



Ozone pollution may limit the benefits of irrigation to wheat productivity in India

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Abstract. Ground level ozone (O_3) pollution, heat and water stress are recognised as key abiotic stresses which threaten the ability of wheat yields to meet the growing demand for food production in India. The magnitude and interplay of O_3 and water-

- 15 stress effects are tightly coupled via stomatal conductance and the transpiration pathway. Existing modelling methods that assess stress response as a function of O₃- and water vapour-stomatal flux are applied to assess O₃'s role in limiting productivity afforded by irrigation. We investigate the effect of these stresses on grain yield of older (HUW-234) vs recently released (HD-3118) Indian wheat cultivars under current and future climates and O₃ precursor emission profiles (using RCP4.5 and RCP8.5 scenarios). Water-stress in rainfed conditions was modelled to analyse the trade-off between O₃-induced vs. water-stress-
- 20 induced yield loss to quantify the extent to which water-stress mitigates O₃ stress via reduced stomatal conductance. Under rainfed conditions for the years 1996-2005, the mean water-stress-induced and O₃-induced yield loss for HUW-234 was 13.3% and 0.6% respectively. The latter was a significant decrease from the mean O₃-induced yield loss of 10.6% modelled under irrigated conditions (i.e. no water stress). Similarly, under RCP4.5 and RCP8.5 scenarios for the mid-century, water-stress induced yield losses under rainfed conditions were 10.1% and 20.0%, while mean O₃-induced yield losses were only 1.0% and
- 0.1% respectively. Under irrigation, O₃-induced yield losses increased to 18.5% and 13.7%, suggesting that O₃ stress will negate the beneficial effects of irrigation. The cultivar HD-3118 suffered on average 0.2% greater O₃ relative yield loss (O₃RYL) than HUW-234 across all scenarios. The O₃RYL increased with climate change under the RCP4.5 scenario by 7.9% and RCP8.5 by 3.0% compared to the current climate. Together these findings suggest that O₃ may continue to substantially limit the productivity benefits of the use of modern cultivars bred for high gas exchange grown under irrigated conditions in

30 India.

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1 Introduction

Wheat is a vital crop for India's economy and food security; India is the second largest wheat producer in the world and most of its population gains >50% of their calorific intake from this staple grain (Tripathi and Mishra, 2017). With India's population of 1.4 billion growing at a rate of 2.23% per year (UNDESA, 2022), wheat will play a major role in ensuring food supply meets the growing demand (Tripathi and Mishra, 2017). However, India's croplands are exposed to particularly high O₃

- concentrations ($[O_3]$) with hotspots occurring across the Indo-Gangetic Plains (IGP) (Roy et al., 2008). The 8-hour daily mean O_3 concentrations often reach up to 100 ppb in hotspots during the Rabi crop growing season (October to April) and are therefore a significant threat to India's wheat productivity (Roy et al., 2009). Currently, there are no air quality standards in
- 40 India to protect crops from surface O_3 , and emissions of O_3 precursors are forecast to continue to rise well into the 21st century, driven by persistent growth in industries, including mining and petroleum industries, vehicular traffic and agricultural activities (Ghude et al., 2014; Sharma et al., 2019; Yadav et al., 2019). Ozone distribution varies spatially and temporally but the IGP often experiences high levels due to the long-distance transport of O_3 and its precursors from urban, industrial or power generation centres located across northern India (Singh and Agrawal, 2017).
- 45 Ozone damages crops when it diffuses into the intracellular airspace of the leaf via the stomata which triggers a cascade of metabolic and physiological responses resulting in reduced carbon assimilation, premature leaf senescence and visible injury. Together, these effects can lead to reductions in overall yield and quality (Emberson et al., 2018). Since O₃ damage relies on stomatal O₃ flux (i.e., O₃ dose), the scale of damage caused by ambient [O₃] varies with stomatal conductance. Stomatal conductance is determined in the short-term, by environmental factors that trigger the closure of the stomata, and in the long
- 50 term, by adaptations to climate change i.e., reduced stomatal density (Emberson et al., 2018). Two other factors also influence a crop's vulnerability to O_3 dose; its detoxification ability and the signal transduction pathway, which regulates the response of cells to the increased oxidative load caused by O_3 (Ainsworth et al., 2008; Kangasjärvi et al., 2005).

It is widely acknowledged that stress conditions including elevated levels of carbon dioxide (CO₂), heat and water vapour pressure deficit (VPD) and soil water deficit (all of which may be associated with climate change) decrease stomatal conductance, thus reducing O₃ flux in wheat and potentially ameliorating O₃ damage to the photosynthetic apparatus (Feng et al., 2008). In addition, several studies have found modern cultivars are more O₃-sensitive due to selection for enhanced gas

- exchange, which could counteract their natural adaptation of lower stomatal conductance resulting from the changing climate. Pleijel et al. (2006) and Yadav et al. (2020) observed greater O₃-related yield loss in a modern wheat cultivar, HD-3118, bred for a higher yield than HUW-234, which was attributed to the cultivar's higher stomatal density and conductance. Climate
- 60 change is expected to increase the use of drought-resistant cultivars which can maintain higher stomatal conductance under drought conditions, this will likely increase crop sensitivity to O₃ (Emberson et al., 2018). However, eliminating this adaptation is unlikely to improve productivity because yield losses due to water-stress out-weigh yield losses due to O₃ (Emberson et al., 2018) and major wheat-producing states in India such as Uttar Pradesh, are in any case, almost fully irrigated (Zaveri and Lobell, 2019).





