Improving ozone damage parameterization in CLM5

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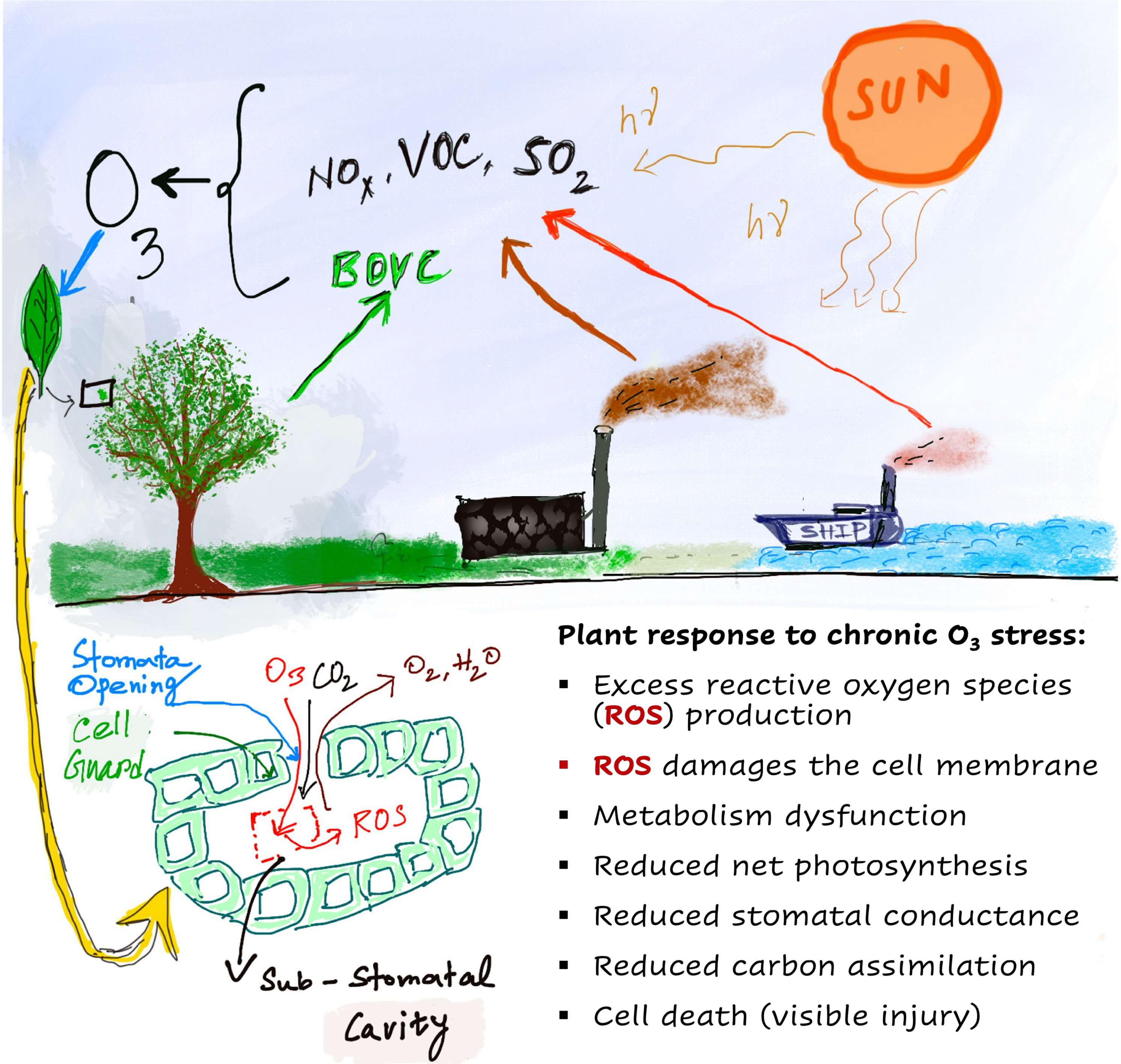


SUN
hν
hν
O3
NOx, VOC, SO2
BOVC
SHIP
Stomata Opening
Cell Guard
O3 CO2
O2, H2O
ROS
Sub-Stomatal Cavity
Plant response to chronic O3 stress:
Excess reactive oxygen species (ROS) production
ROS damages the cell membrane
Metabolism dysfunction
Reduced net photosynthesis
Reduced stomatal conductance
Reduced carbon assimilation
Cell death (visible injury)

