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**Impacts of tropospheric ozone and climate change on Mexico wheat production**

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**Highlights**

* O3 impact will reduce wheat production in Mexico by 7-18% by the 2050s.
* Simulations showed large variability in O3 impact across Mexico.
* The negative O3 impact on wheat production in Mexico is comparable to, or even larger than, the future climate change impact.

**Abstract**

Wheat is an important staple crop sensitive to negative effects from elevated tropospheric ozone (O3) concentrations, but the impacts of future O3 concentrations on wheat production in Mexico are unknown. To determine these impacts, the O3-modified DSSAT-NWheat crop model was used to simulate wheat production in Mexico using a baseline scenario with pre-industrial O3 concentrations from 1980 to 2010 and five Global Climate Models (GCMs) under the Representative Concentration Pathway (RCP) 8.5 scenario from 2041 to 2070 paired with future O3 concentrations from the European Monitoring and Evaluation Programme (EMEP) Meteorological Synthesizing Centre – West (MSC-W) model. Thirty-two representative major wheat-producing locations in Mexico were simulated assuming both irrigated and rainfed conditions for two O3 sensitivity cultivar classifications. The simulations showed large variability (after averaging over 30 years) in yield loss, ranging from 7% to 26% because of O3 impact, depending on the location, irrigation, and climate change emissions scenario. After upscaling and aggregating the simulations to the country scale based on observed irrigated and rainfed production, national wheat production for Mexico is expected to decline by 12% under the future RCP 8.5 climate change scenario with additional losses of 7% to 18% because of O3 impact, depending on the cultivar O3 sensitivity. This yield loss caused by O3 is comparable to, or even larger than, the impact from projected future climatic change in temperature, rainfall, and atmospheric CO2 concentration. Therefore, O3 impacts should be considered in future agricultural impact assessments.

**Key words**

Crop model, wheat yield, emissions scenario, future impact, food security

**1. Introduction**

Tropospheric ozone (O3) is a secondary pollutant formed from photochemical reactions between incoming solar radiation and primary pollutants such as nitrogen oxides (NOx = NO + NO2), volatile organic compounds (VOCs), carbon monoxide (CO), or methane (CH4) (Simpson et al., 2014). O3 is recognized as the most damaging air pollutant to crop growth and development because of its phytotoxicity and ubiquitous transport across the lower atmosphere (Ainsworth et al., 2012; Hauglustaine et al., 2005; Meehl et al., 2007). Future climate models project global O3 concentrations to increase due to growth of O3 precursor emissions. The largest O3 concentration increases are expected in the tropics and subtropics, especially in Southeast Asia, India, and Central America (Cooper et al., 2014; Meehl et al., 2007; Wild et al., 2012). Additionally, global atmospheric carbon dioxide (CO2) concentrations and temperature are expected to continue to increase, causing inevitable future changes in the climate (IPCC, 2013). These future climatic changes can directly affect O3 concentrations, and by 2030 elevated O3 could pose a large threat to global food security (Fowler et al., 2008). Under the Intergovernmental Panel of Climate Change (IPCC) highest emissions scenario, Representative Concentration Pathway (RCP) 8.5, the risk of O3 injury in global vegetation is projected to increase by 70% from 2000 to 2100 (Sicard et al., 2017).

Wheat (*Triticum aestivum* L.) is the second most produced and most harvested crop in the world (FAOSTAT, 2017). Wheat contributes approximately 20% of the global total calories and proteins necessary for human diets (Shiferaw et al., 2013). In Mexico, wheat is one of the five highest produced crops and is a staple food for the population, e.g. 3.8 million tons cultivated on 720,000 ha for the 2015 to 2016 growing season (SAGARPA, 2016b). Wheat production is concentrated in Northwest Mexico. Approximately 65% of the total production comes from the northwestern states of Baja California and Sonora (Lobell et al., 2005), with >90% of the national production requiring irrigation because of the arid and semi-arid climate (SAGARPA, 2016a). Rainfed wheat production occurs in the areas with more moderate temperatures and higher rainfall, usually in the high elevation areas of the central and southern states and the northwestern Mediterranean climate of Baja California (Escobar, 2014).

Depending on the developmental stage of wheat, abiotic stresses such as O3 stress and heat stress can cause severe damage to the crop (Ainsworth, 2017; Porter and Gawith, 1999). This is especially true during the reproductive stage of growth because of the increased sensitivity and higher demand of resources for seed development (Ferris et al., 1998; Leisner and Ainsworth, 2012). Wheat was reported to be the most sensitive crop to O3 exposure when compared to 18 other major agricultural crops (Mills et al., 2007). Many studies have been conducted to determine O3 impacts on wheat production (Feng and Kobayashi, 2009; Heagle, 1989; Mauzerall and Wang, 2001; Wang and Mauzerall, 2004), but few studies have estimated the O3 impact on wheat production in Mexico (Avnery et al., 2011; Mills et al., 2018b; Van Dingenen et al., 2009). Van Dingenen et al. (2009) estimated the impact of O3 on global crop production by 2030, assuming current air quality legislation is implemented, and found a slight improvement of wheat yield in Mexico (1.7%) due to small changes in future O3 concentrations ranging between -3 to 3 parts-per-billion (ppb), depending on the season and area of Mexico. Mills et al. (2018b) used a more biologically relevant estimate based on O3 uptake rather than O3 concentrations to determine O3 impact averaged over 2010 to 2012 on a global scale, and reported a 9.9% decrease in yields in the northern hemisphere with yield decreases in Mexico ranging from 10% to 25%.

