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Contribution of Source Emissions in the Air Pollution Modeling - a WRF/Chem Case Study

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Abstract

We investigate the capability of the WRF/Chem model in the simulation of some criteria air pollutants, during a major air pollution episode between 16 and 21 December 2017. In this study, by employing the EDGAR-HTAP_v2 global emissions data in the WRF/Chem model, we evaluate the simulations of the surface mixing ratios of NO_2, SO_2, and CO. The RADM2 chemical mechanism with MADE-SORGAM aerosol scheme has been used as the chemical option of the WRF/Chem model, to simulate the meteorology-chemistry interactions. The variations of the time series of the pollutants and the comparisons of the results in Tehran with the measurement data showed that although the WRF/Chem simulations in Tehran presented considerable over-estimations, but the model's performance with regard to the time variations of the concentrations of the gaseous agents over the polluted episode is acceptable, and therefore, could be considered in the operational air quality systems. Since emission data are not available for many metropolitan areas over Iran, the HTAP_v2 global dataset could be used as the emissions data with reliable accuracy for the numerical air quality models.

Keywords: WRF/Chem; HTAP_v2 datast; Global emissions; Criteria air pollutants; Numerical modeling.

1. Introduction

Air quality modeling includes several sectors such as simulation of urban and anthropogenic pollutants, biogenic pollutants, and wildfires in the forests. Air pollution in Iran consists of two major challenges: on the one hand, massive dust storms that frequently sweep across vast regions of the country, and on the other hand, the urban air pollution, which are considered as one of the most serious environmental hazards in the megacities, particularly in Tehran. Air pollution episodes are regularly reported by many networks, such as the meteorological organization (IRIMO) and Tehran air quality control company. In Tehran, a trace of air pollution is detectable in most days. But in some cases, due to special atmospheric conditions, such as stability or inversion, this air pollution is intensified. This is the case which is discussed and analyzed in the current study using the relevant meteorological variables and indices, including static stability and planetary boundary layer height (PBLH). The WRF/Chem model (Grell et al., 2005; Fast et al., 2006; Peckham et al., 2011; Powers et al., 2016) as a coupled meteorology-chemistry model has been used in many air quality research projects. In WRF/Chem, the simulation of atmospheric chemistry and air pollution (Zhang et al., 2016; Wang et al., 2015) is carried out simultaneously (online) with the weather modeling. In an online simulation of weather/chemistry, the interaction between the atmospheric variables and air pollutants, such as the secondary effects of aerosols in the formation of clouds, can be considered during the calculation.

Mohan et al. (2018) studied the impact of several atmospheric boundary layer schemes in WRF/Chem in the simulation of PM10 and O_3 concentrations, and found logical results in temperatures lower than 40 °C and wind speed lower than 8 m/s. Using the multi resolution emission inventory for China (MEIC) (Li et al., 2017a, b), Du et al. (2020) studied the impacts from boundary layer mixing and anthropogenic emissions in the diurnal variations of surface PM2.5 concentration over East China with WRF-Chem, with a result that the simulated diurnal $PM_{2.5}$ is sensitive to the PBL schemes (PBL

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height and mixing coefficient) and vertical layer configuration in WRF-Chem. In another study (Wei et al., 2018) in Beijing, the emissions of the volatile organic compounds (VOCs) form petrochemical factories as the main source of VOCs have been analyzed. The results of this study indicate that VOCs have a significant role in the emissions of Ozone. In other words, in the areas surrounded by chemical industries, 30% decrease in the VOC emissions, leads to an average increase in O_3 by 4.7 ppb, while it shows a decrease by 2.5 ppb in the downtown of Beijing.

Emissions data have a major role in the air quality modeling. Apart from how complex is the atmospheric model, if there are considerable uncertainties and errors in the emissions data, an accurate simulation of the pollutants' concentrations cannot be expected. Several studies have been carried out in the analysis and development of emissions data. In the Henan Province of China (Liu et al., 2018), an integrated emission inventory has been provided, and the spatial and temporal variations and the back trajectories of the air pollutants have been analyzed by the WRF/Chem model, concluding that the air pollution in the downtown areas are more related to the high emissions from local sources. In addition, pollutant emissions from the adjacent provinces are the potential sources of $PM_{2.5}$ over this region.

Estimation of emissions and their variability is possible through remote-sensing and atmospheric data-assimilation. For instance, Dai et al. (2021), updated the SO_2 emission over China by assimilating the ground-based hourly SO_2 observations. They revealed that assimilating only the subsequent hourly observations can reveal the diurnal variation of the SO_2 emission, better than updating the magnitude of SO_2 emission within the 12h temporal window. Visser et al. (2019) calculated top-down NOx emissions in WRF/Chem, using the NO_2 column observations from the Ozone Monitoring Instrument (OMI) satellite sensor. In this study, the simulations with satellite-updated NOx emissions caused a reduction of the systematic bias between WRF/Chem and OMI NO_2 ($r^2 = 0.84$), as well as a reduction of the bias against independent surface NO_2 measurement by 1.1 $\mu g\ m^{-3}$ (-56%).

WRF/Chem modeling system based on global emissions data can be set operationally. Although national emissions data are supposed to give the best results for such operational systems, for those regions without national emissions, setting the operational system with global emissions is a reasonable option, with satisfactory results. Spiridonov et al. (2019) configured an air quality system over Macedonia, based on WRF/Chem with the Emission Database for Global Atmospheric Research (EDGAR) system (http://www.mnp.nl/edgar) (Olivier et al., 2005), as well as the Reanalysis of the Troposphere (RETRO) (http://retro.enes.org) (0.50 × 0.50) monthly 1960-2000 emission dataset. The modeled results implied that WRF/Chem is very sensitive to the initial meteorological conditions, grid spacing, and mobile emissions.

In this study, our attempts are focused on the application of global emissions data in urban areas. Contrary to the fact that air pollution modeling without national emissions cannot be accurate enough to be employed in operational systems, we showed that by the virtue of the advanced WRF/Chem regional simulations, and using the EDGAR-HTAP emissions data, regional air pollution modeling systems can be established with satisfactory results for urban areas. This is an important, as well as practical issue, particularly for the urban areas with high rates of pollution that do not have any local emissions data.

