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Study on the variation of air pollutant concentration and its formation mechanism during the COVID-19 period in Wuhan

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HIGHLIGHTS

• Quantitatively analyzed the differences of processes in PM$_{2.5}$ and O$_3$ that were affected by the COVID-19 lockdown in Wuhan.
• Analyzed process budgets to shed light on role of processes dictating increase and decrease in PM$_{2.5}$ and O$_3$ concentrations.
• O$_3$ levels were most impacted during 4–7 P.M. by emission changes associated with COVID lockdowns.

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ABSTRACT

To prevent the spread of COVID-19 (2019 novel coronavirus), from January 23 to April 8 in 2020, the highest Class 1 Response was ordered in Wuhan, requiring all residents to stay at home unless absolutely necessary. This action was implemented to cut down all unnecessary human activities, including industry, agriculture and transportation. Reducing these activities to a very low level during these hard times meant that some unprecedented naturally occurring measures of controlling emissions were executed. Ironically, however, after these measures were implemented, ozone levels increased by 43.9%. Also worthy of note, PM$_{2.5}$ decreased 31.7%, which was found by comparing the observation data in Wuhan during the epidemic from 8th Feb. to 8th Apr. in 2020 with the same periods in 2019. Utilizing CMAQ (The Community Multiscale Air Quality modeling system), this article investigated the reason for these phenomena based on four sets of numerical simulations with different schemes of emission reduction. Comparing the four sets of simulations with observation, it was deduced that the emissions should decrease to approximately 20% from the typical industrial output, and 10% from agriculture and transportation sources, attributed to the COVID-19 lockdown in Wuhan. More importantly, through the CMAQ process analysis, this study quantitatively analyzed differences of the physical and chemical processes that were affected by the COVID-19 lockdown. It then examined the differences of the COVID-19 lockdown impact and determined the physical and chemical processes between when the pollution increased and decreased, determining the most affected period of the day. As a result, this paper found that (1) PM$_{2.5}$ decreased mainly due to the reduction of emission and the contrary contribution of aerosol processes. The North-East wind was also in favor of the decreasing of PM$_{2.5}$. (2) O$_3$ increased mainly due to the slowing down of chemical consumption processes, which made the concentration change of O$_3$ pollution higher at about 4 p.m.–7 p.m. of the day, while increasing the concentration of O$_3$ at night during the COVID-19 lockdown in Wuhan. The higher O$_3$ concentration in the North-East of the main urban area also contributed to the increasing of O$_3$ with unfavorable wind direction.

1. Introduction

The COVID-19 pandemic has significantly challenged our daily life (Lonergan et al., 2020; Shereen et al., 2020). For public health, the Chinese Government ordered its highest Class 1 Response (Hubei Provincial People’s Government, 2020), which is explained in The National Emergency Plan for Public Health Emergencies (The Central People’s Government of the People’s Republic of China, 2006). With this order,
all the unnecessary transportation in and around Wuhan was shut down. All the unnecessary human activities were reduced to the minimum to reduce transmission and avoid cross-infection, including closing down local businesses, schools, colleges and universities (Zhou et al., 2020; Tang et al., 2020).

In another way, the COVID-19 lockdown in Wuhan is also an unprecedented emission mitigation measure that represents opportunities to understand air pollution in extreme cases. It has been widely accepted that PM$_{2.5}$ reduced about 40% in the lockdown conditions in Wuhan compared with the last few years (QAir, 2020; Le et al., 2020; Ministry of Ecology and Environment of the People’s Republic of China, 2020). In addition to the changes to the PM$_{2.5}$, O$_3$ was found to have about a 30% increase during the lockdown (Le et al., 2020; Ministry of Ecology and Environment of the People’s Republic of China, 2020). As for NO$_2$, Le et al. (2020) found a ~93% decrease from satellite data, while the Ministry of Ecology and Environment of the People’s Republic of China (2020) shows about a 40% decrease from the national ground station.

As described in previous studies, one of the main reasons causing the reduction in PM$_{2.5}$ might be the reduction of emissions. Vieno et al. (2015) used the EMEP4UK (UK-scale chemistry-transport model) atmospheric chemistry transport model to investigate the impact of the reductions in PM$_{2.5}$ anthropogenic emissions and found that the reductions of primary PM$_{2.5}$ emissions might be the most effective single-component control on PM$_{2.5}$. Liang et al. (2016) summarized the previous studies and concluded that industrial emission which induced secondary inorganic aerosols were the most dominant sources of PM$_{2.5}$ in urban areas in China. Many emission reduction campaigns were conducted in China to avoid air pollution, with Wang et al. (2009) and Li et al. (2011) having done a study about the emission reduction campaigns during the “Olympics Blue” in 2008. Sun et al. (2016), Huang et al. (2015) completed studies about the “APEC Blue” in 2014 and Han et al. (2016), Chu et al. (2018) and Ren et al. (2019) conducted a study about the “Parade Blue” in 2015. In these cases, China closed factories, industrial plants, construction sites, gas stations and kept vehicles off of the road in order to avoid air pollution, with the emission reduction campaigns proving to be effective. The aerosol extinction coefficient decreased to about 42.3% during the Beijing Olympic Games in 2008 compared with that in 2007. This study indicated the effectiveness of local air pollution control measures in Beijing areas under almost the same meteorological conditions (Yang et al., 2010). During the APEC periods in 2014, air pollutant concentrations had shown significant decreases over the North China Plain, especially over the Jing-Jin-Ji region, with NO$_2$ VCD (vertical column densities), AOD (aerosol optical depth), and AAOD (absorption aerosol optical depth) mostly reduced in Beijing, resulting in percentages of 47%, 34%, and 17% compared with that in the previous three years (Huang, 2015). Lin et al. (2017) found that daily PM$_{2.5}$ concentrations decreased from 98.57 $\mu g/m^2$ to 47.53 $\mu g/m^2$ during “APEC Blue”, and from 59.15 $\mu g/m^3$ to 17.07 $\mu g/m^3$ during the “Parade Blue”, using the same dates from the prior year as a reference. Recently, Wang et al. (2020) used CMAQv5.1.0 to simulate air pollution in China during January 1 to February 12, 2020 and found that the decrease of PM$_{2.5}$ in Wuhan was 30.79 $\mu g/m^3$ when the emissions of transportation, industry and agriculture decreased to 20%.

More specifically, the literature indicates that when O$_3$ production is in a NO$_x$-saturated state (NOx = NO + NO$_2$), a reduction in NO$_x$ leads to an increase in ozone and the lack of NO emissions alleviates ozone titration (Le et al., 2020; Levy et al., 2014; Atkinson et al., 2006). Surface O$_3$ is normally low at night when NO emissions are high. However, during the daytime, the significant removal of ozone via reaction (NO + O$_3$ $\rightarrow$ NO$_2$) occurs in the vicinity of large NO emission sources (Kleinman et al., 2000; Lin et al., 1998). In a recent study, the lack of NO$_x$ due to the reduction of emissions during the COVID lockdown in China led to substantial increases in O$_3$ (Huang et al., 2021). Given that PM$_{2.5}$ decreased and O$_3$ increased during the COVID-19 lockdown period in Wuhan, several questions come to mind. What are the differences and formation mechanisms of their chemical and physical processes in the atmosphere between the pandemic and those of normal years? How can we quantify the impacts of the COVID-19 lockdown on the chemical and physical processes? What are the differences of the COVID-19 lockdown impacts resulting in the pollution increasing or decreasing? How to find the most affected period of the day instigated by the COVID-19 lockdown?