- Khan and Soja (2003) found that well-irrigated wheat plants (i.e. with a 75% soil water capacity (SWC)) suffered grain yield losses of up to 39% when exposed to accumulated O₃ concentrations over a threshold of 40 ppb (AOT40) of ~25ppm/h. Under severe moisture deficit (35% SWC), no O₃-related yield loss was observed as O₃ uptake was reduced by up to 90%. However, the grain yield of water-stressed wheat was significantly less than well-watered wheat. In a similar study by Harmens et al. (2019) on wheat in Africa, grain yield loss due to O₃ exposure was greater in well-watered plants than in crops that received
- reduced irrigation suggesting controlled irrigation as a management tool to reduce O_3 impact. Whilst drought reduces yields at all stages of development, drought stress during anthesis and grain-filling cause the greatest yield reductions (Farooq et al., 2014). Additionally, anthesis and grain filling is when wheat is most sensitive to $[O_3]$ and is the period of time when the $[O_3]$ are highest during the Indian growing season (Gelang et al., 2000; Pleijel et al., 1998; Rathore et al., 2023). Several experimental studies have investigated the interaction between O_3 and drought stress in wheat. While some studies have
- observed no significant interactions between increased $[O_3]$ and water stress (Broberg et al., 2023; Fangmeier et al., 1994), others have observed an interaction. Ghosh et al., (2020) observed an additive effect of O_3 and drought stress, with a greater reduction in grain yield when both stressors occurred simultaneously due to the reduction in nutrient uptake and assimilation. As a result of these contrasting findings, it is evident the trade-offs between O_3 exposure and water stress require further study. Irrigation has the potential to maximise O_3 -stress by providing conditions likely to enhance stomatal conductance such as
- 80 plentiful soil and leaf water, transpirational cooling and low leaf-to-air VPD. Irrigation is widespread across the IGP, particularly in the states of Punjab, Haryana and Uttar Pradesh; the area irrigated as a percentage of the total area of wheat was 99.1%, 99.9% and 99% respectively in 2018-19 (Ministry of Agriculture & Farmers Welfare, 2022), which means that current wheat crop management practices are likely to enhance sensitivity to O_3 . Modifying irrigation practices has been suggested as a strategy to reduce O_3 damage, but caution is needed to avoid introducing water stress, which could also negatively affect
- 95 yield (Harmens et al., 2019; Teixeira et al., 2011). Irrigation has additional benefits and has often been implemented to offset heat-related yield losses which occur when temperatures exceed 35°C (Zaveri and Lobell, 2019). However, studies suggest that sustainable use of India's future groundwater availability with current irrigation practices would mitigate less than 10% of the climate change impact on crop yield (Fishman, 2018). Additionally, water for irrigation purposes is limited; for example, Zaveri et al. (2016) found Uttar Pradesh will lack scope for further increasing irrigation as groundwater depletion escalates
- 90 due to climate change and increased unsustainable water demand. With irrigation accounting for up to 90% of India's total water demand, water efficiency in agriculture is a priority in the IGP to achieve better environmental and economic performance (Fischer et al., 2007; Wada et al., 2013). Here, we explore the interplay between O₃- and water-stressed induced yield losses which will help inform whether water efficiencies could also provide some benefits in terms of the decreased sensitivity of staple crops to O₃.
- 95 There have been an increasing number of studies exploring the effect of O_3 on wheat yields using a cumulative stomatal O_3 flux metric (POD_Y; phytotoxic O_3 dose over a flux threshold Y) which accounts for the stomatal response to environmental conditions and plant growth stages that alter O_3 uptake. By comparison, concentration-based exposure metrics such as AOT40 only account for atmospheric $[O_3]$ which may be decoupled from O_3 uptake under environmental conditions that limit stomatal





conductance; they also omit O₃ below 40 ppb which are known to be capable of causing damage (CLRTAP, 2017; Emberson 100 et al., 2018). Mills et al. (2018a) estimated an O_3 -induced yield loss that incorporated the effects of irrigation to be in the range of 15-20% for wheat growing in Uttar Pradesh between 2010-2012 using POD₃IAM (POD above 3nmol $m^{-2}s^{-1}$, parameterised for integrated assessment modelling) (CLRTAP, 2017). This parameterisation was based on European wheat cultivars and a broad-scale assessment of India's wheat growing season with the POD₃IAM metric being applied according to the formulations of the Deposition of Ozone for Stomatal Exchange (DO₃SE) model (Büker et al., 2012; CLRTAP, 2017; Emberson et al.,

105 2000a, 2018).

> Application of the stomatal O_3 flux method allows exploration of the relative effects of both O_3 and water stress on yield since the DO₃SE model also estimates water vapour fluxes from which potential and actual evapotranspiration can be calculated (Büker et al., 2012). In this study, we parameterise the DO₃SE 3.1.0 version model for two late-sown Indian wheat cultivars for the estimation of POD₆SPEC metric intended for local to regional scale O_3 risk assessment (CLRTAP, 2017). We apply

- the Weather Research and Forecasting model with Chemistry (WRF-Chem) (Grell et al., 2005) to obtain $[O_3]$ and climate 110 variable data for Varanasi, Uttar Pradesh. We compare O₃ effect yield losses (using the wheat grain yield flux-effect relationship (CLRTAP, 2017) with yield losses due to water stress based on yield responses to the ratio of actual vs potential evapotranspiration (cf. FAO (2012)). This modelling set-up allows us to explore the relative magnitude of yield losses from O₃ and water stress; how these are likely to change in the future and the relative sensitivities of older vs more recently released
- 115 Indian cultivars to damage from O₃ pollution.

2 Methods

For this study, Varanasi was selected as the study area due to (i) its location in the important wheat-growing IGP and, (ii) the availability of observed crop and O₃ data.

2.1 Experimental data

- Experimental data from 2016-2018 were obtained for two late sown Indian spring wheat (Triticum aestivum L.) cultivars 120 grown at the Botanical Garden, Banaras Hindu University (BHU), Varanasi (25°16' N, 82°59' E; 81.0m above sea level). HUW-234 (released in 1986 by BHU, Varanasi) and HD-3118 (released in 2014 by IARI, New Delhi) were selected based on their heat tolerance and extensive cultivation in the North East Plain Zone of India (Joshi et al., 2007; Yadav et al., 2019). The recently released cultivar, HD-3118 is more high-yielding (6.64 tons ha⁻¹) compared to HUW-234 (4.5–5 tons ha⁻¹), most
- likely due to its enhanced capacity for gas exchange. This enhanced capacity for gas exchange is the likely reason for the HD-125 3118 cultivar having a greater sensitivity to O₃ than the HUW-234 cultivar (Yadav et al., 2020).