In this study, the application of global emissions data in air pollution modeling, with an emphasis on urban areas, has been assessed. In section 2, we introduce the WRF modeling system and its capability to be coupled with atmospheric chemistry (the so-called WRF/Chem model). Some important technical steps, regarding the WRF atmospheric modeling and ingestion of emissions data have been explained. Moreover, the EDGAR-HTAP global emissions data and its structure are discussed. Finally, some technical steps regarding the incorporation of the emissions data and the run process are summarized.

2. Materials and methods

Air quality modeling is dependent on two primary issues: simulations of the main atmospheric variables (wind speed, temperature, etc.), and provision of emissions data. Although the numerical modeling system itself has a key role in the simulations of air pollutants, the provision and accuracy of the emissions data have the same importance in air quality modeling. No matter how complex and sophisticated is a modeling system, if the emissions data are not accurate enough, model results for the simulations of the pollutants concentrations will not be reliable. This issue is more pronounced when it comes to air quality modeling over regions with lack of emissions measurement data, which is the main challenge of air quality modeling in developing and less developed countries.

2-1. Synoptic maps from ERA-Interim data

Figure 1 shows the synoptic conditions over the polluted period between 16 and 21 of December 2017. Sea surface pressure during 16 to 21 of December 2017 indicates the settling of high pressure systems from north east of Iran, which is gradually intensified by about 4 hPa, over north-west and central parts of Iran. In other words, it is increased from 1024 hPa on December 16 to 1028 hPa on December 21. Variations of surface humidity over the study period are not significant. Dew point deficit over the northwest is about 2 °C and over the central parts of Iran is about 7 °C. Furthermore, 10 m wind speed does not show considerable variation and is generally less than 10 knots.

Geopotential heights on 700 hPa show an increase from 3100 m to 3190 m during the study period (16 to 21 of December 2017), which is a considerable rise during four days. This pattern is accompanied with a cold advection, indicating an increase in atmospheric stability at 700 hPa. Moreover, wind speed is estimated about 20 to 25 knots at this layer over the study period. The vertical velocity over the north-west reaches a maximum value of 0.4 Pa/s, and in other parts of the study area, it reaches maximum value of 0.2 Pa/s, whereas from December 23, the vertical velocity shows an increase of 0.4 Pa/s. These results show that from December 21 onwards, the stable atmospheric patterns over Iran are weakening, leading to lower air pollutant concentration.

2-2. WRF/Chem modeling system

The Advanced Research WRF (ARW) dynamical core considers several approaches in atmospheric simulations, including model initialization, boundary conditions, physics options, and grid-nesting techniques in the numerical modeling (Skamarock and Klemp, 2008). Physics and planetary boundary layer (PBL) parameterizations are required for the modelling of small scale processes such as precipitation, which generally cannot be numerically solved by the model. WRF/Chem modelling system can be configured to include indirect aerosol effects in the modeling process, which can enhance the simulation of precipitation (Wang et al., 2015; Carvalho et al., 2014). This option, which is beyond the scope of this paper, is especially beneficial for the modelling of the spatio-temporal variation of gaseous concentrations in the urban areas that can from acidic particles in acid rains events.

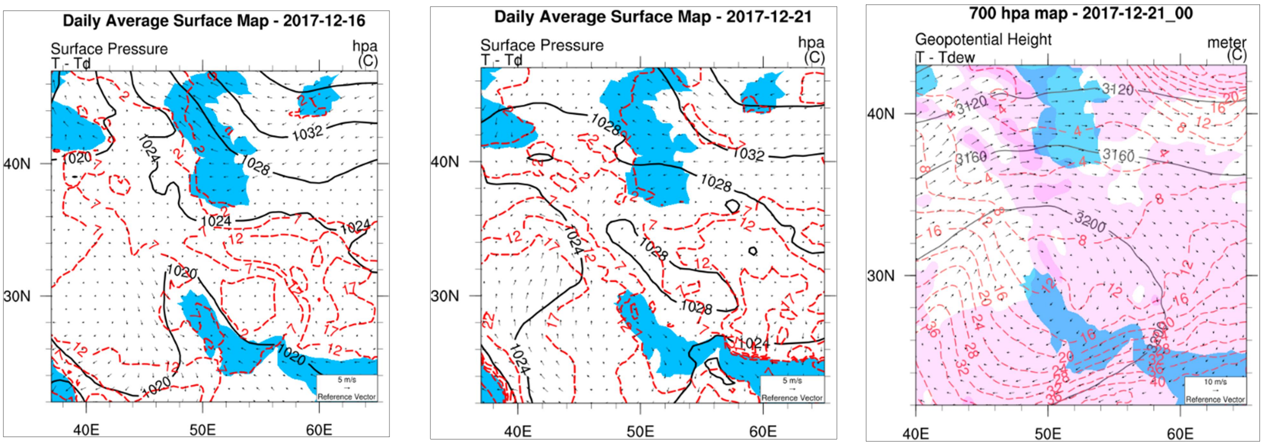


Figure 1. General weather conditions during the air pollution episode (16-21 December 2017); the pink areas are with negative vertical velocity (data from ECMWF ERA-Interim).

Figure 2 illustrates the different stages of setting up and running the model WRF/Chem for the urban air quality modeling. The run process can be divided into two stages: preparing meteorological and geographical data, and preparing and ingesting the emissions data. At the first step, using the static geographical data and the global meteorological data, the initial and boundary conditions over the model domains for the simulation time is prepared. At the second step, using a special tool (anthro_emiss or prep_chem_sources), the emissions data are extracted from the global data (Freitas et al., 2011) and interpolated over the simulation grid points. These data are ingested through the modeling process, to simulate the air pollutants trajectories and concentrations. WRF/Chem for dust modeling could be run without any emissions data. For dust simulations, the dust emissions are calculated based on some special geographical data, particularly soil erosion. In this study, since the air pollution episode was not a dust outbreak, the pollutants in the studied megacities could be mostly considered as non-dust particles, originated from the anthropogenic sources.