Future climate change projections for Mexico vary in severity, but all projections estimate a warmer and drier climate by mid-century (Conde et al., 2011; Karmalkar et al., 2011). These warmer and drier conditions will likely result in more active photochemistry and higher O3 concentrations (Zhang and Wang, 2016). An analysis of historical climate data found that the increased global mean temperature from 1980 to 2008 caused a 5.5% decline in global aggregated wheat production (Lobell et al., 2011). The increasing global temperature trend suggests a warming of up to 2°C by mid-century (IPCC, 2013), and global wheat production is estimated to decrease by 6% per 1°C increase if no adaptation strategies are applied (Asseng et al., 2015). Additionally, heat waves are expected to become more frequent in the future (Semenov and Shewry, 2011; Trnka et al., 2014), which may increase the likelihood of extreme O3 concentration events (Hou and Wu, 2016). In Mexico, warming trends in Obregon, Sonora and Toluca, Mexico State have resulted in wheat yield declines of 2% to 3% per decade from 1980 to 2010 (Asseng et al., 2015). Hernandez-Ochoa et al. (2018) simulated the impact of climate change on wheat production in Mexico using five Global Climate Models (GCMs) under two RCPs, 4.5 and 8.5, with two wheat crop models, DSSAT-CROPSIM and DSSAT-NWheat, and projected that national wheat production is expected to decline by 7.2% for RCP 8.5 by mid-century.

The aim of this study is to determine the impact of O3, in addition to climate change, on wheat production in Mexico using five GCMs under the highest emissions scenario, RCP 8.5, paired with two O3 emissions scenarios using the Decision Support System for Agrotechnology Transfer (DSSAT) O3-modified wheat model, DSSAT-NWheat v.4.6.1.01. DSSAT is a crop modeling platform that provides software that facilitates evaluation and application of crop models for various objectives (Jones et al., 2003). DSSAT-NWheat is a well-known and widely used model that was originally derived and validated as part of the Agricultural Production Systems Simulator (APSIM) framework (Asseng et al., 2004; Asseng et al., 1998; Asseng et al., 2000). NWheat has also been validated with controlled field experiments and various agronomic treatments at many global locations (Kassie et al., 2016; Liu et al., 2016). Recently, NWheat was modified with an O3 impact subroutine that accounts for photosynthetic reduction and accelerated leaf senescence associated with O3 stress (Guarin et al., 2018). Building on the study by Hernandez-Ochoa et al. (2018), we extend the climate change impact assessment by including the impact of O3 stress on wheat production in Mexico.

**2. Materials and Methods**

2.1 Mexico wheat production representative locations

Wheat production in Mexico was simulated using 32 point-based representative locations across major wheat-producing areas. Locations were chosen based on observed five year (2010-2014) average yield levels that captured various environmental conditions for irrigated and rainfed wheat production (SAGARPA, 2016a). Many of the locations were in the northwestern states of Mexico because of the high volume of wheat production in that area. Table 1 shows the soil texture, temperature, and rainfall for both winter and summer wheat-growing seasons at the 32 representative locations. Soil data was based on the HC27 global soil profile distribution map from Koo and Dimes (2010) and was derived from the combination of three major texture types (clay, loam, sand), organic carbon levels (high, medium, low), and depths (shallow, medium, deep) (Hernandez-Ochoa et al., 2018). Most soils for the 32 representative locations were considered loamy and clay soils, with variable organic carbon content and depth.

