₁₀ measurements in January and July 2012.

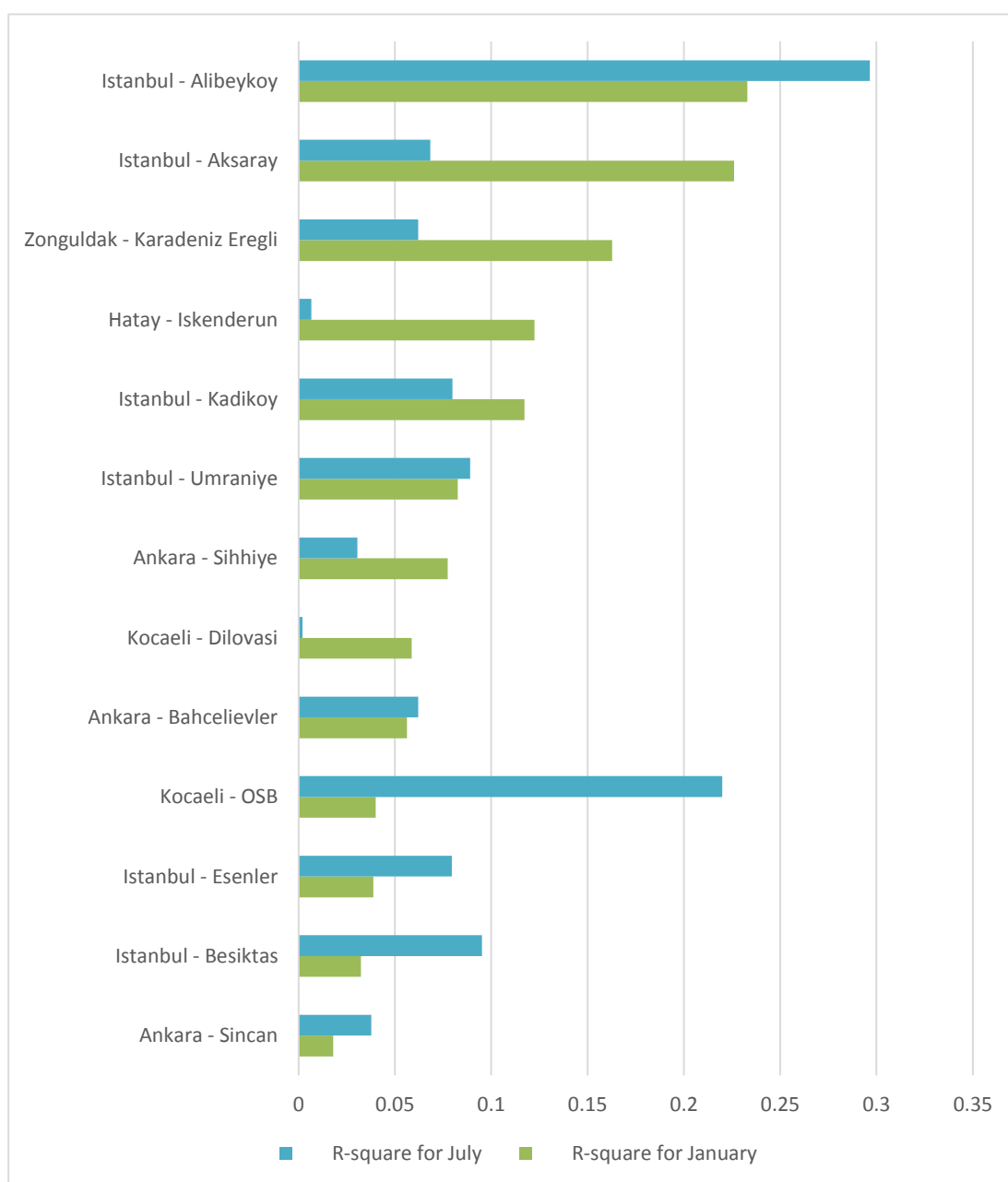


Figure 3.21 : The coefficients of determination of CMAQ and ground observations for NO₂ measurements in January and July 2012.

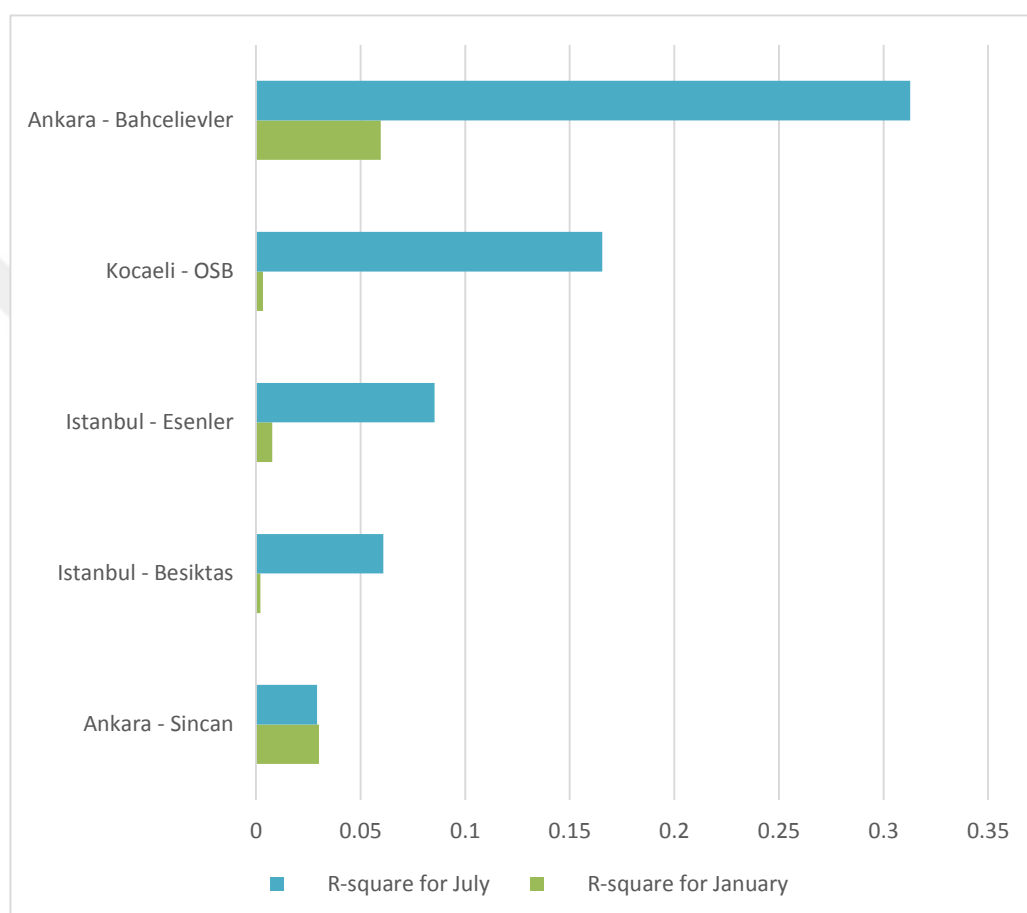


Figure 3.22 : The coefficients of determination of CMAQ and ground observations for NO measurements in January and July 2012.