To fill a literature gap in studying the influence of the COVID-19 lockdown (Huang et al., 2021; Le et al., 2020; Wang et al., 2020), this study focused on emission reduction ratio through examining partial differentiations in individual species chemical and physical processes. The study utilized the CMAQv5.3.1 (Byun and Schere, 2006) to conduct sensitivity simulation tests with four sets of emission data collected in Wuhan during the lockdown period. The study, which the individual pollutant actions show is more complicated than the previous studies, was demonstrated through implementing the PROCAN (Process Analysis Preprocessor) module (Byun and Ching, 1999). This module further revealed the quantitative effects of the individual chemical and physical processes, which instigated the mechanism for the changes in PM$_{2.5}$ and O$_3$ in Wuhan during the COVID-19 lockdown time. This paper found that PM$_{2.5}$ decreased mainly due to the reduction of emission and the positive contribution of aerosol processes. O$_3$ increased mainly due to the slowing down of chemical consumption processes, which made the concentration change of O$_3$ pollution higher at about 4 p.m.–7 p.m. of the day, and increased the concentration of O$_3$ at night during the COVID-19 lockdown in Wuhan.

2. Data and method

2.1. Data

This study used data from the 10 air quality stations in Wuhan from China National Environmental Monitoring Center. The FNL (Final Operational Global Analyses) $1^\circ \times 1^\circ$ data that was produced by the National Centers for Environmental Prediction (NCEP), was used in this simulation to initialize the WRF (The Weather Research and Forecasting) model, which can be downloaded from the website in https://rd.a.ucar.edu/datasets/ds083.2/. The MEIC (Multi-resolution Emission Inventory for China) was developed and maintained by Tsinghua University (Zhang et al., 2009), which can be downloaded from this website in https://meicmodel.org.

3. Method

In this study, a WRF-CMAQ modeling system was applied to simulate the pollution. The Weather Research and Forecasting (WRF) Model was developed at the National Center for Atmospheric Research (NCAR), which is operated by the University Corporation for Atmospheric Research (UCAR) (Chen et al., 2007). The WRFv3.7.1 was used to generate the meteorological background for air quality simulation. The Community Multiscale Air Quality (CMAQ) modeling system is an active open-source development project of the U.S. EPA that consists of a suite of programs for conducting air quality model simulations (United States Environmental Protection Agency, 2020; Byun and Schere, 2006; Pye et al., 2017; Fahey et al., 2017). The CMAQv5.3.1 was used to simulate the spatial distribution and temporal variation of pollution within the study region from Dec. 13, 2019 to Jan. 15, 2020 and from Feb. 5, 2020 to Apr. 8, 2020. A twenty-days gap from 15th Jan. to Feb. 5, 2020, around Jan. 23, 2020 when the lockdown occurred, was left to better analyze the influence of the lockdown.

The PROCAN (Process Analysis Preprocessor) module was implemented in CMAQ by Byun and Ching (1999) which is an accounting system that tracks the quantitative effects of the individual chemical and physical processes, which were combined to explain the predicted hourly species concentrations from a simulation. The PROCAN module helped calculate integrated process rates and integrated reaction rates, which can then be used for diagnosing the physical and chemical
behavior of these pollution processes. PROCAN has two components: Integrated Process Rate (IPR) analysis, and Integrated Reaction Rate (IRR) analysis, IPR was mainly used in this study.

The detailed WRF-CMAQ model configurations can be found in Table 1(a) and Table 1(b). The model simulation domain and topography height are shown in Fig. 1. The scheme we used to calculate PM$_{2.5}$ followed the CMAQv5.3.1 mechanism cb6r3 ae7 aq rules, can be found at https://github.com/USEPA/CMAQ/blob/master/CCTM/src/MECHs/cb6r3 ae7 aq/SpecDef cb6r3 ae7 aq.txt. There are 9 p.m. chemical or physical processes assigned by PROCAN, including HADV(horizontal advection), ZADV(vertical advection), HDFI(horizontal diffusion), VDFI(vertical diffusion), DDEP(dry deposition of species), CLDS(change due to cloud processes; includes aqueous reaction and removal by clouds and rain), AERO(change due to aerosol processes), CHEM(net sum of all chemical processes for species over output step) and EMIS(emissions contribution to concentration). The CHEM of PM$_{2.5}$ process analysis in the CMAQ model represents the heterogeneous reactions. The aerosol species involved in reactions in the mechanism definition file are listed here: https://github.com/USEPA/CMAQ/blob/master/CCTM/src/gas/ebi_cb6r3_ae7 aq/Mech cb6r3 ae7 aq.def. The production and loss of each of these reactions can be found in https://github.com/USEPA/CMAQ/blob/master/CCTM/src/MECHs/cb6r3 ae7 aq/SpecDef cb6r3 ae7 aq.txt.

There are seven O$_3$ chemical or physical processes signed by PROCAN, including HADV, ZADV, HDFI, VDFI, DDEP, CLDS, CHEM.

### 4. Observation analysis and model assessment

#### 4.1. Observation analysis

Literature was reviewed to report the studies on the behavior of air pollution when the lockdowns were implemented (Table 2). Please note that all the observation data came from the national ground station except no.6, which used the data from TROPOMI (The Tropospheric Monitoring Instrument). As shown in Table 2, these studies reached a consensus that PM$_{2.5}$ reduced 50%-50% in the lockdown conditions. Compared with the preceding years, in contrast to the changes to the PM$_{2.5}$, Le et al. (2020) and Ministry of Ecology and Environment of the People’s Republic of China (2020) found an approximately 30% increase in O$_3$ during the lockdown. As for NO$_2$, Le et al. (2020) found a ~93% decrease using the satellite, and other reports (Ministry of Ecology and Environment of the People’s Republic of China, 2020) which show about a 40% decrease from the national ground station.

In this paper, the observations of ten air quality stations average over space and time were compared in Wuhan from the China National Environmental Monitoring Center. Considering that there must have been some changes in emissions between 2019 and 2020 in Wuhan, we separated the observations to four time periods. Then the observations periods: Dec. 15, 2018 to 15th; Jan. 2019 and Feb. 08, 2019; Apr. 08, 2019 were used to do comparative analysis. The observations from Dec.

| Table 1(a) | WRF model configurations. |
|------------|--------------------------|
| **Model**  | **Vertical resolution**   |
| WRFv3.7.1  | 33 vertical levels        |
| Microphysics scheme | WSM 3-class simple ice scheme |
| Boundary layer scheme | YSU scheme |
| Surface layer scheme | MM5 scheme |
| Land-surface scheme | Unified Noah land-surface model |
| Longwave radiation scheme | rerm scheme |
| Shortwave radiation scheme | Dudhia scheme |
| Grid-nudging fdda | on |
| Domain center | 31.0°N,112.5°E |
| Domain id | 1 2 3 |
| Domain size | 57 × 57 91 × 67 64 × 70 |
| Starting L-indexes from the parent domain | (13,19) (57,13) |
| Horizontal resolution | 27 km 9 km 3 km |