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2.2 Modelled data

Hourly meteorological data for the Varanasi grid box (45 km x 45 km horizontal resolution) were obtained by running WRF-Chem v.3.8.1 for years 1996-2005 (considered the 'current' climate) and 2046-2055 using both RCP4.5 and RCP8.5 climate

- 130 scenarios. The 45 km resolution model domain is the same as in Daloz et al. (2021), and the meteorological initial and boundary conditions come from global climate model simulations with the Community Earth System Model (CESM) v.1.0.4 (Gent et al., 2011), documented in Hodnebrog et al. (2019). The WRF-Chem simulations are set up with the RADM2 gas-phase chemistry scheme (Stockwell et al., 1990) and O₃ precursor emissions are from Lamarque et al. (2010) for the historical period and from Lamarque et al. (2011) for the future RCPs. Global mean CO₂ mixing ratios (ppm) for 1996-2005 were obtained
- 135 from NASA (using Tans and Conway (no date) for 1983-2003 and Conway (no date) for 2004-2007). For future scenarios, RCP4.5 and RCP8.5 [CO₂] for 2046-2055 were acquired (Meinshausen et al., 2011).

The RCP climate scenarios are selected to provide a range of climate and pollution futures for India from which a consequent range in yield responses can be estimated. RCPs are possible greenhouse gas (GHG) emission pathways designed to aid research into climate change impacts (Riahi et al., 2011). RCP8.5 is a very high baseline, representing the highest GHG

emission pathway in a 'business as usual' scenario resulting in a radiative forcing of 8.5 Wm⁻² at the close of the 21st century; equivalent to 1370 ppm [CO₂] (He and Zhou, 2015; Riahi et al., 2011). RCP4.5 is a medium stabilisation scenario where global climate policy values the role of natural carbon sequestration and land use, resulting in a radiative forcing target of 4.5 Wm⁻² (650ppm [CO₂] equivalent) for 2100 (Riahi et al., 2011; van Vuuren et al., 2011).

These data provided input to the DO₃SE model which was used to simulate stomatal O₃ flux values and water stress characteristics for the two cultivars for each year. The modelled climate, O₃ and CO₂ data for the current climate and both RCP scenarios are summarised in Table 1. The modelled temperature data are on average 1.3°C warmer in the RCP4.5 scenario and 1.9°C warmer in the RCP8.5 scenario than the current modelled climate.

Table 1: Modelled climate, [O₃] and [CO₂] data for the Varanasi grid box, used for the current climate and both future RCP scenarios (expressed as the range of 24-hour mean values, value in brackets indicates mean). The length of growing season is shown in days over two years and can be visualised in Fig. 2.

| Parameter | Current climate (1996-2005) | RCP4.5 (2046-2055) | RCP8.5 (2046-2055) |
|---|-----------------------------|-----------------------|-----------------------|
| Temperature (°c) | 17.4-20.6 (18.9) | 19.1-21.3 (20.2) | 19.6-21.8 (20.8) |
| VPD (hPa) | 8.3-14.4 (11.0) | 12.5-17.5 (14.5) | 11.1-18.1 (15.1) |
| Precipitation (total over growing season; mm) | 72.4-393.4 (235.5) | 35.1-184.4 (101.7) | 0.93-234.0 (92.5) |
| [O ₃] (24 hour mean; ppb) | 47.1-50.6 (48.6) | 57.9-62.2 (60.5) | 54.6-63.0 (59.7) |





| [CO ₂] (pp | n) | | | 362.6-379.5 (370.7) | 476.3-498.5 (487.6) | 518.6-570.5 (543.9) | |
|------------------------|--------|-------|------|---------------------|---------------------|---------------------|--|
| Growing | season | (Days | over | 220 469 | 220 466 | 330 473 | |
| 2 years) | | | | 339-400 | 559-400 | 557-475 | |

2.3 Model formulation

The DO₃SE 3.1.0 version model (<u>https://www.sei.org/projects-and-tools/tools/do3se-deposition-ozone-stomatal-exchange/</u>) was used to estimate stomatal O₃ flux and subsequent O₃-induced yield loss for wheat. DO₃SE is a dry deposition model which takes into account the influence of climatic, soil and plant factors on stomatal conductance to estimate stomatal O₃ flux and determine the accumulated stomatal O₃ uptake during a specified growth period; POD_Y (CLRTAP, 2017). The stomatal

- 155 determine the accumulated stomatal O₃ uptake during a specified growth period; POD_Y (CLRTAP, 2017). The stomatal conductance (g_{sto}) multiplicative algorithm Eq. (1) used in DO₃SE estimates hourly g_{sto} to O₃ by modifying a species-specific maximum g_{sto} (g_{max}) according to environmental variables and is described in Emberson et al. (2000a, b). $g_{sto} = g_{max} \times [min(f_{phen}, f_{O3})] \times f_{light} \times max\{f_{min}, (f_{temp} \times f_{VPD} \times f_{sw})\}$ [1]
- where g_{sto} and g_{max} are expressed as mmol O₃ m⁻² PLA s⁻¹. The factors f_{phen} , f_{03} , f_{light} , f_{temp} , f_{VPD} , f_{sw} and f_{min} represent the influence of phenology, [O₃], light, air temperature, VPD, soil water potential and minimum g_{sto} and are expressed in relative terms as a proportion of g_{max} (so have a value between 0-1). Functions describing these factors for environmental conditions are described in CLRTAP (2017) based on European wheat varieties; for f_{sw} (and to simulate g_{sto} for rainfed wheat) we assume a linear relationship between a relative g_{sto} of 1 and f_{min} at soil water potentials (SW) of -0.3 and -1.1 MPa (Ali et al., 1999; Morgan, 1984). To simulate the g_{sto} of irrigated wheat we simply assume that f_{sw} is always equal to 1.
- 165 Stomatal O₃ flux (F_{st} ; nmol m⁻² PLA s⁻¹) was calculated using Eq. (2).

$$F_{st} = c(zi) \times g_{sto} \times \frac{rc}{(rb+rc)}$$
[2]

where c(zi) is [O₃] at the top of the canopy height *i* (m), *rc* and *rb* represent leaf surface and quasi-laminar leaf boundary layer resistances respectively, based on leaf dimension and wind speed (CLRTAP, 2017).