Ozone damage parameterization in CLM5

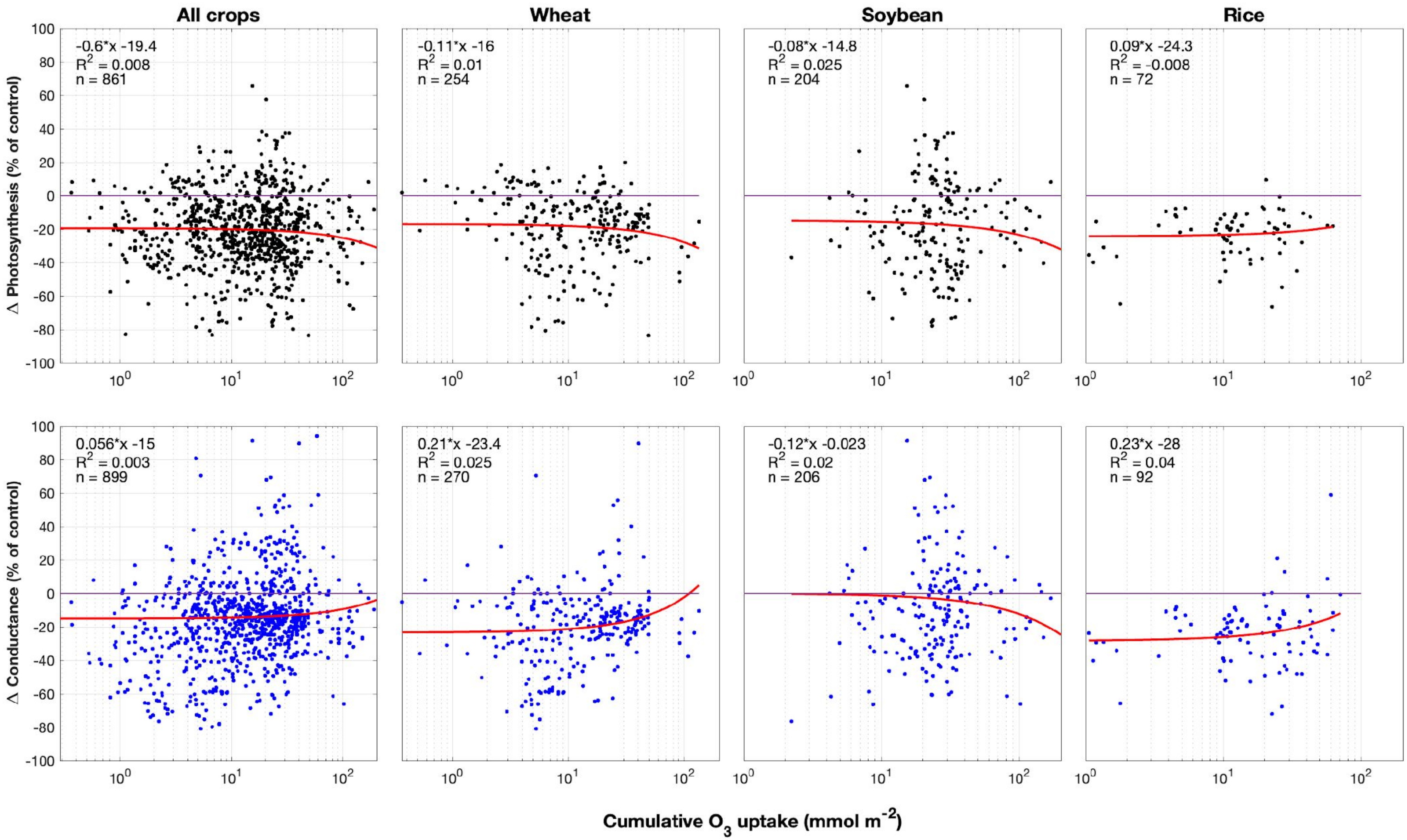
- Ozone damage on vegetation in CLM5 is directly and independently influenced by **photosynthesis** and **stomatal conductance** based on the cumulative uptake of ozone (**CUO**) through stomata (Lombardozzi et al., 2015; Lombardozzi et al., 2013; Lawrence, 2019).
- The impact of ozone is estimated for three broad plant functional types (PFTs):
  1. Broadleaf trees and shrubs
  2. Needleleaf trees and shrubs, and
  3. Crops and grasses
- Through this study, our goal is to improve the ozone damage function by analyzing peer-reviewed ozone damage experimental data.
- We gathered ozone damage experiments for various plants, crops, grasses, pulses etc., therefore, another goal is to develop unique ozone damage parameterization for different PFTs (e.g., wheat, rice, soybean, tropical evergreen trees, C4 crops).