### Table 1(b)

CMAQ model configurations.

| CMAQv5.3.1 | Horizontal advection | Yamo |
|------------|----------------------|-----|
| Vertical advection | WRF |
| Horizontal diffusion | Multiscale |
| Vertical diffusion | ACM2 |
| Deposition | M3Dry |
| Chemistry solver | EBI |
| Aerosol module | AERO7 |
| Cloud module | ACM |
| Mechanism | cb6r3 ae7 aq |

Domain id | 1 2 3 |
Domain size | 54 × 54 93 × 93 61 × 67 |

15, 2019 to Jan. 15, 2020 were considered, however, as there was no emission influence from COVID-19 lockdown which had not yet begun, we only noted the differences between 2020 and 2019. For the other observation periods, were reviewed through the lens that there was causality from the COVID-19 lockdown compared to the observations in the same period in 2019. Table 3 shows the differences of PM$_{2.5}$, PM$_{10}$(inhalable particles), the ratio of PM$_{2.5}$/PM$_{10}$, O$_3$ and NO$_2$ between these 4 time periods. The calculate method is used as follows:

$$D = \frac{\sum_{Data1}^{Data2} - \sum_{Data1}^{Data2}}{\sum_{Data1}^{Data2}} \times 100\%$$ (1)

where Data1, Data2 represents the observations (PM$_{2.5}$, PM$_{10}$, the ratio of PM$_{2.5}$/PM$_{10}$, O$_3$ and NO$_2$) from different time periods, N$_1$, N$_2$ represents the number of samples in Data1, Data2.

Table 3 shows the differences of observations, A1 represents the differences of the air pollutant concentration during the COVID-19 lockdown in 2020 and the same time period in 2019. A2 represented the differences before the COVID-19 lockdown in 2020 and the same time period in 2019. B1 represented the differences before and during the COVID-19 lockdown in 2020. B2 represented the differences of the same time period as B1 in 2019. PM$_{2.5}$ decreased 31.7% from Feb. 08, 2020 to Apr. 08, 2020 compared with 2019, and O$_3$ increased 43.9%, NO$_2$ decreased 51.8%. The concentration of PM$_{2.5}$, PM$_{10}$ and NO$_2$ were lower in lockdown time period A2 than before the lockdown time period A1, meanwhile O$_3$ was higher. The results above show that the lockdown in Wuhan had a great influence on air pollution. Compared with B1 and B2, it’s clear that PM$_{2.5}$ and PM$_{10}$ had a downward trend from December to April, and it’s going down more in 2020. O$_3$ continually had an upward trend from December to April, but it’s going up much more in 2020. NO$_2$ should not have changed much from December to April, but it decreased 53.1% in 2020. Our results are in alignment with the previous studies that PM$_{2.5}$ reduced 30%-50%. Beyond that, O$_3$ in our results increased 43.9%, much more than previous studies. The reasons might be that our observation periods lasted much longer until the lockdown was over in Wuhan. The results of observations show that the influence to O$_3$ of the lockdown in Wuhan was more significant when the concentration of O$_3$ is higher. There is an upward trend of O$_3$ from February to April in both 2019 and 2020, with the concentration of O$_3$ being higher in April compared to February, therefore there is a larger inferred increase in O$_3$ levels when a longer observational period was compared.

Fig. 2 shows the concentrations of the four species pollutants from December 2018–April 2019 and December 2019–April 2020(considering that 2020 is a leap year, we used the Julian date here). It is clear that PM$_{2.5}$ and PM$_{10}$ had a continuing downward trend and O$_3$ had a continuing upward trend from December to April in both 2019 and 2020. The concentration of PM$_{2.5}$, PM$_{10}$ and NO$_2$ was lower in 2020.
after February. Meanwhile the concentration of O$_3$ was much higher.

4.2. Model assessment

In order to assess the performance of the CMAQ simulation and make this study more convincing, the Eva experiment scenario was carried out to simulate the pollution from Dec. 15, 2019 to Jan. 15, 2020, before the COVID-19 lockdown. This experiment used an adjusted anthropogenic emission inventory that is based on MEIC 2016. It was multiplied by coefficients compared with observations to be an alternative solution when the real-time emission inventory is unavailable. The simulated pollutants concentrations of the Eva experiment were compared to the observations of the ten air quality stations. We cannot directly evaluate our simulation during the COVID-19 lockdown in Wuhan because we cannot get the accurate emission inventory during that time. Therefore, the Eva experiment was used to evaluate the simulation of the CMAQ model and find out the suitable emission inventory, which confirmed that the simulation presented a reliable performance before the COVID-19 lockdown in Wuhan. The Emission Control module in CMAQv5.3.1 was used here to adjust the emission inventories in 2020. First of all, NO$_x$ and SO$_2$ was adjusted in the emission inventory and compared to the simulation results with the observation of NO$_2$ and SO$_2$ (Formula 2~5 were used here).Then, the total amount of VOC and PM$_{2.5}$ was adjusted.

Table S1 listed the adjust ratios and Table S2 listed the performance of EVA0 (without adjustment) and EVA6 (the emission inventory we used in the following paper) simulation from Nov. 15, 2019 to Jan. 14, 2020 compared with the observation in the average of the ten stations. The correlation coefficient (COR), root mean squared error (RMSE), normalized mean bias (NMB) and normalized mean error (NME) were calculated as follows:

\[
\text{COR} = \frac{\text{Cov}(C_m, C_0)}{\sqrt{D(C_m)}\sqrt{D(C_0)}}
\]

\[
\text{RMSE} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (C_m - C_0)^2}
\]

\[
\text{NMB} = \frac{\sum_{i=1}^{N} (C_m - C_0)}{\sum_{i=1}^{N} C_0} \times 100\%
\]

\[
\text{NME} = \frac{\sum_{i=1}^{N} |C_m - C_0|}{\sum_{i=1}^{N} C_0} \times 100\%
\]

where $C_m$ is the simulated concentration, $C_0$ is the observed data, $N$ represents the number of samples, Cov($x$) means the covariation of $x$ and $D(x)$ means the variance of $x$. 

All the data in this study we simulated by the WRF-CMAQ model was in the surface layer and analyzed by the daily average of the ten stations’
in Wuhan. Table 4 shows the detailed model assessment. Fig. 3 compared the observation and simulation of the Eva experiment of PM$_{2.5}$, PM$_{10}$, O$_3$ and NO$_2$ from Dec. 15, 2019 to Jan. 15, 2020. Compared with the observations, our simulation presented a strong performance.

5. Simulation and results analysis

5.1. The average characteristics of meteorological factors during the COVID-19 lockdown

Fig. 4 shows the average temperature, sea level pressure and relative humidity with wind in Wuhan from Feb. 08, 2020 to Apr. 08, 2020 simulated using CMAQ model. The average wind direction during the COVID-19 lockdown was from North-East to South-West. The temperature was approximately 12$^\circ$C in the main urban area of Wuhan, and the temperature was lower where the surface is water (including the Yangtze River, Hanjiang River and lakes in Wuhan). The sea level pressure was approximately 1020.2hpa in the main urban area of Wuhan. The relative humidity was approximately 67% in the main urban area of Wuhan, and was higher where the surface is water.