**Table 1.** Locations representing wheat-growing areas in Mexico. Modified after: Hernandez-Ochoa et al. (2018).

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| # | State | Coordinates |  | Wintera | Summerb |
| Latitude | Longitude | Soil Texture | Tmean (oC) | Rainfall (mm) | Tmean (oC) | Rainfall (mm) |
| 1 | Sonora | 32.25 | -114.75 | Loam | 13.6 | 26 | 27.5 | 12 |
| 2 | Baja California  | 31.75 | -116.25 | Loam | 13.7 | 200 | 24.0 | 14 |
| 3 | Chihuahua | 31.25 | -108.25 | Loam | 8.7 | 52 | 23.6 | 171 |
| 4 | Sonora | 30.75 | -112.75 | Loam | 13.2 | 49 | 28.8 | 75 |
| 5 | Chihuahua | 30.75 | -106.75 | Loam | 8.5 | 40 | 22.5 | 205 |
| 6 | Sonora | 30.25 | -111.25 | Loam | 14.1 | 64 | 28.5 | 205 |
| 7 | Baja California  | 29.25 | -114.25 | Loam | 15.4 | 60 | 27.1 | 18 |
| 8 | Sonora | 29.25 | -111.25 | Loam | 14.1 | 50 | 28.5 | 209 |
| 9 | Coahuila | 29.25 | -102.25 | Loam | 12.6 | 51 | 24.6 | 139 |
| 10 | Chihuahua | 28.75 | -106.25 | Loam | 9.4 | 33 | 21.6 | 307 |
| 11 | Chihuahua | 28.25 | -104.25 | Clay | 10.4 | 32 | 19.3 | 245 |
| 12 | Coahuila | 28.25 | -101.75 | Loam | 15.1 | 65 | 25.5 | 198 |
| 13 | Coahuila | 28.25 | -101.25 | Loam | 15.1 | 67 | 25.5 | 208 |
| 14 | Sonora | 28.25 | -109.25 | Loam | 13.7 | 110 | 24.9 | 468 |
| 15 | Sonora | 27.75 | -110.25 | Loam | 16.7 | 55 | 28.7 | 195 |
| 16 | Coahuila | 27.75 | -103.25 | Loam | 13.0 | 37 | 22.2 | 150 |
| 17 | Chihuahua | 27.75 | -108.25 | Loam | 13.7 | 116 | 24.9 | 558 |
| 18 | Sinaloa | 26.25 | -108.25 | Clay | 17.7 | 87 | 25.8 | 566 |
| 19 | Baja California Sur | 25.25 | -111.25 | Loam | 19.1 | 36 | 27.5 | 153 |
| 20 | Coahuila | 25.25 | -101.75 | Loam | 14.9 | 36 | 22.1 | 221 |
| 21 | Durango | 25.25 | -106.25 | Clay | 14.2 | 133 | 21.3 | 705 |
| 22 | Nuevo Leon | 25.25 | -98.75 | Clay | 17.8 | 86 | 25.5 | 325 |
| 23 | Nuevo Leon | 24.25 | -100.25 | Loam | 18.0 | 61 | 22.7 | 212 |
| 24 | Durango | 24.25 | -104.75 | Clay | 15.2 | 40 | 19.6 | 350 |
| 25 | Zacatecas | 24.25 | -102.25 | Loam | 12.6 | 27 | 16.8 | 189 |
| 26 | Zacatecas | 23.75 | -103.25 | Loam | 12.6 | 27 | 16.8 | 276 |
| 27 | Michoacán | 20.25 | -100.25 | Clay | 13.8 | 38 | 16.3 | 459 |
| 28 | Hidalgo | 20.25 | -99.25 | Clay | 13.8 | 32 | 16.3 | 234 |
| 29 | Michoacán | 19.75 | -101.25 | Loam | 14.9 | 42 | 16.4 | 539 |
| 30 | Puebla | 18.25 | -97.25 | Sand | 16.0 | 92 | 19.0 | 681 |
| 31 | Oaxaca | 17.25 | -96.75 | Clay | 16.0 | 94 | 19.0 | 692 |
| 32 | Chiapas | 15.25 | -92.25 | Loam | 22.3 | 57 | 22.4 | 1111 |

a Winter season period from December 10 to March 30 for the baseline scenario (1980-2010).

b Summer season from July 1 to Sept 7 for the baseline scenario (1980-2010).

2.2 Future climate change impact

Climate change impact was estimated by comparing future scenarios from five GCMs (Table 2) to a historical baseline scenario. The climate change data was based on the methodology from Hernandez-Ochoa et al. (2018). The period from 1980 to 2010 was chosen as the historical baseline scenario based on protocols from the Agricultural Model Intercomparison and Improvement Project (AgMIP) (Guttman, 1989; Rosenzweig et al., 2013; WMO, 2017). The climate data for the baseline scenario was collected from climate datasets within the MINK gridded crop modeling system for the coordinates of the 32 representative locations (Robertson, 2017). For the future scenarios, five downscaled and bias-corrected GCM scenarios from the Inter-Sectoral Impact Model Intercomparison Project (ISI-MIP) were obtained from the Potsdam Climate Institute for the 2041 to 2070 period (Mueller and Robertson, 2014). The future climate change scenario selected, RCP 8.5, was the highest projected greenhouse gas concentration trajectory for future climate adopted by the IPCC (IPCC, 2013). Daily maximum and minimum temperature, rainfall, and solar radiation were collected for both the baseline and future scenarios. Solar radiation remained unchanged for the future scenarios. The baseline scenario used an atmospheric CO2 concentration of 362 parts-per-million (ppm), corresponding to the 30-year mean of the baseline period (1980 to 2010), while the future scenarios used an atmospheric CO2 concentration of 572 ppm based on the report from IPCC (IPCC, 2013).

2.3 Future O3 concentration

O3 impact was estimated by simulating wheat production for the baseline and future climate change scenarios with added O3 concentrations, and then comparing the simulated production from the future emissions scenarios to the simulated production of the baseline scenario with pre-industrial O3 levels (< 25 ppb). The EMEP MSC-W model (Table 2), version 4.17 (Simpson et al., 2012; Simpson et al., 2017), was used to simulate hourly O3 data at each of the 32 representative locations for the 2010 and 2050 emissions scenarios. The EMEP model has previously been shown to provide good estimates of O3-relevant metrics such as daily maximum or M7 (defined below) across a range of sites around the globe (Mills et al., 2018b; Stadtler et al., 2018). In order to allow for year-to-year variability, five years of meteorological data from 2008 to 2012 were used for each emissions scenario, creating a total of 10 different annual O3 precursor emissions scenarios (referred to as O3 emissions scenarios). These meteorological data were obtained from the European Centre for Medium Range Weather Forecasts Integrated Forecasting System (ECMWF-IFS) model (<https://www.ecmwf.int/en/research/modelling-and-prediction>). For each annual O3 emissions scenario, daily 7-hour (9:00 – 15:59 h) mean (M7) O3 concentration was calculated and repeated for 29 additional years. The 30 years of M7 O3 concentrations were then added to the 30-year baseline scenario and RCP 8.5 scenario of the 5 GCMs, for each annual O3 emissions scenario (Table 3). The M7 O3 exposure index was used because it is the most commonly used O3 index (Ashmore, 2005), and is the standard input for the NWheat crop model (Guarin et al., 2018). Figure 1 shows the annual average M7 O3 concentrations for the two O3 emissions scenarios (averaged for the five years) at the 32 representative locations in Mexico.

