Evaluating impact of tropospheric ozone on plants with improved ozone damage parameterization in CLM5

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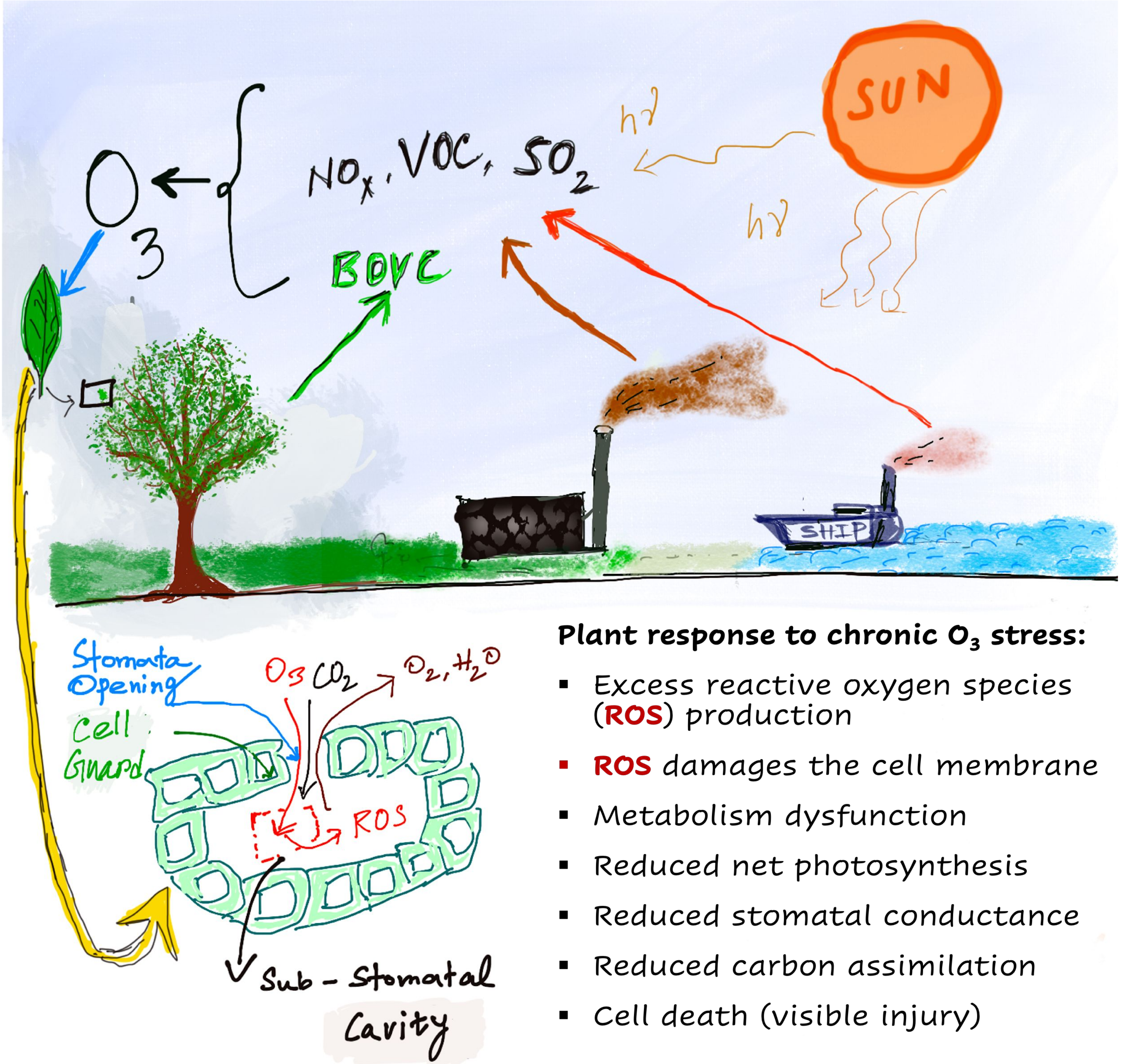


Plant response to chronic O_3 stress:

- Excess reactive oxygen species (**ROS**) production
- **ROS** damages the cell membrane
- Metabolism dysfunction
- Reduced net photosynthesis
- Reduced stomatal conductance
- Reduced carbon assimilation
- Cell death (visible injury)

Ozone damage parameterization in CLM5

- Ozone damage on vegetation in CLM5 is directly and independently influenced by **photosynthesis** and **stomatal conductance** based on the cumulative uptake of ozone (**CUO**) through stomata (Lombardozzi et al., 2015; Lombardozzi et al., 2013; Lawrence, 2019).

- The impact of ozone is estimated for three broad plant functional types (PFTs):
  1. Broadleaf trees and shrubs
  2. Needleleaf trees and shrubs, and
  3. Crops and grasses

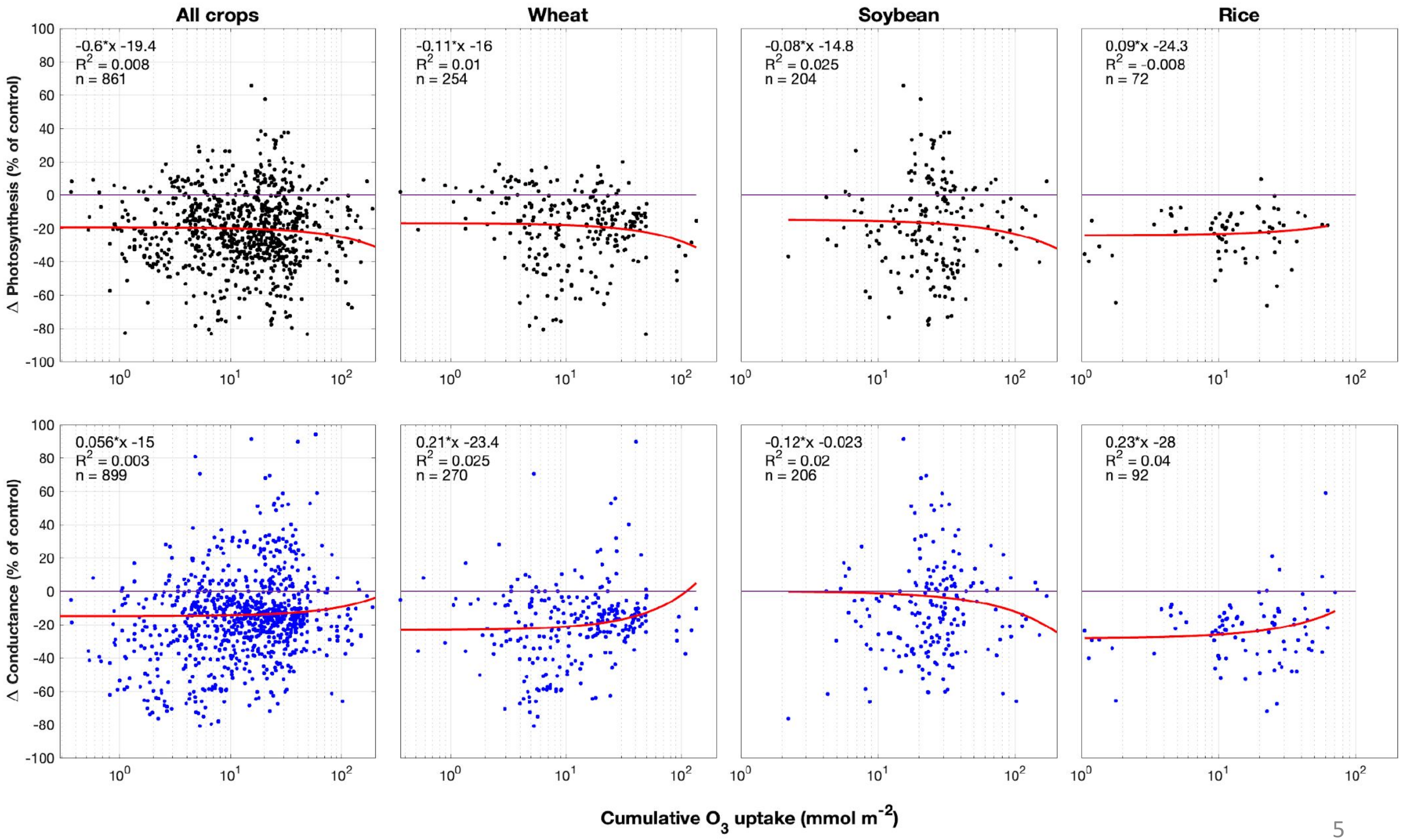
Impact of ozone on photosynthesis in CLM5 Lombardozzi et al. (2013)

Charcoal-filtered air, medium or high confidence data: photosynthesis	n	Mean	p value	Regression	r^2	p value
All data	345	82.1	$<0.001^*$	$84.34-0.10^*x$	0.02	0.01^*
Plant type						
Crop	134	77.22	0.05^*	$80.21-0.09^*x$	0.08	$<0.001^*$
Evergreen shrub	0	NA	NA	NA	NA	NA
Grasses (C_3 and C_4)	8	80.18	0.87	NS	0.27	0.18
Herbaceous	41	83.27	0.8	NS	0.04	0.2
Temperate deciduous tree	113	87.52	0.22	NS	0.003	0.58
Temperate evergreen tree	47	83.9	0.66	NS	0.08	0.06
Tropical tree	2	44.13	0.19	NA	NA	NA
Plant age (years)						
<1	234	79.71	0.29	$82.55-0.11^*x$	0.06	$<0.001^*$
1–5	95	89.14	0.18	NS	0.002	0.64
>5	7	81.41	0.93	NS	0.01	0.8
Exposure system						
Greenhouse	24	76.38	0.08	NS	0.08	0.18
Branch chamber	18	88.68	0.07	NS	0.12	0.16
Growth chamber	157	83.54	0.69	NS	0.00002	0.96
Open-top chamber	146	80.68	0.59	$84.48-0.11^*x$	0.08	$<0.001^*$
Free-air enrichment	NA	NA	NA	NA	NA	NA
Rooting Environment						
Pot	271	81.64	0.87	$83.55-0.09^*x$	0.01	0.05^*
Ground	65	85.63	0.2	$91.74-0.19^*x$	0.17	$<0.001^*$
Vulnerability						
Low	58	86.19	0.34	NS	0.01	0.42
High	135	81.52	0.88	NS	0.01	0.16