5.2. Simulation schemes and results for emission control

5.2.1. Simulation schemes for emission control

In order to investigate the greatest possible emissions reduction ratio caused by the COVID-19 lockdown, Eva and the other four simulation scenarios were performed and compared. As seen in Table 5, the Base (stand for baseline) experiment was regarded as the benchmark experiment, and Exp1 (stand for experiment 1), Exp2 (stand for experiment 2), Exp3 (stand for experiment 3) were regarded as the sensitivity experiments with different decreasing ratios in different emission categories. The MEIC emission inventory was used here and the ratios of PM$_{2.5}$, PM$_{10}$, NO$_X$, and VOC in MEIC emission inventory can be found in Fig. S1.

First, the Base experiment scenario used the same emission inventory as the Eva experiment in section 3.2 but simulated the time period in COVID-19 lockdown from Feb. 8, 2020 to Apr. 8, 2020, assuming that COVID-19 lockdown had no effect on the emissions in Wuhan. As seen in Fig. 5, the concentration of PM$_{2.5}$, PM$_{10}$, and NO$_2$ was much higher than observation, meanwhile the concentration of O$_3$ was much lower. Then, Exp1 was carried out and the emissions were decreased to 50% in agriculture, industry and transportation in Wuhan compared with the Base experiment. Considering that with the highest Class 1 Response, all the unnecessary transportation were shut down and all the unnecessary human activities were reduced to the minimum, including closing down
local business, schools, colleges, universities, restricting the movement of people (Hubei Provincial People’s Government, 2020) and carrying out agricultural production in different periods and batches (Agricultural and rural Bureau of Wuhan, 2020). The results in Fig. 5 shows that the decreasing ratio of agriculture, industry and transportation was still low.

Next, Exp2 was carried out, the emissions were decreased to 20% in agriculture, industry and transportation in Wuhan compared with the Base experiment. It is obvious that the concentration of PM$_{2.5}$ and PM$_{10}$ was similar to observation, but the concentration of NO$_2$ was still a little high, while O$_3$ was still a little low. Wang et al. (2020) did the similar experiment but cut the emissions in Hubei.
Finally, in order to get a better performance in simulating $O_3$, Exp3 was carried out and the emissions were decreased to 20% in industry and 10% in transportation and agriculture in Wuhan compared with the Base experiment. Considering that $PM_{2.5}$ and $PM_{10}$ were well simulated and the differences of ratios in the MEIC emission inventory between $PM_{2.5}$, $PM_{10}$ and $NO_2$ mainly came from transportation and agriculture, Exp3 cut more in transportation and agriculture compared with Exp2.

The results of emission control experiments demonstrated that Exp3 had the best performance on both $PM_{2.5}$ and $O_3$. The COR, RMSE, NMB and NME of $PM_{2.5}$ were 0.28, 17.07(ug/m$^3$), 1.9% and 38.1%. The COR, RMSE, NMB and NME of $O_3$ were 0.62, 14.45(ug/m$^3$), −7.1% and 18.1% compared with observation. Our results were better than the previous study (Wang et al., 2020). As the results show, Exp3 presented great performance in simulating $PM_{2.5}$ and $O_3$ during the COVID-19 lockdown in Wuhan. Therefore, in our study, the greatest possible emissions were decreased to 20% in industry and 10% in agriculture and transportation during the COVID-19 lockdown period compared with the emissions before the lockdown period in Wuhan.

5.2.2. Variety characteristics of pollutant concentration for emission control

The horizontal distribution of the average simulated $PM_{2.5}$, $PM_{10}$, $O_3$, $O_2$ and $NO_2$ concentration from Feb. 08, 2020 to Apr. 08, 2020 in Wuhan are represented in Fig. 6(c), (f), Fig. 6(i), (o). The results reflect that the COVID-19 lockdown increased the pollution more in urban areas in Wuhan. The spatial and concentration differences of $O_3$ and $O_2$-8H revealed that the COVID-19 lockdown increased more on the low level of $O_3$ in the urban area of Wuhan. As the max 8-h average $O_3$ usually occurs in the afternoon of the day, and the low level of $O_3$ always occurs at night, it can be deduced that COVID-19 had more influence on the low level of $O_3$ at night. The further analysis was carried out in section 4.2.5.

5.3. Formation mechanism study baselined on processes analysis

5.3.1. Formula of processes analysis

In order to find out the formation mechanism that caused significant changes in $PM_{2.5}$ and $O_3$ during the lockdown time period, the Process Analysis module was used in CMAQv5.3.1. Formula 6~9 shows how to calculate the concentration of $PM_{2.5}$ and $O_3$ using process analysis. Table S3 shows the species index used in process analysis of $PM_{2.5}$ and $O_3$.

\[
CH_{A_{d}} = \sum_{r=24(d-1)}^{24} CH_{A_{r}}
\]

\[
C_{d} = \frac{\sum_{r=24(d-1)}^{24} \sum_{t=24(r-1)}^{24} C_{t} + \sum_{r=24(d-1)}^{24} \sum_{t=24(r-1)}^{24} CH_{A_{r}}}{24}
\]

where $CH_{A_{r}}$ means the total concentration change of all processes in hour $t$, $P_{process}$ means the change due to process in hour $t$, $CH_{A_{d}}$ means the total daily concentration change of all processes in day $d$, $C_{d}$ means the concentration of $PM_{2.5}$ or $O_3$ in hour $t$, $C_{d}$ means the daily average concentration of $PM_{2.5}$ or $O_3$.

5.3.2. Daily average processes analysis

Fig. 7 shows the daily average process analysis of $PM_{2.5}$ and $O_3$ of Base and Exp3. As declared in section 2.2, for example, ZADV PM$_{2.5}$ means the daily summation of $PM_{2.5}$ changes due to vertical advection in every hour, whereas, $CHA_{d}$ means the daily change of $PM_{2.5}$, which is the summation of each hour and each process, where $PM_{2.5}$ means the daily average $PM_{2.5}$. It should be noted that the hourly concentration of $PM_{2.5}$ is equal to the summation of the initial concentration and changes of all the processes in this hour, which can be seen in Fig. S2.

As for $PM_{2.5}$, it’s clear that emissions contributions always play an important role in increasing the concentration (Vieno et al., 2015) and had a stable performance during the whole simulation. Vertical diffusion, horizontal advection and vertical advection dominated the decreasing of $PM_{2.5}$, and it is clear that pollution always occurs while VIFD or HADV slows down (Hua et al., 2016). ZADV often had the
Fig. 6. The averaged simulated concentration horizontal distribution during Feb. 08, 2020 to Apr. 08, 2020. PM$_{2.5}$ of Base (a), Exp3 (b) and differences (c). PM$_{10}$ of Base (d), Exp3 (e) and differences (f). O$_3$ of Base (g), Exp3 (h) and differences (i). O$_3$–8H of Base (j), Exp3 (k) and differences (l). NO$_2$ of Base (m), Exp3 (n) and differences (o). The differences were defined as Exp3 minus Base. The vector indicate wind, the black points means the location of 10 air quality stations.
opposite tendency compared with VDIF and HADV, and it influenced much more in Exp3 compared to Base. Aerosol processes increased pollution in the Base experiment, but on the contrary, reduced the pollution in Exp3 on average, and AERO was lower on the decreasing time of PM$_{2.5}$ and even reduced the pollution in Exp3. HDIF, DDEP, CLDS and CHEM gave a little contribution to PM$_{2.5}$. HDIF decreased the concentration a little while PM$_{2.5}$ increased and almost equal 0 while PM$_{2.5}$ decreased. The DDEP was higher, though it’s similar in the Base
and Exp3. CLDS is always equal to 0, but it decreased the concentration while there was rain or high humidity. The CHEM always increased the concentration and higher while PM$_{2.5}$ increased, and it’s similar in the Base and Exp3. The CHEM of PM$_{2.5}$ is connected with heterogeneous reactions. The heterogeneous reactions can increase the concentration of PM$_{2.5}$.