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

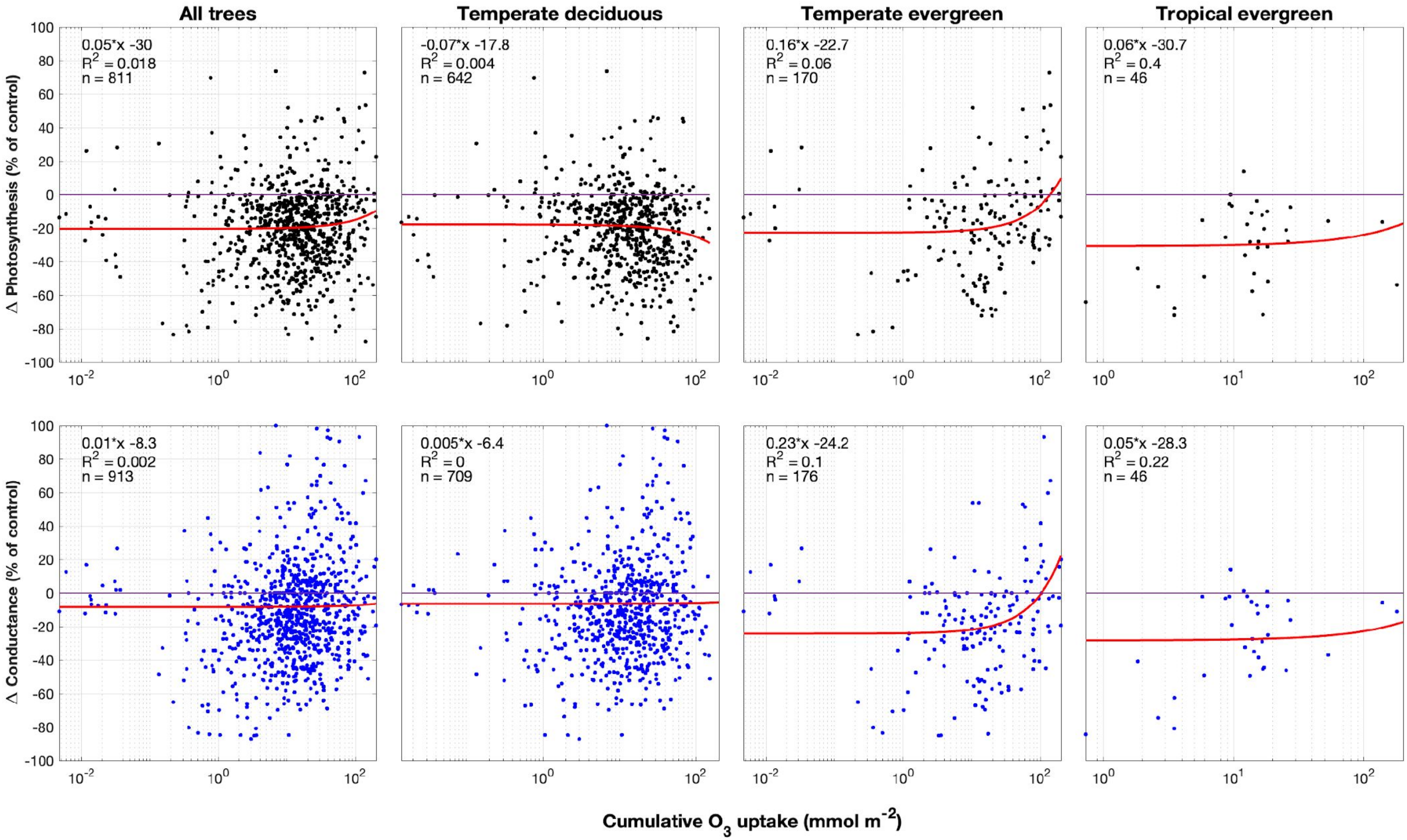
Category	Categorical Level						
Plant Type	Crop (81, 903)	Shrub (9, 35)	Grasses (C3 & C4) (5, 11)	Herbaceous (13, 49)	Temperate deciduous tree (84, 775)	Temperate evergreen tree (21, 180)	Tropical evergreen tree (9,48)
Crop Type	Wheat (30, 276)	Soybean (13, 209)	Rice (9, 94)	Maize (2, 26)	Pulses (8, 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).

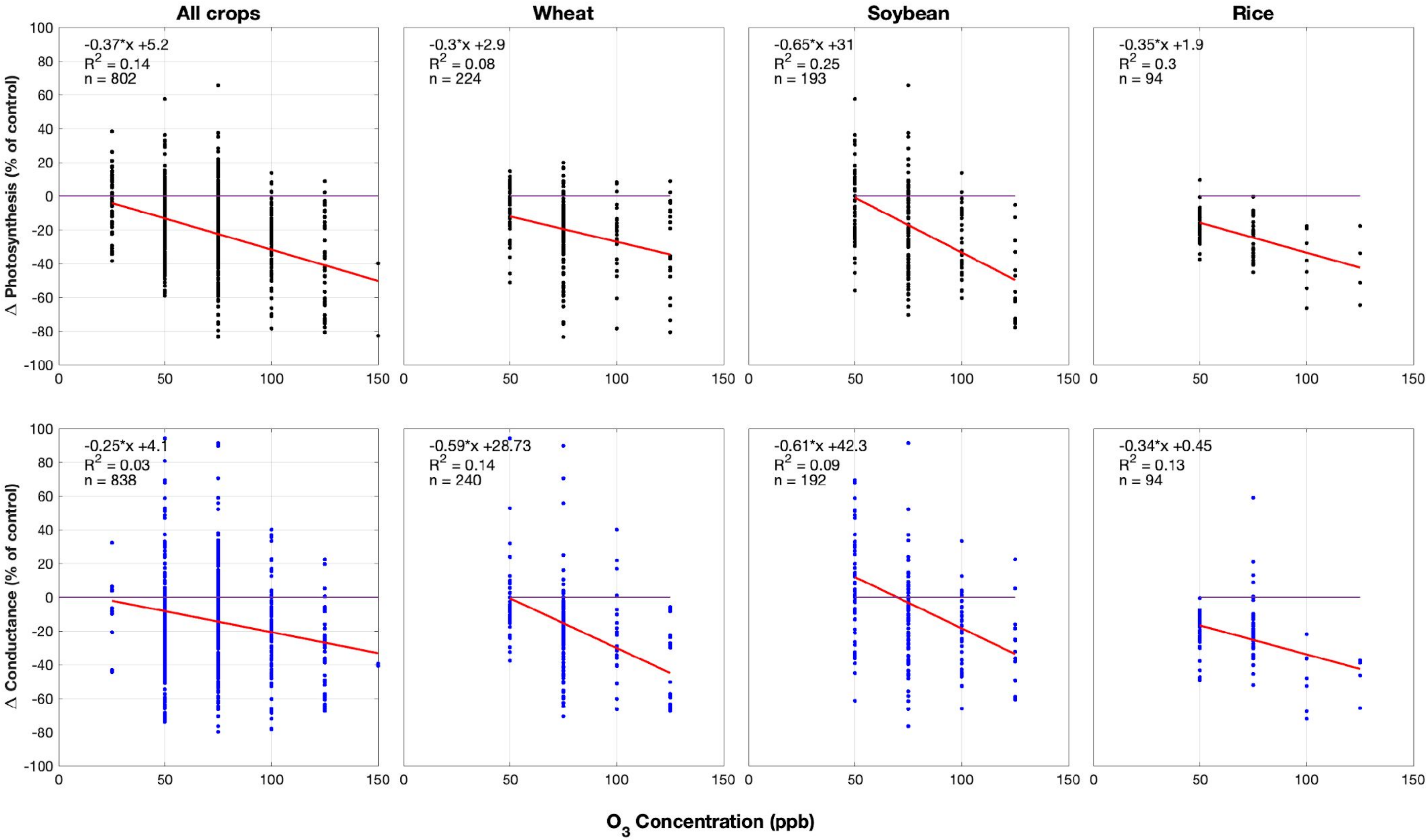
The correlation of **photosynthesis** and **stomatal conductance** to **cumulative uptake of O_3 (CUO)** across **category crop types** for all other categories (1970-2022)