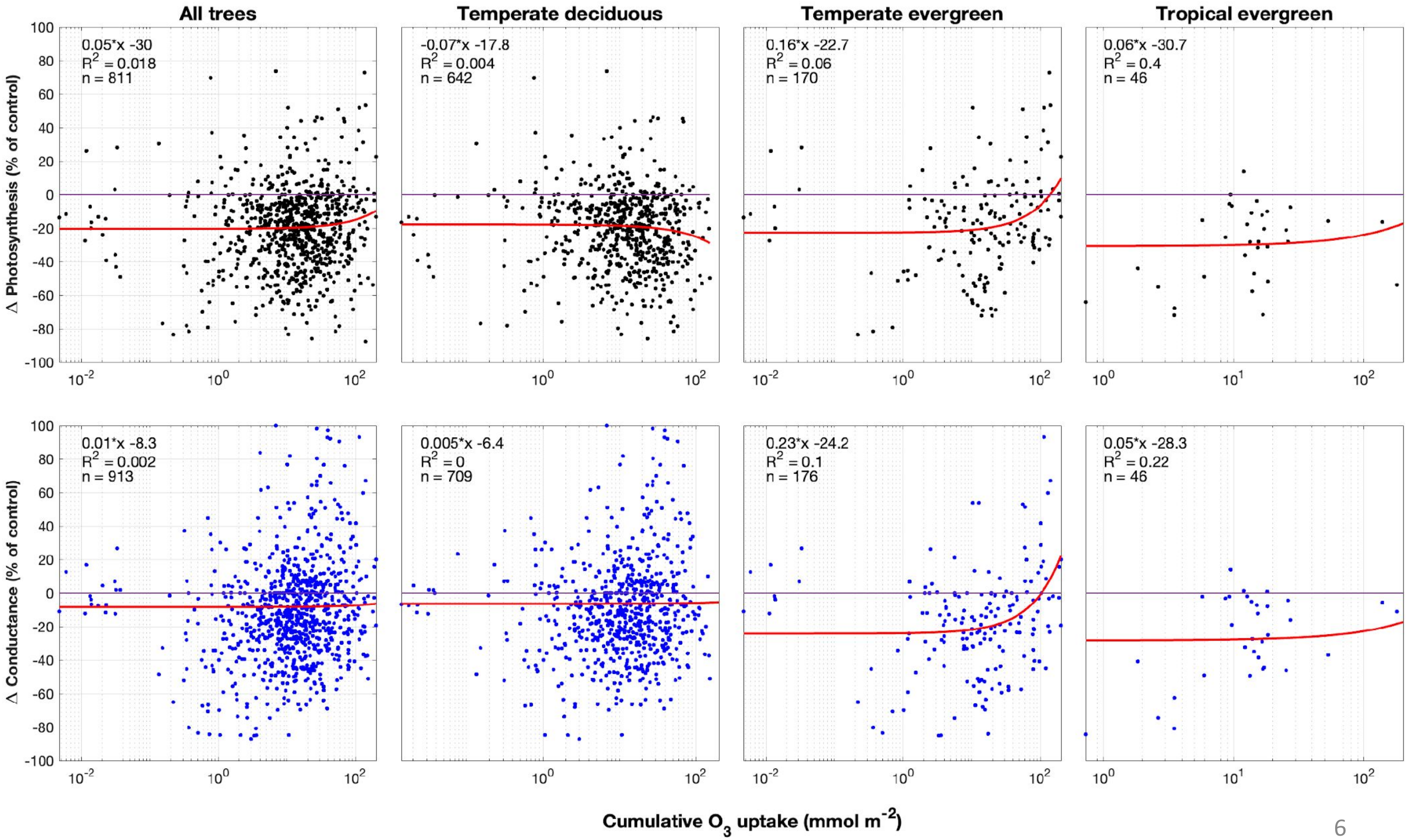
OzoneMod.F90

```fortran
  ! !PRIVATE TYPES:
  integer, parameter :: stress_method_lombardozzi2015 = 1
  integer, parameter :: stress_method_falk = 2

  ! TODO(wjs, 2014-09-29) The following parameters should eventually be moved to the
  ! params file. Parameters differentiated on veg type should be put on the params file
  ! with a pft dimension.

  ! o3:h2o resistance ratio defined by Sitch et al. 2007
  real(r8), parameter :: ko3 = 1.67_r8

  ! LAI threshold for LAIs that asymptote and don't reach 0
  real(r8), parameter :: lai_thresh = 0.5_r8

  ! threshold below which o3flux is set to 0 (nmol m^-2 s^-1)
  real(r8), parameter :: o3_flux_threshold = 0.8_r8

  ! o3 intercepts and slopes for photosynthesis
  real(r8), parameter :: needleleafPhotoInt   = 0.8390_r8  ! units = unitless
  real(r8), parameter :: needleleafPhotoSlope = 0._r8      ! units = per mmol m^-2
  real(r8), parameter :: broadleafPhotoInt    = 0.8752_r8  ! units = unitless
  real(r8), parameter :: broadleafPhotoSlope  = 0._r8      ! units = per mmol m^-2
  real(r8), parameter :: nonwoodyPhotoInt     = 0.8021_r8  ! units = unitless
  real(r8), parameter :: nonwoodyPhotoSlope   = -0.0009_r8 ! units = per mmol m^-2

  ! o3 intercepts and slopes for conductance
  real(r8), parameter :: needleleafCondInt    = 0.7823_r8  ! units = unitless
  real(r8), parameter :: needleleafCondSlope  = 0.0048_r8  ! units = per mmol m^-2
  real(r8), parameter :: broadleafCondInt     = 0.9125_r8  ! units = unitless
  real(r8), parameter :: broadleafCondSlope   = 0._r8      ! units = per mmol m^-2
  real(r8), parameter :: nonwoodyCondInt      = 0.7511_r8  ! units = unitless
  real(r8), parameter :: nonwoodyCondSlope    = 0._r8      ! units = per mmol m^-2

  ! Data is currently only available for broadleaf species (Dec 2020)
  ! o3 intercepts and slopes for JmaxO3/Jmax0
  real(r8), parameter :: needleleafJmaxInt   = 1._r8                ! units = unitless
  real(r8), parameter :: needleleafJmaxSlope = 0._r8                ! units = per mmol m^-2
  real(r8), parameter :: broadleafJmaxInt    = 1._r8                ! units = unitless
  real(r8), parameter :: broadleafJmaxSlope  = -0.0037_r8           ! units = per mmol m^-2
  real(r8), parameter :: nonwoodyJmaxInt     = 1._r8                ! units = unitless
  real(r8), parameter :: nonwoodyJmaxSlope   = 0._r8                ! units = per mmol m^-2
```

The correlation of **photosynthesis** and **stomatal conductance** to **cumulative uptake of O_3 (CUO)** across **category crop types** for all other categories (1970-2022)

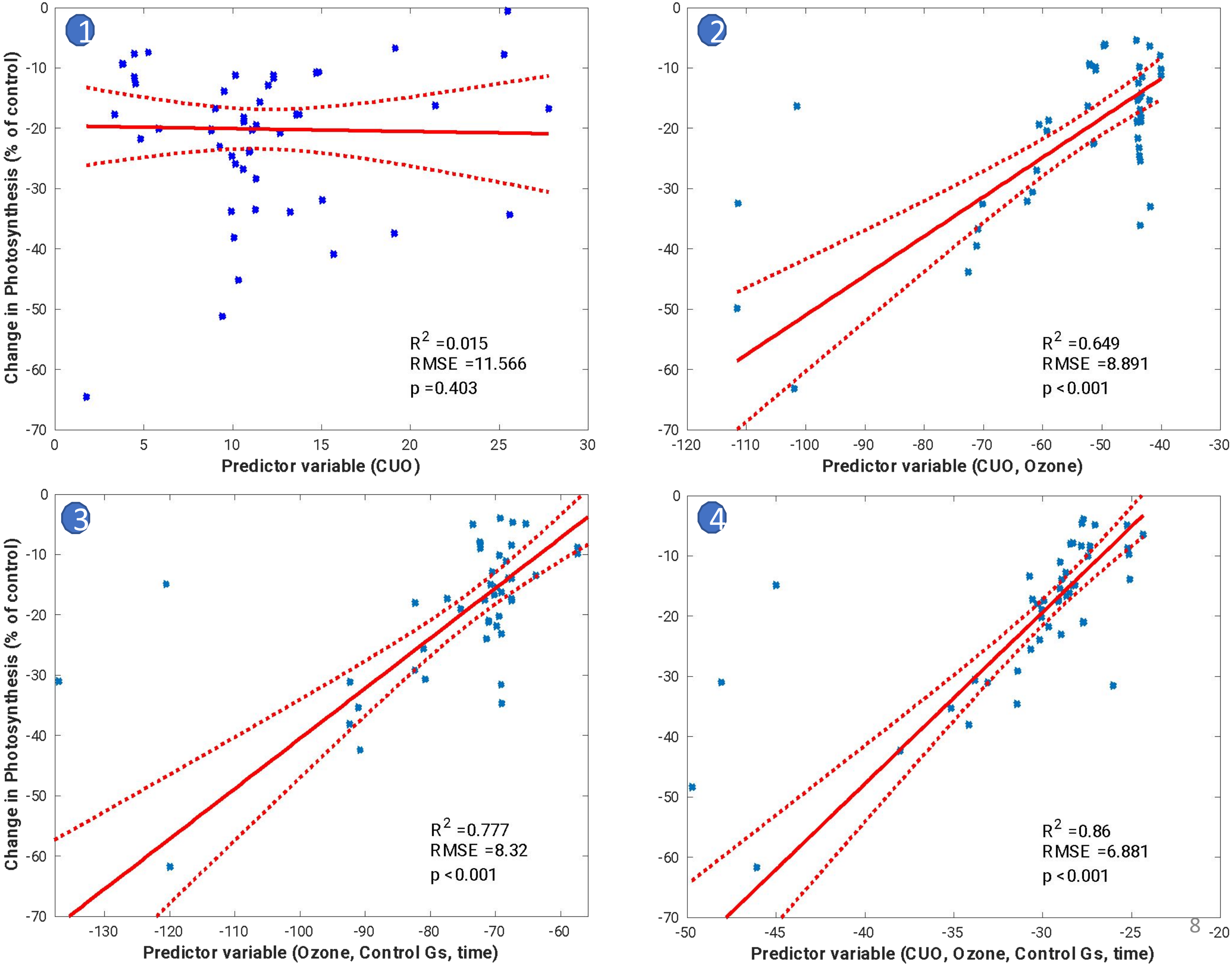


The correlation of **photosynthesis** and **stomatal conductance** to **cumulative uptake of O_3 (CUO)** across **category tree types** for all other categories (1970-2022)