Comparing Exp3 with the Base experiment, there is a conspicuous decrease in EMIS contributions that then lead to the decreasing of all processes. Under the influence of all the decreasing processes, the concentration of PM$_{2.5}$ stayed low during the lockdown in Wuhan.

As for other findings of note, in terms of O$_3$, vertical diffusion and horizontal advection dominated the increase of O$_3$ while the chemical processes dominated the decrease, as Hgreghe et al. (2018) and Tzella (1983) described in their studies. CHEM always had the similar tendency but had an opposite contribution compared with the summation of VDIF and HADV. Also, dry deposition always decreased the concentration of O$_3$. Strikingly, the cloud processes and horizontal diffusion gave little contribution. As seen in Fig. 7, the concentration change of O$_3$ mainly connects with the summation of HADV, VDIF and CHEM processes. However, compared with the Base experiment, although the emissions were cut down in Exp3, the concentration of O$_3$ was higher. It is important to note that the results were disproportionate in the decreasing CHEM and increasing HADV and VDIF.

5.3.3. Total contribution of each process

In order to quantify the impacts of the COVID-19 lockdown on the chemical and physical processes, analysis was conducted to examine the total contribution of each process for PM$_{2.5}$ and O$_3$ during Feb. 08, 2020 to Apr. 08, 2020, including concentration changes and their proportion as summarized in Table 6. TOT means the total concentration contribution of all the processes. The proportion of each process were calculated as:

$$S_{jt} = \sum_{j=1}^{n} C_{jt}$$

(10)

$$P_{jt} = \frac{S_{jt}}{\sum_{j=1}^{n} S_{jt}}$$

(11)

where $C_{jt}$ means the changes due to process $j$ in hour $t$, and $S_{jt}$ means the sum of concentration changes of process $j$ in hour $t$ from $t=1$ to $t$.

while $P_{jt}$ means the proportion of process $j$ in time $t$.

The total contribution of each process for PM$_{2.5}$ in Base, Exp3, as well as the differences between Exp3 and Base (Exp3-Base), and the decline ratio from Base to Exp3(Exp3/Base) were shown in Table 6(a). The summation of all the processes, demonstrating the differences of concentration between the first hour and last hour in the simulation, was 124 μg/m$^3$ in Base, 50 μg/m$^3$ in Exp3. The difference was 32.5 μg/m$^3$ in observation, with Exp3 much closer to the observation comparatively to Base, so Exp3 can better reflect the authentic situation for PM$_{2.5}$.

The proportion of each process in the differences between Exp3 and Base (Exp3-Base) shows us that EMIS and AERO dominate the decreasing changes, attributed to the COVID-19 lockdown, and VDIF, HADV dominate the increasing changes. The data indicated significant differences in each process as follows; EMIS is a dominant physical increasing process and accounts for approximately 44% of the contribution for all the processes in Base and 50% in Exp3. The changes attributed to the COVID-19 lockdown were about 42%. AERO increased pollution (6%) in the Base experiment, but on the contrary reduced the pollution (−2%) in the Exp3. The changes attributed to the COVID-19 lockdown were about −12%, which can be explained through analysis of the condensation processes that changed aerosol species in different emission levels (Zhang, 2017). VDIF is a dominant physical decreasing process and accounts for approximately 20% of the contribution of all the processes in Base and 23% in Exp3, with the changes attributed to the COVID-19 lockdown being about 43%. HADV also contributed significantly and accounts for approximately 22% of the contribution of all the processes, including 13% in Exp3, with the changes attributed to the COVID-19 lockdown being about 21%.

In our simulation, we conclude that the PM$_{2.5}$ reduced during the COVID-19 lockdown period in Wuhan because of the contributions of EMIS and AERO decreased more than HADV and VDIF. The contribution of EMIS decreased to 42%, which always increased the concentration. And AERO had an opposite trend from increasing concentration to decreasing concentration and changed to −12%. HADV and VDIF decreased to 21% and 43% respectfully, which always decreased the concentration.

The total contribution of each process for O$_3$ in Base, Exp3, the differences between Exp3 and Base (Exp3-Base), as well as the decline ratio from Base to Exp3(Exp3/Base) were shown in Table 6(b). The summation of all the processes, demonstrated by the differences of concentration between the first hour and last hour in the simulation was 5.8 μg/m$^3$ in Base, 21.4 μg/m$^3$ in Exp3. The difference was 19.2 μg/m$^3$ in

| $a$.PM$_{2.5}$(μg/m$^3$) | TOT | ZADV | HADV | HDIF | VDIF | EMIS | DDEP | CLDS | CHEM | AERO |
|------------------------|-----|------|------|------|------|------|------|------|------|------|
| Base 123.5             | −5511 | −19132 | −36 | −16860 | 37341 | −1171 | −21 | 71 | 5442 |
| Exp3 50.5              | −6% | −22% | 0% | −20% | 44% | −1% | 0% | 0% | 6% |
| Exp3-Base −74.0        | −8% | −13% | 0% | −23% | 50% | −2% | −1% | 0% | −2% |
| Exp3/Base              | 5% | 27% | 0% | 17% | −38% | 1% | −1% | 0% | −11% |

| $b$.O$_3$(μg/m$^3$) | TOT | CHEM | DDEP | CLDS | ZADV | HADV | HDIF | VDIF |
|---------------------|-----|------|------|------|------|------|------|------|
| Base 5.8            | −32282 | −3573 | −380 | 2259 | 9547 | 33 | 24402 |
| Exp3 21.4           | −45% | −5% | −1% | 3% | 13% | 0% | 34% |
| Exp3-Base 15.5      | −34% | −15% | 0% | 3% | 16% | 0% | 32% |
| Exp3/Base           | 49% | −4% | 1% | −3% | −10% | 0% | −33% |

Table 6
Total contribution of each process in the average over 10 stations in Wuhan from Feb. 08, 2020 to Apr. 08, 2020 (a. PM$_{2.5}$, b. O$_3$). (The symbol + means the tendency that increase the concentration, − means the tendency that decrease the concentration.)
observation, so Exp3 better reflects the real situation for $O_3$.

The proportion of each process in the differences between Exp3 and Base (Exp3-Base) shows that VDIF and HADV dominate the decreasing changes, while CHEM dominates the increasing changes. The data indicated significant differences in each process as follows; VDIF is a dominant physical increasing process and accounts for approximately 34% of all the processes in Base and 32% in Exp3, as the changes attributed to the COVID-19 lockdown is about 45%. HADV also contributed significantly and accounts for approximately 13% of all the processes in Base and 16% in Exp3, with the changes attributed to the COVID-19 lockdown about 57%. CHEM dominated the decreasing of $O_3$ and accounted for approximately 45% of all the processes in Base and 34% in Exp3, with the changes attributed to the COVID-19 lockdown being about 37%.