**Table 2.** The five Global Climate Models (GCMs) and the O3 model used for the different scenario simulations. The GCMs provided daily maximum and minimum temperature, rainfall, and solar radiation. The O3 model provided hourly O3 concentrations used to calculate daily 7-hour mean (M7) O3 concentrations. Modified after Hernandez-Ochoa et al. (2018).

|  |  |  |
| --- | --- | --- |
| **Model Name** | **Model Acronym** | **Type** |
| Geophysical Fluid Dynamics Laboratory – Earth System Model | GFDL-ESM2M | GCM 1 |
| Institute Pierre Simon Laplace – Coupled Model | IPSL-CM5A-LR | GCM 2 |
| Hadley Centre Global Environment Earth System Model | HadGEM2-ES | GCM 3 |
| Model for Interdisciplinary Research on Climate – Earth System Model | MIROC-ESM-CHEM | GCM 4 |
| The Norwegian Earth System Model | NorESM1-M | GCM 5 |
| European Monitoring and Evaluation Programme Meteorological Synthesizing Centre – West Model | EMEP MSC-W | O3 |

**Table 3.** Methodology for combining the baseline and future RCP 8.5 climate change scenarios with the 2010 and 2050 O3 emissions scenarios. The 2010 and 2050 combined emissions scenarios were used as input for the NWheat crop model simulations.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Baseline Scenario with Pre-industrial O3** |  | **2010 O3 Emissions Scenario** |  | **2010 Combined Emissions Scenarios** |
| 1980 | **+** | Year 1 | **=** | 1980 + Year 1 |   | 1980 + Year 2 |   | 1980 + Year 3 |   | 1980 + Year 4 |   | 1980 + Year 5 |
| ⁞ | Year 2 | ⁞ |  | ⁞ |  | ⁞ |  | ⁞ |  | ⁞ |
| 2010 | Year 3 | 2010 + Year 1 |   | 2010 + Year 2 |   | 2010 + Year 3 |   | 2010 + Year 4 |   | 2010 + Year 5 |
|  |  |  |  |  |  | Year 4 |  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  | Year 5 |  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| **Future RCP 8.5 Scenario with Pre-industrial O3** |  | **2050 O3 Emissions Scenario** |  | **2050 Combined Emissions Scenarios** |
| GCM 1 | GCM 2 | GCM 3 | GCM 4 | GCM 5 | **+** | Year 1 | **=** | GCM 1 |
| 2041 | 2041 | 2041 | 2041 | 2041 | Year 2 | 2041 + Year 1 |  | 2041 + Year 2 |  | 2041 + Year 3 |  | 2041 + Year 4 |  | 2041 + Year 5 |
| ⁞ | ⁞ | ⁞ | ⁞ | ⁞ | Year 3 | ⁞ |  | ⁞ |  | ⁞ |  | ⁞ |  | ⁞ |
| 2070 | 2070 | 2070 | 2070 | 2070 | Year 4 | 2070 + Year 1 |   | 2070 + Year 2 |   | 2070 + Year 3 |   | 2070 + Year 4 |   | 2070 + Year 5 |
|  |  |  |  |  |  | Year 5 |  | GCM 2 |
|  |  |  |  |  |  |  |  | 2041 + Year 1 |  | 2041 + Year 2 |  | 2041 + Year 3 |  | 2041 + Year 4 |  | 2041 + Year 5 |
|  |  |  |  |  |  |  |  | ⁞ |  | ⁞ |  | ⁞ |  | ⁞ |  | ⁞ |
|  |  |  |  |  |  |  |  | 2070 + Year 1 |   | 2070 + Year 2 |   | 2070 + Year 3 |   | 2070 + Year 4 |   | 2070 + Year 5 |
|  |  |  |  |  |  |  |  | GCM 3 |
|  |  |  |  |  |  |  |  | 2041 + Year 1 |  | 2041 + Year 2 |  | 2041 + Year 3 |  | 2041 + Year 4 |  | 2041 + Year 5 |
|  |  |  |  |  |  |  |  | ⁞ |  | ⁞ |  | ⁞ |  | ⁞ |  | ⁞ |
|  |  |  |  |  |  |  |  | 2070 + Year 1 |   | 2070 + Year 2 |   | 2070 + Year 3 |   | 2070 + Year 4 |   | 2070 + Year 5 |
|  |  |  |  |  |  |  |  | GCM 4 |
|  |  |  |  |  |  |  |  | 2041 + Year 1 |  | 2041 + Year 2 |  | 2041 + Year 3 |  | 2041 + Year 4 |  | 2041 + Year 5 |
|  |  |  |  |  |  |  |  | ⁞ |  | ⁞ |  | ⁞ |  | ⁞ |  | ⁞ |
|  |  |  |  |  |  |  |  | 2070 + Year 1 |   | 2070 + Year 2 |   | 2070 + Year 3 |   | 2070 + Year 4 |   | 2070 + Year 5 |
|  |  |  |  |  |  |  |  | GCM 5 |
|  |  |  |  |  |  |  |  | 2041 + Year 1 |  | 2041 + Year 2 |  | 2041 + Year 3 |  | 2041 + Year 4 |  | 2041 + Year 5 |
|  |  |  |  |  |  |  |  | ⁞ |  | ⁞ |  | ⁞ |  | ⁞ |  | ⁞ |
|  |  |  |  |  |  |  |  | 2070 + Year 1 |   | 2070 + Year 2 |   | 2070 + Year 3 |   | 2070 + Year 4 |   | 2070 + Year 5 |