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



The correlation of **photosynthesis** and **stomatal conductance** to **O_3 concentration-bins** across **category crop types** for all categories (1970-2022)



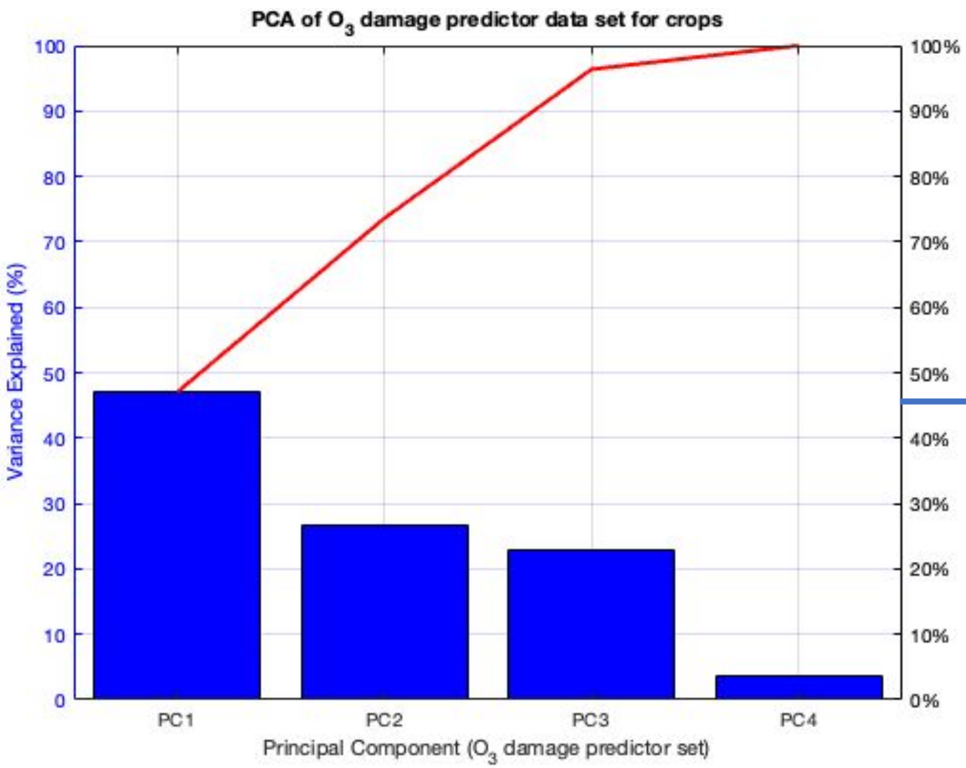
Conclusions from the data analysis using Lombardozzi et al. (2013) methodology

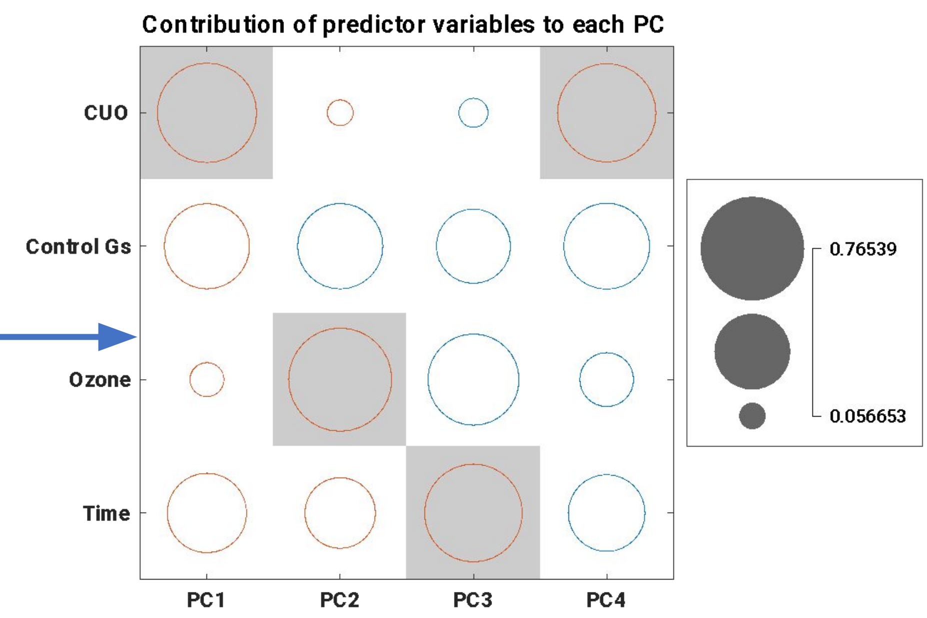
- On average all the crops shows reduction in photosynthesis (21%) and stomatal conductance (14%), highest for rice (23% and 24%, respectively).
- On average crops are more sensitive to chronic ozone exposure than trees.
- The correlation between **CUO (*Cumulative ozone uptake)***and change in photosynthesis and conductance is not significant, the correlation improves if predictor variable is **Ozone concentrations.**
- The experimental data shows different crops and trees are affected differently and hence should have unique ozone damage function in CLM5.
- ***CUO*** is integrated O_3 flux into leaves through time and is an indicator of ozone uptake but taking **Ozone *concentration*** into account while deriving plant damage is crucial.
- **CUO** calculation is directly proportional to **stomatal conductance (Gs)** of the plant, **ozone concentration** and **total exposure time**.
- **However, a plant can have similar CUO values for various condition, e.g.,**