In our simulation, the reason why $O_3$ increased during the COVID-19 lockdown period in Wuhan was that the contribution of CHEM decreased more than HADV and VDIF. The contribution of CHEM decreased to 37%, which always decreased the concentration. And the contribution of HADV and VDIF decreased to 57% and 45%, which always increased the concentration.

The two dominated physical processes HADV and VDIF in the CMAQ model were highly connected with the meteorological parameters. The HADV and VDIF were solved in the science algorithms of CMAQ model (Byun et al., 1999) and shown as:

$$
\frac{\partial (\sqrt{\gamma} \varphi_i)}{\partial t} = - \nabla \bullet (\sqrt{\gamma} \varphi_i \hat{V}) \quad \text{(HADV)}
$$

$$
\frac{\partial \eta}{\partial t} = - \frac{\partial \mathcal{F}_\alpha (\varphi)}{\partial \xi} \bigg|_{\xi = \rho(T)} + \frac{Q_o}{\frac{\eta}{\rho(T)}} \mathcal{G}_0 \mathcal{F}_0 \frac{\partial \ln(\sqrt{\gamma} \varphi(T))}{\partial \xi} \quad \text{(VDIF)}
$$

where $\gamma$ is the Jacobian of coordinate transformation, $\varphi_i$ is the trace species concentration in density units, $t$ is the time step, $\hat{V}$ is horizontal wind components in the coordinates $\xi$, $\xi$ is the terrain-influenced vertical coordinate, whose value is increasing monotonically with height, $q_i = \rho \varphi_i$ the species mass mixing ratio, $\rho(T)$ is air density connected with temperature $T$, $\mathcal{F}_0$ represents frictional forcing terms, $Q_o$ is the source or sink term.

In formula 12, the HADV is mainly connected with the horizontal wind. As shown in Fig. 6, the average wind direction during the COVID-19 lockdown in Wuhan is North-East wind, and in Fig. 6(a) and (b), the concentration of PM$_{2.5}$ in the North-East of Wuhan was much lower than the main urban area. The favorable wind direction led to lower concentration in PM$_{2.5}$. In Fig. 6(g) and (b), it is different for $O_3$ that the concentration was always lower in the main urban area. Therefore, instead of decreasing, HADV increased the concentration of $O_3$ in the main urban area.

In formula 13, the formula used the eddy diffusion concept (K-theory) (Stouton, 1932), and as the theory proved, the species mass mixing ratio is highly connected with temperature $\rho(T)$ and the trace species concentration in different vertical coordinate $\varphi_i$. The simulation of PM$_{2.5}$ and $O_3$ had the same temperature gradient but different concentration gradient. The recent observation results in China has proved that the concentration of PM$_{2.5}$ generally decreased with height and the concentration of $O_3$ increased with height (Li et al., 2020). Therefore, the different tendency of VDIF between PM$_{2.5}$ and $O_3$ in our study can be explained by that VDIF decreased the surface concentration of PM$_{2.5}$ as a flux from the surface to upper layers and increased the surface concentration of $O_3$ as the flux from upper layers to the surface, in consistent with the study of Li et al. (2016) and Hogrefe et al. (2018).

In order to investigate why the AERO of PM$_{2.5}$ had an opposite trend in Base and Exp3 and why the HADV of $O_3$ was always positive in the average of ten stations in Wuhan, the horizontal distribution of the average rates of AERO of PM$_{2.5}$ from Feb. 08, 2020 to Apr. 08, 2020 in Base, Exp3 and their difference was shown in Fig. 8. In Fig. 8, the AERO of PM$_{2.5}$ had positive impact on the main urban area and negative impact on the other areas in Wuhan. The COVID-19 lockdown slowed down the positive rates of AERO but speed up the negative rates. Fig. S3 shows the rates of divided aerosol processes. The results in Fig. S3 revealed that the changes in aerosol species due to condensation was the main cause. The low emissions in the north-east of the main urban area in Wuhan became lower due to the COVID-19 lockdown. The AERO of PM$_{2.5}$ around the stations in the North-East of the urban area increased the concentration of PM$_{2.5}$ in Base but changed to decrease the concentration in Exp3. Then led to the opposite trend of the AERO of PM$_{2.5}$ in Base and Exp3.

### 5.3.4. Performances of each process while the pollution increased or decreased

In order to determine the impact of the COVID-19 lockdown regarding the pollution metrics during periods of increasing and decreasing pollution rates, analysis was conducted to examine the average contribution of each process and whether the concentration of pollutants increased or decreased from the previous hour (increasing and decreasing stages) as summarized in Table 7. The positive value of increasing and decreasing stages means the concentration increased in the average of the whole simulation. The negative value of increasing and decreasing stages means the concentration decreased in the average of the whole simulation. The ratio means the concentration changed while the pollution increased compared with the concentration changed while the pollution decreased. The ratio reflects the difference between the periods of increasing and decreasing pollution in Base and Exp3, providing a direct target to find out the influences of COVID-19 lockdown to air pollution in Wuhan. As for PM$_{2.5}$, the ratio of EMIS was 1.07 in Base and 1.08 in Exp3. The results proved that the EMIS plays a similar role in increasing and decreasing stages. It decreased in almost equal proportion with the increasing and decreasing stages during the COVID-19 lockdown. The ratio of HADV was 1.01 in Base and 2.63 in Exp3. The results show that HADV played a similar role in the increasing and decreasing stages in Base but it contributed more in increasing stages than decreasing stages in Exp3.

It is clear that the COVID-19 lockdown had more impact on the decreasing stages of HADV. The ratio of VDIF was 0.29 in Base and 0.24 in Exp3. The results show that VDIF contributed more in dissipating stages, and it decreased in almost equal proportion in increasing and decreasing stages during the COVID-19 lockdown. The ratio of AERO was 3.02 in Base and −0.48 in Exp3. The results also show that AERO contributed more in increasing the concentration during decreasing stages in Base, then changed to contribute more in decreasing the concentration during increasing stages in Exp3. It is also evident that the COVID-19 lockdown had a significant impact on AERO in decreasing stages. As for other findings of note, in terms of $O_3$, the ratio of HADV was 0.75 in Base and 0.86 in Exp3. The results show that HADV contributed more in decreasing stages. In addition, the COVID-19 lockdown had a little more impact on the decreasing stages of HADV. The ratio of VDIF was 1.79 in Base and 1.97 in Exp3. The results show that VDIF contributed more in increasing stages, and the COVID-19 lockdown had a little more impact on the decreasing stages of VDIF. The ratio was 0.70 in Base and 0.28 in Exp3. The results show that VDIF contributed more in decreasing stages, but the COVID-19 had a significant impact on the increasing stages of CHEM.

In conclusion, the COVID-19 lockdown had a greater impact on the decreasing stages of horizontal advection and aerosol processes of PM$_{2.5}$, and the increasing stages of chemical processes of $O_3$, which might be caused by the lack of NO$_2$ and NO and explained in section 4.2.5.