The species-specific POD_Y (POD_YSPEC) is estimated for the wheat accumulation period according to Eq. (3).

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$$POD_YSPEC = \sum \left[(F_{st} - Y) \times \left(\frac{3600}{10^6} \right) \right]$$
 [3]

where *Y* (nmol O₃ m⁻² PLA s⁻¹) is subtracted from F_{st} (in nmol m⁻² PLA s⁻¹) when $F_{st}>Y$, during daylight hours; this *Y* value represents the assumed detoxification capacity of wheat to O₃ flux. The value is then converted to hourly fluxes by multiplying by 3600 and to mmol by dividing by 10⁶ to give *POD_YSPEC* in mmol O₃ m⁻² PLA (CLRTAP, 2017). A *Y* value of 6 nmol m⁻²

² PLA s⁻¹ was used based on values for European wheat (CLRTAP, 2017). The resulting *POD*₆*SPEC* values were used to
 estimate the percentage grain yield (relative to 100% grain yield under pre-industrial O₃ conditions) based on the dose-response relationship Eq. (4).

$$\%$$
Grain Yield = 100.3 - (3.85 × POD₆SPEC) [4]





2.4 Model formulation

- The DO₃SE 3.1.0 model was used to model the effect of water stress on yield through the provision of estimates of potential (ET_m) and actual (ET_a) evapotranspiration following the DO₃SE model algorithms used to estimate soil-plant-atmosphere cycling of water described in Büker et al. (2012). These DO₃SE algorithms essentially estimate the total loss of soil water through ET_a (and the equivalent ET_m) using the method of Shuttleworth and Wallace (1985) modified to incorporate the atmospheric, boundary layer and stomatal resistances to water vapour flux as calculated within DO₃SE. Resistances are scaled from leaf to canopy using LAI and upscaling methods described in Büker et al. (2012). LAI is modelled to vary over the course
- of the wheat growing season between a value of 0 and $3.5 \text{ m}^2/\text{m}^2$ (consistent with average maximum LAI values frequently found across the IGP region as observed from satellite data (Nigam et al., 2017). The DO₃SE soil moisture module was developed based on the Penman-Monteith model of evapotranspiration (*Et*), which is described in Eq. (5) (Büker et al., 2012; Montieth, 1965; Shuttleworth and Wallace, 1985):

$$Et = \frac{\Delta \left(\Phi n - G \right) + \rho_a c_p \left(\frac{D}{R_{bH_2O}} \right)}{\lambda \left\{ \Delta + \gamma \left(1 + \frac{R_{stoH_2O}}{R_{bH_2O}} \right) \right\}}$$
[5]

- 190 where Δ is the slope of the relationship between the saturation vapour pressure and temperature, Φn is the net radiation at the top of the canopy, *G* is the soil surface heat flux, ρ_a is the air density, c_p is the specific heat of air, *D* is the vapour pressure deficit of air, R_{bH_2O} is the canopy boundary layer resistance to water vapour exchange, R_{stoH_2O} is the stomatal canopy resistance to the transfer of water vapour, γ is the psychrometric constant, and λ is the latent heat of vaporisation.
- The effect of ET_a (and hence water-stress) on wheat yield was estimated according to the relationship between relative yield and the corresponding relative evapotranspiration (*Et*) described in Doorenbos and Kassam (1979) for spring wheat. When a crop is not water-stressed, ET_a is equal to ET_m however in drought conditions, $ET_a < ET_m$ (Yao, 1974). The ET_a and ET_m values produced by DO₃SE were used in Eq. (6).

$$1 - \frac{Y_a}{Y_m} = K_y \left(1 - \frac{ET_a}{ET_m} \right)$$
^[6]

where Y_a is the actual relative grain yield and Y_m is the potential relative grain yield. K_y is the crop-specific yield response 200 factor assumed to be 1.15 for the whole growing season, in accordance with the value for spring wheat from the FAO (Steduto et al., 2012).

2.5 Model parameterisation

The DO₃SE model was parameterised for the HD-3118 and HUW-234 cultivars by (Yadav et al. (2021) using data from a series of O₃ exposure experiments at the Banaras Hindu University, Varanasi, Uttar Pradesh. For this study, we use the same parameterisation except for the f_{phen} term (which we allow to vary as a function of effective temperature sum (ETS) during

205 parameterisation except for the f_{phen} term (which we allow to vary as a function of effective temperature sum (ETS) during the growing season) and the inclusion of the f_{03} term (which accounts for O₃ inducing early onset senescence). The parameterisations used for both cultivars are given in Table 2.