  1. **low ozone concentration, for a long duration**
  2. **high ozone concentration, for a shorter duration**
  3. **high ozone concentration, for a longer duration but, have low Gs**

Analyzing the properties of the ozone experimental data for category crop:

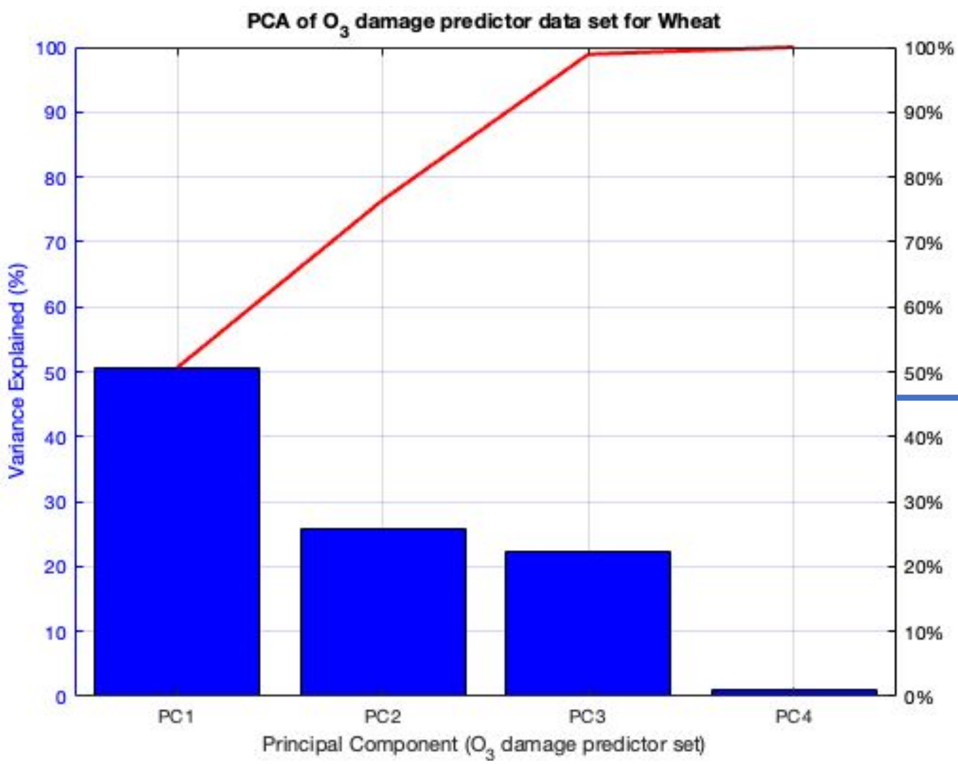
1. Almost 95% variance in the data can be explained by 3 principal components (PC).
2. However, all predictor variables (**CUO** ,$\mathbf{G_s}$, **ozone concentration** and **total exposure time**) have significance contribution in each PC with varying weight.
3. This might be the reason that no significant correlation of CUO alone could not be seen with change in photosynthesis or stomatal conductance.

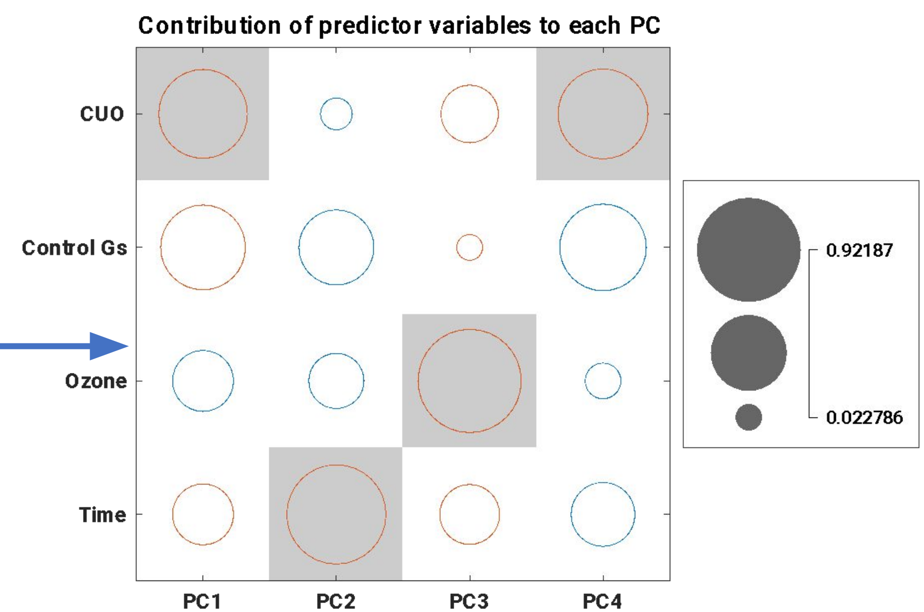




Verifying if the different weight of variables in different PCs are due to different crops categories:

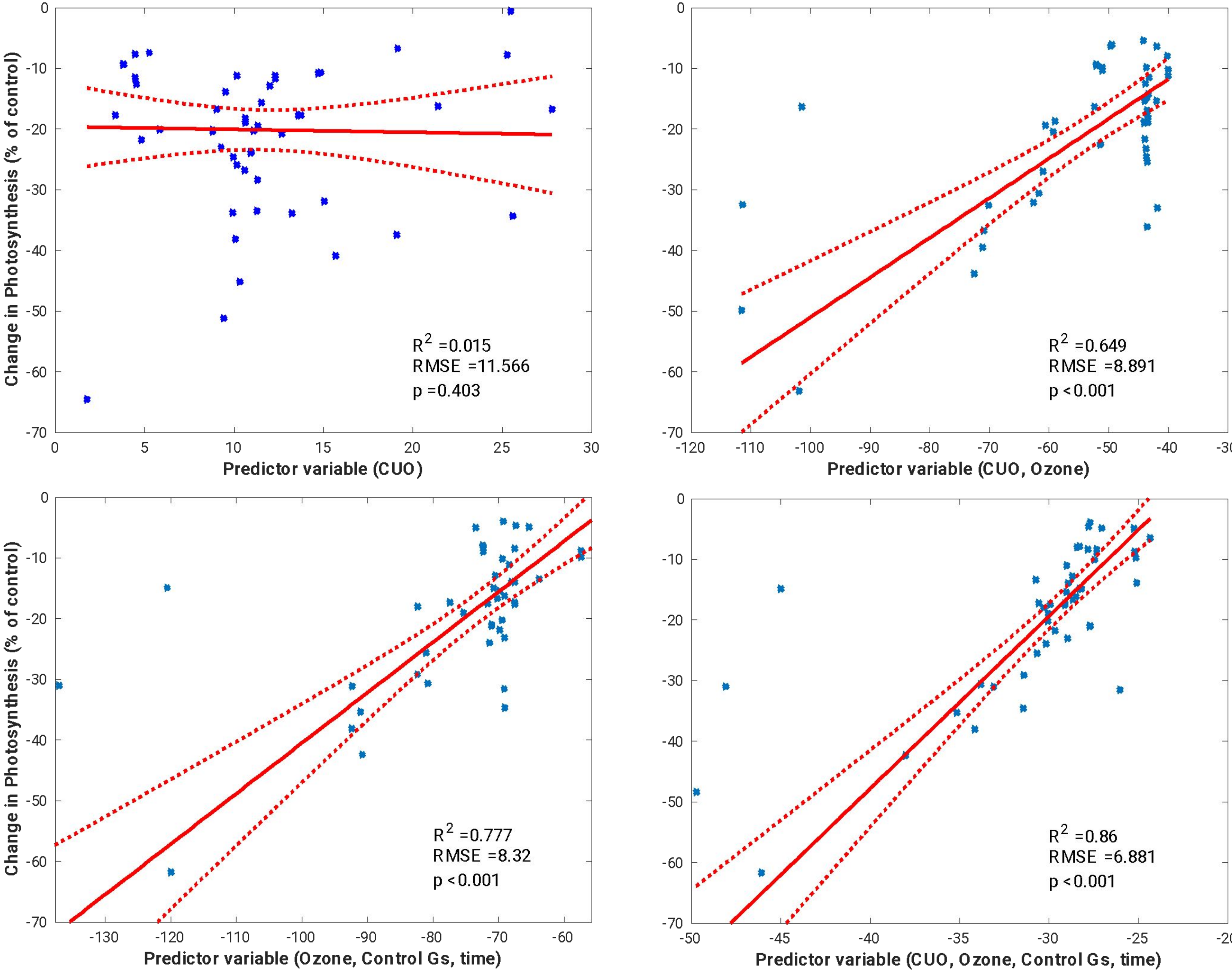
- The ozone experimental data for wheat also have different contribution of variables to each PC.
- This strongly indicates **CUO** alone can not explain the impact of chronic ozone exposure to plants.
- This may be because the experimental data is from different climates, crop varieties and experimental setting.