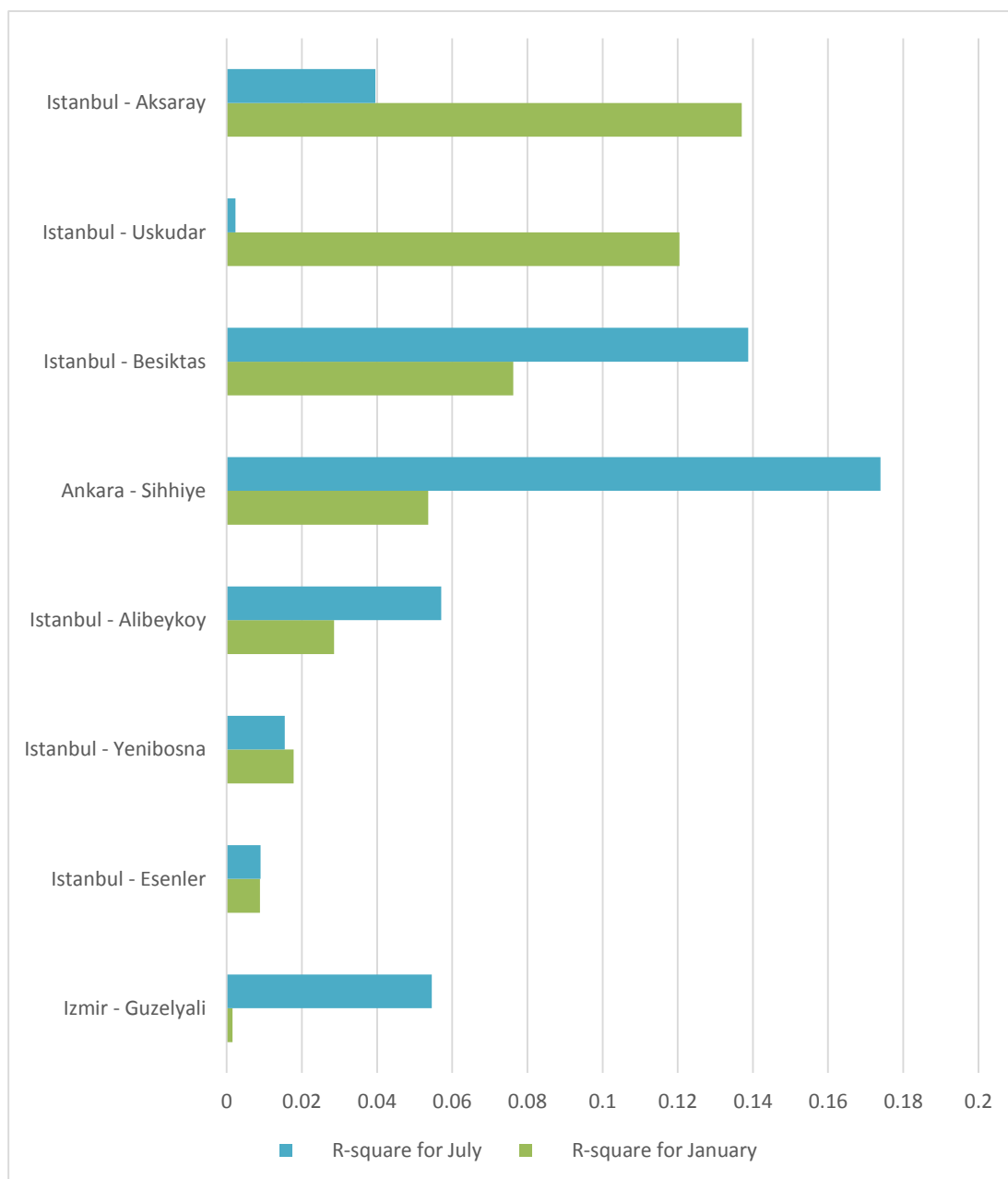


Figure 3.23 : The coefficients of determination of CMAQ and ground observations for CO measurements in January and July 2012.

3.5 Overall Comparison for SO₂

The investigation on MNB and MNE statistical measures of SO₂ for satellite-based and ground-based comparisons showed that the model captured ground-based trend better than satellite observations. The model has better predictions for ground observation locations which are usually in urban regions. But for satellite where all areas included have worse performance.

On the other hand, although the bias of the modeled-ground SO₂ was lower comparing with the modeled-satellite SO₂ comparison, the difference between biases for January and July was higher in modeled-ground SO₂ comparison. This can indicate winter specific sources at the ground such as residential heating using coal.

In some regions like Afsin Elbisan power plant, the comparison of modeled SO₂ and satellite retrievals during July showed that the model underestimated SO₂ at that time episode while the model-ground comparison indicated an overestimation in that place. It could be because of the distance of measuring stations to the pollution point source. This actually indicates the effect of elevated point sources, and the performance is effected depending on where the model allocates the SO₂ around that source. For these sources, satellite column amounts give more representative information because the total pollution can be seen not only the surface level.



4. CONCLUSIONS AND RECOMMENDATIONS

Inter-comparison of CMAQ with available satellite SO₂, ground SO₂, NO, NO₂, PM₁₀, and CO observations for a 2-month period from the summer and winter of 2012 (July-January) found general agreement, but important differences as well.

Modeled SO₂ showed a reasonable bias (31.5% for July and -27.19% for January) between simulated levels and ground-based observations over Turkey. The contribution of EMEP SO₂ emissions indicates underestimations in January.

The results showed underestimations for NO₂, NO, CO and PM₁₀. For CO, the negative bias was lower than other species so it had a better agreement with the observations.

Satellite-based SO₂ observations had a negative bias that could be because of the negative values in the satellite retrievals. The model-satellite comparison indicated the underestimation of the model in both January and July. The comparison between model and ground-based observations showed underestimation in the model predictions in January and overestimation in July. NO was underestimated in comparison with the ground-based observations.

Inter-comparison of SO₂ model-ground observations and model-satellite retrievals showed higher negative bias in the model results with satellite retrievals for January.

Here, the representativeness of the ground observations for the scan area becomes important. This result showed that the model underestimates the total SO₂ column and the surface observations of SO₂ over power plants and also overestimates the western part of Turkey. Moreover, the model underestimated average monthly SO₂ concentration in the eastern part of Turkey with respect to ground observations for January. The contribution of EMEP SO₂ emission in uncertainty could be discussed in January with respect to the underestimations.

This comparison could be improved if additional investigation performed including improvement of satellite observations quality combined with more ground observation stations. However, neither of the comparisons contradicted the findings from separate evaluations of the model.



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APPENDICES

Appendix A

In this study some MATLAB, FORTRAN and Shell Scripting was written for emission processing and other tasks. Some of them are available here.