Table 2: Parameterisation of the DO₃SE model for POD₆SPEC for wheat flag leaves for Indian bread wheat (Triticum aestivum L.) cultivars. European bread wheat parameters reported by CLRTAP (2017) have been included for comparative purposes. Parameters are highlighted where there are differences between Indian and European cultivars.

| Parameter | Units | Indo-Gangetic Plains | | Atlantic, Boreal, |
|---------------------------|---|----------------------|---------|--|
| | | HUW-234 | HD-3118 | Continental bread wheat (CLRTAP, 2017) |
| g _{max} | mmol O ₃ m ⁻² PLA s ⁻¹ | 500 | 521 | 500 |
| \mathbf{f}_{\min} | fraction | 0.13 | 0.13 | 0.01 |
| light_a | - | 0.011 | 0.011 | 0.011 |
| T_{min} | °C | 12 | 12 | 12 |
| T _{opt} | °C | 26 | 26 | 26 |
| T _{max} | °C | 40 | 40 | 40 |
| VPD _{max} | kPa | 3.2 | 3.2 | 1.2 |
| VDP _{min} | kPa | 4.6 | 4.6 | 3.2 |
| $\sum VPD_{crit}$ | kPa | 16 | 16 | 8 |
| PAW [*] | % | 50 | 50 | 50 |
| f_{O3} | POD ₀ mmol O ₃ m ⁻² PLA s ⁻¹ | 14 | 14 | 14 |
| Leaf dimension | cm | 2 | 2 | 2 |
| Canopy height | m | 1 | 1 | 1 |
| f _{phen_a} | fraction | 0.3 | 0.3 | 0.3 |
| f_{phen_e} | fraction | 0.7 | 0.7 | 0.7 |

Bread wheat cultivar parameterisation - POD₆SPEC





| $f_{phen_1_ETS}$ | °C day | -616.6 | -553 | -200 |
|-------------------------|--------|--------|------|------|
| $f_{phen_2_ETS}$ | °C day | 0 | 0 | 0 |
| fphen_3_ETS | °C day | 621.5 | 553 | 100 |
| $f_{phen_4_ETS}$ | °C day | 182.75 | 238 | 525 |
| f _{phen_5_ETS} | °C day | 959 | 1000 | 700 |

*PAW_t is the threshold for plant available water (PAW) above which stomatal conductance is at a maximum

The ETS model (see Eq. 7) was calibrated using experimental data for HUW-234 and HD-3118 that provided the timing (as day of year) of key crop development stages (sowing, emergence, flag leaf emergence, fully expanded flag leaf, start of seed

215 setting, start of senescence and harvest) for both cultivars for 3 years (2016 to 2018 inclusive). Corresponding 3-hourly temperature data were used to estimate daily mean temperature from which ETS values could be determined according to Eq. (7).

$$ETS = \sum (T_i - T_b)$$
^[7]

- Where T_i is the mean daily temperature and T_b is the base temperature assumed 0°C for wheat. This is equivalent to the 220 method of thermal time accumulation recommended by CLRTAP (2017) and assumes that there is no upper threshold temperature for phenology and that thermal time increases linearly across the entire temperature range. The ETS components of the f_{phen} function from flag leaf emergence were estimated by assuming that $f_{phen}1_ETS$ and $f_{phen}3_ETS$ together were equivalent to thermal time equally divided between the emerging flag leaf and seed setting. This precaution ensured f_{phen} was not allowed to decrease too early; that $f_{phen}5_ETS$ less $f_{phen}4_ETS$ was equivalent to the
- thermal time at seed setting less the thermal time at flag leaf emergence and that $f_{phen}1_ETS$ and $f_{phen}5_ETS$ together were equivalent to the thermal time at harvest less the thermal time at flag leaf emergence; these basic assumptions allowed the derivation of f_{phen}_ETS parameters 1-5 given in Table 2. Supplement Figure S1 gives an indication of the year-to-year variability in the timing of these key growth stages used to parameterise the f_{phen} function. This f_{phen} function is subsequently used to represent the phenological influence on g_{max} and to define the seasonal accumulation period for
- 230 POD_YSPEC (see also CLRTAP (2017)). Parameterisation of the f_{phen} _ETS model shows little difference in phenology between these cultivars, although HUW-234 had a greater range in dates of flag leaf emergence and fully expanded flag leaf. Seed setting and the start of senescence occurred ~3 days earlier in HD-3118 than HUW-234. The Indian cultivar f_{phen} _ETS values differ from the European Continental bread wheat values (also shown in Table 2). In part, this is related to the precautionary approach taken in defining the length of the period during which f_{phen} will equal 1 to ensure we capture the
- 235 period when O_3 may be taken up by the stomata in the absence of growth stage data more specific to the f_{phen} -ETS stages.





The resulting f_{phen} _ETS parameterization suggests that Indian cultivars take more thermal time to reach mid-anthesis and less thermal time between the start of senescence and harvest than would bread wheat from the European region.

2.6 Model runs

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DO₃SE 3.1.0 model runs were made for each cultivar described in Table 2 using the WRF-Chem modelled O₃ and met data for 1996-2005 which was assumed to represent the current climate. The DO₃SE model runs were repeated for future scenarios using the WRF-Chem modelled O₃ and meteorological data for 2046-2055 based on the two scenarios; RCP4.5 and RCP8.5 to explore the influence of changes in climate and O₃ precursor emissions on O₃ uptake. We assume a sowing data of early November since October to December represent the main sowing months of wheat across the most productive wheat growing states in the IGP (Lobell et al., 2013).

245 3 Results and discussion

3.1 Phenology

Accurate modelling of the growing season and the f_{phen} period in relation to the prevailing O₃ climate is crucial for realistic estimates of O₃ damage to wheat. The ETS model for late-sown cultivars is variable in its ability to simulate key growth stages between years and cultivars. For each growth stage, the minimum and maximum °Cday values between years are 63 to

- 250 426°Cday for HUW-234 and 63 to 317°Cday for HD-3118 respectively. Given that the mean daily temperature during the Indian wheat growing season is ~25°C this would suggest the ETS model may have a maximum error of 17 and 13 days for HUW-234 and HD-3118 respectively. These values are likely at the high end of the uncertainty range as temperatures increase during the growing season and the greatest uncertainty was found for the flag leaf emergence and fully expanded flag leaf growth stages. The inclusion of the 'emerging flag leaf' in the f_{phen} period helps to capture the full period when the
- 255 flag leaf may be vulnerable to O_3 as a precaution given the uncertainty in the ETS model defining the timing of the period from full flag leaf expansion and senescence.