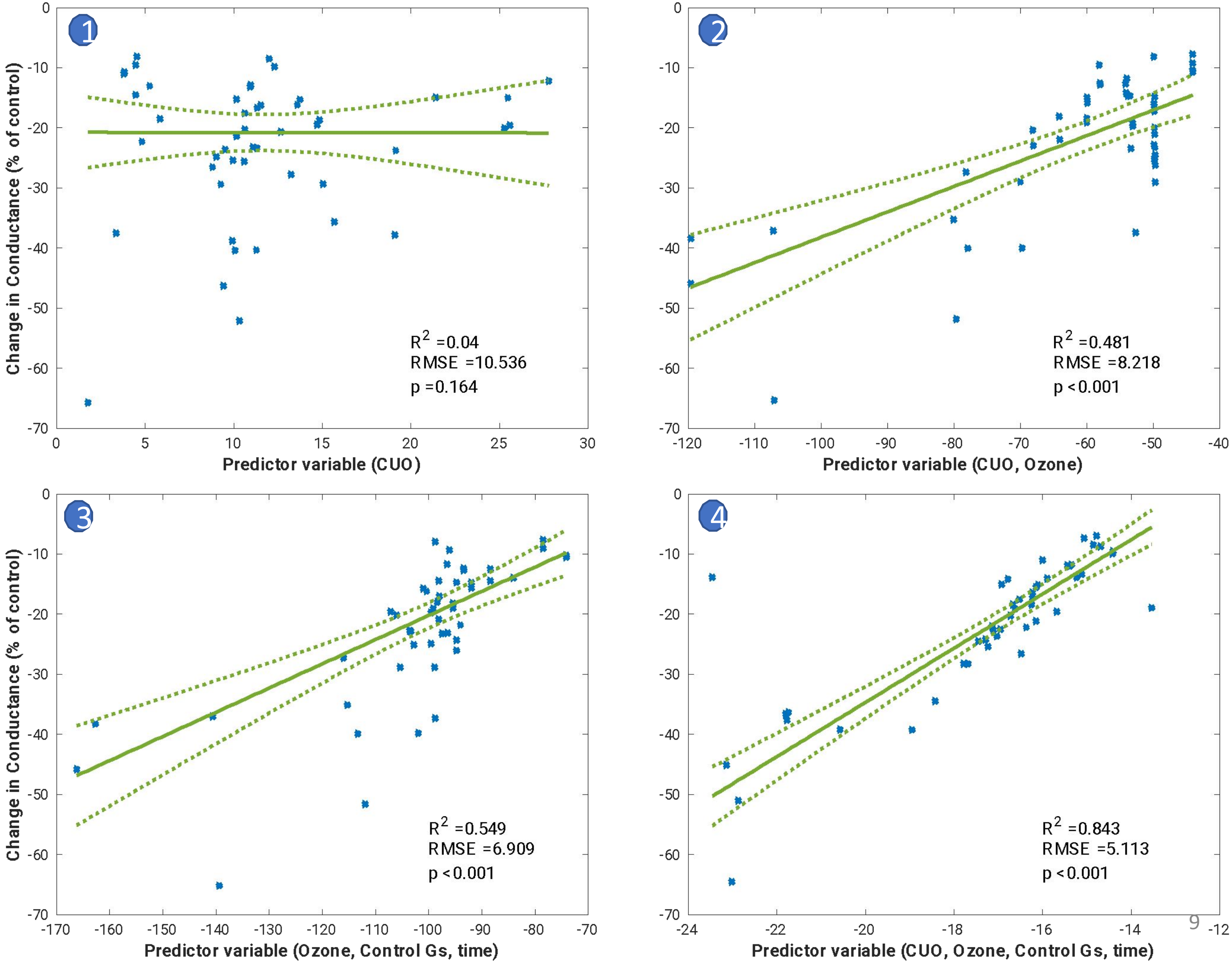


Improved correlation with to predict changes in photosynthesis and stomatal conductance under chronic ozone exposure

Regression for change in photosynthesis due to chronic ozone exposure in **Rice**



Regression for change in conductance due to chronic ozone exposure in **Rice**



Improved correlation with to predict changes in photosynthesis

Plant type	**CUO**			**CUO, Ozone**			**Ozone, Gs, time**			**CUO, Ozone, Gs, time**		
	R^2	RMSE	*p*	**R^2**	RMSE	*p*	**R^2**	RMSE	*p*	**R^2**	RMSE	*p*
Trees												
All trees	**0.01**	19.9	*	**0.045**	20.1	**	**0.047**	20.2	**	**0.046**	20.1	**
Temperate deciduous tree	**0.012**	19.3	0.08	**0.045**	18.9	*	**0.045**	19.02	*	**0.059**	18.8	*
Temperate evergreen tree	**0.085**	24.1	*	**0.086**	25.0	*	**0.103**	26.1	*	**0.391**	22.4	**
Tropical evergreen tree	**0.021**	21.6	0.42	**0.034**	21.9	0.6	**0.381**	17.8	*	**0.752**	15.4	**
Crops												
All crops	**0**	21.4	0.71	**0.231**	18.8	**	**0.258**	18.4	**	**0.381**	17.2	**
Wheat	**0.05**	18.8	*	**0.144**	18.1	**	**0.222**	16.9	**	**0.401**	14.9	**
Soybean	**0.005**	28.5	0.35	**0.307**	23.6	**	**0.370**	22.1	**	**0.457**	20.5	**
Rice	**0.015**	11.6	0.40	**0.649**	8.9	**	**0.777**	8.2	**	**0.860**	6.9	**

Improved correlation with to predict changes in photosynthesis

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Insights from the preliminary results from the testing of new ozone damage parameterization:

Test experimental Set up:

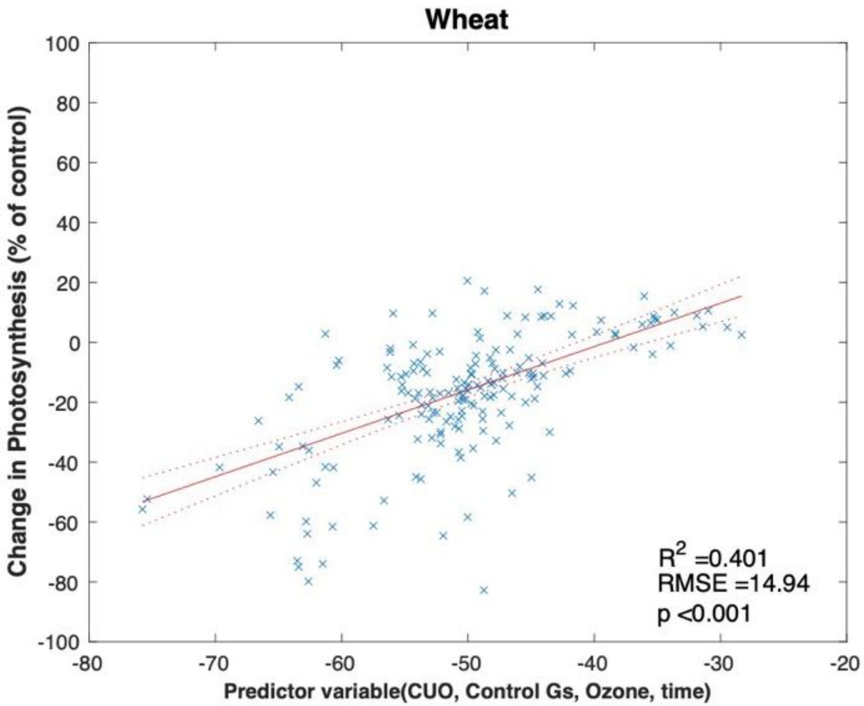
- Single point (41.63° N, 96.65° W) simulation for 2011-2013
- Spring wheat as dominant PFT
- Ozone damage parametrization for wheat
- For ozone concentrations of 100ppb, 70 ppb and 40 ppb

Ozone Parameterization in CLM5

$$photocoef = intercept + CUO * coef$$

New Ozone Parameterization in CLM5

$$photocoef = intercept + CUO * coef1 + Gs * coef2 + O_3 * coef3 + time * coef4$$

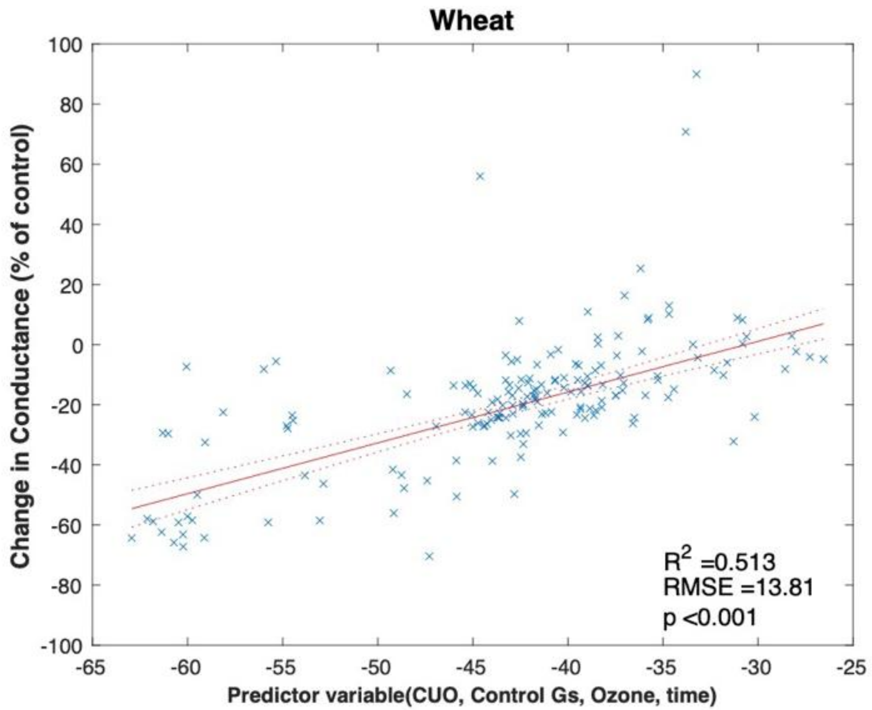



```
Linear regression model (robust fit):
    y ~ 1 + x1 + x2 + x3 + x4
```

Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	56.437	7.5074	7.5175	3.3793e-12
x1	1.3485	0.19623	6.8719	1.237e-10
x2	-0.063854	0.0095745	-6.6692	3.7002e-10
x3	-0.5154	0.057702	-8.9322	7.9151e-16
x4	-0.091575	0.011044	-8.2917	3.7344e-14

```
Number of observations: 170, Error degrees of freedom: 165
Root Mean Squared Error: 14.9
R-squared: 0.401,  Adjusted R-Squared: 0.387
F-statistic vs. constant model: 27.6, p-value = 1.46e-17
```