A.1 Calculation of mean and standard deviation for different pollutants and months from CMAQ results (MATLAB code)

```
function cmaq_poll_jan_daily_monthly_ave_std(poll,m,MW)
ncid=['/mnt/INT_HDD_2/amir/MCIP/10km/0',num2str(m),'2012/METCRO3D_0',num2str(m),'2012'];
P=ncread(ncid,'PRES');
T=ncread(ncid,'TA');
load('obs_st_cmaq_col_row.mat');
mat=NaN(6417,36);
monthly_ave=NaN(207,5);
R=8.3144598;
st0=1;
d0=1;
for st=1:207
st1=st0+30;
mat(st0:st1,1)=st;
pp=[1:31];pp=pp' ;
mat(st0:st1,2)=pp;
mat(st0:st1,3)=obs_st_cmaq_col_row(st,4);
st0=st1+1;
for d=1:31
DAY=['The process is being done for:',num2str(d),' ',num2str(m),' 2012'];
disp(DAY);
if d < 10

ncid1=['/mnt/EXT_HDD_1/amir/CMAQ_outputs/20120',num2str(m),'0',num2str(d),'
/CCTM_D502a_Linux2_x86_64pgi.ACONC.10km_20120',num2str(m),'0',num2str(d)];
else

ncid1=['/mnt/EXT_HDD_1/amir/CMAQ_outputs/20120',num2str(m),num2str(d),'C
CTM_D502a_Linux2_x86_64pgi.ACONC.10km_20120',num2str(m),num2str(d)];
end
POLL1=ncread(ncid1,poll);
```

```

for t=1:24
    t1=(d-1)*24+t;

    POLL_INT=POLL1(obs_st_cmaq_col_row(st,1),obs_st_cmaq_col_row(st,2),:,t)*(P(
    obs_st_cmaq_col_row(:,1),obs_st_cmaq_col_row(:,2),1,t1)/(T(obs_st_cmaq_col_ro
    w(:,1),obs_st_cmaq_col_row(:,2),1,t1)*R))*MW;
    POLL_hourly(t)=POLL_INT;
    end
    POLL_daily_mean=nanmean(POLL_hourly);
    POLL_daily_std=nanstd(POLL_hourly);
    POLL_daily_max=max(POLL_hourly);
    POLL_daily_min=min(POLL_hourly);
    POLL_daily_mean=squeeze(POLL_daily_mean);
    POLL_daily_std=squeeze(POLL_daily_std);
    POLL_daily_max=squeeze(POLL_daily_max);
    POLL_daily_min=squeeze(POLL_daily_min);
    qq=(st-1)*31+d;
    mat(qq,5)=POLL_daily_mean;
    mat(qq,7)=POLL_daily_std;
    mat(qq,9)=POLL_daily_min;
    mat(qq,11)=POLL_daily_max;
    mat(qq,13:36)=POLL_hourly;
    end
    monthly_ave(st,4)=nanmean(POLL_hourly);
    monthly_ave(st,5)=nanstd(POLL_hourly);
end
fileout=['/mnt/INT_HDD_2/amir/DUMAN/obs_loc_CMAQ/ACONC_T_P/',poll,'_M
',num2str(m),'_Daily_monthly_ACON.mat'];
cmd=['save ',fileout,' mat monthly_ave'];
eval(cmd);
disp('finished!');

```

A.2 Calculation of SO₂ from CMAQ results (MATLAB code)

```
R=8.3144598;

ncid=('/mnt/INT_HDD_2/amir/MCIP/10km/012012/METCRO3D_012012');

P=ncread(ncid,'PRES');

T=ncread(ncid,'TA');

for d=1:31

    if d < 10

        ncid1=['/mnt/EXT_HDD_1/amir/CMAQ_outputs/2012010',num2str(d),'/CCTM_D5
02a_Linux2_x86_64pgi.CONC.10km_2012010',num2str(d)];

    else

        ncid1=['/mnt/EXT_HDD_1/amir/CMAQ_outputs/201201',num2str(d),'/CCTM_D50
2a_Linux2_x86_64pgi.CONC.10km_201201',num2str(d)];

    end

    SO2=ncread(ncid1,'SO2');

    SO2=SO2(:,:,,1:24);

    ZF=ncread(ncid,'ZF');

    for i=1:241

        for j=1:154

            for l=1:15

                for h1=1:24

                    h2=24*(d-1)+h1;

                    INT(i,j,l,h1)=SO2(i,j,l,h1)*(1e-6)*P(i,j,l,h2)*(6.022140857e23)/(R*T(i,j,l,h2));-

                    if l==1

                        dH(l)=ZF(:,:,l,:);

                    else
```

```
    dH(l)=ZF(:,l,:)-ZF(:,l-1,:);  
    end  
    DU(i,j,l,h1)=INT(i,j,l,h1)*dH(l)*(1e-6);  
    end  
end  
end  
end  
end
```



A.3 Calculation of monthly SO₂ averages from ground-based observations

(MATLAB code)

```
aver=NaN(70680,4);
for st=1:95
    indx=isnan(Ground(st,2:744));
    indx1=size(find(indx==0),1);
    if indx1 > 223
        h1=1;
        for h=1:31
            h2=h1+23;
            for hr=1:24
                counter=(st-1)*31*24+(h-1)*24+hr;
                aver(counter,1)=l(st);
                aver(counter,2)=h;
                aver(counter,3)=hr;
                G_int=Ground(h1+1:h2+1,st);
                aver(counter,4)=G_int(hr);
            end
            h1=h2+1;
        end
    end
end
```

A.4 Calculation and plotting the statistical parameters and factors for SO₂

CMAQ vs. ground-based observations (MATLAB code)

```
da=4368;%0
ssn=size(Ground,2);
ssn2=size(Ground,1);
stn=24*31*ssn;
aver=NaN(stn,4);
l=Ground(1,:);
for st=1:ssn
    indx=isnan(Ground(2+da:745+da,st));
    indx1=size(find(indx==0),1);
    if indx1 > 223
        h1=1;
        for h=1:31
            h2=h1+23;
            G_int=Ground(h1+1+da:h2+1+da,st);
            for hr=1:24
                counter=(st-1)*31*24+(h-1)*24+hr;
                aver(counter,1)=l(st);
                aver(counter,2)=h;
                aver(counter,3)=hr;
                aver(counter,4)=G_int(hr);
            end
            h1=h2+1;
        end
    end
end
a=find(isnan(aver(:,1))==1);
aver(a,:)=[] ;
sts=unique(aver(:,1));
ssts=size(sts,1);
for p=1:ssts
    matadd=find(mat(:,1)==sts(p));
    averadd=find(aver(:,1)==sts(p));
    mat2= mat(matadd,13:36)' ;
    mat2=mat2(:);
    aver(averadd,5)=mat2;
end
b=find(isnan(aver(:,4))==1);
aver(b,:)=[] ;
sts=unique(aver(:,1));
ssts=size(sts,1);
clear indx indx1 counter;
x=aver(:,4);
y=aver(:,5);
coefficients=NaN(ssts,10);
for i=1:ssts
    c=1;
```

```

kk=find(aver(:,1)==sts(i));
x=aver(kk,4);
y=aver(kk,5);
cftool(x,y);
name=['Station ',num2str(sts(i))];
[ff,g]=createFit(x,y,name);
gof=struct2array(g);
slopes=coeffvalues(ff);
coefficients(i,3:7)=gof(:,:);
coefficients(i,9:10)=slopes(:,:);
coefficients(i,1)=i;
coefficients(i,2)=sts(i);
l=['PM10_Jul_Station_',num2str(sts(i))];
print(l,'-djpeg');
close(c);
end

```



A.5 Extracting the arbitrary ground observation data from the raw pollutant data and performing statistical calculations for different days and months

(MATLAB code)

```
function poll_obs(poll,m,ind,fd);

%m=1;fd=31;ind=4;

ep=fd-ind+1;

int_matrix=NaN(10,2,173);

load('obs_col_row.mat');

final_table=NaN(10,173,ep);

for d=ind-3:fd-3

DAY=['The process is being done for:',num2str(d),' ',num2str(m),' 2012'];

disp(DAY);

D=d+3;

    if D < 10

ncid1=['/mnt/EXT_HDD_1/amir/CMAQ_outputs/20120',num2str(m),'0',num2str(D),'
/CCTM_D502a_Linux2_x86_64pgi.CONC.10km_20120',num2str(m),'0',num2str(D)
];

    else

ncid1=['/mnt/EXT_HDD_1/amir/CMAQ_outputs/20120',num2str(m),num2str(D),'C
CTM_D502a_Linux2_x86_64pgi.CONC.10km_20120',num2str(m),num2str(D)];

    end

    SO2=ncread(ncid1,poll);

    for i=1:173

l=squeeze(SO2(obs_col_row(i,1),obs_col_row(i,2),1:10,14:15));

int_matrix(:,i)=l;
```

```

end

disp(size(int_matrix));

ME=mean(int_matrix,2);

disp(size(ME));

final_table(:,d)=ME;

end

MEAN=mean(final_table,3);

STD=std(final_table,3);

MIN=min(int_matrix,3);

MAX=max(int_matrix,3);

statmat=NaN(10,173,4);

statmat(:,1)=MEAN;

statmat(:,2)=STD;

statmat(:,3)=MIN;

statmat(:,4)=MAX;

ME=squeeze(ME);

fileout=['/mnt/INT_HDD_2/amir/DUMAN/obs/',poll,'_M',num2str(m),'_D_1
3_14_avg.mat'];

cmd=['save ',fileout,' final_table statmat'];

eval(cmd);

clear cmd final_table ME int_matrix STD MIN MAX MEAN statmat SO2;

disp('finished!');