Fig. 1: The evolution of ETS and associated growth stages for the observed (2016-18) climate (to which the ETS model is calibrated with a sowing date of 5th Dec) and the WFR-Chem modelled current (1986-2005) and future (2046-2055; RCP4.5 and 8.0) climates
 (for which the model is applied with a sowing date of 5th Nov) for the HUW-234 cultivar.

When the parameterisation was applied to the WRF-Chem modelled 1996-2005 climate temperature data, with a sowing date of 5th November, maturity is simulated to occur around the end of March (consistent with our observed maturity date of the late sown variety under the relatively high temperatures for years 2016-2018 used for parameterisation) – see Fig. 1. Thus our *f*_{phen} parameterisation, when using standard, early November, sowing dates gives realistic maturity dates for IGP grown
wheat when used with current year WRF-Chem modelled data (Fig. 2). Since the WRF-Chem data are consistent between climate periods (i.e., 1996-2005 and 2046-2055) they can be deemed to provide a means of comparing the relative effect of changes in temperature on the growing season, O₃ uptake and the evolution of soil moisture deficit. The empirical data used for model parameterisation collected in years 2016-18, consistently produced higher temperatures

270 climate change; average air temperatures in India for 2016, 2017 and 2018 were in the top ten on record since 1901 (ESSO, 2019). However, on average, 2016-18 was only +0.72°C, +0.55°C and +0.41°C warmer than the 1981-2010 annual air temperature average respectively (Earth System Science Organisation et al., 2019), therefore it is likely that uncertainties in the modelled values caused the greater part of these discrepancies in temperatures. Since the WRF-Chem model at this resolution may not consider some urban heat island effects, a finer model resolution may have led to better agreement with

than the WRF-Chem model-based met data, which was collected from 1996-2005 (Fig. 3). This could be in part due to

275 observations for this urban site. Despite this, the nature of the ETS model is that it can provide comparative estimates of the influence of temperature profiles on the timing and length of the growing season.







Fig. 2: The ETS model parameterised for HUW-234 based on observed current temperatures (2016-2018; black). The ETS model for the modelled current temperatures (years 1996-2005) are in blue. The range of observed dates of sowing, germination, flag leaf emergence, fully expanded flag leaf, start of seed setting, start of senescence and harvest from the experimental data (Agrawal, pers. comm.) are marked with arrows. Astart to Aend represent the start of anthesis to the end of anthesis.

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Fig. 3: Temperature changes over the growing season for observed calibration data (2016-18) and WRF-Chem modelled data for the current climate (1996-2005).

285 **3.2 Effect of O₃ stress on the yield benefits of irrigation**

Water-stress induced yield loss under rainfed conditions modelled under the climate scenario for 1996-2005 was found to exceed O₃-related yield loss (O₃RYL) under irrigated conditions for the majority of the 10 years investigated. Under this climate, rainfed conditions produced a mean water-stress related yield loss (WSRYL) of 13.3% for HUW-234, with a range of 2.8-31.3% (Fig. 4a). Under rainfed conditions, mean O₃RYL was projected to be negligible (0.6%), significantly lower than

290 the mean O_3RYL when no water-stress is assumed under irrigation (10.7% with a range of 4.8-15.4%). This demonstrates the importance of irrigation for wheat production in India and highlights the substantial influence on the yield of O_3 for irrigated wheat.

 O_3 RYL under irrigated conditions exceeded WSRYL in 80% of the 10 years investigated in the RCP4.5 scenario (Fig. 4b). This highlights how O_3 stress negates some of the increased productivity that arises from reducing water stress through

295 irrigation. In the RCP8.5 scenario, WSRYL under rainfed conditions exceeded O₃RYL under irrigated conditions in all but one year (2051), when precipitation totaled 234.0mm for the growing season (Fig. 4c). In this scenario, precipitation during





the growing season ranges from 0.9-234.0 mm, with a mean of 94 ± 82.97 mm, and as a result the WSRYL fluctuates within the 10 years.

Whilst irrigation has played an important role in increasing yields for India's wheat, these results show that O_3 is likely to 300 negate some of the yield benefits of irrigation. Based on the results of simulations of future climates, irrigation will have less of an effect on yield increases as $[O_3]$ levels rise.











Fig. 4: The water-stress and ozone-related relative yield loss modelled for HUW-234 under rainfed conditions (water stress) and with no water stress (f_{sw} set to 1 in DO₃SE) for (a) the current climate 1996-2005; (b) RCP4.5 scenario 2046-2055; (c) RCP8.5 scenario 2046-2055.

The mean total precipitation for the growing season under the 1996-2005 climate scenario was higher than the median values in the RCP4.5 and RCP8.5 scenarios for 2046-2055, meaning Uttar Pradesh's crops will receive less rainfall in the future. In addition, the RCP8.5 scenario had a larger interquartile range (IQR) of 131.0mm than the 1996-2005 climate (54.8mm) and the smallest lower quartile (22.3mm), demonstrating less and more irregular precipitation in the future climate. Whilst RCP4.5

- 310 was less extreme; it had a larger IQR of 90.1mm. This irregularity and increased risk of low precipitation over the growing season demonstrates the continuing importance of irrigation for wheat productivity. In all modelled climate scenarios, water stress tends to be a much greater threat to crop yields than O₃ and therefore, some level of irrigation is crucial for sustained wheat productivity in India. However, these findings clearly show that O₃ is a limiting factor to yield under irrigated conditions meaning that the full potential benefit of irrigation is not being realised and hence will lead to inefficiencies in the use of
- 315 irrigation water. Further research should be carried out to find the 'sweet spot' for irrigation, that will minimise O_3 stress without inducing water stress, to practice more responsible water management.