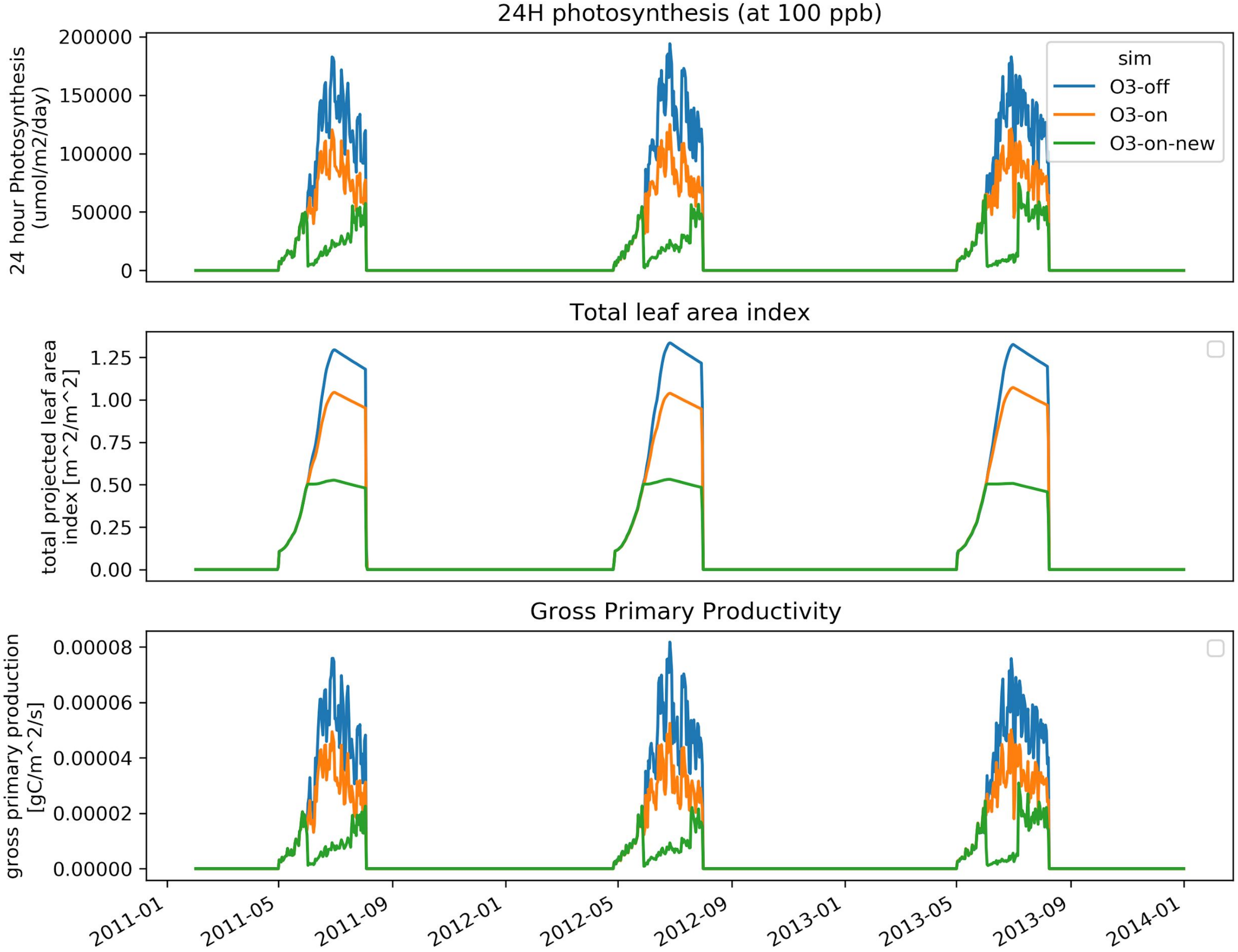

```
Linear regression model (robust fit):
    y ~ 1 + x1 + x2 + x3 + x4
```

Estimated Coefficients:

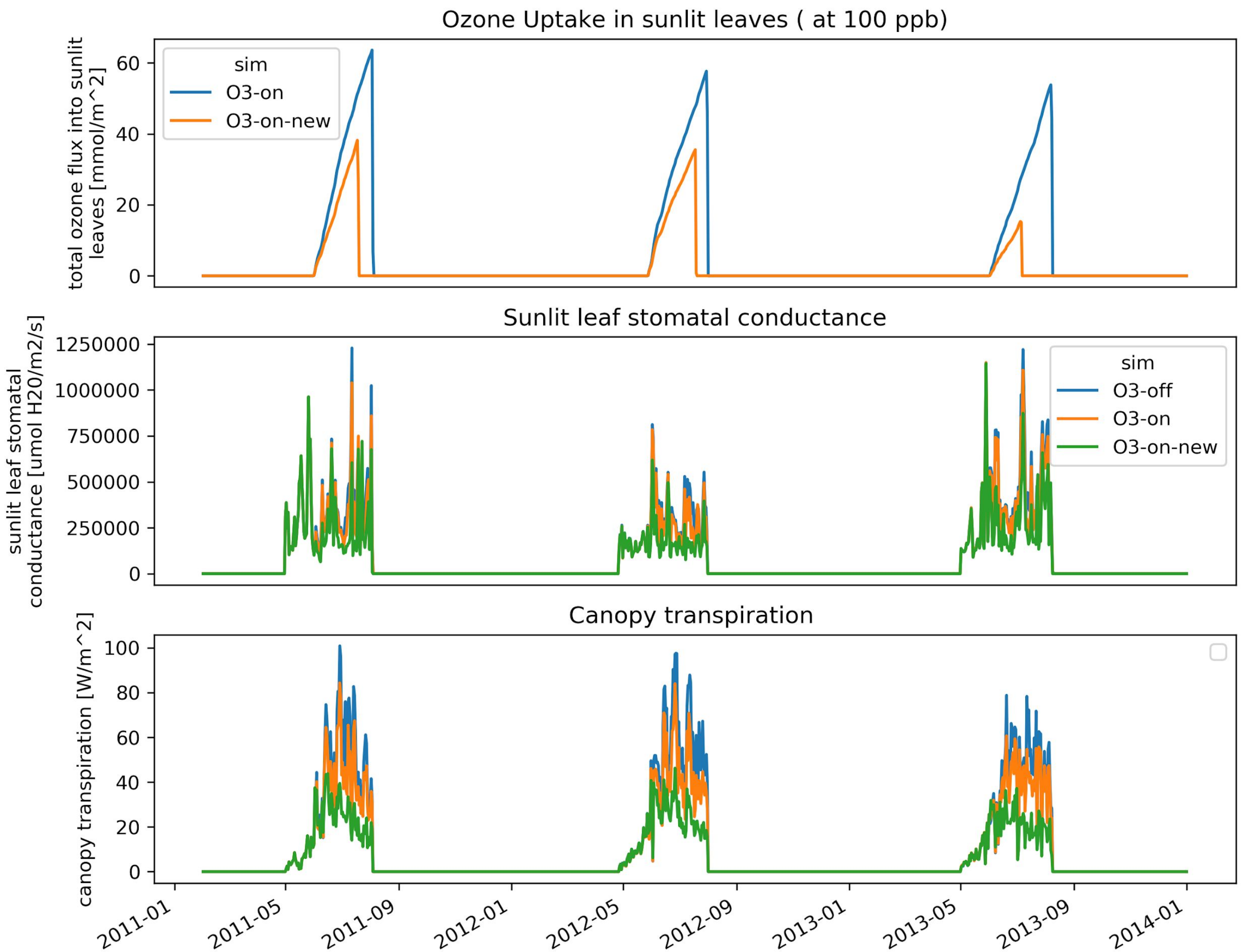
	Estimate	SE	tStat	pValue
(Intercept)	51.789	6.9394	7.4631	4.605e-12
x1	1.5624	0.18138	8.6135	5.4553e-15
x2	-0.060244	0.00885	-6.8072	1.7577e-10
x3	-0.63506	0.053336	-11.907	5.4591e-24
x4	-0.082425	0.010209	-8.0741	1.3495e-13

```
Number of observations: 170, Error degrees of freedom: 165
Root Mean Squared Error: 13.8
R-squared: 0.513,  Adjusted R-Squared: 0.501
F-statistic vs. constant model: 43.4, p-value = 7.51e-25
```

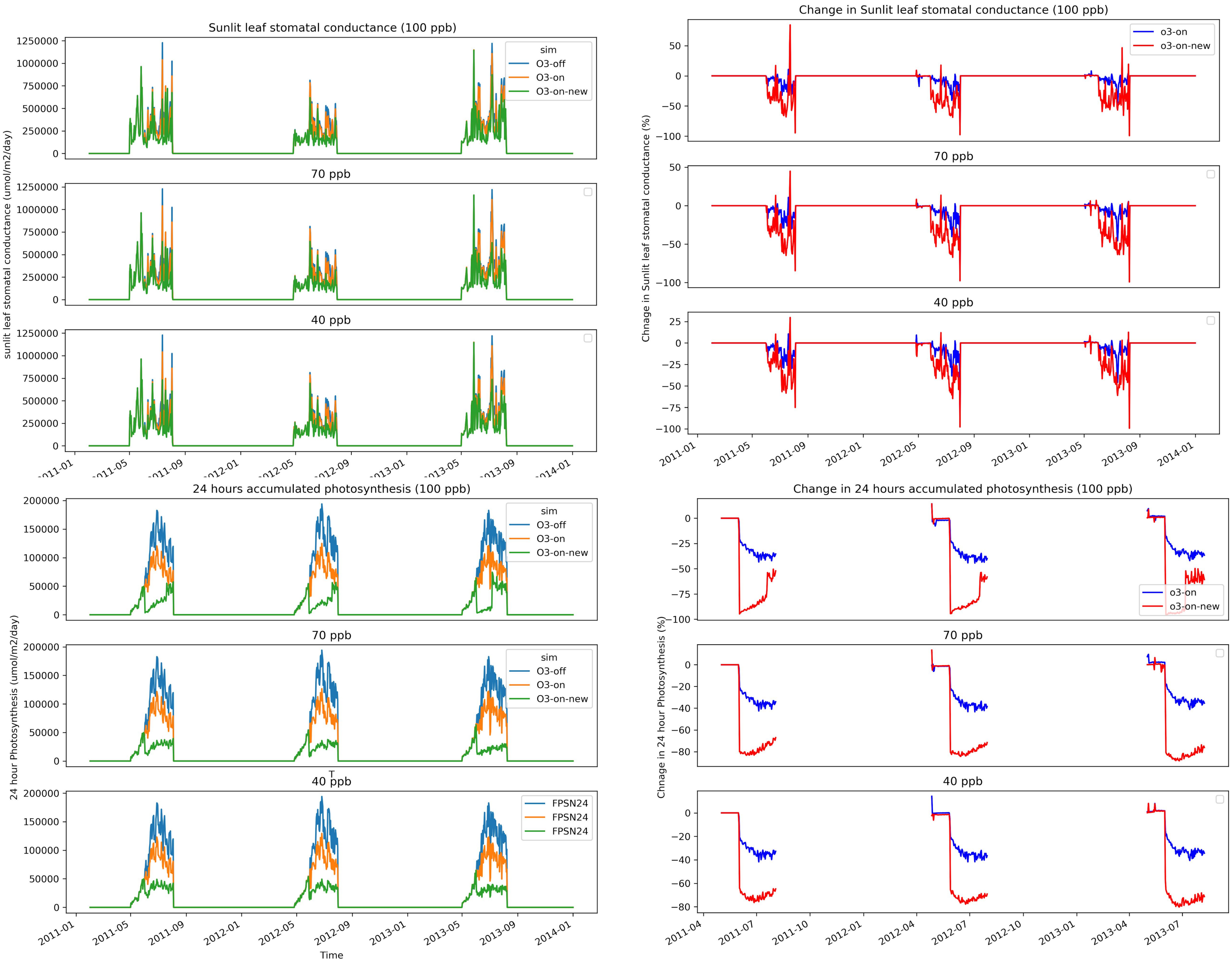
Photosynthesis, TLAI and GPP at 100 pb



O_3 uptake, conductance and canopy transpiration at 100 ppb



Changes under different ozone concentrations



Findings from the preliminary simulations

- The new ozone parameterization is not very sensitive to change in O_3 for change in photosynthesis and stomatal conductance
- The decrease in photosynthesis is very large compared to stomatal conductance
- One reason might be mismatch between timestep (and possibly variable units) in the parametrization and model
- The sudden drop in photosynthesis seems to be related with spike in plant stomatal conductance
- These might be due to lack of sufficient stomatal conductance data in the observation dataset used to derive the parameterization