2-2-1. RADM2 chemical mechanism

The RADM2 (Stockwell et al., 1990) chemical option besides the MADE/SORGAM aerosol scheme (Ackermann et al., 1998) has been set to simulate the meteorology-chemistry interactions. The MADE aerosol scheme has been developed to treat aerosol effects in atmospheric models, by considering a lognormal distribution for aerosol sizes. The Regional Acid Deposition Model (RADM) is a chemical and transport scheme for the troposphere, designed to model episodic events on a time scale up to several days (Chang et al., 1987). The second generation RADM or RADM2 is part of the RADM1 model, which is incorporated into the meteorology-chemistry models, such as WRF/Chem and EURAD (Ebel et al., 1991). RADM2 is a nonlinear model, since predicted ozone, sulfate, and nitric acid concentrations are complicated functions of NOx and non-methane hydrocarbon concentrations.

2-3. Emissions data

Measuring the air pollutants emissions is a demanding task, requiring special equipment and sensors. The lack of measured emissions data is a major challenge in many urban areas. Fortunately, there are some data, providing global emissions that could be used in the regional air quality models. The HTAP_V2 emissions dataset (Janssens-Maenhout et al., 2015) with a spatial resolution of 0.1°×0.1° in geographical scale, consists of several air pollutants, such as CH_4, CO, SO_2, NOx, PM_{10}, and $PM_{2.5}$, for the years 2008 and 2010. HTAP_V2 are gridded dataset based on the reports of national emissions, which have been scientifically analyzed. The HTAP dataset involves several sectors, such as industry, transport, and residential areas. Figure 3 illustrates the HTAP_v2 global emissions data corresponding to the industry sector. Many hot spots, especially East Asia with dark blue color, represent industrial regions.

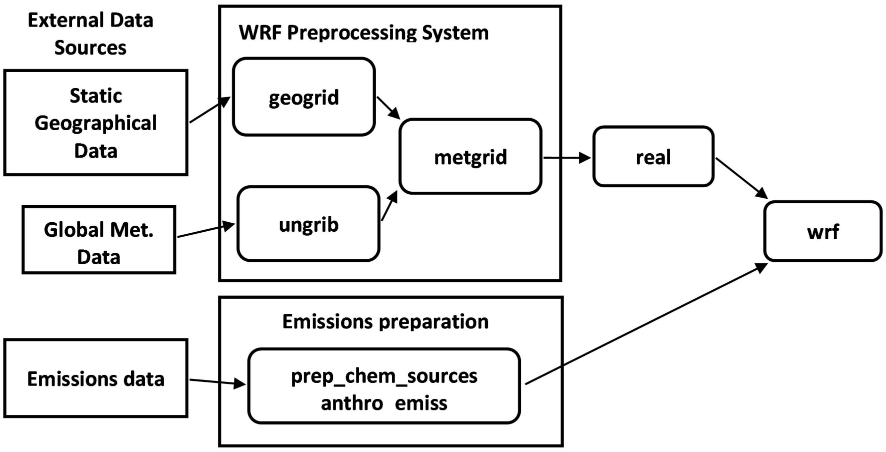


Figure 2. WRF/Chem structure in the air quality modeling.

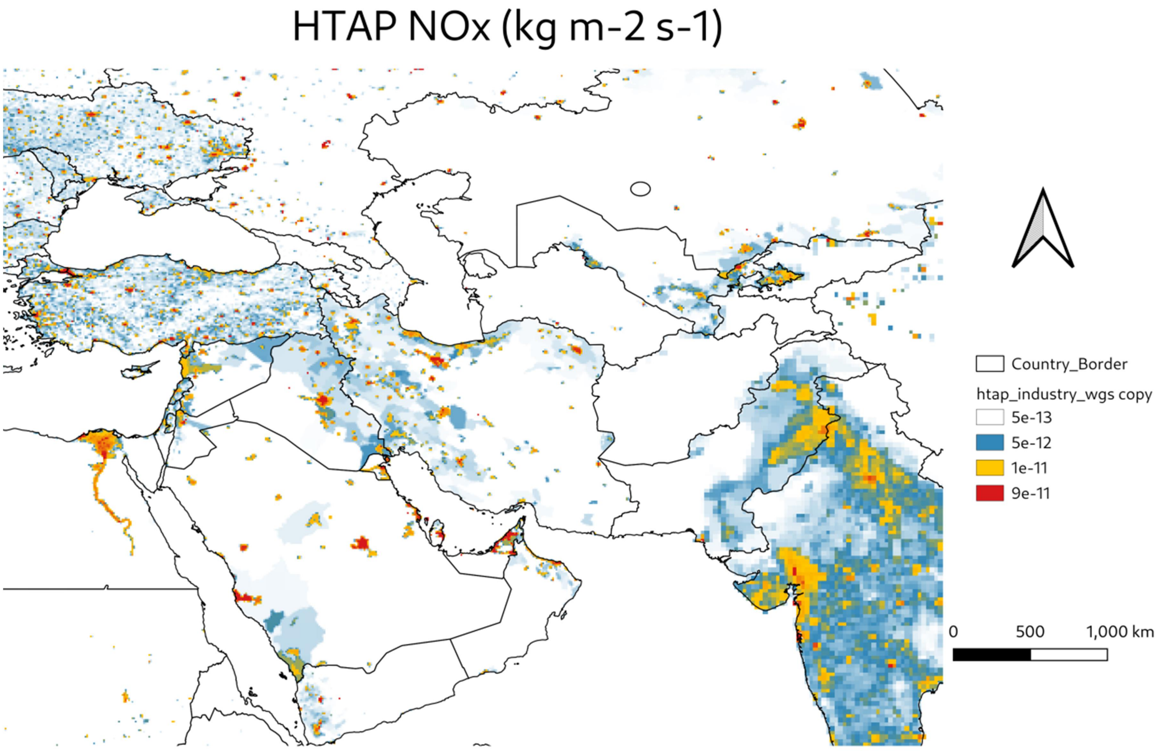


Figure 3. HTAP_v2 global emissions data from industry sector, in West Asia.

In this study, the HTAP global emissions data have been employed to identify the emissions of the gaseous air pollutants, including NO_2, SO_2, and CO, with the unit of mole/km^2/s. The second version of HTAP emissions data with the spatial resolution of 0.1°×0.1° and monthly temporal resolution, provide the emissions of several air pollutants, such as CH_4, CO, NOx, and NH_3. The HTAP emissions data incorporating several air pollution sectors, including industry, transportation, and residential areas, are based on the years 2008 and 2010 measurements, and a combination of national emissions data and satellite measurements.