Future studies should investigate how short, sharp high O_3 periods could be mitigated with temporary reductions in irrigation, if the efficacy of such approaches can be demonstrated they could be practically applied in the future with the advent of new technologies such as accurate pollution forecasting via machine learning models (Jumin et al., 2020; Wang et al., 2020). A

320 holistic approach that considers the trade-offs between other abiotic stressors such as heat stress is needed, as irrigation plays a significant role in mitigating such stress (Zaveri and Lobell, 2019) and higher temperatures are a precursor of higher O_3 levels with the chance that O_3 effects are erroneously attributed to heat stress (Tai et al., 2014).

3.3 Effect of climate change on O₃ sensitivity

Higher O₃-induced yield losses were modelled under future scenarios (Fig. 5). For HUW234, a statistically significant increase in yield loss of 7.9±5.56% and 3.1±5.08% was modelled for RCP4.5 and RCP8.5 respectively, compared to the current climate.

- Similarly, for RCP4.5 and RCP8.5, an increase of $8.0\pm5.71\%$ and $3.0\pm4.87\%$ yield loss was predicted for HD-3118, respectively. This suggests that the increase in O₃ impact due to future emissions/climate is larger than the year-to-year variability in O₃ impact for the RCP4.5 (but not RCP8.5 where [O₃] were lower, see below) scenario. The current climate represents the lowest mean O₃, suggesting O₃, rather than other environmental conditions that might influence sensitivity to
- O_3 , is the most important factor in determining O_3 -induced yield loss. These findings imply that the changing climate (i.e., higher frequency of temperatures that exceed the T_{opt} with consequent reductions in stomatal conductance and hence O_3 flux) will be insufficient at ameliorating the increase in O_3 -induced yield loss. This contrasts with several studies that have shown the potential of elevated temperatures to lead to reductions in O_3 flux via reduced stomatal conductance, thus reducing O_3 damage (Emberson et al., 2018; Feng et al., 2008). This could be due differences in the timing and duration of periods of more
- 335 extreme temperatures that exist between studies; a possibility that would benefit from further study.







Fig. 5: Mean O₃-induced relative yield losses (RYL) ±SD modelled for the current climate (1996-2005), and two future climate scenarios for 2046-2055; RCP4.5 and RCP8.5 for two Indian spring wheat cultivars; HUW-234 and HD-3118.

The results from this study are within the range published by Mills et al. (2018b) for O₃-induced yield losses for wheat in Uttar Pradesh, which were modelled for 2010-2012 using POD₃IAM with European wheat parameterisation and a broadscale assessment of India's wheat growing season. The Mills et al. (2018b) study used the most recent methodology from CLRTAP (2017) to calculate O₃-induced yield loss for wheat, as a reference POD₃IAM value representing O₃ uptake at pre-industrial conditions was subtracted before crop loss was calculated. Whilst this study also uses a stomatal flux-based metric, POD₃IAM is vegetation-type specific suited for large-scale modelling (CLRTAP, 2017). The POD₆SPEC was used in this current study

since we were able to define a cultivar-specific growth period with some certainty thereby allowing greater confidence in the use of the more biologically relevant metric than POD₃IAM (CLRTAP, 2017).
 Mean relative O_ induced yield losses for both cultivare modelled under PCP4 5 (18.7+3.82%) were significantly bicker than

Mean relative O_3 induced yield losses for both cultivars modelled under RCP4.5 (18.7±3.83%) were significantly higher than the RCP8.5 (13.8±3.22%). This is likely due to a combination of slightly higher [O₃] in RCP4.5 (Table 1) and the WRF-Chem





model projections of higher temperatures (limiting O_3 flux as temperatures have a tendency to exceed T_{opt}) under RCP8.5. 350 Whilst the RCP4.5 scenario sees a global reduction in $[O_3]$ due to pollution regulation, the South Asian region is an exception to this rule, where $[O_3]$ continues to increase at a similar rate as occurred in previous decades (Tai and Martin, 2017). RCP8.5 projects a worldwide increase in [O₃] due to the lack of regulation of precursor emissions except in parts of the US, East and Southeast Asia (Tai and Martin, 2017). Therefore, mean $[O_3]$ during the growing season is lowest in the current climate at 48.6ppb but similar, at least in South Asia, in both the RCP4.5 and RCP8.5 scenarios (60.5ppb and 59.7ppb respectively; Table 1).

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The O₃-induced yield loss will increase from current levels, regardless of whether global emissions follow a business-as-usual or medium stabilisation scenario. We predict that O3-induced yield losses will continue to increase in South Asia with climate change, given the co-emission of radiative forcers and O_3 precursors and the two-way causality that exists between O_3 formation and climate change, i.e., hot, sunny conditions likely to be enhanced under climate change encourages O₃ formation,

- whilst O_3 itself is a radiative forcer (Fu and Tian, 2019). This means that O_3 and climate variable stress are likely to co-occur 360 in the future which becomes especially problematic for crop productivity when environmental thresholds (e.g. due to temperature extremes) for plant productivity are exceeded. South Asia and the IGP are important agricultural regions where O₃ thresholds are being exceeded now (Mills et al., 2018c), with the likelihood that the extent of such exceedance will only worsen in the future and with climate change (Cooper et al., 2014; Fowler et al., 2008; Fu and Tian, 2019; Rathore et al., 2023).
- 365 It should be noted that there are uncertainties in the WRF-Chem model used in modelling meteorological and $[O_3]$ data. There are important criticisms that the WRF-Chem model is limited in its ability in capturing true wind speeds, which influences temperature and O_3 mixing ratios (Rydsaa et al., 2016). Despite this, these findings serve as a useful insight into the future risk of O₃ on wheat yields relative to early 21st-century conditions. Ideally, future research should consider the use of model ensembles to more robustly capture ranges in future meteorological and $[O_3]$ data.