```

A.6 Performing the intersection between EMEP and WRF grids (MATLAB code)

```
yyyyddd=2012002;
year=2012;
m=1;
for d=1:10
poll={'CO' 'NH3' 'NMVOC' 'NOx' 'SOx' 'PMco' 'PM2_5'};
npoll=size(poll,2);
load('/mnt/INT_HDD_2/amir/intersection/30km/FinalAreasFrac2_REF_EU_EMEP_30km_25sub.mat');
load('/mnt/INT_HDD_2/amir/intersection/30km/FinalCol_REF_EU_EMEP_30km_25sub.mat');
load('/mnt/INT_HDD_2/amir/intersection/30km/FinalRow_REF_EU_EMEP_30km_25sub.mat');
for p=1:npoll
    if      strcmp(poll{p},'NOx')==1      |      strcmp(poll{p},'PM2_5')==1      |
    strcmp(poll{p},'PMcoarse')==1
        sector={'A_PublicPower' 'B_Industry' 'C_OtherStationaryComb' 'D_Fugitive'
'F_RoadTransport' 'G_Shipping' 'H_Aviation' ...
'I_Offroad' 'J_Waste' 'K_AgriLivestock' 'L_AgriOther' };
        s={'1' '3' '2' '6' '7' '8' '8' '8' '9' '10' '10'};
        nsector=size(s,2);
    elseif      strcmp(poll{p},'NMVOC')==1      |      strcmp(poll{p},'SOx')==1      |
    strcmp(poll{p},'CO')==1
        sector={'A_PublicPower' 'B_Industry' 'C_OtherStationaryComb' 'D_Fugitive'
'F_RoadTransport' 'G_Shipping' 'H_Aviation' ...
'I_Offroad' 'J_Waste' 'L_AgriOther'};
```

```

s={'1' '3' '2' '6' '7' '8' '8' '8' '9' '10'};

nsector=size(s,2);

else

sector={'A_PublicPower' 'B_Industry' 'C_OtherStationaryComb' 'F_RoadTransport'
'G_Shipping' 'H_Aviation' ...

'I_Offroad' 'J_Waste' 'K_AgriLivestock' 'L_AgriOther' };

s={'1' '3' '2' '7' '8' '8' '8' '9' '10' '10'};

nsector=size(s,2);

end

for t=1:10

    %create directory if needed

    if

exist(['/mnt/INT_HDD_2/amir/DUMAN/EMEP/',num2str(year),'/hourly/',poll{p},'/S'
,num2str(t),'/d01/'])==0

        cmd=['mkdir

/mnt/INT_HDD_2/amir/DUMAN/EMEP/',num2str(year),'/hourly/',poll{p},'/S',num2
str(t),'/d01/'];

        system(cmd);

        disp(cmd);

    end

end

for g=1:nsector

file=['/mnt/INT_HDD_2/amir/DUMAN/EMEP/',num2str(year),'/hourly/',poll{p},'/S',
s{g},'/d01/',EMEP_gridded_d01_',num2str(year), ...

'_M',num2str(m),'_D',num2str(d),'_',poll{p},'_S',s{g},'_0_1deg.mat'];

if exist(file)==0

```

```
extract_all_hr_layer(year,m,d,poll{p},str2num(s{g}));
```

```
end
```

```
end
```

```
end
```

```
end
```



A.7 Summation of the EMEP snaps for a specific pollutant (MATLAB code)

```
function sum_sectors(year,m,d)

poll={'CO'}; %'NH3' 'NMVOC' 'NOx' 'SOx' 'PMco' 'PM2_5'};

npoll=size(poll,2);

s=1:10;

i=m;

summation=zeros(188,156,24,16);

j=d;

for p=1:npoll
for g=1:10
fileout=['/mnt/INT_HDD_2/amir/DUMAN/EMEP/',num2str(year),'/hourly/',poll{p},'
/S',num2str(s(g)),'/d01/EMEP_EMIS_d01_',num2str(year), ...
'_M',num2str(i),'_D',num2str(j),'_',poll{p},'_'_S',num2str(s(g)),'_0_1deg.mat'];
if exist(fileout)==1
disp(fileout);
load(fileout);
for l=1:16
summation(:,:,,l)=summation(:,:,,l)+emi_emep_orig_hh(:,:,,l);
end
end
end
cmd=['save summation emi_emep_orig_hh;'];
eval(cmd);
end
```

A.8 Plotting the spatial distribution of pollutants (MATLAB code)

```
map_title=['Spatial distribution of ',INT1,' averages from CMAQ simulations',' for  
,mo,' 2012'];  
  
load('D:\my_matlab_EMEP\Observations\thesis\lat_lon_REF_EU_10_CSB.mat');  
  
figure  
  
colormap(flipud(parula));  
  
axesm('lambert','MapLatLimit',[35.1 43],'MapLonLimit',[25 45.1]);  
  
axis off; framem on; gridm on; mlabel off; plabel off;  
  
geoshow(OurLat,OurLon,mapping(:,:),'DisplayType','texturemap');  
  
SL=shaperead('tr.shp');  
  
hold on  
  
geoshow([SL.Y],[SL.X],'Color','black');  
  
set(gca,'Clim',[0 80]);  
  
xlabel('Longitude');  
  
ylabel('Latitude');  
  
title(map_title);  
  
xlabel('Longitude');  
  
ylabel('Latitude');  
  
c = colorbar;  
  
c.Label.String = '?g/m^3';
```

Appendix B

B.1 Temperature statistical parameters in different stations in January and July

Table B.1 : Statistical indices for Temperature in different stations for January 2012.
[1] the coefficient of determination, [2] the slope of the trend line, [3] the interception of the trend line, [4] number of data for each station and [5] Root Mean Square Error of the model and ground observations.

Station name	R-square ^[1]	m ^[2]	h ^[3]	DFE ^[4]	RMSE ^[5]
Aksaray	0.77	0.71	-0.04	705	2.09
Ankara - Cebeci	0.80	1.50	-9.66	707	2.00
Ankara - Demetevler	0.85	1.56	-10.23	485	2.08
Ankara - Dikmen	0.84	1.01	0.40	632	2.03
Ankara - Kayas	0.80	0.90	-1.82	733	2.21
Ankara - Kecioren	0.85	0.78	0.88	665	1.83
Ankara - Sihhiye	0.74	1.15	-4.01	467	2.53
Ankara - Sincan	0.78	0.88	0.78	654	2.20
Antalya	0.60	0.82	-2.89	742	2.10
Artvin	0.66	0.84	-3.59	656	2.12
Balikesir	0.62	0.69	0.11	630	2.22
Bayburt	0.65	0.50	-4.77	717	2.23
Bitlis	0.75	0.59	-3.37	741	1.28
Burdur	0.64	0.89	-4.16	740	2.79
Canakkale - Biga Icdas	0.90	0.93	0.31	740	1.30
Duzce	0.58	0.55	0.62	740	2.58
Erzincan	0.68	0.53	-6.17	742	2.11
Giresun	0.75	0.75	0.94	485	2.24
Hakkari	0.01	-0.03	-5.63	577	2.53
Hatay - Antakya	0.44	0.54	4.51	741	2.01
Igdir	0.00	-0.08	8.99	426	2.53
Icel	0.27	0.75	-9.88	741	3.91
Izmir - Gaziemir	0.50	0.62	1.68	272	1.83
Kahramanmaras - Elbistan	0.65	0.59	-0.84	742	2.20
Karaman	0.70	0.63	-0.09	717	2.28
Kastamonu	0.57	0.66	-1.54	742	2.92
Kayseri - OSB	0.86	0.66	-6.32	742	1.71
Kirikkale	0.23	0.27	3.87	737	2.54
Kilis	0.19	0.67	-6.69	733	4.45
Kocaeli	0.71	0.67	-0.62	699	1.99
Mus	0.47	0.44	-0.51	742	2.69
Nevsehir	0.92	0.74	-2.47	741	1.36
Ordu - Stadyum	0.77	0.79	0.29	741	1.88
Osmaniye	0.55	0.58	0.32	741	1.88
Rize	0.68	0.74	1.38	742	2.00
Sakarya	0.84	0.74	-0.71	741	1.45
Siirt	0.69	0.74	0.91	742	1.68
Sinop	0.09	0.22	1.86	741	2.63
Sanliurfa	0.37	0.93	-8.22	724	3.49
Sirnak	0.49	1.13	-6.40	739	3.15
Tokat	0.74	0.60	-3.18	742	2.38
Tunceli	0.62	1.11	-11.89	742	2.28
Yalova	0.83	0.74	0.04	741	1.41
Zonguldak - Karadeniz Eregli	0.81	0.77	-0.08	695	1.54