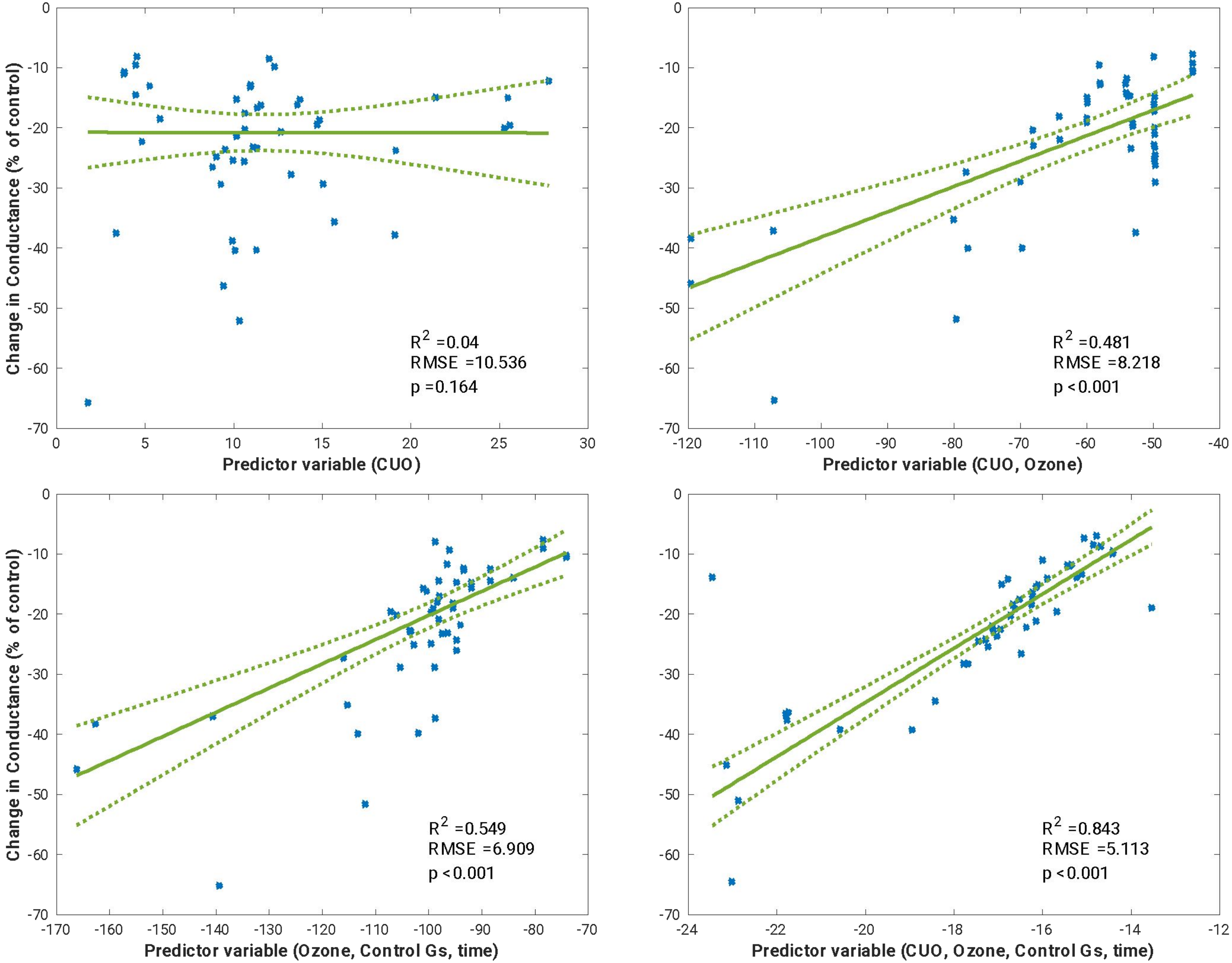


Incorporating multiple predictor variables other than CUO to prediction of change in photosynthesis and stomatal conductance under chronic ozone exposure

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



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



Takeaways

CUO alone does not explain ozone damage on plants

CUO combined with control Gs, O_3, and time explain the ozone damage significantly

The predictor variables interact differently for different crop types

Next Step:

- Adding and testing the new and improved ozone parameterizations in CLM5.
- Adding the parameterizations for new PFTs (wheat, rice, soybean, tropical evergreen trees, and C4 crops) in CLM5.


Thank You

Appendices

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
```

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

Charcoal-filtered air, medium or high confidence Data: Condutance	n	Mean	p value	Regression	r^2	p value
All data	393	84.44	< 0.001*	NS	0.0006	0.63
Plant type						
Crop	136	75.11	0.007*	NS	0.005	0.43
Evergreen shrub	0	NA	NA	NA	NA	NA
Grasses (C_3 and C_4)	8	89.15	0.53	NS	0.2	0.27
Herbaceous	41	88.19	0.37	NS	0.02	0.33
Temperate deciduous tree	153	91.25	0.02*	NS	0.0001	0.9
Temperate evergreen tree	53	86.45	0.54	78.23 + 0.48*x	0.32	< 0.001*
Tropical tree	2	48.3	0.17	NA	NA	NA
Plant age (years)						
< 1	236	82.02	0.36	NS	0.00001	0.93
1–5	133	89.9	0.08	84.95 + 0.33*x	0.05	0.009*
> 5	15	79.56	0.6	108.37 − 3.14*x	0.34	0.02*
Exposure system						
Greenhouse	30	89.1	0.31	NS	0.02	0.43
Branch chamber	18	90.97	0.05*	NS	0.17	0.09
Growth chamber	163	82.69	0.62	74.25 + 0.57*x	0.12	< 0.001*
Open-top chamber	182	84.59	0.95	86.69 − 0.07*x	0.03	0.02*
Free-air enrichment	NA	NA	NA	NA	NA	NA
Rooting environment						
Pot	310	84.14	0.9	NS	0.0008	0.61
Ground	74	86.8	0.39	NS	0.004	0.61
Vulnerability						
Low	106	91.11	0.13	78.24 + 1.13*x	0.23	< 0.001*
High	135	79.14	0.04*	NS	0.004	0.49

OzoneMod.F90

```
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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