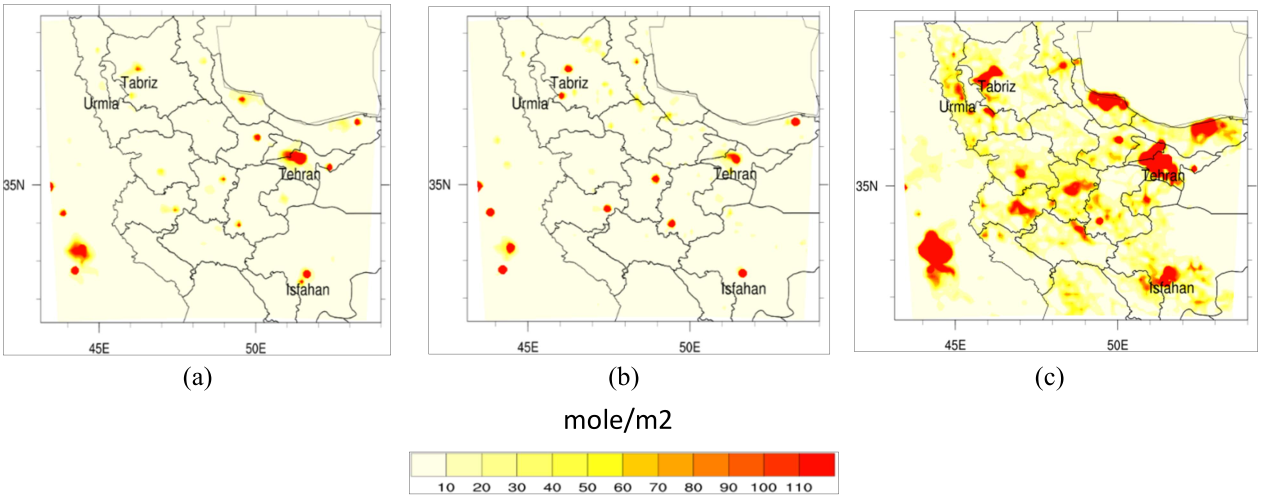

(a) (b) (c)

Figure 4. Air pollutant emissions from the HTAP_v2 global dataset for (a) NO_2, (b) SO_2, and (c) CO.

The emissions data of three air pollutants (SO_2, NO_2, and CO) have been prepared in a separate input file to be ingested in a WRF/Chem simulation for the study period, between 16 and 21 of December 2017. Figure 4 illustrates the spatial pattern of the emissions data over the WRF/Chm simulation domain. The urban areas could be noticed as hot spots with higher emission values.

2-4. OMI and AIRS Satellite data

The WRF/Chem outputs for CO and NO_2 have been compared with satellite data (AIRS and OMI data, respectively) to evaluate the model's capability in the simulation of the distribution of the pollutant concentrations. The Ozone Monitoring Instrument (OMI) (Levelt et al., 2006) is a UV and visible spectrometer designed to monitor the ozone and other atmospheric species, installed on EOS AURA satellite. OMI measures some of the criteria air pollutants defined by the US Environmental Protection Agency (EPA), including O_3, NO_2, and SO_2, with a spatial resolution of 36x48 km.

AIRS (Chahine et al., 2006) is the atmospheric infrared sounder on NASA's Aqua satellite, which gathers infrared energy emitted from Earth's surface and atmosphere globally. The AIRS data provides 3D measurements of temperature and water vapor through the atmospheric column. In this study, the average values of the OMI and AIRS (700 hpa) data during 16 and 21 December 2017 has been used to compare with the WRF/Chem's outputs.

2-5. Run process

Two nested domains with 30×30 km and 10×10 km in horizontal spatial resolutions have been set to run the WRF/Chem model. Simulation results for the sub-domain with finer spatial resolution (10×10 km) have been analyzed as the model results over the locations of Tehran, Tabriz, and Hamedan. Figure 5 illustrates the positions of the domains.

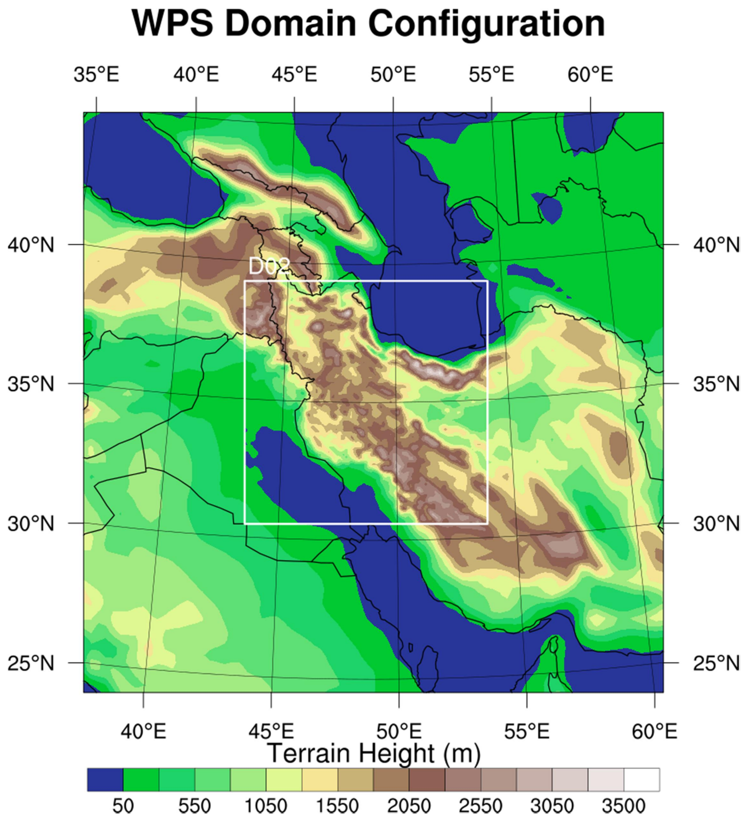


Figure 5. Model domains with spatial resolution of 30×30 km and 10×10 km, for parent domain and subdomain, respectively.