Table B.2 : Statistical indices for Temperature in different stations for July 2012. [1] the coefficient of determination, [2] the slope of the trend line, [3] the interception of the trend line, [4] number of data for each station and [5] Root Mean Square Error of the model and ground observations.

Station name	R-square ^[1]	m ^[2]	h ^[3]	DFE ^[4]	RMSE ^[5]
Aksaray	0.52	0.72	5.79	741	3.87
Ankara - Cebeci	0.65	1.21	-2.47	742	3.20
Ankara - Demetevler	0.67	1.28	-3.80	715	3.06
Ankara - Dikmen	0.67	0.84	4.97	665	3.06
Ankara - Kayas	0.65	0.71	5.53	730	3.09
Ankara - Kecioren	0.66	0.68	6.11	742	3.17
Ankara - Sihhiye	0.65	0.90	2.61	742	3.10
Ankara - Sincan	0.64	0.83	5.65	742	3.25
Antalya	0.41	0.71	6.92	739	3.06
Artvin	0.60	0.92	0.69	734	3.34
Balikesir	0.53	0.76	4.37	742	3.00
Bayburt	0.57	0.61	3.60	740	3.61
Bitlis	0.74	0.63	5.42	739	2.15
Burdur	0.48	0.66	4.07	742	3.79
Canakkale - Biga Icdas	0.62	0.71	7.55	742	1.78
Duzce	0.49	0.51	10.70	739	2.88
Erzincan	0.51	0.59	2.50	740	3.86
Giresun	0.41	0.49	10.25	740	2.24
Hakkari	0.38	1.29	-1.20	636	3.05
Hatay - Antakya	0.43	0.74	5.64	740	2.87
Igdir	0.02	0.04	28.53	639	1.86
Icel	0.44	1.34	-18.80	732	3.82
Izmir - Gaziemir	0.30	0.56	9.90	497	3.30
Kahramanmaras - Elbistan	0.46	0.57	10.51	740	4.36
Karaman	0.56	0.67	7.20	741	3.62
Kastamonu	0.40	0.46	9.23	741	3.98
Kayseri - OSB	0.67	0.88	-0.27	742	3.42
Kirikkale	0.25	0.40	17.07	742	4.25
Kirklareli	0.36	0.67	3.90	739	4.08
Kilis	0.42	0.62	2.25	741	4.03
Kocaeli - OSB	0.36	0.69	6.69	729	2.86
Mus	0.45	1.49	-15.51	732	3.84
Nevsehir	0.57	0.63	4.92	741	3.72
Ordu - Stadyum	0.45	0.52	8.53	733	2.29
Osmaniye	0.37	0.59	7.45	737	3.13
Rize	0.42	0.45	11.00	742	1.99
Sakarya	0.32	0.52	10.76	739	3.09
Siirt	0.59	0.72	8.62	742	3.04
Sinop	0.42	1.71	-10.67	361	3.91
Sanliurfa	0.42	0.76	-5.11	742	4.62
Sirnak	0.51	1.14	-12.81	711	4.20
Tokat	0.35	0.54	5.15	738	4.47
Tunceli	0.47	0.83	2.55	656	3.94
Yalova	0.29	0.48	12.72	742	2.75
Zonguldak - Karadeniz Eregli	0.34	0.32	15.96	738	2.62

Appendix C

C.1 Sigma pressure layers for WRF and CMAQ

Table C.1 : Sigma pressure layers for WRF and CMAQ.

CMAQ Layers		Sigma Pressure Layer
Layer Number	Layer Height (m)	
0	0	1
1	41	0.995
2	61	0.9925
3	81	0.99
4	122	0.985
5	204	0.975
6	413	0.95
7	627	0.925
8	845	0.9
9	1298	0.85
10	2804	0.7
11	5283	0.5
12	8703	0.3
13	11168	0.2
14	15166	0.1
15	29283	0

C.2 Vertical distribution of anthropogenic emissions

Table C.2 : Vertical Distribution of Anthropogenic Emissions (EMEP, 2003).

Layer	SNAP									
	1	2	3	4	5	6	7	8	9	10
0m – 41m	-	0.44	0.09	0.08	0.04	0.44	0.44	0.44	-	0.44
41m – 61m	-	0.22	0.05	0.04	0.02	0.22	0.22	0.22	-	0.22
61m – 81m	-	0.22	0.05	0.04	0.02	0.22	0.22	0.22	-	0.22
81m – 122m	-	0.12	0.27	0.25	0.21	0.12	0.12	0.12	0.13	0.12
122m – 204m	0.07	-	0.51	0.49	0.45	-	-	-	0.36	-
204m – 413m	0.64	-	0.03	0.09	0.26	-	-	-	0.5	-
413m – 627m	0.26	-	-	-	-	-	-	-	0.01	-
627m – 845m	0.02	-	-	-	-	-	-	-	-	-
845m – 1298m	-	-	-	-	-	-	-	-	-	-
1298m – 2804m	-	-	-	-	-	-	-	-	-	-
2804-5283m	-	-	-	-	-	-	-	-	-	-
5283-8703m	-	-	-	-	-	-	-	-	-	-
8703-11168m	-	-	-	-	-	-	-	-	-	-
11168-15166m	-	-	-	-	-	-	-	-	-	-
15166-29283m	-	-	-	-	-	-	-	-	-	-

Appendix D

The temporal profiles which were used in the emission processing are available in this section. All of the profiles are sector specific.

D.1 Monthly temporal profile of each pollutant separately

Table D.1 : Monthly temporal profile of CO for Turkey.

SNAP	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
1	1.339	1.239	1.12	1.084	0.903	0.766	0.72	0.693	0.779	0.975	1.131	1.265
2	2.021	2.242	1.864	1.207	0.582	0.377	0.209	0.188	0.25	0.579	0.977	1.587
3	1.102	1.153	1.148	1.057	0.979	0.947	0.858	0.779	0.86	0.987	1.052	1.092
4	0.981	1.04	1.071	1.044	1.027	1.025	0.969	0.875	0.933	1.025	1.022	0.992
5	0.993	1.001	1.001	0.999	1	0.999	1.001	1.001	1.001	1.001	1.001	1.001
6	0.989	0.961	0.982	1.021	1.036	1.036	0.969	0.891	0.961	1.042	1.056	1.056
7	0.9	0.943	0.992	1.02	1.04	1.039	1.02	1.006	1.013	1.058	1.017	0.95
8	0.899	0.944	1.01	1.037	1.039	1.08	1.045	0.97	1.016	1.047	0.988	0.923
9	1	1	1	1	1	1	1	1	1	1	1	1
10	0	0.03	0.37	0.521	0.297	0.209	0.583	1.043	2.586	3.629	2.158	0.528
11	1	1	1	1	1	1	1	1	1	1	1	1

Table D.2 : Monthly temporal profile of NH₃ for Turkey.