370 3.4 Influence of cultivar physiology on O₃ sensitivity

The O₃RYL modelled for HUW-234 were similar to HD-3118 in the current climate and both the RCP4.5 and RCP8.5 scenarios (Fig. 5). This is due to the similarity in g_{max} values for HUW-234 and HD-3118 which were estimated, from empirical data at 500mmol O₃ m⁻² PLA s⁻¹ and 520.9 mmol O₃ m⁻² PLA s⁻¹ respectively. The mean yield losses for current climate and RCP scenarios combined, modelled for HD-3118 (14.5±0.05%) were similar to HUW-234 (14.3±0.05%), a difference of

- 375 0.2%. Despite the similar mean yield losses observed for HD-3118 and HUW-234, these results align with concerns that modern wheat cultivars are more susceptible to O₃-damage as they are bred for maximum gas exchange or heat tolerance rather than O₃ tolerance (Emberson et al., 2018; Pleijel et al., 2006; Yadav et al., 2020). Typically, plant traits bred for heat tolerance and maximum gas exchange conflict with traits for O_3 tolerance and may increase irrigation requirements; i.e. higher stomatal conductance enhances transpiration rates, allowing for higher rates of photosynthesis (Pleijel et al., 2007; Yadav et al., 2020).
- 380 Despite the potential for HD-3118 to produce higher yields due to a high stomatal conductance, HUW-234 performs better in terms of O_3 tolerance for Varanasi's current conditions and projections for the future climate and $[O_3]$. This is also observed



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in the empirical data for Varanasi from 2016-18, which was used to parameterisation the ETS model. The empirical data observed lower relative yield loss under elevated [O₃] compared to ambient [O₃] for HUW-234 than HD-3118 (21.2% and 23.2% respectively; see Table S1). Absolute yields failed to observe the higher yielding potential expected of HD-3118 even under ambient conditions; the mean absolute grain yield for HUW-234 under ambient [O₃] was 533.4g/m compared to

432.8g/m for HD-3118. Under elevated $[O_3]$, the yield gap widens; HUW-234 has an absolute grain yield of 420.4g/m whilst HD-3118 has a yield of 332.3g/m. This suggests O_3 has a greater impact on yield in HD-3118 than HUW-234, possibly even under ambient concentrations.

Despite corroborating literature for the DO₃SE model results (Yadav et al., 2020), there is some limitation in the ability to accurately parameterise the model for specific cultivars. Here we have been able to parameterise key parameters that will influence stomatal O₃ flux (g_{max} and f_{phen}) for Indian varieties, however, the remaining parameters that determine the modification of g_{max} by environmental conditions rely on European parameterisations. Similarly, the DO₃SE model estimates O₃-induced crop yield losses based on a dose-response relationship configured using five European wheat cultivars (CLRTAP, 2017). Whilst the DO₃SE model is a valuable tool for risk assessment, the use of appropriately calibrated and evaluated crop

- 395 models will provide mechanisms to fully explore the interplay between stresses such as O₃ and water stress on yield (Emberson et al., 2018). The results of this paper make clear the need for such modelling to improve our understanding of how these different stresses act over the course of the growing season to determine changes in productivity. A new generation of crop models that are being developed to incorporate the O₃ effect, as well as other stresses (Emberson et al., 2018), will be able to explore trade-offs between stresses related to soil water, extreme temperatures, and soil fertility. Such advances in crop modelling will be crucial in assessing future wheat productivity under a range of abiotic stress conditions.
- In this Indian study, the mid-anthesis and grain filling period occurred in March (Fig.'s 1 and 2) which corresponds to peak O_3 in Uttar Pradesh (Jain et al., 2023; Mukherjee et al., 2019; Shukla et al., 2017). However, a study on timely-sown Chinese winter wheat cultivars found that elevated O_3 only had a significant effect during the mid-grain filling stage, suggesting that timing mid-grain filling with O_3 troughs could be a mitigation strategy, which may be achieved by earlier sowing (Feng et al.,
- 405 2016). Late planting results in reduced productivity of the wheat crop, with earlier, timely sowing of wheat in the third week of November yielding the best productivity in Eastern Uttar Pradesh (Chandna et al., 2004). Past studies have reported that delays in sowing after mid-November leads to reduction in yield of wheat, often at a rate of 1-1.5% per day (McDonald et al., 2022; Ortiz-Monasterio R. et al., 1994). In addition, Kumar et al. (2014) claimed conversion from late to timely-sown would offset the impacts of climate change. A multi-tolerance approach like early sowing could mitigate heat and O₃ stress however,
- 410 late sowing is often due to delays in harvesting rice in Rice-Wheat systems, a cropping sequence which provides income for tens of millions of farm families (Jain et al., 2017; Mishra et al., 2021). Further investigation of the inter-play between [O₃] profiles over the growing season and targeted crop phenology of different cultivar types should be conducted.





4 Conclusion

- Whilst irrigation has played a pivotal role in increasing wheat production in India through maximising yields, O₃ is likely to 415 negate some of the yield benefits of irrigation, which will reduce irrigation efficiency. Based on the POD₆SPEC values obtained via the DO_3SE model and associated flux-response relationships, O_3 concentrations prevalent in the IGP region of India are high enough to cause grain yield losses in Indian wheat. This paper demonstrates the complexity of avoiding O₃-stress and the importance of taking a multi-stress approach to mitigation. Since high levels of O_3 typically coincide with other abiotic stressors such as heat stress, the approach taken to maximise crop yield must consider multiple stressors and their interactions.
- 420 Rather than altering irrigation patterns to mitigate O_3 stress and risk increasing the effect of other stressors such as water stress or heat stress, earlier sowing to avoid peak O₃ and temperatures in March may benefit irrigated wheat growing in India. Given that modern wheat cultivars are more O_3 -sensitive, wheat growers should reconsider using modern cultivars bred for optimal gas exchange.

425 **Competing interests**

The contact author has declared that none of the authors has any competing interests

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