The initial steps in air pollution modeling with WRF/Chem, is not different from a regular WRF simulation. After configuring the domains of simulation by using the constant geographical data, the initial and boundary conditions must be generated by incorporating the atmospheric global data into the domains of simulations. For the current study, the ECMWF ERA-Interim data have been used in the WRF pre-processing package. After finishing the initial required steps and before running the model, the emissions data are ingested into the domain grids. Emissions data are available for the ground surface; therefore, the ingestion process is actually the interpolation of emissions data on the domain grids. Beside the "prep_chem_sources" utility for preparing the emissions data in separate files, there are other utilities such as "anthro_emiss", which can carry out the same task, but have some limitations and do not support all emissions data.

Generated emissions files can be variable through the run process; however, this is usually the case when national emissions with high temporal/spatial resolutions are available. Since EDGAR-HTAP is monthly data, it is not necessary to make multiple emissions files for a single simulation in a specific month. However, for the simulations in different months, different emissions files are required to be generated. After preparing the emission data in separate file, which include variables with emissions values for each air pollutants (NO_2, SO_2, and CO), run process is started and the emissions data are read from the files generated by "prep_chem_sources", or "anthro_emiss", and ingested in the simulation.

Some important model settings, including the microphysics and PBL physics options are summarized in Table 1. The description part has been taken from the WRF user guide, which can be downloaded for various WRF versions (https://www2.mmm.ucar.edu/wrf/users/docs/user_guide_V3/contents.html).

3. Results and discussion

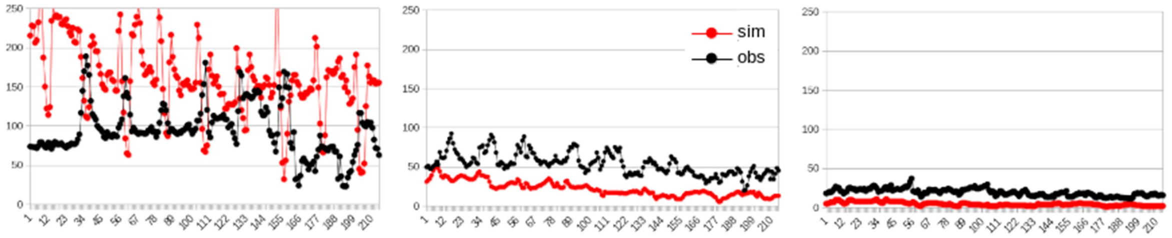
In this section, WRF/Chem's results for the selected criteria pollutants (NO_2, SO_2, and CO) are presented in forms of time-series diagrams and contour maps, and their variations, and distributions are discussed and the outputs are evaluated by comparing to station data and satellite observations. Moreover, using some primary atmospheric variables and indices, including atmospheric stability and PBLH, the model's capability in the simulations of atmospheric conditions leading to air pollution is discussed.

3-1. WRF/Chem model results

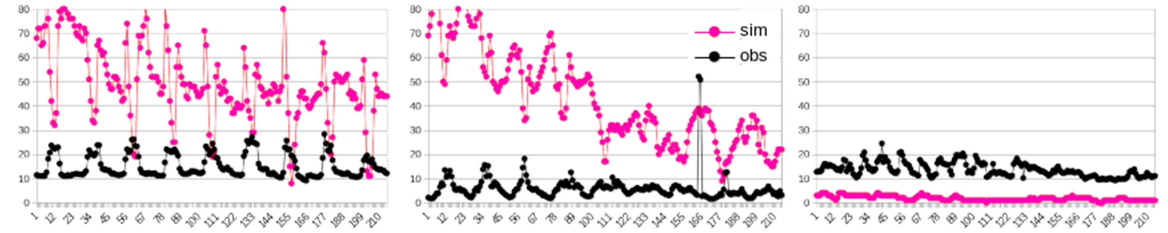
Simulation results for some major urban areas in Iran were extracted from the model's subdomain. WRF/Chem has been run for 10 days, from 14 to 23 December 2017. The first day of simulation has been ignored as the spin-up time, and the model results have been analyzed from the 15th of December.

Table 1. WRF/Chem configuration.

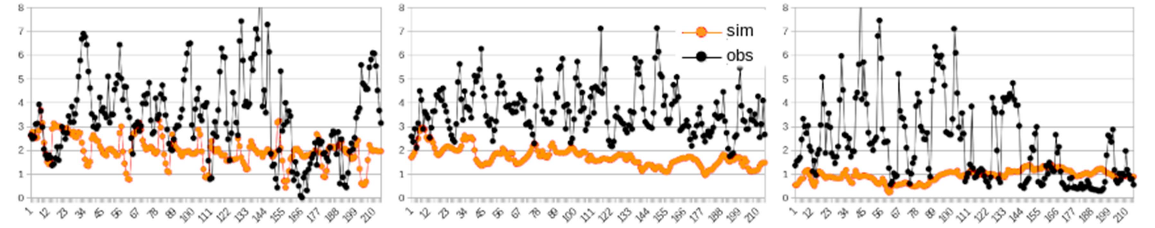
Setting	Option	Description
Microphysics	Lin et al. scheme	A sophisticated scheme that has ice, snow and graupel processes, suitable for real-data high-resolution simulations
Surface Layer	Eta similarity	Used in Eta model. Based on Monin-Obukhov with Zilitinkevich thermal roughness length and standard similarity functions from look-up tables
Planetary Boundary layer	Mellor-Yamada-Janjic scheme	Eta operational scheme. One-dimensional prognostic turbulent kinetic energy scheme with local vertical mixing
Longwave Radiation	RRTM scheme	Rapid Radiative Transfer Model. An accurate scheme using look-up tables for efficiency. Accounts for multiple bands, and microphysics species
Shortwave Radiation	Dudhia scheme	Simple downward integration allowing efficiently for clouds and clear-sky absorption and scattering