SNAP	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
1	1.332	1.255	1.137	1.089	0.903	0.736	0.675	0.679	0.807	1.011	1.141	1.253
2	1.983	2.282	1.892	1.292	0.57	0.357	0.207	0.185	0.229	0.593	0.96	1.535
3	1.123	1.159	1.151	1.062	0.983	0.945	0.845	0.743	0.834	0.993	1.061	1.116
4	0.98	1.046	1.075	1.043	1.025	1.024	0.959	0.883	0.945	1.022	1.019	0.984
5	1	1	1	1	1	1	1	1	1	1	1	1
6	0.926	0.928	0.969	1.012	1.027	1.055	1.043	1.018	1.044	1.036	0.985	0.953
7	0.906	0.945	0.986	1.017	1.038	1.038	1.023	1.009	1.014	1.056	1.018	0.948
8	0.874	0.924	1.004	1.038	1.04	1.093	1.076	1.014	1.047	1.045	0.957	0.886
9	1	1	1	1	1	1	1	1	1	1	1	1
10	0.525	0.689	1.313	1.57	1.244	1.05	0.869	0.871	1.001	1.077	1.038	0.744
11	1	1	1	1	1	1	1	1	1	1	1	1

Table D.3 : Monthly temporal profile of NO_x for Turkey.

SNAP	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
1	1.307	1.216	1.087	1.05	0.899	0.788	0.752	0.74	0.823	0.996	1.124	1.232
2	2.019	2.243	1.865	1.21	0.581	0.376	0.209	0.188	0.249	0.579	0.977	1.585
3	1.103	1.153	1.148	1.057	0.979	0.947	0.858	0.777	0.859	0.987	1.052	1.092
4	0.978	1.035	1.071	1.041	1.024	1.026	0.963	0.879	0.944	1.027	1.025	0.992
5	0.994	1.001	1.001	0.999	1	0.999	1.001	1.001	1.001	1.001	1.001	1.001
6	0.889	0.898	0.957	1.013	1.032	1.076	1.077	1.059	1.08	1.044	0.96	0.91
7	0.898	0.933	0.974	1.008	1.031	1.037	1.03	1.021	1.025	1.067	1.024	0.947
8	0.898	0.943	1.01	1.037	1.039	1.081	1.046	0.972	1.017	1.047	0.986	0.922
9	1	1	1	1	1	1	1	1	1	1	1	1
10	0.06	0.126	0.724	0.987	0.602	0.444	0.593	0.921	2.135	2.98	1.872	0.518
11	1	1	1	1	1	1	1	1	1	1	1	1

Table D.4 : Monthly temporal profile of PM_{2.5} for Turkey.

SNAP	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
1	1.307	1.216	1.087	1.05	0.899	0.788	0.752	0.74	0.823	0.996	1.124	1.232
2	2.019	2.243	1.865	1.21	0.581	0.376	0.209	0.188	0.249	0.579	0.977	1.585
3	1.103	1.153	1.148	1.057	0.979	0.947	0.858	0.777	0.859	0.987	1.052	1.092
4	0.978	1.035	1.071	1.041	1.024	1.026	0.963	0.879	0.944	1.027	1.025	0.992
5	0.994	1.001	1.001	0.999	1	0.999	1.001	1.001	1.001	1.001	1.001	1.001
6	0.889	0.898	0.957	1.013	1.032	1.076	1.077	1.059	1.08	1.044	0.96	0.91
7	0.898	0.933	0.974	1.008	1.031	1.037	1.03	1.021	1.025	1.067	1.024	0.947
8	0.898	0.943	1.01	1.037	1.039	1.081	1.046	0.972	1.017	1.047	0.986	0.922
9	1	1	1	1	1	1	1	1	1	1	1	1
10	0.06	0.126	0.724	0.987	0.602	0.444	0.593	0.921	2.135	2.98	1.872	0.518
11	1	1	1	1	1	1	1	1	1	1	1	1

Table D.5 : Monthly temporal profile of PM_{co} for Turkey.

SNAP	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
1	1.307	1.216	1.087	1.05	0.899	0.788	0.752	0.74	0.823	0.996	1.124	1.232
2	2.019	2.243	1.865	1.21	0.581	0.376	0.209	0.188	0.249	0.579	0.977	1.585
3	1.103	1.153	1.148	1.057	0.979	0.947	0.858	0.777	0.859	0.987	1.052	1.092
4	0.978	1.035	1.071	1.041	1.024	1.026	0.963	0.879	0.944	1.027	1.025	0.992
5	0.994	1.001	1.001	0.999	1	0.999	1.001	1.001	1.001	1.001	1.001	1.001
6	0.889	0.898	0.957	1.013	1.032	1.076	1.077	1.059	1.08	1.044	0.96	0.91
7	0.898	0.933	0.974	1.008	1.031	1.037	1.03	1.021	1.025	1.067	1.024	0.947
8	0.898	0.943	1.01	1.037	1.039	1.081	1.046	0.972	1.017	1.047	0.986	0.922
9	1	1	1	1	1	1	1	1	1	1	1	1
10	0.06	0.126	0.724	0.987	0.602	0.444	0.593	0.921	2.135	2.98	1.872	0.518
11	1	1	1	1	1	1	1	1	1	1	1	1

Table D.6 : Monthly temporal profile of SO_x for Turkey.

SNAP	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
1	1.301	1.21	1.084	1.049	0.901	0.792	0.755	0.741	0.824	0.999	1.127	1.23
2	2.021	2.242	1.864	1.207	0.581	0.377	0.209	0.188	0.25	0.579	0.977	1.587
3	1.102	1.153	1.148	1.057	0.979	0.947	0.858	0.779	0.86	0.987	1.052	1.092
4	0.979	1.038	1.071	1.04	1.023	1.024	0.958	0.884	0.95	1.025	1.023	0.99
5	0.993	1.001	1.001	0.999	1	0.999	1.001	1.001	1.001	1.001	1.001	1.001
6	0.876	0.887	0.952	1.014	1.034	1.083	1.089	1.074	1.093	1.047	0.951	0.895
7	0.901	0.931	0.966	1.001	1.025	1.033	1.032	1.028	1.029	1.072	1.029	0.949
8	0.899	0.944	1.01	1.037	1.039	1.08	1.045	0.97	1.016	1.047	0.988	0.923
9	1	1	1	1	1	1	1	1	1	1	1	1
10	0.022	0.182	1.915	2.687	1.545	1.094	0.454	0.407	0.865	1.335	1.146	0.327
11	1	1	1	1	1	1	1	1	1	1	1	1

D.2 Daily temporal profile of each pollutant separately

Table D.7 : Daily temporal profile of CO for Turkey.

SNAP	Mon	Tue	Wed	Thu	Fri	Sat	Sun
1	1.03	1.034	1.069	1.073	1.05	0.906	0.838
2	1.02	0.988	0.994	1.005	1.015	0.966	1.012
3	1.074	1.082	1.087	1.079	1.068	0.805	0.807
4	1.074	1.085	1.09	1.083	1.066	0.801	0.802
5	1.016	1.017	1.016	0.962	0.962	1.012	1.015
6	1.207	1.208	1.21	1.21	1.211	0.715	0.239
7	1.005	0.995	0.997	0.996	0.999	1.001	1.007
8	1	1.003	1.004	1.002	0.999	0.992	1
9	1	1	1	1	1	1	1
10	0.997	0.982	0.982	1.005	1.02	1.001	1.013
11	1	1	1	1	1	1	1

Table D.8 : Daily temporal profile of NH₃ for Turkey.