**Figure 1.** Annual average M7 O3 concentrations for 5 years of data at each of the 32 Mexico locations for a) 2010 O3 emissions scenario and b) 2050 O3 emissions scenario from the EMEP MSC-W model. The shaded area indicates wheat-growing areas in Mexico.

2.4 O3-modified crop model

The NWheat crop model simulates wheat development and growth, water and nitrogen (N) dynamics, and multiple stress responses in daily time steps using inputs of daily maximum and minimum temperature, rainfall, solar radiation, and M7 O3 concentrations (Asseng et al., 2004; Keating et al., 2001). The life cycle of the crop is based on Zadoks growth scale and uses the radiation-use efficiency (RUE) approach for biomass accumulation (Asseng et al., 2004; Zadoks et al., 1974). To calculate the effects of abiotic stresses on crop growth, NWheat uses two subroutines to reduce photosynthesis and accelerate leaf senescence because these processes can affect crop growth at different rates depending on the duration and severity of the stress. The O3 function in NWheat includes the two main responses of O3 stress via stomatal uptake directly affecting photosynthesis by limiting daily dry matter (carbohydrate) production and via accelerated leaf senescence, which also indirectly impacts photosynthesis (Guarin et al., 2018). These two O3 stress responses and their rate of impact can be influenced by other growing conditions. For example, water deficit stress may cause stomatal closure which limits O3 uptake, or elevated atmospheric CO2 may reduce the direct O3 impact on photosynthesis but not leaf senescence (Biswas and Jiang, 2011; Biswas et al., 2013; Khan and Soja, 2003). The photosynthetic reduction effect of O3 stress considers the interactive effects of O3 concentrations with water deficit stress and CO2 concentrations. The effect of O3 stress accelerating leaf senescence operates in a similar way as the NWheat heat stress function where leaf senescence is accelerated above a set threshold. NWheat uses a minimum O3 stress threshold of 25 ppb based on pre-industrial O3 concentrations and previous National Crop Loss Assessment Network of the United States (NCLAN) studies indicating that O3 damage usually occurs above this base threshold (Feng and Kobayashi, 2009; Heck et al., 1984; Lesser et al., 1990).

2.5 Crop model initial conditions and experimental setting

The crop model simulations were initialized one day before sowing every year. Sowing date was based on previous observations (Sayre et al., 1997) and expert knowledge. The sowing date was set on December 10th for the winter growing season and on July 1st for the summer growing season. All irrigated wheat simulations were sown in winter and the majority of rainfed simulations were sown in summer, except in Northwest Mexico (Baja California, Baja California Sur, Sonora, Chihuahua, and Sinaloa) where temperature and rainfall are more suitable for winter sowing. Planting density was 300 plants m-2 at a depth of 5 cm. Due to limited soil water content data, initial water content was set at 100% field capacity (FC) in the first 30 cm of the soil profile to ensure germination and at 10% FC for the rest of the soil profile.

Initial mineral soil N was set to 25 kg ha-1 with initial surface residue and root mass set to 3000 kg ha-1 and 1000 kg ha-1, respectively, for all simulations. The N fertilizer amounts for the irrigated wheat simulations ranged from 90 to 140 kg ha-1 depending on location, and the N fertilizer amount for rainfed wheat was 10 kg ha-1 at all representative locations. For the irrigated wheat simulations, two N fertilizer applications were split equally on day of sowing and 40 days after sowing. For the rainfed wheat simulations, a single application was applied on the day of sowing. The fertilizer applied was urea-N banded beneath the surface and incorporated at 5 cm. The irrigated treatment used automatic irrigation, set at 80% of maximum water available in the first 30 cm of the soil profile, to reduce the risk of water deficit stress in the crop. The wheat cultivars and genetic coefficients used were based on the site-specific cultivar selection and adapted coefficients from Hernandez-Ochoa et al. (2018). All cultivars were simulated with the two most common O3 sensitivity cultivar classifications included in NWheat, O3 tolerant and O3 intermediate, based on previous O3 exposure experiments (Guarin et al., 2018).

2.6 Sensitivity analysis and upscaling impacts to national level

To estimate the impact of various O3 concentrations on national wheat production, a sensitivity analysis was conducted using the climate change data (section 2.2) paired with six different treatments consisting of constant daily M7 O3 concentrations of 25, 40, 60, 80, 100, and 120 ppb for the entire growing season of each year. The pre-industrial M7 O3 concentration of 25 ppb was considered as the control to evaluate the model with negligible effects of O3 stress (i.e., same output as simulation with 0 ppb O3).