(a) NO_2 (ppb)- Tehran (b) NO_2 (ppb)- Tabriz (c) NO_2 (ppb)- Hamedan



(d) SO_2 (ppb)- Tehran (e) SO_2 (ppb)- Tabriz (f) SO_2 (ppb)- Hamedan



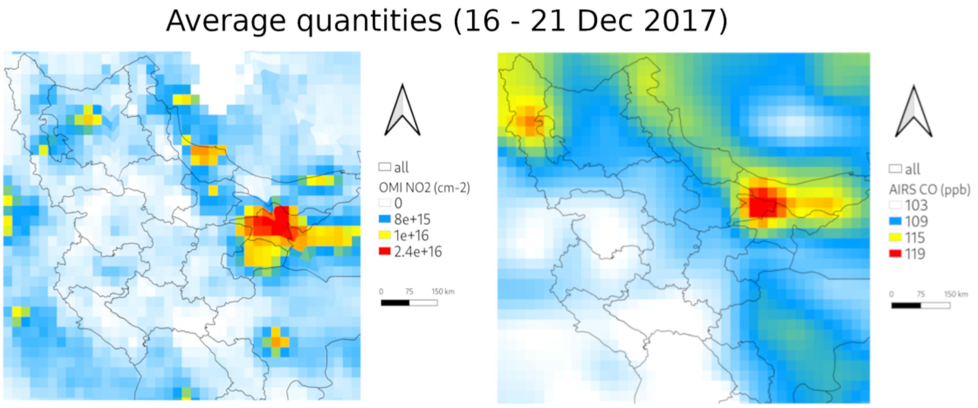
(g) CO (ppm)- Tehran (h) CO (ppm)- Tabriz (i) CO (ppm)- Hamedan

Figure 6. Time series of the WRF/Chem outputs for NO_2 for (a) Tehran, (b) Tabriz, and (c) Hamedan - SO_2 for (d) Tehran, (e) Tabriz, and (f) Hamedan - and CO for (g) Tehran (h) Tabriz, and (i) Hamedan.

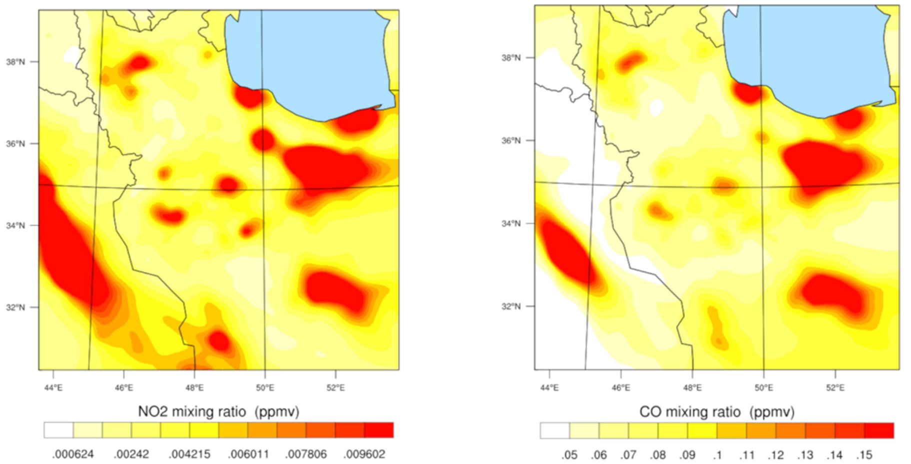
The main aim of the study was to simulate the concentrations of the gaseous air pollutants; therefore, dust modeling has been deactivated in the running process. Figure 6 shows the WRF/Chem results for SO_2, NO_2, and CO for Tehran (35.69, 51.39), Tabriz (38.10, 46.27), and Hamedan (37.55, 45.08). Figure 6 can be discussed in two ways; first, the rate of concentrations, which are proportional to the location's air quality. In other words, Tehran shows the highest pollutants concentrations, which is followed by Tabriz and Hamedan, respectively. The logical proportions of the time-series magnitude, demonstrate a convincing proof of the accuracy of the EDGAR-HTAP emissions data. The second discussion regarding Figure 6 is the trends, which slightly decrease by approaching to the end of time series (end of the air pollution period).

The difference between the magnitudes of simulation/observation concentrations can be explained due to the global emissions data used in a regional modeling, so the small scale atmospheric motions cannot be modeled in the simulation. At the end of each time series (reaching to the end of the polluted period), a decreasing trend (particularly for Tabriz and Hamedan) can be noticed, presenting a convincing performance. This result proves the satisfactory quality of the EDGAR-HTAP emissions data in regional air pollution modeling.

Figure 7 shows the WRF/Chem outputs for the average daily concentrations of NO_2, SO_2, and CO over the simulation domain. Wind fields as the main factor in the dispersion of the trace gases, play a primary role in the simulation of pollutant mixing ratios. In other words, wind fields are the main dispersing factor for the trace gases, and simulation of secondary aerosols were not among our aims. Therefore, in this study, the WRF/Chem's capability in the simulation of atmospheric variables is a key factor in air pollution modeling. Figure 7 shows a reasonable agreement between the WRF/Chem's outputs for NO_2 and CO and the observations from OMI and AIRS satellite data. Tehran, Tabriz and Isfahan are most noticeable as the hot spots of pollutanted areas, which are shown both by the model and the satellite data.



(a) Tropospheric NO_2 (OMI) (b) CO mixing ratios (AIRS)



(c) NO_2 mixing ratios (WRF/Chem) (d) CO mixing ratios (WRF/Chem)

Figure 7. Comparisons of the corresponding satellite images of (a) OMI tropospheric NO_2 and (b) AIRS CO mixing ratio with WRF/Chem outputs for the average diurnal concentrations of (c) NO_2 and (d) CO.

It should be mentioned that in our simulation, the radiation effect, modeling of secondary aerosols (needed for ozone simulations), and running with indirect effects were not used, and our aim was focused on the model's capability in the simulation of the main driving forces and chemical mechanisms in photolysis, as well as the dispersion modeling, which according to Figure 6, the output time-series of concentrations could satisfactorily show the diurnal variability in the pollutants concentrations. Considering the model's capability in the simulation of atmospheric driving factors in atmospheric dispersion, we added supplementary part to discuss these factors (stability, PBLH, and model's scores in the simulation of main atmospheric variables).

3-2. Further discussion

To further evaluate the model performance, with regard to air pollution modeling, two additional simulated variables, which have significant impact on the model results, have been analyzed.

3-2-1. Simulated static stability

Static stability is a primary variable in air pollution conditions. Atmospheric pollutants accumulate in concentration, while the atmosphere is statically stable. In other words, the more the atmosphere is stable, the more it is resistant to vertical mixing (less turbulent), and hence, the pollutants are less able to be dispersed. Stability can be formulated as below (Young, J.A.; 2003):

$$N^2 = (g/\theta_{v0})\partial\, \theta_{v0}/\partial\, z \qquad (1)$$

Also known as the Brunt–Vaisalla frequency, N is mainly determined by the vertical gradient of potential temperature.