Step forward from the preliminary simulations

- Fine-tuning of the parameterization to ensure accurate translation of the derived parameterization from observational data to the model
- The new parameterization introduces four variables, adding complexity to tune the model
- Considering the model's variable units and time frequency to fine tune tune the parameterization
- Regional and global simulations to further refine and tune the parameterization
- Defining upper and lower limit coefficients for the variables in the parameterization
- These limits will help ensure that the parameterization remains within a realistic and feasible range

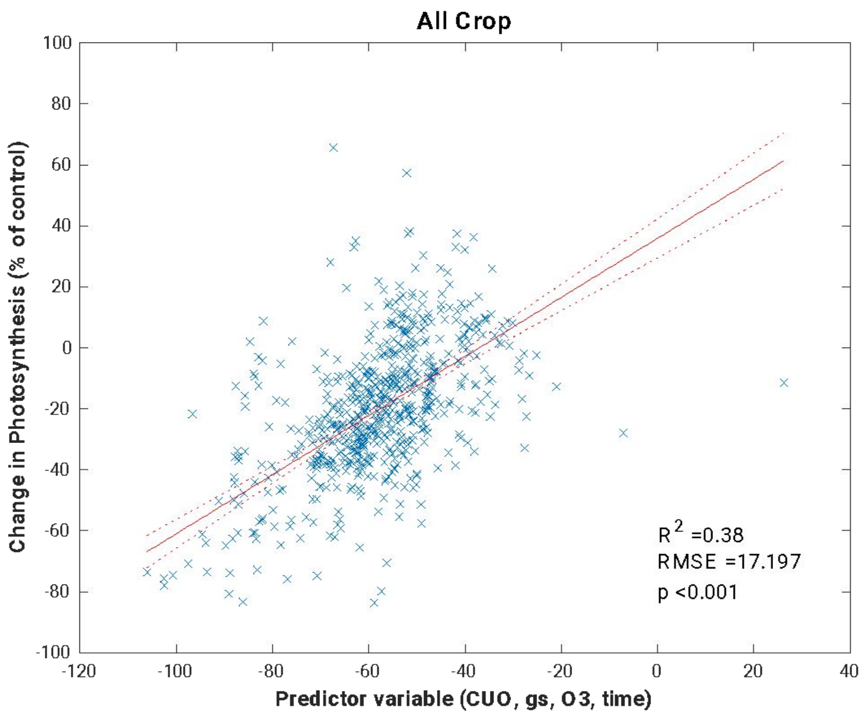

Thank You

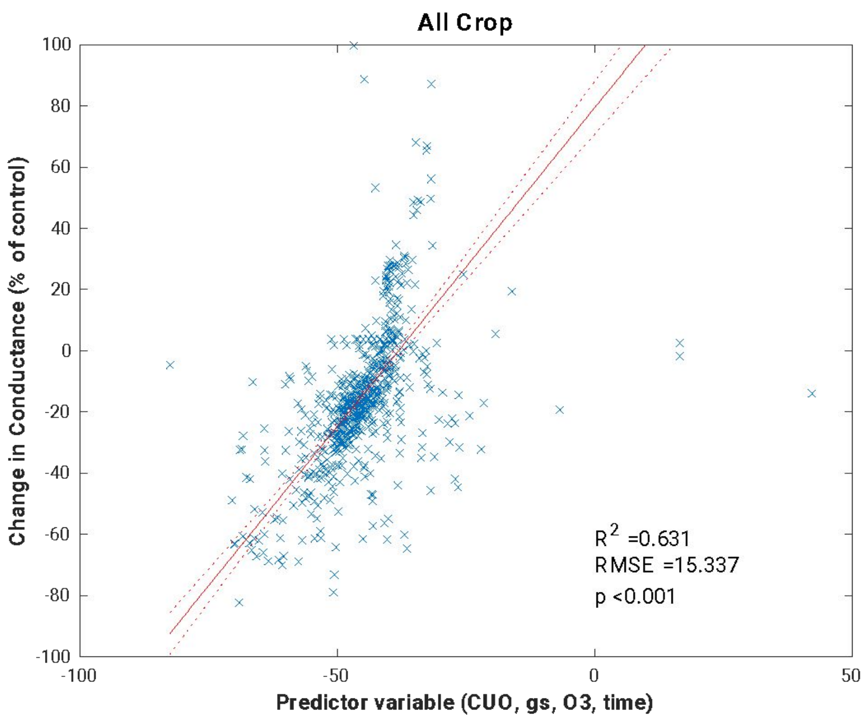
Appendices

Categories and levels describing the data collected from experiments studying ozone effects on photosynthesis and stomatal conductance

Category	Categorical Level					
Plant Type	Crop (81, 903)	Shrub (9, 35)	Grasses (C3 & C4) (5, 11)	Herbaceous (13, 49)	Temperate deciduous tree (84, 775)	Temperate evergreen tree (21, 180)	Tropical evergreen tree (9,48)
Crop Type	Wheat (30, 276)	Soybean (13, 209)	Rice (9, 94)	Maize (2, 26)	Pulses (8, 202)	Sugarcane (1,8)	Cotton (1,4)
Control Air	Ambient (56,716)	Charcoal filtered (166, 1225)					
Exposure System	Greenhouse (9, 125)	Growth chamber (69, 505)	Open-top chamber (92, 935)	Free-air enrichment (52, 382)			
Ozone conc. bins (ppb)	25 to 50 (11, 159)	50-75 (76, 421)	75-100 (74, 751)	100-125 (13, 197)	125-150 (12, 64)	>150 (7, 44)	
Rooting environment	Pot (163, 1316)	Ground (72, 626)					
Vulnerability to Ozone	Low (42, 230)	Med (99, 890)	High (81, 765)				
Data Confidence	Low (98, 698)	Med (104, 919)	High (14, 84)				

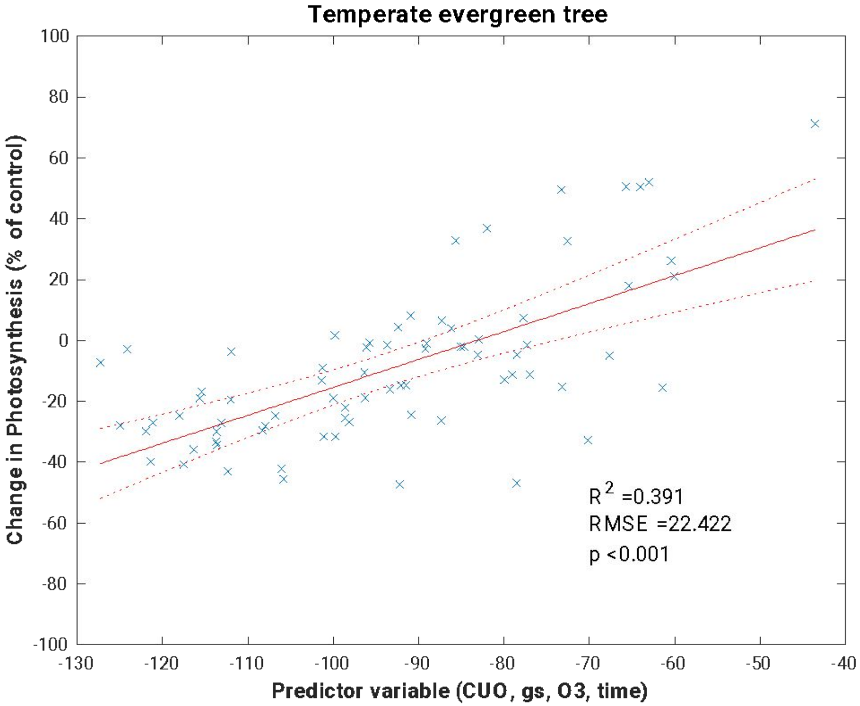
- Data from 235 papers (almost 1600 data points) published from 1970 till the present.
- Data points within the associated categorical level: (# of studies, # of data points).
- For details see Lombardozzi et al. (2013)

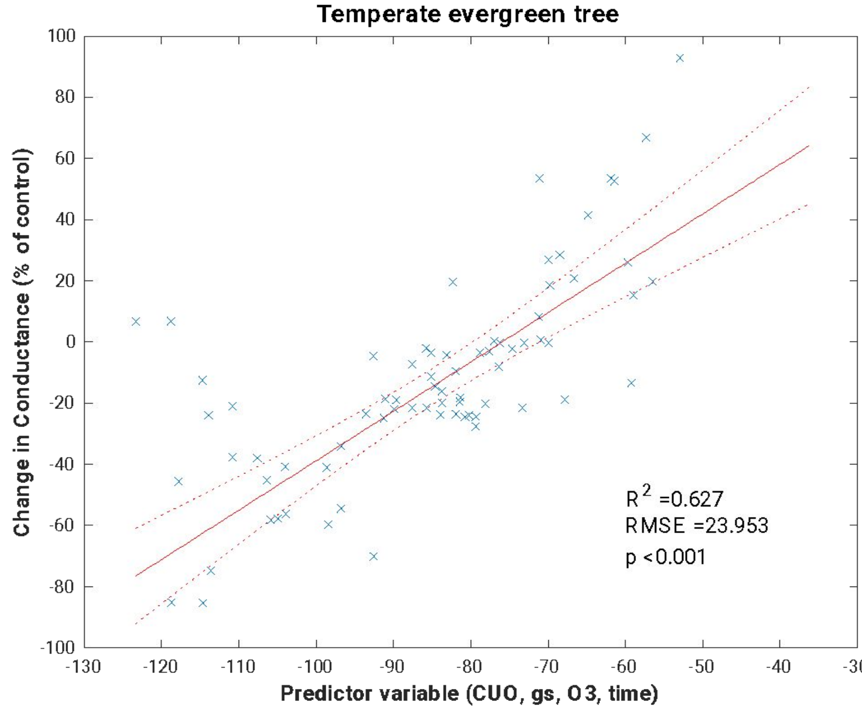





```
Linear regression model (robust fit):
    y ~ 1 + x1 + x2 + x3 + x4

Estimated Coefficients:
                   Estimate        SE         tStat       pValue
                   _________    _________    _______    __________

    (Intercept)       35.916        3.899     9.2114    4.5635e-19
    x1                0.7571     0.069149     10.949    1.0932e-25
    x2             -0.022521    0.0051473    -4.3754    1.4154e-05
    x3              -0.60271     0.034128    -17.661    3.8364e-57
    x4             -0.052714    0.0046008    -11.458    8.9825e-28


Number of observations: 644, Error degrees of freedom: 639
Root Mean Squared Error: 17.2
R-squared: 0.38,  Adjusted R-Squared: 0.376
F-statistic vs. constant model: 97.7, p-value = 7.34e-65
```