Observed irrigated and rainfed 2015 district wheat production data in Mexico from SAGARPA (2016a) were used to upscale production from the 32 representative locations to the national scale. Each of the 32 representative locations was assigned to a wheat-producing district, depending on proximity and yield level. Wheat production change for each representative location was calculated by finding the percentage change of the simulated emissions scenario output versus the baseline scenario output. These calculated production changes were then applied to the observed 2015 district wheat production based on the assigned representative location. Future irrigated and rainfed wheat production were added together to report an aggregated national production for each emissions scenario. This process was done using both O3 tolerant and O3 intermediate cultivar classifications to estimate the O3 impact on national production with different cultivar O3 sensitivities.

**3. Results**

3.1 Simulated O3 model concentrations

The simulated O3 concentrations of the two emissions scenarios from the EMEP model were compared to 2010 observed O3 data (Figure 2). Observed hourly O3 data for 2010 were collected from the Red Automática de Monitoreo Atmosférico (RAMA) database for 22 weather stations in Mexico City located within approximately a 75 km radius. Observed O3 data were collected only for Mexico City due to limited availability of national hourly O3 data. Any missing daily M7 O3 concentrations were filled with monthly average M7 O3 concentrations. The annual average M7 O3 concentrations of the simulated 2010 and 2050 O3 emissions scenarios were 49 and 50 ppb, respectively, while the annual average of the 2010 observed data was 53 ppb. All three M7 O3 concentrations had a standard error of approximately ±2 ppb. The higher observed M7 O3 is likely the result of the data being solely from Mexico City, which has the highest air pollution emissions in the country (Molina et al., 2007; Molina and Molina, 2004).



**Figure 2.** Daily M7 O3 concentrations for 2010 observed O3 averaged over 22 weather stations in Mexico City (all stations within ~75 km radius), and two simulated O3 emissions scenarios averaged over five years of data for each scenario from the EMEP MSC-W model for the 32 representative wheat-growing locations in Mexico. The shaded area shows the standard error of the mean from the five years of data for each emissions scenario and from the 22 weather stations for the observed data.

3.2 Sensitivity analysis of seasonal M7 O3 concentrations

Figure 3 shows the simulated national wheat production from the sensitivity analysis using the RCP 8.5 emissions scenario with various M7 O3 concentrations ranging from 0 ppb to 120 ppb for the two O3 sensitivity cultivar classifications. As seasonal M7 O3 increased from 25 ppb to 120 ppb, the simulated total wheat production using the O3 tolerant cultivar classification decreased from 3.28 Mt to 2.64 Mt (19.5% loss), and the simulated total production using the O3 intermediate cultivar classification decreased from 3.28 Mt to 1.75 Mt (46.6% loss).



**Figure 3.** Sensitivity analysis showing the simulated total aggregated wheat production for Mexico using the RCP 8.5 emissions scenario with different seasonal M7 O3 concentrations for two different O3 sensitivity cultivar classifications. Aggregated production was upscaled from 32 representative wheat-growing locations based on 2015 Mexico production data.

3.3 Crop model simulated output

The NWheat simulations used the described experimental setting with varying irrigation and N management, cultivar O3 sensitivities, and emissions scenarios (depending on the GCM and O3 emissions). Figure 4 shows an example of the simulated yield and biomass at representative location 1, Sonora, for the year 2043 using the GFDL-ESM2M GCM emissions scenario with O3 concentrations averaged over the five years of 2050 O3 emissions scenarios for both irrigated and rainfed treatments using the “Bacanora” winter cultivar with both O3 tolerant and O3 intermediate cultivar classifications. The year 2043 with the “Bacanora” cultivar was chosen as an example because it was the highest yielding year and cultivar of the GFDL-ESM2M GCM 30-year scenario for both the irrigated and rainfed treatments. Location 1, Sonora, was selected because it is in Northwest Mexico, where the majority of wheat production is concentrated.

The high biomass and yield in the irrigated treatment compared to the rainfed treatment is caused by higher water and N availability throughout the growing season. The simulated yield and biomass differences between the O3 tolerant (solid lines) and O3 intermediate (dashed lines) cultivar classifications are the O3 effect for the year 2043. The irrigated treatment had a larger negative effect from O3 than the rainfed treatment because increased water availability can increase stomatal conductance, leading to higher O3 uptake (Khan and Soja, 2003).



**Figure 4.** Simulated average biomass and yield for a) irrigated and b) rainfed treatments at location 1, Sonora, using the “Bacanora” cultivar under the O3 tolerant (solid line) and O3 intermediate (dashed line) cultivar classifications for the year 2043 using the GFDL-ESM2M GCM; averaged for all five of the 2050 O3 emissions scenarios. Sowing date was December 10th. The standard error of the mean of the O3 emissions scenarios is too small to visualize.

3.4 Simulated O3 impact

Each of the 30-year combined climate change and O3 emissions scenarios were input into NWheat to simulate wheat growth per year (Table 3). For the 2010 combined emissions scenarios, annual yields were averaged by representative location for the five years of O3 emissions scenarios. For the 2050 combined emissions scenarios, annual yields of all five GCMs were first combined and then averaged by representative location for the five years of O3 emissions scenarios. Wheat production change for the 32 representative locations was obtained by calculating the percent change from the yields of the baseline scenario with pre-industrial M7 O3 concentration and the yields of each of the five years of O3 emissions scenarios (Figure 5). These calculated production changes from the 32 representative locations were upscaled and aggregated using the 2015 observed district wheat production as described in the sensitivity analysis to obtain the national wheat production for the five years of O3 emissions scenarios. The national wheat production of the five years of O3 emissions scenarios was then averaged and compared to the national production of the baseline scenario with pre-industrial O3 to determine total production loss (Figure 6). The national production change from the 2050 emissions scenario with pre-industrial O3 was also compared to the baseline scenario with pre-industrial O3 to determine the production change from climate change only, without an O3 effect (Figure 6). Both O3 sensitivity cultivar classifications were used to determine the different severity of O3 effects at the representative locations (Figure 5) and at the national scale (Figure 6).