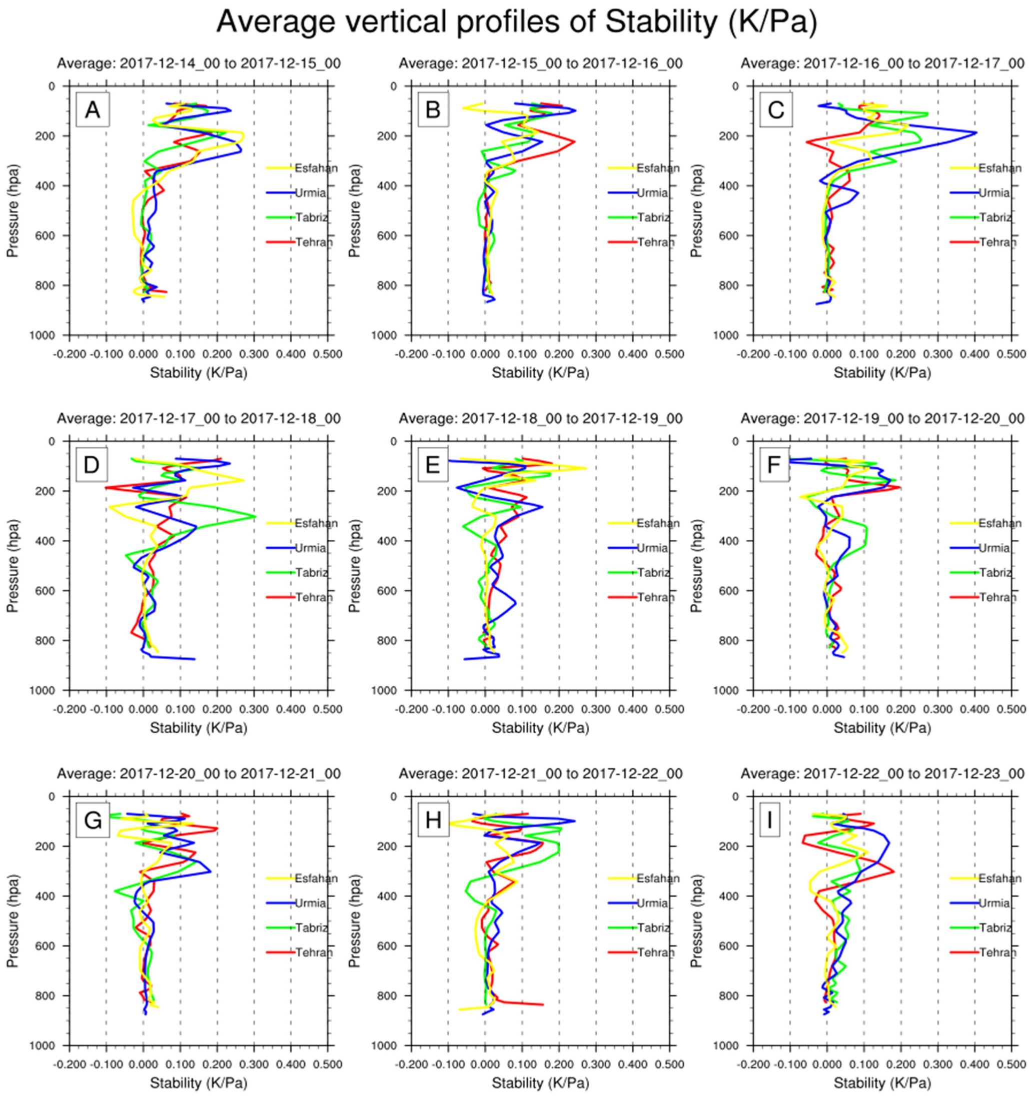


Figure 8. Vertical profiles of hourly static stability in the studied locations.

Figure 8 shows the model's capability in simulating the static stability for four locations of Tehran, Esfahan, Urmia and Tabriz, over the simulation period. From Figure 9C to Figure 9F (polluted period), a slightly more positive values for the average diurnal static stability, especially over the lower atmospheric levels, is noticeable, which makes the pollution concentrations to be higher in the study region.

3-2-2. Simulated PBLH

Planetary Boundary Layer Height (PBLH) has a significant role in the formation of air pollution episodes. Like the static stability, PBLH (with lower values) can suppress the atmospheric vertical mixing, and therefore, hinders the dilution of pollutants near the ground surface, leading to the accumulation of pollutants concentrations.

Figure 9 presents the contour maps of the average simulated PBLH over the middle of the simulation period (between 15 and 20 December, 2017). Regarding Figures 10A to 10C, an overall decrease in the average diurnal PBL heights (shallower PBL) can be noticed, leading to higher pollutants concentrations and more stable environment. Considering Figures 9D to 9F, the PBLH is showing a significant increase, which is a sign of reaching to the end of the polluted period.