### 5.3.5. Daily change of $O_3$

In order to find the most affected period of the day during the COVID-19 lockdown, Fig. 9 was carried out and shows the daily change of $O_3$ in observation, Base, Exp3 and the differences of each process between
Table 7
Average contribution of each process while the pollution increased or decreased (a. PM$_{2.5}$, b. O$_3$). (The symbol + means the tendency that increase the concentration, - means the tendency that decrease the concentration.)

| a. PM$_{2.5}$(μg/m$^3$) | Increasing stages | Decreasing stages | Ratio (Increasing stages/Decreasing stages) |
|-------------------------|-----------------|-----------------|--------------------------------------------|
| Base                    | Hours           |                 |                                            |
|                         | 783h            | 657h            | 1.19                                       |
| ZADV                    | −4.47           | −3.06           | 1.46                                       |
| HADV                    | −13.36          | −13.20          | 1.01                                       |
| HDF                     | −0.05           | +0.00           | 0                                           |
| VDIF                    | +5.26           | −19.15          | 0.29                                       |
| EMIS                    | +26.69          | −25.03          | 1.07                                       |
| DDEP                    | +0.68           | −0.97           | 0.70                                       |
| CLDS                    | +0.28           | −0.36           | −0.78                                      |
| CHEM                    | +0.04           | +0.06           | 0.67                                       |
| AERO                    | +5.44           | +1.80           | 3.02                                       |
| Total                   | +8.42           | −9.85           | −0.85                                      |
| Exp3                    | Hours           |                 |                                            |
|                         | 812h            | 628h            | 1.29                                       |
| ZADV                    | −2.10           | −1.46           | 1.44                                       |
| HADV                    | −3.74           | −1.42           | 2.63                                       |
| HDF                     | −0.02           | +0.00           | 0                                           |
| VDIF                    | +2.11           | −8.71           | 0.24                                       |
| EMIS                    | +11.13          | +10.29          | 1.08                                       |
| DDEP                    | −0.34           | −0.57           | 0.60                                       |
| CLDS                    | −0.13           | −0.55           | 0.24                                       |
| CHEM                    | +0.01           | +0.02           | 0.50                                       |
| AERO                    | +1.24           | −2.78           | −0.48                                      |
| Total                   | +4.06           | −5.16           | −0.79                                      |

| b. O$_3$(μg/m$^3$) | Increasing stages | Decreasing stages | Ratio (Increasing stages/Decreasing stages) |
|-------------------|-----------------|-----------------|--------------------------------------------|
| Base              | Hours           |                 |                                            |
|                   | 604h            | 836h            | 0.72                                       |
| CHEM              | −17.87          | −25.70          | 0.70                                       |
| DDEP              | −3.14           | −2.00           | 1.57                                       |
| CLDS              | −0.33           | −0.21           | 1.57                                       |
| ZADV              | +1.40           | +1.69           | 0.83                                       |
| HADV              | +5.56           | +7.40           | 0.75                                       |
| HDF               | +0.00           | +0.04           | 0.00                                       |
| VDIF              | +22.76          | +12.75          | 1.79                                       |
| Total             | +8.36           | −6.04           | −1.38                                      |
| Exp3              | Hours           |                 |                                            |
|                   | 816h            | 824h            | 0.75                                       |
| CHEM              | −3.36           | −11.96          | 0.28                                       |
| DDEP              | −4.14           | −3.36           | 1.23                                       |
| CLDS              | −0.07           | −0.04           | 1.75                                       |
| ZADV              | +0.55           | +0.71           | 0.77                                       |
| HADV              | +3.48           | +4.05           | 0.86                                       |
| HDF               | +0.00           | +0.02           | 0.00                                       |
| VDIF              | +10.56          | +5.36           | 1.97                                       |
| Total             | +7.02           | −5.22           | −1.34                                      |

Exp3 and Base from the average of Feb. 08, 2020–Apr. 08, 2020. Fig. 9 represents the average of the whole COVID-19 lockdown period. TOT means total contribution of all the processes, while OBS means the observations. There is no doubt that Exp3 had a better performance in simulating daily change of O$_3$. In our simulation, it is apparent that Base had a lower O$_3$ concentration at night compared to Exp3. As seen in Fig. 9, for most of the day, the total contribution of all processes was a bit lower except 4 p.m.–7 p.m. The significant total differences of all the processes during the time of 4 p.m.–7 p.m. between Base and Exp3 resulted in higher O$_3$ levels at night during the COVID-19 lockdown period in Wuhan. The difference between the maximum and minimum concentration of the day change from the average during Feb. 08, 2020–Apr. 08, 2020, which was 63.38 μg/m$^3$ in Exp3 and 77.23 μg/m$^3$ in Base. The results here were in alignment with the results in section 4.2.4. These results reached an agreement that the COVID-19 lockdown made the differences smaller between the high concentration and low concentration of O$_3$. The COVID-19 lockdown had a greater impact on the increasing stages of chemical processes in O$_3$ as an hourly average. Beyond that, the results in Fig. 9 shows that the biggest difference of chemical processes attributed to the COVID-19 lockdown was about 4 p.m.–7 p.m. in the decreasing stages.

For future consideration, what causes the significant differences between Base and Exp3? Fig. 9 shows that the declining rates of decreasing the concentration that are mainly due to chemical processes, were much higher than the declining rates of increasing the concentration by vertical diffusion and horizontal advection decreased. The differences in Base and Exp3 around 6 p.m. lead to the different rate of the consumption of O$_3$, and then made O$_3$ higher at night. Chemical processes at about 4 p.m.–7 p.m. were the main factors that led to the high O$_3$ pollution during the COVID-19 lockdown in Wuhan. As described in the previous study, the main chemical processes of O$_3$ is that O$_3$ produced directly by photolysis of NO$_2$ (R1), where the oxygen atom (O) rapidly recombines with molecular oxygen to produce ozone (O$_3$). Normally, this reaction is counterbalanced by the reaction of NO with ozone(R2):

$$\text{NO} + h\rightarrow \text{NO} + \text{O} \quad \text{(R1)}$$

$$\text{NO} + \text{O}_3 \rightarrow \text{NO}_2 + \text{O}_2 \quad \text{(R2)}$$

There is always net removal of ozone at nighttime. Surface O$_3$ is normally low when NO emissions are high. The significant daytime removal of ozone via reaction (R2) occurs in the vicinity of large NO emission sources (Kleiman et al., 2000; Lin et al., 1998). In our situation, NO$_2$ had decreased in the lockdown, leading to lower rates of ozone titration, which led to higher O$_3$ at night, leading to a higher daily concentration of O$_3$. One could easily hypothesize then, that the causes of the high O$_3$ conditions during the lockdown might be that the
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increased 43.9% from Feb. 8, 2020 to Apr. 8, 2020 compared to the same time period in 2019. The observation results from this study were in order to properly calibrate the initial emission source of the model, the Eva experiment was used to assess the performance of the CMAQ simulation. The Base experiment was designed as a baseline without considering the COVID-19 lockdown in Wuhan. The other three experiments which considered the COVID-19 lockdown in Wuhan show that Exp3 had the best performances in simulating PM$_{2.5}$ and O$_3$, by a decrease of 20% in industry and 10% in agriculture and transportation. Therefore, Exp3 might reflect the most possible reduction of emissions caused by the COVID-19 lockdown in Wuhan.