SNAP	Mon	Tue	Wed	Thu	Fri	Sat	Sun
1	1.028	1.039	1.058	1.054	1.049	0.92	0.852
2	1.025	1.007	0.995	0.989	1.001	0.979	1.005
3	1.07	1.078	1.08	1.072	1.08	0.808	0.811
4	1.074	1.085	1.09	1.083	1.066	0.801	0.802
5	1	1	1	1	1	1	1
6	1.211	1.212	1.213	1.213	1.212	0.647	0.292
7	1.004	0.997	0.998	0.996	1	1	1.006
8	1	1.003	1.004	1.002	0.999	0.992	1
9	1	1	1	1	1	1	1
10	1.001	1.001	1.001	1.001	1.001	0.994	1.001
11	1	1	1	1	1	1	1

Table D.9 : Daily temporal profile of NO_x for Turkey.

SNAP	Mon	Tue	Wed	Thu	Fri	Sat	Sun
1	1.031	1.035	1.071	1.073	1.051	0.904	0.835
2	1.02	0.988	0.994	1.005	1.015	0.966	1.012
3	1.074	1.082	1.087	1.079	1.068	0.805	0.807
4	1.074	1.085	1.09	1.083	1.066	0.801	0.802
5	1.016	1.017	1.016	0.962	0.962	1.012	1.015
6	1.213	1.214	1.215	1.215	1.214	0.607	0.324
7	1.007	0.992	0.994	0.995	0.999	1.004	1.01
8	1	1.003	1.004	1.002	0.999	0.992	1
9	1	1	1	1	1	1	1
10	0.997	0.982	0.982	1.005	1.02	1.001	1.013
11	1	1	1	1	1	1	1

Table D.10 : Daily temporal profile of PM_{2.5} for Turkey.

SNAP	Mon	Tue	Wed	Thu	Fri	Sat	Sun
1	1.031	1.035	1.071	1.073	1.051	0.904	0.835
2	1.02	0.988	0.994	1.005	1.015	0.966	1.012
3	1.074	1.082	1.087	1.079	1.068	0.805	0.807
4	1.074	1.085	1.09	1.083	1.066	0.801	0.802
5	1.016	1.017	1.016	0.962	0.962	1.012	1.015
6	1.213	1.214	1.215	1.215	1.214	0.607	0.324
7	1.007	0.992	0.994	0.995	0.999	1.004	1.01
8	1	1.003	1.004	1.002	0.999	0.992	1
9	1	1	1	1	1	1	1
10	0.997	0.982	0.982	1.005	1.02	1.001	1.013
11	1	1	1	1	1	1	1

Table D.11 : Daily temporal profile of PM_{co} for Turkey.

SNAP	Mon	Tue	Wed	Thu	Fri	Sat	Sun
1	1.031	1.035	1.071	1.073	1.051	0.904	0.835
2	1.02	0.988	0.994	1.005	1.015	0.966	1.012
3	1.074	1.082	1.087	1.079	1.068	0.805	0.807
4	1.074	1.085	1.09	1.083	1.066	0.801	0.802
5	1.016	1.017	1.016	0.962	0.962	1.012	1.015
6	1.213	1.214	1.215	1.215	1.214	0.607	0.324
7	1.007	0.992	0.994	0.995	0.999	1.004	1.01
8	1	1.003	1.004	1.002	0.999	0.992	1
9	1	1	1	1	1	1	1
10	0.997	0.982	0.982	1.005	1.02	1.001	1.013
11	1	1	1	1	1	1	1

Table D.12 : Daily temporal profile of SO_x for Turkey.

SNAP	Mon	Tue	Wed	Thu	Fri	Sat	Sun
1	1.038	1.047	1.083	1.079	1.055	0.887	0.812
2	1.02	0.988	0.994	1.005	1.015	0.966	1.012
3	1.074	1.082	1.087	1.079	1.068	0.805	0.807
4	1.074	1.085	1.09	1.083	1.066	0.801	0.802
5	1.016	1.017	1.016	0.962	0.962	1.012	1.015
6	1.213	1.214	1.215	1.215	1.214	0.592	0.335
7	1.008	0.991	0.992	0.995	0.998	1.005	1.011
8	1	1.003	1.004	1.002	0.999	0.992	1
9	1	1	1	1	1	1	1
10	1.001	0.998	0.998	1.003	1.007	0.988	1.005
11	1	1	1	1	1	1	1

D.3 Hourly temporal profile for various days and SNAPs

Table D.13 : Hourly temporal profile of Monday for Turkey.

SNAP	Hour																							
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
1	0.79	0.72	0.72	0.71	0.74	0.8	0.92	1.08	1.19	1.22	1.21	1.21	1.17	1.15	1.14	1.13	1.1	1.07	1.04	1.02	1.02	1.01	0.96	0.88
2	0.38	0.36	0.36	0.36	0.37	0.5	1.19	1.53	1.57	1.56	1.35	1.16	1.07	1.06	1	0.98	0.99	1.12	1.41	1.52	1.39	1.35	1	0.42
3	0.75	0.75	0.78	0.82	0.88	0.95	1.02	1.09	1.16	1.22	1.28	1.3	1.22	1.24	1.25	1.16	1.08	1.01	0.95	0.9	0.85	0.81	0.78	0.75
4	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
5	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
6	0.5	0.35	0.2	0.1	0.1	0.2	0.75	1.25	1.4	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.4	1.25	1.1	1	0.9	0.8	0.7
7	0.19	0.09	0.06	0.05	0.09	0.22	0.86	1.84	1.86	1.41	1.24	1.2	1.32	1.44	1.45	1.59	2.03	2.08	1.51	1.06	0.74	0.62	0.61	0.44
8	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
9	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
10	0.6	0.6	0.6	0.6	0.6	0.65	0.75	0.9	1.1	1.35	1.45	1.6	1.8	1.75	1.7	1.55	1.35	1.1	0.9	0.75	0.65	0.6	0.6	0.6
11	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

Table D.14 : Hourly temporal profile of Tuesday for Turkey.

SNAP	Hour																							
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
1	0.79	0.72	0.72	0.71	0.74	0.8	0.92	1.08	1.19	1.22	1.21	1.21	1.17	1.15	1.14	1.13	1.1	1.07	1.04	1.02	1.02	1.01	0.96	0.88
2	0.38	0.36	0.36	0.36	0.37	0.5	1.19	1.53	1.57	1.56	1.35	1.16	1.07	1.06	1	0.98	0.99	1.12	1.41	1.52	1.39	1.35	1	0.42
3	0.75	0.75	0.78	0.82	0.88	0.95	1.02	1.09	1.16	1.22	1.28	1.3	1.22	1.24	1.25	1.16	1.08	1.01	0.95	0.9	0.85	0.81	0.78	0.75
4	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
5	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
6	0.5	0.35	0.2	0.1	0.1	0.2	0.75	1.25	1.4	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.4	1.25	1.1	1	0.9	0.8	0.7
7	0.19	0.09	0.06	0.05	0.09	0.22	0.86	1.84	1.86	1.41	1.24	1.2	1.32	1.44	1.45	1.59	2.03	2.08	1.51	1.06	0.74	0.62	0.61	0.44
8	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
9	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
10	0.6	0.6	0.6	0.6	0.6	0.65	0.75	0.9	1.1	1.35	1.45	1.6	1.8	1.75	1.7	1.55	1.35	1.1	0.9	0.75	0.65	0.6	0.6	0.6
11	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

Table D.15 : Hourly temporal profile of Wednesday for Turkey.