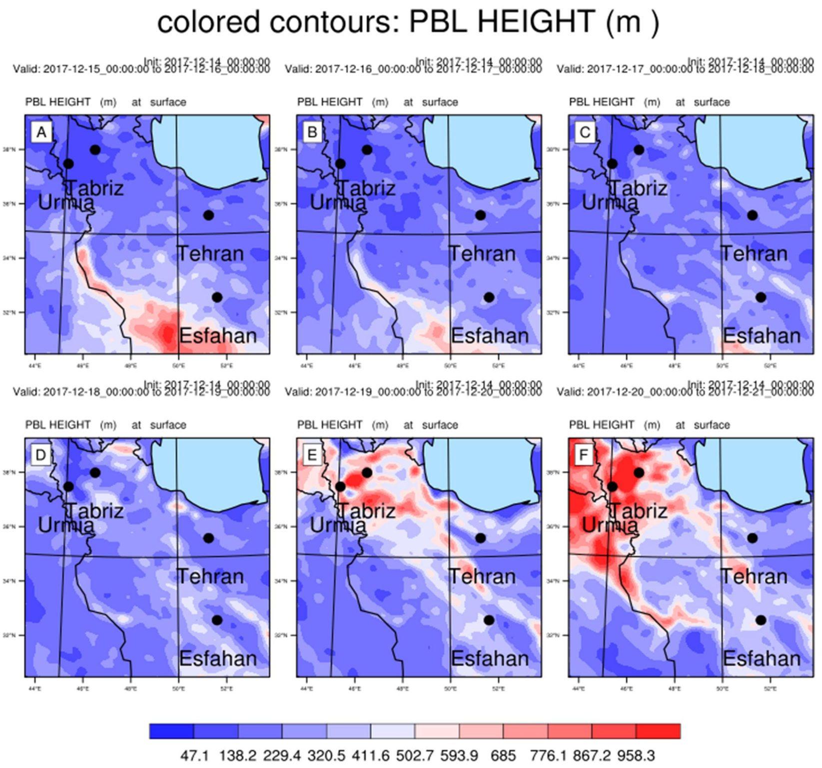
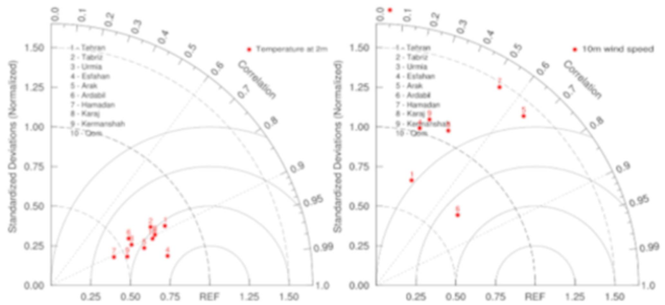


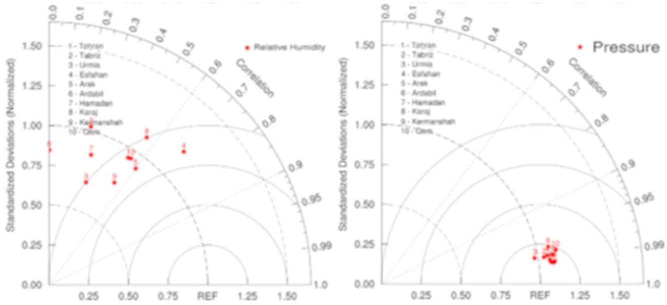
Figure 9. Average PBLH over the middle of the simulation period (between 15 and 20 December, 2017).

3-2-3. Model verification for atmospheric variables

Temperature, relative humidity, pressure, and wind speed are the primary variables among the simulated atmospheric variables by the WRF/Chem model. Using the data provided by the Iran Meteorological Organization (IRIMO), the model results for the aforementioned variables have been compared with observations, presented by Figure 10, in forms of Taylor diagrams.



(a) Temperature at 2m (b) 10m wind sped



(c) Surface relative humidity (d) Surface air pressure

Figure 10. Taylor diagrams for (a) 2m temperature, (b) 10m wind speed (c) surface relative humidity, and (d) surface pressure.

As shown in Figure 10A and Figure 10D, model's performance (RMSE and correlation) for 2m temperature and (especially) surface pressure is considerable. However, for surface relative humidity and more importantly, 10m wind speed, the model results are not accurate. This result is more significant for 10m wind speed, which affectes the turbulence inside the atmospheric boundary layer. Turbulence in the lower levels of atmospheric boundary layer is a major factor in air pollution dispersion, and requires high-resolution grid points to be accurately simulated.

4. Conclusions

Quantitative comparisons between the WRF/Chem results for air pollutants and measurements show a considerable overestimation for Tehran. Considering the increase of the pollutants over the beginning and the middle of simulation period and its decrease over the end of the simulation period, the temporal variations of the model results, especially for Tehran, present a good agreement with regard to the variations of the pollutants for this episode. Regarding the WRF/Chem results run by the EDGAR-HTAP global emissions data, these dataset are accurate enough to be used in the regional models. Therefore, for the mesoscale simulations (less than 1000 km), the HTAP global dataset provide reliable and valid emissions data, which are highly valuable, especially for those regions and urban areas without any local measured emissions data. Regarding that the WRF performance for atmospheric variables in the regional scale, it is quite satisfactory, and considering that air pollution is highly sensitive to atmospheric variables, WRF/Chem, even with global emissions, can present valid results for the air pollution simulations. However, the more accurate are the emissions data, the more accurate will be the model's results.

Air pollution modeling, especially when it comes to urban air quality with high-resolution grids, is usually computationally demanding. However, in this study, by the aim of the WRF/Chem model, we showed that, not only the urban air quality is plausible with regular hardware and model configuration, but it can even give us valuable simulations with reasonable outputs for aerosol concentrations. Considering the WRF's good performance in simulating the atmospheric variables and indices relevant to air quality (static stability and BLH), even a regular WRF modeling system without chemistry and emissions data, can be used to simulate the atmospheric conditions, which can lead to air pollution events. This task can be carried out by the post-processing of the model outputs and calculating the relevant indices.

Although the WRF/Chem model is a regional model, the model's grid points could be set with a high spatial resolution to simulate the urban air pollutants. Since the model WRF/Chem in this study has shown a good performance in estimation of the variations in the air pollutant concentrations over the urban areas, this capability could be used to set up operational air quality models for the urban areas, as an air quality warning and advisory system. If any national emissions data are provided, they could be used instead of the global emissions to reach more accurate model results in air quality modeling. Model's output for the pollutant's concentrations can be analyzed even further, by defining some threshold values with regard to air pollution (air quality index, for instance), these threshold values can be set in the operational models, to be used as warning advisory systems for the urban areas.

The next studies can be focused on the performance of the WRF/Chem outputs with global emissions, in simulating the secondary aerosols (ozone for instance), which is a required step in simulating ozone mixing ratios. Furthermore running the model with different spatial/temporal resolutions can be assessed to reach an optimum model configuration, with regard to the accuracy and simulation time. Another plan worth mentioning is the correction of the emissions data over regional scale. According to the results of this study, WRF/Chem outputs for SO_2 concentrations show considerable over-estimations for Tehran, while the diurnal variations in the time-series of the concentrations are reasonable. By adjusting the emissions data over the study area to reach more accurate simulated concentrations, it is possible to correct the emissions values for a specific area. This is quite an advanced topic in air pollution studies, which is technically called inverse modeling, and needs other scientific methods, such as advanced statistical analysis and machine learning.

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