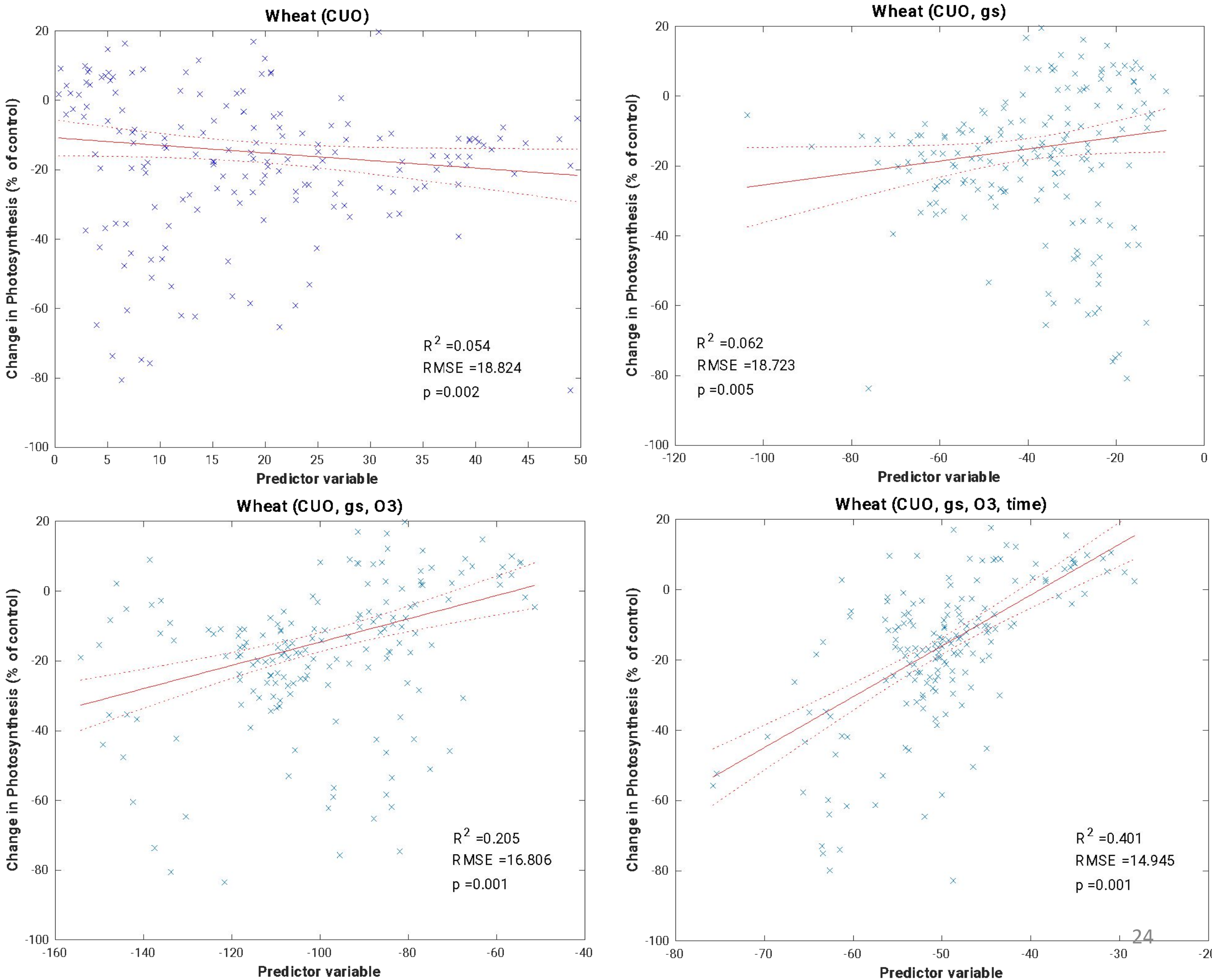
```
Linear regression model (robust fit):
    y ~ 1 + x1 + x2 + x3 + x4

Estimated Coefficients:
                   Estimate        SE         tStat        pValue
                   _________    _________    _______    ___________

    (Intercept)       79.447       3.4774     22.847      6.583e-85
    x1                1.9443     0.061671     31.527    2.6104e-132
    x2              -0.11146    0.0045906    -24.279     9.1678e-93
    x3              -0.73252     0.030437    -24.067     1.3452e-91
    x4             -0.090727    0.0041032    -22.111     6.8613e-81


Number of observations: 644, Error degrees of freedom: 639
Root Mean Squared Error: 15.3
R-squared: 0.631,  Adjusted R-Squared: 0.629
F-statistic vs. constant model: 274, p-value = 7.03e-137
```