SNAP	Hour																							
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
1	0.79	0.72	0.72	0.71	0.74	0.8	0.92	1.08	1.19	1.22	1.21	1.21	1.17	1.15	1.14	1.13	1.1	1.07	1.04	1.02	1.02	1.01	0.96	0.88
2	0.38	0.36	0.36	0.36	0.37	0.5	1.19	1.53	1.57	1.56	1.35	1.16	1.07	1.06	1	0.98	0.99	1.12	1.41	1.52	1.39	1.35	1	0.42
3	0.75	0.75	0.78	0.82	0.88	0.95	1.02	1.09	1.16	1.22	1.28	1.3	1.22	1.24	1.25	1.16	1.08	1.01	0.95	0.9	0.85	0.81	0.78	0.75
4	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
5	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
6	0.5	0.35	0.2	0.1	0.1	0.2	0.75	1.25	1.4	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.4	1.25	1.1	1	0.9	0.8	0.7
7	0.19	0.09	0.06	0.05	0.09	0.22	0.86	1.84	1.86	1.41	1.24	1.2	1.32	1.44	1.45	1.59	2.03	2.08	1.51	1.06	0.74	0.62	0.61	0.44
8	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
9	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
10	0.6	0.6	0.6	0.6	0.6	0.65	0.75	0.9	1.1	1.35	1.45	1.6	1.8	1.75	1.7	1.55	1.35	1.1	0.9	0.75	0.65	0.6	0.6	0.6
11	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

Table D.16 : Hourly temporal profile of Thursday for Turkey.

SNAP	Hour																							
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
1	0.79	0.72	0.72	0.71	0.74	0.8	0.92	1.08	1.19	1.22	1.21	1.21	1.17	1.15	1.14	1.13	1.1	1.07	1.04	1.02	1.02	1.01	0.96	0.88
2	0.38	0.36	0.36	0.36	0.37	0.5	1.19	1.53	1.57	1.56	1.35	1.16	1.07	1.06	1	0.98	0.99	1.12	1.41	1.52	1.39	1.35	1	0.42
3	0.75	0.75	0.78	0.82	0.88	0.95	1.02	1.09	1.16	1.22	1.28	1.3	1.22	1.24	1.25	1.16	1.08	1.01	0.95	0.9	0.85	0.81	0.78	0.75
4	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
5	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
6	0.5	0.35	0.2	0.1	0.1	0.2	0.75	1.25	1.4	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.4	1.25	1.1	1	0.9	0.8	0.7
7	0.19	0.09	0.06	0.05	0.09	0.22	0.86	1.84	1.86	1.41	1.24	1.2	1.32	1.44	1.45	1.59	2.03	2.08	1.51	1.06	0.74	0.62	0.61	0.44
8	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
9	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
10	0.6	0.6	0.6	0.6	0.6	0.65	0.75	0.9	1.1	1.35	1.45	1.6	1.8	1.75	1.7	1.55	1.35	1.1	0.9	0.75	0.65	0.6	0.6	0.6
11	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

Table D.17 : Hourly temporal profile of Friday for Turkey.

SNAP	Hour																							
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
1	0.79	0.72	0.72	0.71	0.74	0.8	0.92	1.08	1.19	1.22	1.21	1.21	1.17	1.15	1.14	1.13	1.1	1.07	1.04	1.02	1.02	1.01	0.96	0.88
2	0.38	0.36	0.36	0.36	0.37	0.5	1.19	1.53	1.57	1.56	1.35	1.16	1.07	1.06	1	0.98	0.99	1.12	1.41	1.52	1.39	1.35	1	0.42
3	0.75	0.75	0.78	0.82	0.88	0.95	1.02	1.09	1.16	1.22	1.28	1.3	1.22	1.24	1.25	1.16	1.08	1.01	0.95	0.9	0.85	0.81	0.78	0.75
4	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
5	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
6	0.5	0.35	0.2	0.1	0.1	0.2	0.75	1.25	1.4	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.4	1.25	1.1	1	0.9	0.8	0.7
7	0.19	0.09	0.06	0.05	0.09	0.22	0.86	1.84	1.86	1.41	1.24	1.2	1.32	1.44	1.45	1.59	2.03	2.08	1.51	1.06	0.74	0.62	0.61	0.44
8	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
9	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
10	0.6	0.6	0.6	0.6	0.6	0.65	0.75	0.9	1.1	1.35	1.45	1.6	1.8	1.75	1.7	1.55	1.35	1.1	0.9	0.75	0.65	0.6	0.6	0.6
11	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

Table D.18 : Hourly temporal profile of Saturday for Turkey.

SNAP	Hour																							
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
1	0.79	0.72	0.72	0.71	0.74	0.8	0.92	1.08	1.19	1.22	1.21	1.21	1.17	1.15	1.14	1.13	1.1	1.07	1.04	1.02	1.02	1.01	0.96	0.88
2	0.38	0.36	0.36	0.36	0.37	0.5	1.19	1.53	1.57	1.56	1.35	1.16	1.07	1.06	1	0.98	0.99	1.12	1.41	1.52	1.39	1.35	1	0.42
3	0.75	0.75	0.78	0.82	0.88	0.95	1.02	1.09	1.16	1.22	1.28	1.3	1.22	1.24	1.25	1.16	1.08	1.01	0.95	0.9	0.85	0.81	0.78	0.75
4	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
5	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
6	0.5	0.35	0.2	0.1	0.1	0.2	0.75	1.25	1.4	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.4	1.25	1.1	1	0.9	0.8	0.7
7	0.60	0.55	0.50	0.51	0.58	0.74	0.92	1.15	1.33	1.43	1.46	1.44	1.39	1.37	1.36	1.29	1.25	1.19	1.09	0.97	0.83	0.73	0.69	0.63
8	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
9	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
10	0.6	0.6	0.6	0.6	0.6	0.65	0.75	0.9	1.1	1.35	1.45	1.6	1.8	1.75	1.7	1.55	1.35	1.1	0.9	0.75	0.65	0.6	0.6	0.6
11	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

Table D.19 : Hourly temporal profile of Sunday for Turkey.

SNAP	Hour																							
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
1	0.79	0.72	0.72	0.71	0.74	0.8	0.92	1.08	1.19	1.22	1.21	1.21	1.17	1.15	1.14	1.13	1.1	1.07	1.04	1.02	1.02	1.01	0.96	0.88
2	0.38	0.36	0.36	0.36	0.37	0.5	1.19	1.53	1.57	1.56	1.35	1.16	1.07	1.06	1	0.98	0.99	1.12	1.41	1.52	1.39	1.35	1	0.42
3	0.75	0.75	0.78	0.82	0.88	0.95	1.02	1.09	1.16	1.22	1.28	1.3	1.22	1.24	1.25	1.16	1.08	1.01	0.95	0.9	0.85	0.81	0.78	0.75
4	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
5	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
6	0.5	0.35	0.2	0.1	0.1	0.2	0.75	1.25	1.4	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.4	1.25	1.1	1	0.9	0.8	0.7
7	0.61	0.56	0.49	0.47	0.48	0.57	0.67	0.81	0.97	1.13	1.23	1.27	1.29	1.38	1.46	1.47	1.46	1.46	1.38	1.24	1.08	0.94	0.85	0.72
8	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
9	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
10	0.6	0.6	0.6	0.6	0.6	0.65	0.75	0.9	1.1	1.35	1.45	1.6	1.8	1.75	1.7	1.55	1.35	1.1	0.9	0.75	0.65	0.6	0.6	0.6
11	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1



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