**Figure 5.** Simulated irrigated (left semi-circle) and rainfed (right semi-circle) total yield change from the baseline scenario with pre-industrial O3 at 32 Mexico locations for (a) 2050 climate change scenario (RCP 8.5) with pre-industrial O3, (b, c) 2010 combined emissions scenario (baseline + 2010 O3), and (d, e) 2050 combined emissions scenario (RCP 8.5 + 2050 O­3) using both (b, d) O3 tolerant and (c, e) O3 intermediate cultivar classifications. The yield change for the 2050 climate change scenario with pre-industrial O3 was the same for both the O3 tolerant and O3 intermediate cultivar classifications because there was no O3 effect. The shaded areas indicate wheat-growing areas in Mexico.



**Figure 6.** Simulated total aggregated production change from the baseline scenario with pre-industrial O3 for Mexico using the 2010 combined emissions scenario (baseline + 2010 O3), 2050 combined emissions scenario (RCP 8.5 + 2050 O3), and the 2050 climate change scenario (RCP 8.5) with pre-industrial O3 for two different O3 sensitive cultivar classifications. Aggregated production was upscaled from 32 representative wheat-growing locations based on 2015 Mexico production data. 2010 and 2050 combined emissions were averaged over five years of O3 emissions data. Error bars show the standard error of the mean of the five years of the 2010 and 2050 combined emissions scenarios and the five GCMs for the 2050 scenario with pre-industrial O3.

**4. Discussion**

4.1 Simulated O3 concentrations

The simulated M7 O3 concentrations of the two O3 emissions scenarios from the EMEP model (Figure 2) agree reasonably well with previously observed seasonal O3 temporal trends for Mexico. In these trends, April and May had the highest O3 concentrations followed by a decrease over the summer months because of increased precipitation and cloud cover (Barrett and Raga, 2016; Hernandez Paniagua et al., 2017). The elevated O3 concentrations in April and May also agree with the observed peak O3 season in the Northern Hemisphere (Cooper et al., 2014). The daily variability of the 2010 observed M7 O3 concentrations was much higher than the daily variability of the M7 O3 concentrations from the two simulated O3 emissions scenarios. The high variability in the observed data was likely influenced by local NO sources (which titrate O3 to NO2), complex topography, and generally elevated air pollution in Mexico City resulting in more active photochemistry and increased O3 concentration extremes compared to other areas of Mexico. Also, roughly 10% of the observed hourly O3 data were missing, adding uncertainty to the observations. However, despite the high variability and uncertainty, the observed data support the temporal trends of the two simulated O3 emissions scenarios.

4.2 Sensitivity analysis of Mexico wheat production

The sensitivity analysis showed that simulated total wheat production for Mexico decreased for both O3 sensitivity cultivar classifications as seasonal M7 O3 concentrations increased above 25 ppb (Figure 3). Under the O3 tolerant cultivar classification, simulated total production loss increased from 4.0% to 19.5% as seasonal M7 O3 increased from 40 ppb to 120 ppb, with an average production loss of 0.23% per ppb M7 O3 increase above 25 ppb. The average production loss for the O3 intermediate cultivar classification was 0.59% per ppb M7 O3 increase above 25 ppb. These simulated production losses due to M7 O3 agree with previous wheat production O3 impact studies. For example, Guarin et al. (2018) found a 0.26% increase in yield loss using the O3 tolerant cultivar classification and a 0.54% increase in yield loss using the O3 intermediate cultivar classification. Ollerenshaw and Lyons (1999) reported an average yield loss of 0.26% per ppb M7 O3 increase, Feng and Kobayashi (2009) reported an average yield loss of 0.67% per ppb M7 O3 increase, and Pleijel et al. (2018) reported an average yield loss of 0.38% per ppb M7 O3 increase. These studies covered different ranges of O3 concentrations, treatments, and cultivar O3 sensitivities so the exact yield loss per ppb O3 will not be constant, especially over a large range of O3 concentrations. The yield loss will depend on the O3 sensitivity of the cultivar and the environmental growing conditions (Feng et al., 2010). Also, studies using daily O3 indices, such as M7, estimate daily average changes in stomatal uptake, photosynthesis, and leaf senescence which may miss some co-variation in environmental interactions that occur at an hourly time step. However, most crop models only simulate interactions on daily time steps, and simulating crop growth and environmental interactions on an hourly time step requires additional computing power and time.

4.3 Future climate change and O3 impact

Mexico national wheat production is estimated to decline by 11.7% because of future climate change (Figure 6), which is higher than the estimated decline of 7.2% from Hernandez-Ochoa et al. (2018) using two crop models. However, when using only the NWheat model, Hernandez-Ochoa et al. (2018) reported a similar production decline of 11.2% (this difference is due to slight adjustments in representative location coordinates). The larger production decrease is because the NWheat model places a higher emphasis on sensitivity to heat stress than other wheat crop models, which can lead to slightly larger simulated negative yield impacts in heat stress environments (Asseng et al., 2015).