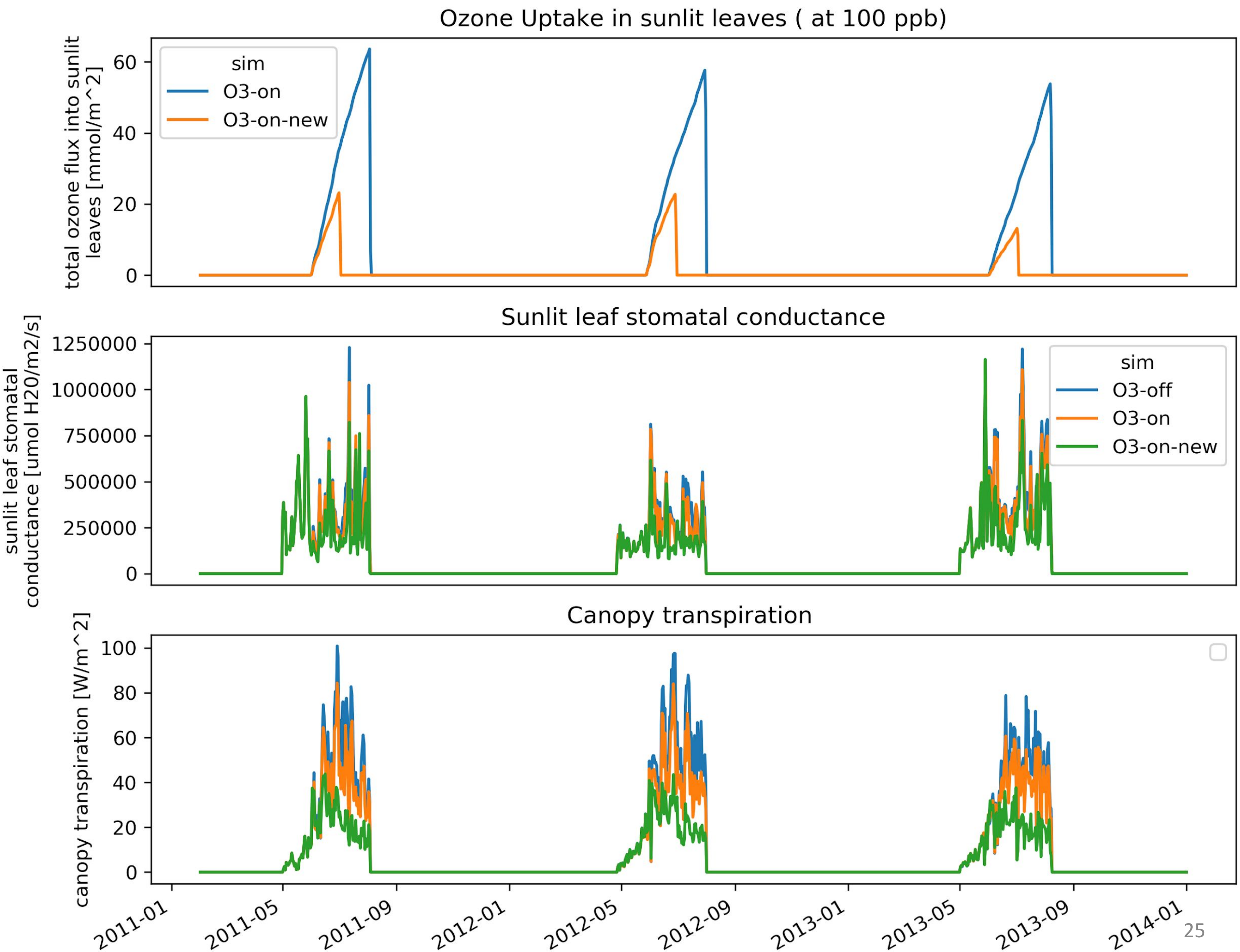


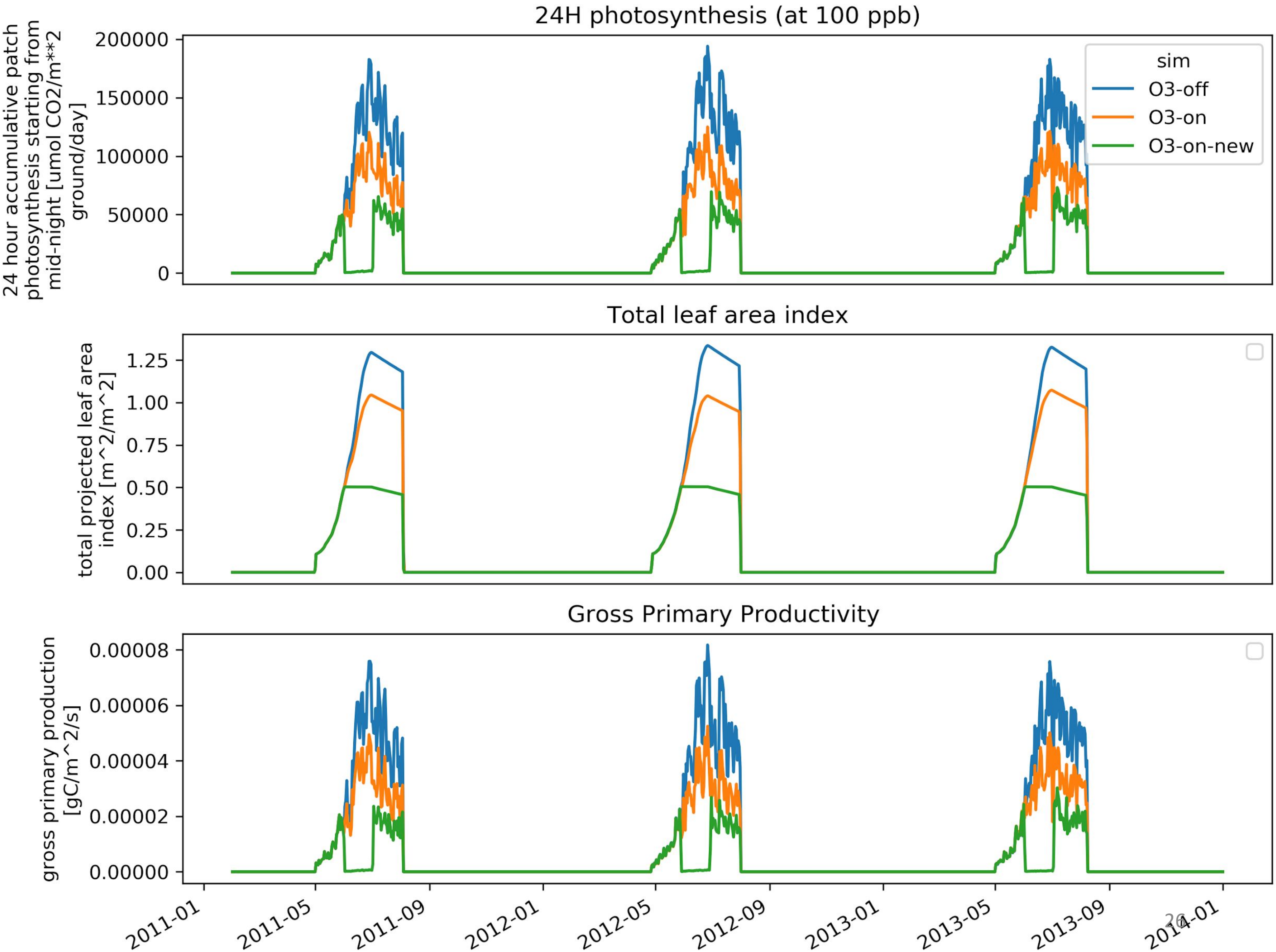


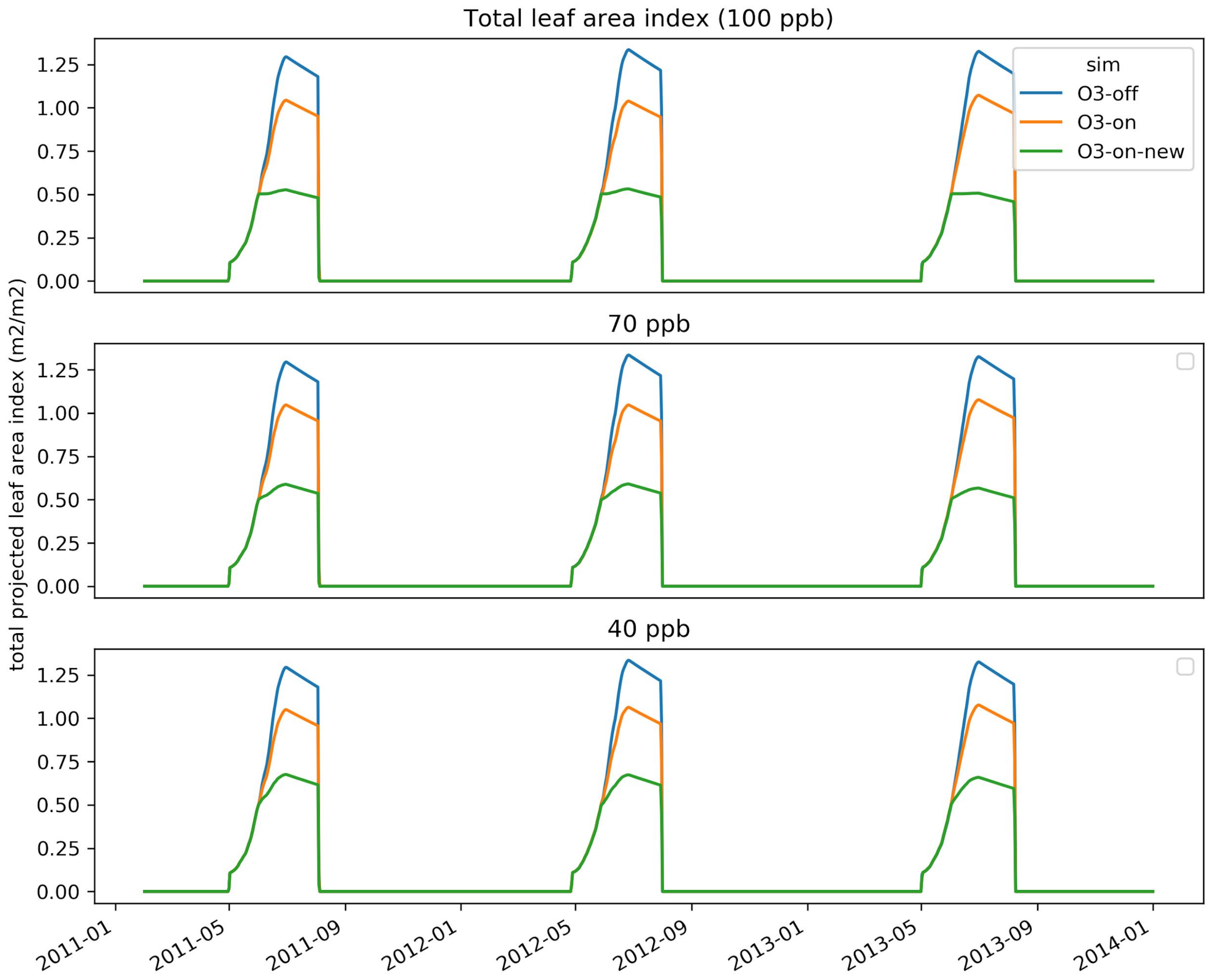

```
Linear regression model (robust fit):
    y ~ 1 + x1 + x2 + x3 + x4

Estimated Coefficients:
                   Estimate        SE         tStat       pValue
                  __________    _________    _______    __________

    (Intercept)       76.377       18.765     4.0702    0.00012032
    x1               0.45913     0.084145     5.4564    6.7214e-07
    x2              -0.26435     0.042701    -6.1908    3.4436e-08
    x3              -0.74932      0.23411    -3.2007     0.0020512
    x4            -0.0074396    0.0018736    -3.9707    0.00016967


Number of observations: 76, Error degrees of freedom: 71
Root Mean Squared Error: 22.4
R-squared: 0.391,  Adjusted R-Squared: 0.357
F-statistic vs. constant model: 11.4, p-value = 3.37e-07
```

```
Linear regression model (robust fit):
    y ~ 1 + x1 + x2 + x3 + x4

Estimated Coefficients:
                   Estimate        SE         tStat       pValue
                  __________    _________    _______    __________

    (Intercept)       122.64       20.046     6.1179     4.647e-08
    x1               0.69696      0.08989     7.7535    4.7888e-11
    x2              -0.43097     0.045616    -9.4479    3.5107e-14
    x3                -1.391       0.2501    -5.5618    4.4192e-07
    x4            -0.0093298    0.0020015    -4.6613    1.4317e-05


Number of observations: 76, Error degrees of freedom: 71
Root Mean Squared Error: 24
R-squared: 0.627,  Adjusted R-Squared: 0.606
F-statistic vs. constant model: 29.8, p-value = 1.5e-14
```

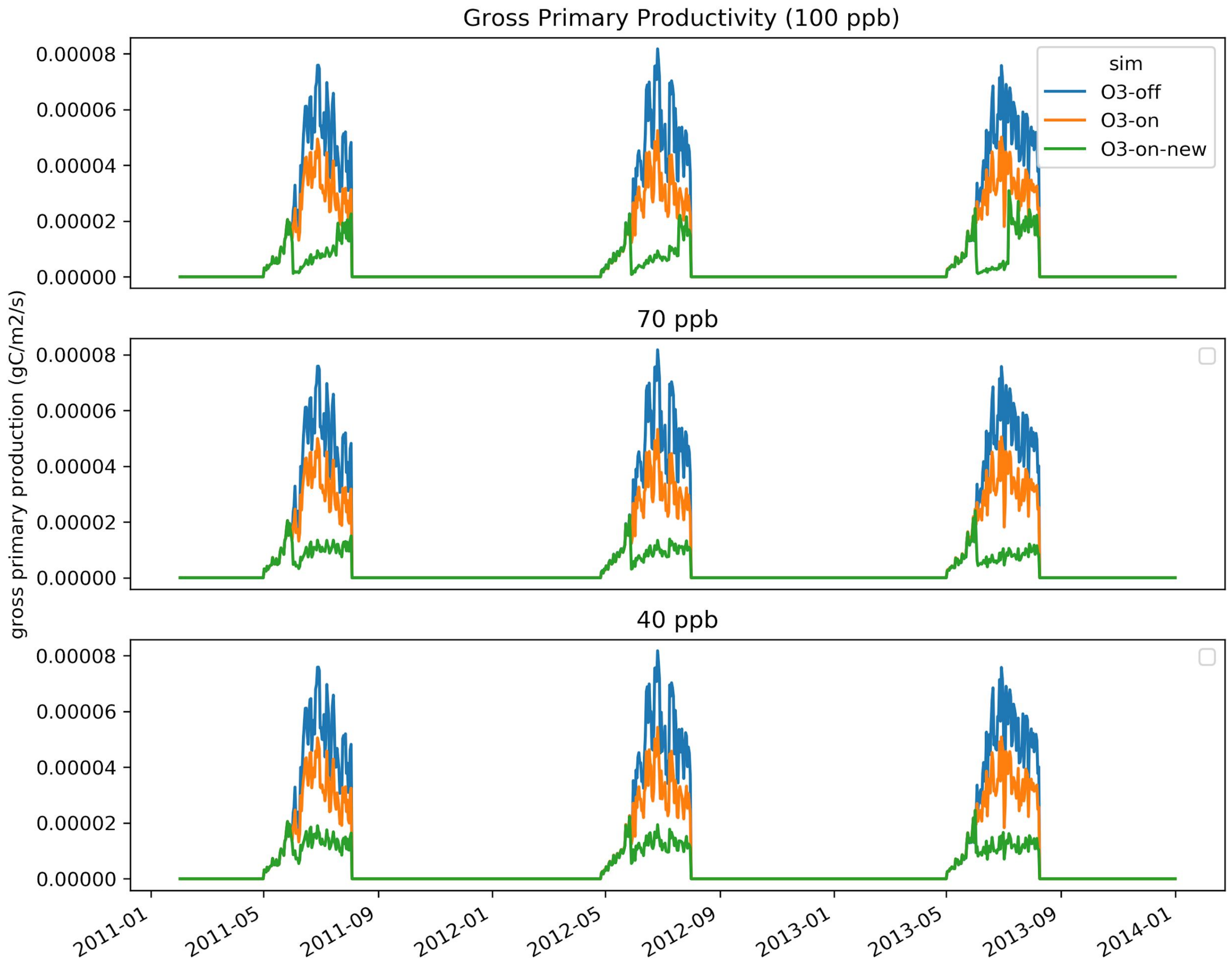

Wheat (CUO)
Change in Photosynthesis (% of control)
Predictor variable
R 2 =0.054
RMSE =18.824
p =0.002
Wheat (CUO, gs)
Change in Photosynthesis (% of control)
Predictor variable
R 2 =0.062
RMSE =18.723
p =0.005
Wheat (CUO, gs, O3)
Change in Photosynthesis (% of control)
Predictor variable
R 2 =0.205
RMSE =16.806
p =0.001
Wheat (CUO, gs, O3, time)
Change in Photosynthesis (% of control)
Predictor variable
R 2 =0.401
RMSE =14.945
p =0.001