Thirdly, analysis was conducted to examine the impacts of the COVID-19 lockdown on the chemical and physical processes as summarized in Table 6. While comparing the results of process analysis of PM$_{2.5}$ and O$_3$ between Exp3 and Base, it was found that (1) the reduction of PM$_{2.5}$ was mainly due to the reduction of emissions, which dropped to 42% in Exp3 compared with Base. The concentration contribution of the aerosol process in Exp3 changed to −12%, meaning that the aerosol process had an opposite tendency in changing PM$_{2.5}$ concentration in Exp3 compared with Base. In addition, the rates of concentration contribution in Exp3 are reduced to 43% for vertical diffusion and 21% for horizontal advection. (2) The increase of O$_3$ was mainly due to the weakening of the chemical process (weaken to 37% compared with the base), which was unfavorable to consumption, although the rates of diffusion and advection increasing O$_3$ concentration were reduced to 45% and 57% respectively.

As for the horizontal advection, it is mainly connected with the horizontal wind. The average wind direction during the COVID-19 lockdown in Wuhan is North-East wind, the concentration of PM$_{2.5}$ in the North-East of Wuhan was much lower than the main urban area. The favorable wind direction led to lower concentration in PM$_{2.5}$. It is different for O$_3$ that the concentration was always lower in the main urban area. Therefore, instead of decreasing, the horizontal advection increased the concentration of O$_3$ in the main urban area. The North-East wind was in favor of the decreasing of PM$_{2.5}$. The higher O$_3$ concentration in the North-East of the main urban area contributed to the increasing of O$_3$ with unfavorable wind direction. As for the vertical diffusion, the eddy diffusion concept (K-theory) (Sutton, 1932) has proved that the species mass mixing ratio is highly connected with

![Fig. 9. The daily change of O$_3$ in observation, Base and Exp3(line) and the differences of each process between Exp3 and Base(bar) in the average over 10 stations in Wuhan from the average of Feb. 08, 2020–Apr. 08, 2020.](image-url)
temperature and the trace species concentration in different vertical coordinate. The simulation of PM\textsubscript{2.5} and O\textsubscript{3} had the same temperature gradient but different concentration gradient. The recent observation results in China has proved that the concentration of PM\textsubscript{2.5} generally decreased with height and the concentration of O\textsubscript{3} increased with height (Li et al., 2020). Therefore, the different tendency of VDIF of PM\textsubscript{2.5} and O\textsubscript{3} in our study can be explained by that VDIF decreased the concentration of PM\textsubscript{2.5} as a flux from the surface to upper layers and increased the concentration of O\textsubscript{3} as the flux from upper layers to the surface, in consistent with the study of Li et al. (2016) and Hogrefe et al. (2018).

As for the aerosol process of PM\textsubscript{2.5}, it had an opposite tendency during the COVID-19 lockdown. The aerosol process had positive impact on the main urban area and negative impact on the other areas in Wuhan. The COVID-19 lockdown slowed down the positive rates of aerosol processes but speed up the negative rates, changed the rates from increasing the concentration of PM\textsubscript{2.5} to decrease in the North-East of the urban area. The results also revealed that the changes in aerosol species due to condensation was the main cause.

The results of this study quantified the impacts of the COVID-19 lockdown to air pollution, and offered an answer in what and how an unprecedented emission mitigation measure can be done to prevent air pollution. The results show that although an unprecedented emission mitigation measure was carried out, the concentration of PM\textsubscript{2.5} decreased significantly, the concentration of O\textsubscript{3} increased on the contrary. This result pointed out that to prevent O\textsubscript{3} and PM\textsubscript{2.5} pollution at the same time is more difficult than existing proposed measures (Wang et al., 2009; Li et al., 2011) in the field, that primarily were emission reduction campaigns including closing factories, industrial plants, construction sites, gas stations and keeping vehicles off of the road.

Fourth, in order to find out the differences of the COVID-19 lockdown impacts between the pollution that increased and decreased, analysis was conducted to examine the performances of processes changed while pollution increased or decreased due to the COVID-19 lockdown in Wuhan as summarized in Table 7. The concentration contribution ratios were used here. Through dividing the average process rates of increasing periods by decreasing periods in Base and Exp3, the ratios reflect the difference between the periods of increasing and decreasing pollution in Base and Exp3, providing a directly target to find the influences of COVID-19 lockdown to air pollution in Wuhan. (1) As for PM\textsubscript{2.5}, the concentration contribution ratios of horizontal advection were 2.63 in Exp3 and 1.01 in Base while the pollution increase compared to decrease. The ratio shows that horizontal advection demonstrated more differences between the pollution which increased and decreased in Exp3. (2) The ratio of aerosol processes was –0.48 in Exp3 and 3.02 in Base, indicating that aerosol processes were more likely to decrease the concentration while the pollution decreased in Exp3, rather than increasing the concentration. (3) As for O\textsubscript{3}, the ratio of chemical processes was 0.28 in Exp3 and 0.75 in Base, showing that chemical processes demonstrated more differences between the pollution which increased or decreased in Exp3.

The COVID-19 lockdown had a greater impact on the decreasing stages of horizontal advection and aerosol processes in PM\textsubscript{2.5}, and on the increasing stages of chemical processes in O\textsubscript{3}. The results can help better understand the differences of pollution increasing stages and pollution decreasing stages when an emission mitigation measure is carried out. This can further help the government to consider how to prevent O\textsubscript{3} and PM\textsubscript{2.5} pollution at the same time. According to the results of this paper, focusing on the decreasing stages of PM\textsubscript{2.5}, and increasing stages of O\textsubscript{3} might be more effective when air pollution needs to be avoided.

Finally, in order to find the most affected period of the day by the COVID-19 lockdown, Fig. 9 was carried out and found the significant differences at about 4 p.m.–7 p.m. between Base and Exp3, which might be caused by the O\textsubscript{3} being higher at night during the COVID-19 lockdown period in Wuhan. The causes of the significant differences might be that the restriction of traffic leads to the reduction of NO concentration, which weakens the reaction between O\textsubscript{3} and NO, NO\textsubscript{2} an NO, stimulating a reduction of fresh NO emissions and alleviating ozone titration.

This study further pointed out the exact time period of the day that was most affected in addition to its similar results to previous studies (Huang et al., 2021; Le et al., 2020) that the reduction of fresh NO emissions alleviates ozone titration leading to the higher O\textsubscript{3} during the COVID-19 lockdown. Beyond that this result further confirms the previous conclusions through quantitative analysis and provides a new possible way that enhances ozone titration at about 4 p.m.–7 p.m. of the day to avoid O\textsubscript{3} pollution.
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Abbreviations

COVID-19: 2019 novel coronavirus
CMAQ: The Community Multiscale Air Quality modeling system
PM2.5: fine particulate matter
PM10: inhalable particles
PROCAN: Process Analysis Preprocessor
HADV: horizontal advection
ZADV: vertical advection
HDF: horizontal diffusion
VDIP: vertical diffusion
DDEP: dry deposition of species
CLDS: change due to cloud processes; includes aqueous reaction and removal by clouds and rain
AERO: change due to aerosol processes
CHEMS: net sum of all chemical processes for species over output step
EMIS: emissions contribution to concentration
COR: correlation coefficient
RMSE: root mean squared error
NMB: normalized mean bias
NME: normalized mean error