After including O3 concentrations in the model simulations, average production loss of all 32 representative locations varied from 7.4% to 26.2%. The lowest average losses (7.4%) were under the 2010 combined emissions scenario using the O3 tolerant cultivar classification (Figure 5b) and the highest average losses (26.2%) were under the 2050 combined emissions scenario using the O3 intermediate cultivar classification (Figure 5e). Irrigated production decreased in all locations for all emissions scenarios (left semi-circles of Figure 5), with the larger decreases under the emissions scenarios using the O3 intermediate cultivar classification. This agrees with previous findings that increased stomatal conductance from increased water availability results in high yield loss from increased O3 uptake (Biswas and Jiang, 2011; Khan and Soja, 2003).

Some locations in the southern states of Mexico had high rainfed production under the future emissions scenarios (Figure 5a, 5d, and 5e). This occurred due to simulated low rainfed yields for both the baseline and future emissions scenarios. For example, in Figure 5d at location 30, Puebla, the average simulated baseline rainfed yield was 530 kg ha-1 and the average simulated emissions scenario rainfed yield was 780 kg ha-1, which led to a production gain of approximately 47%. Although the percent increase is large, it is difficult to justify differences in small yield changes due to uncertainties in the input data and models. Puebla is one of the lower yielding representative locations, and the 250 kg ha-1 yield difference is relatively small compared to other higher yielding areas. For some years, it is possible that O3 stress reduced biomass earlier in the season leading to higher available water and N later in the season, resulting in higher yields, as shown with variable fertilizer N affecting water availability later in the season (Asseng and van Herwaarden, 2003; Fischer, 1979). It is also possible that low levels of O3 stress (i.e., M7 O3 concentrations slightly above 25 ppb) benefitted crop growth through hormesis (Calabrese, 2014). Overall, simulated rainfed production only contributed a small percent to the national aggregated production because of the low country production in rainfed areas (~ 9%) compared to irrigated areas (>90%).

After upscaling and aggregating production to the national scale, all emissions scenarios showed national wheat production losses (Figure 6). The simulated production losses from the 2010 combined emissions scenario using the O3 tolerant and O3 intermediate cultivar classifications, 9.2% and 24% respectively, strongly agree with the findings from Mills et al. (2018b) in which yield losses for Mexico were reported between 10% to 25% using averaged 2010 to 2012 M7 O3 concentrations and a stomatal uptake model. This agreement is because the stomatal uptake model provides a stomatal flux-based metric that can be used to estimate yield losses using established flux-response metrics, similar to the M7 response relationship used in this study. The simulated production losses from the 2050 combined emissions scenario using the O3 tolerant and O3 intermediate cultivar classifications are 19.0% and 30.1%, respectively. These losses disagree with the estimated small wheat yield improvement in Mexico from 2000 to 2030 reported by Van Dingenen et al. (2009). However, this study assumed highest emissions scenarios while Van Dingenen et al. (2009) assumed scenarios using full implementation of air quality legislation. Figure 6 shows that future O3 concentrations are estimated to further reduce the production loss from the RCP 8.5 emissions scenario (11.7%) by 7.3% and 18.5% for the O3 tolerant and O3 intermediate cultivar classifications, respectively. These results suggest that future O3 impacts could be larger than future climate change impacts, emphasizing the need to account for O3 effects in agricultural impact assessments and adaptation strategies. Additionally, simulations using the O3 intermediate cultivar classification had additional 14.8% and 11.2% losses in total production compared to simulations using the O3 tolerant cultivar classification for the 2010 and 2050 O3 emissions scenarios, respectively (Figure 6). The additional national production losses of >10% due to higher cultivar O3 sensitivity support the need for adaptive strategies to include O3 resistant cultivars.

**5. Conclusion**

The O3 impact on wheat production varied in severity depending on location, irrigation, O3 emissions scenario, and cultivar O3 sensitivity, but overall, the inclusion of O3 concentrations in simulations decreased average production for all emissions scenarios. The national simulated wheat production loss due to future O3 effects is equal to, or even larger than, the simulated production loss from future climatic changes in temperature, rainfall, and atmospheric CO2 in Mexico. This suggests that potential yield benefits from increased irrigation practices in response to climate change (Roche, 2015) may be mitigated by increased O3 impact on yield. This also emphasizes the importance of including O3 effects in future decision making and the development of adaptation strategies. To reduce the future negative O3 impact on Mexico wheat production, future adaptation strategies should focus on breeding O3 resistant wheat cultivars, limiting emissions of O3 precursors, and managing irrigation in high O3 conditions.

For future assessments of O3 impact, additional O3 monitoring data and O3 effects data should be collected for testing and evaluating O3-modified crop models and the simulated impacts of elevated O3 stress on growth and productivity. Limited O3 data availability is often an issue in O3 impact studies and is a main reason that O3 effects are often not included in many crop simulation models (Lobell and Asseng, 2017). However, the Tropospheric Ozone Assessment Report (TOAR) is a new global database for O3 observations that can help reduce O3 data limitations (Mills et al., 2018a; Schultz et al., 2017). Additionally, the AgMIP (<http://www.agmip.org/>) collaborative modeling community allows for multi-model ensemble studies, which can reduce uncertainties within O3 impact assessments (Martre et al., 2015) when multiple models that consider O3 impacts become available.

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