Ozone Uptake in sunlit leaves (at 100 ppb)
total ozone flux into sunlit leaves [mmol/m^2]
sim
O3-on
O3-on-new
Sunlit leaf stomatal conductance
sunlit leaf stomatal conductance [umol H20/m2/s]
sim
O3-off
O3-on
O3-on-new
Canopy transpiration
canopy transpiration [W/m^2]
2011-01
2011-05
2011-09
2012-01
2012-05
2012-09
2013-01
2013-05
2013-09
2014-01


24H photosynthesis (at 100 ppb)
24 hour accumulative patch photosynthesis starting from mid-night [umol CO2/m**2 ground/day]
200000
150000
100000
50000
0
sim
O3-off
O3-on
O3-on-new
Total leaf area index
total projected leaf area index [m^2/m^2]
1.25
1.00
0.75
0.50
0.25
0.00
Gross Primary Productivity
gross primary production [gC/m^2/s]
0.00008
0.00006
0.00004
0.00002
0.00000
2011-01
2011-05
2011-09
2012-01
2012-05
2012-09
2013-01
2013-05
2013-09
2014-01

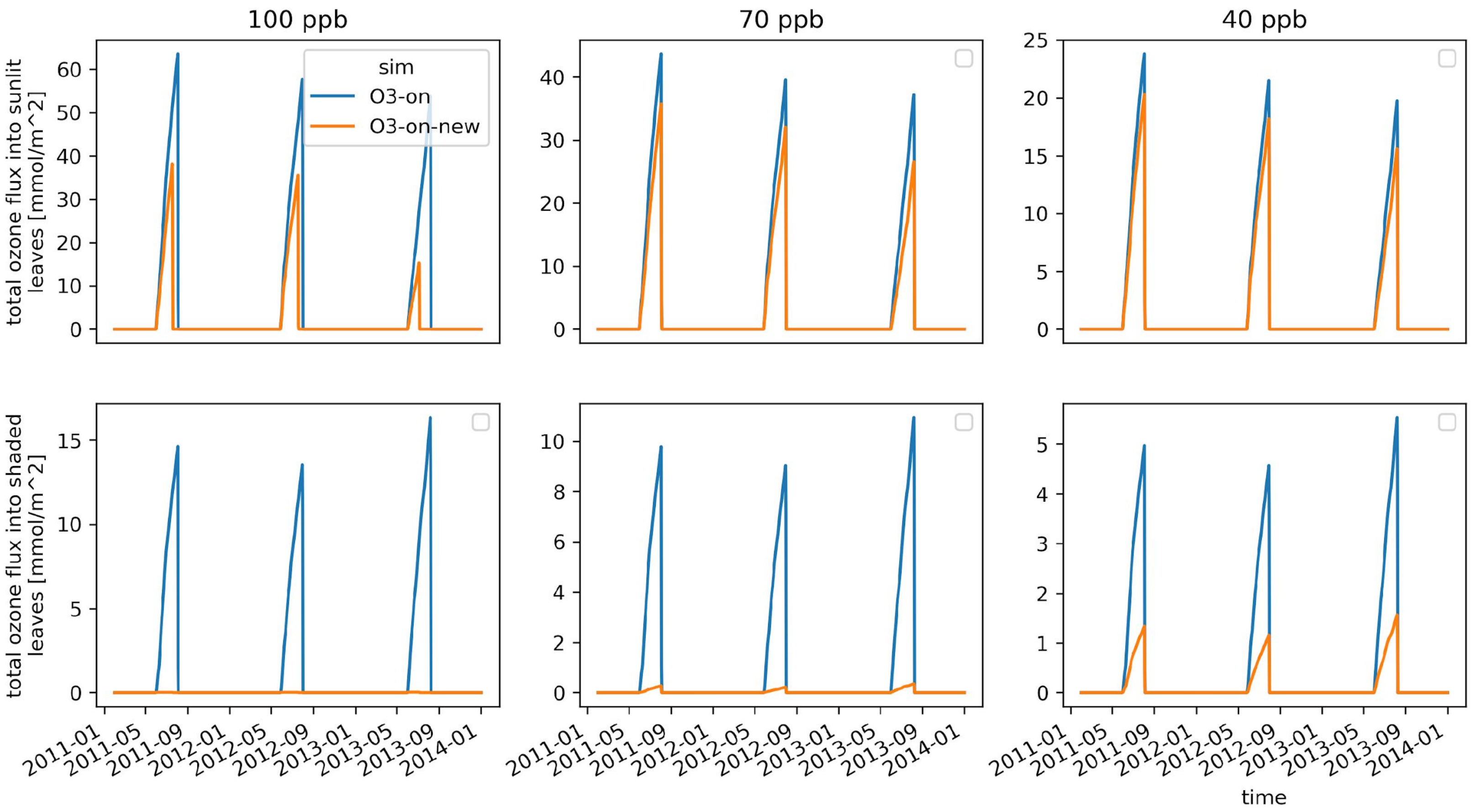


Total leaf area index (100 ppb)
70 ppb
40 ppb
sim
O3-off
O3-on
O3-on-new
total projected leaf area index (m2/m2)
0.00
0.25
0.50
0.75
1.00
1.25
2011-01
2011-05
2011-09
2012-01
2012-05
2012-09
2013-01
2013-05
2013-09
2014-01

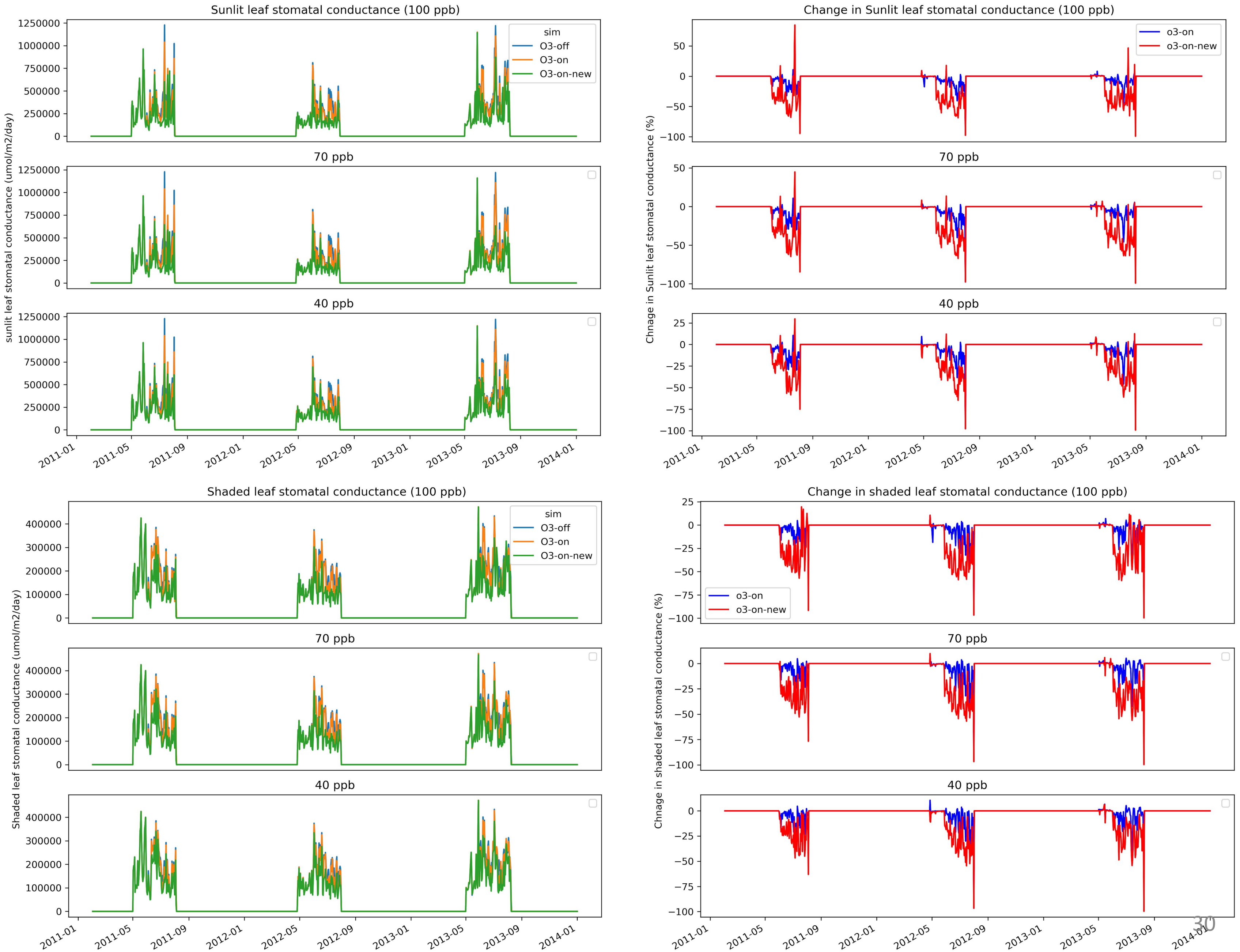


Gross Primary Productivity (100 ppb)
70 ppb
40 ppb
gross primary production (gC/m2/s)
0.00008
0.00006
0.00004
0.00002
0.00000
sim
O3-off
O3-on
O3-on-new
2011-01
2011-05
2011-09
2012-01
2012-05
2012-09
2013-01
2013-05
2013-09
2014-01

Total Ozone flux in sunlit and shaded leaves



Change in sunlit and shaded Stomatal conductance



```fortran
  ! o3:h2o resistance ratio defined by Sitch et al. 2007
  real(r8), parameter :: ko3 = 1.67_r8

  ! LAI threshold for LAIs that asymptote and don't reach 0
  real(r8), parameter :: lai_thresh = 0.5_r8

  ! threshold below which o3flux is set to 0 (nmol m^-2 s^-1)
  real(r8), parameter :: o3_flux_threshold = 0.8_r8

  ! o3 intercepts and slopes for photosynthesis
  real(r8), parameter :: needleleafPhotoInt   = 0.8390_r8  ! units = unitless
  real(r8), parameter :: needleleafPhotoSlope = 0._r8      ! units = per mmol m^-2
  real(r8), parameter :: broadleafPhotoInt    = 0.8752_r8  ! units = unitless
  real(r8), parameter :: broadleafPhotoSlope  = 0._r8      ! units = per mmol m^-2
  real(r8), parameter :: nonwoodyPhotoInt     = 0.8021_r8  ! units = unitless
  real(r8), parameter :: nonwoodyPhotoSlope   = -0.0009_r8 ! units = per mmol m^-2

  ! o3 intercepts and slopes for conductance
  real(r8), parameter :: needleleafCondInt    = 0.7823_r8  ! units = unitless
  real(r8), parameter :: needleleafCondSlope  = 0.0048_r8  ! units = per mmol m^-2
  real(r8), parameter :: broadleafCondInt     = 0.9125_r8  ! units = unitless
  real(r8), parameter :: broadleafCondSlope   = 0._r8      ! units = per mmol m^-2
  real(r8), parameter :: nonwoodyCondInt      = 0.7511_r8  ! units = unitless
  real(r8), parameter :: nonwoodyCondSlope    = 0._r8      ! units = per mmol m^-2

  character(len=*), parameter, private :: sourcefile = &
       __FILE__

contains

  ! ========================================================================
```