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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
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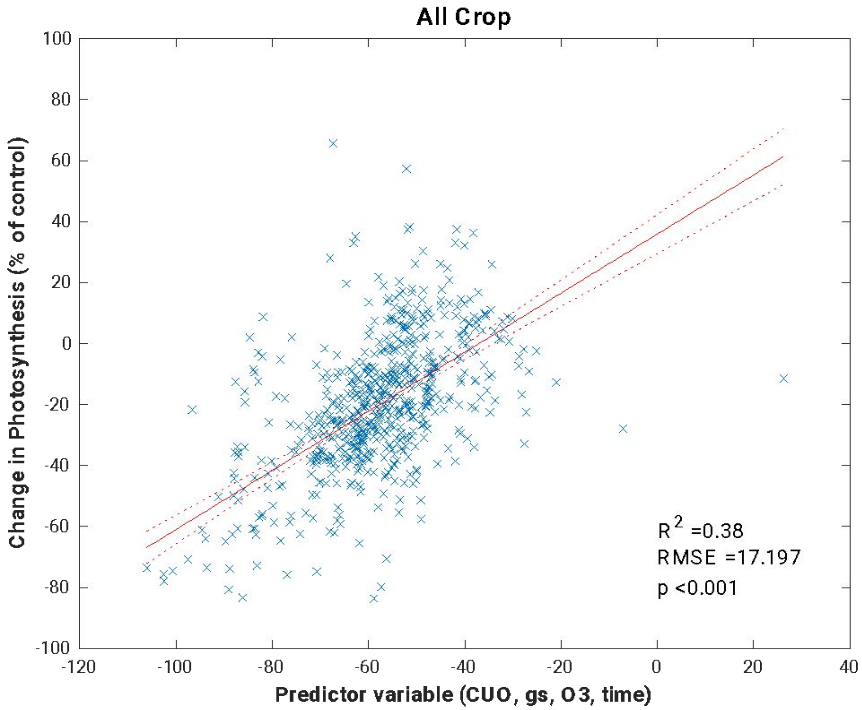
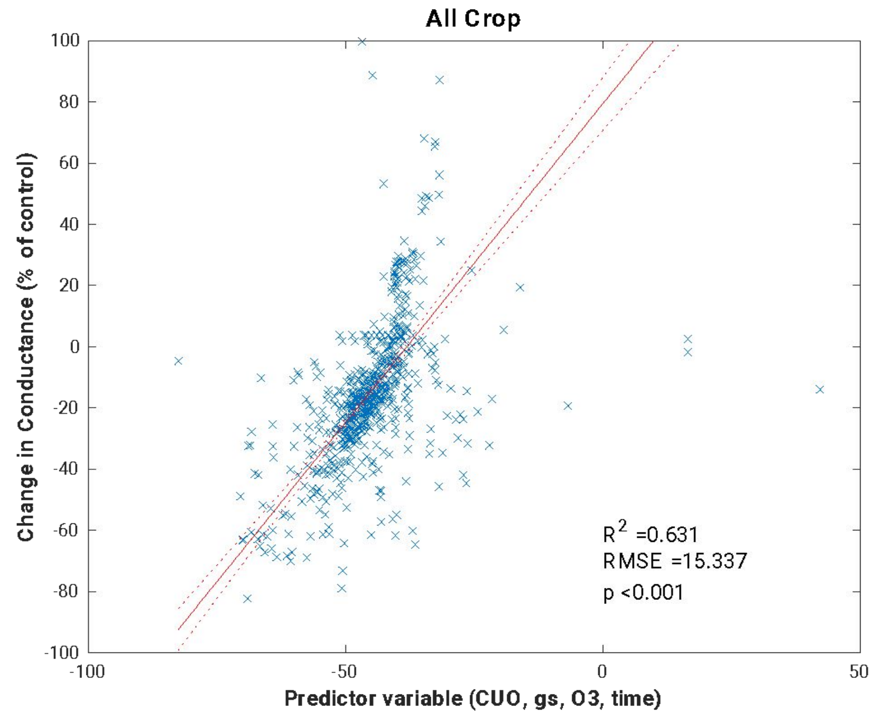





```
Linear regression model (robust fit):
    y ~ 1 + x1 + x2 + x3 + x4

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

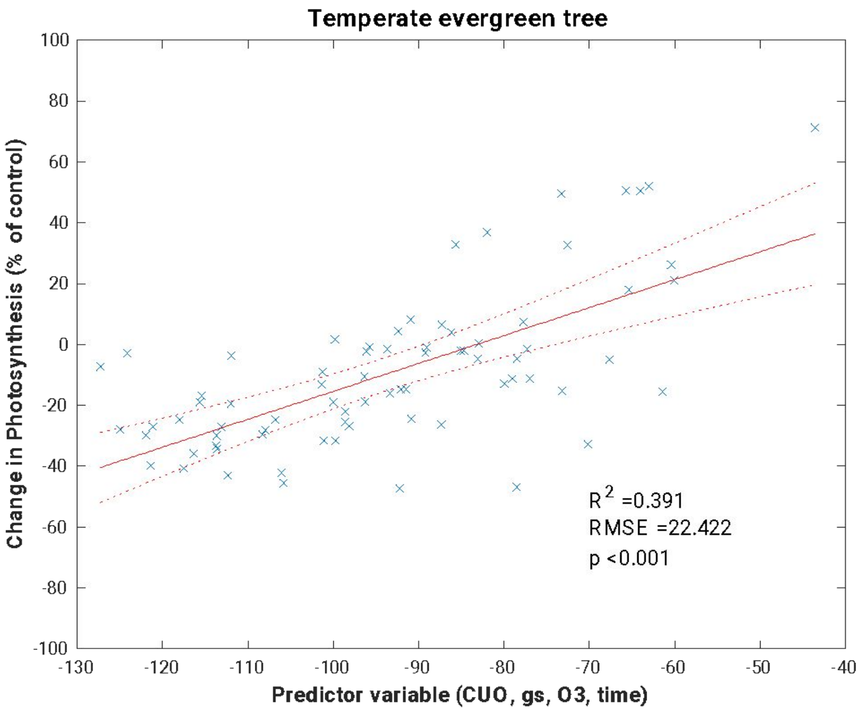

Number of observations: 644, Error degrees of freedom: 639
Root Mean Squared Error: 17.2
R-squared: 0.38,  Adjusted R-Squared: 0.376
F-statistic vs. constant model: 97.7, p-value = 7.34e-65
```

```
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
```

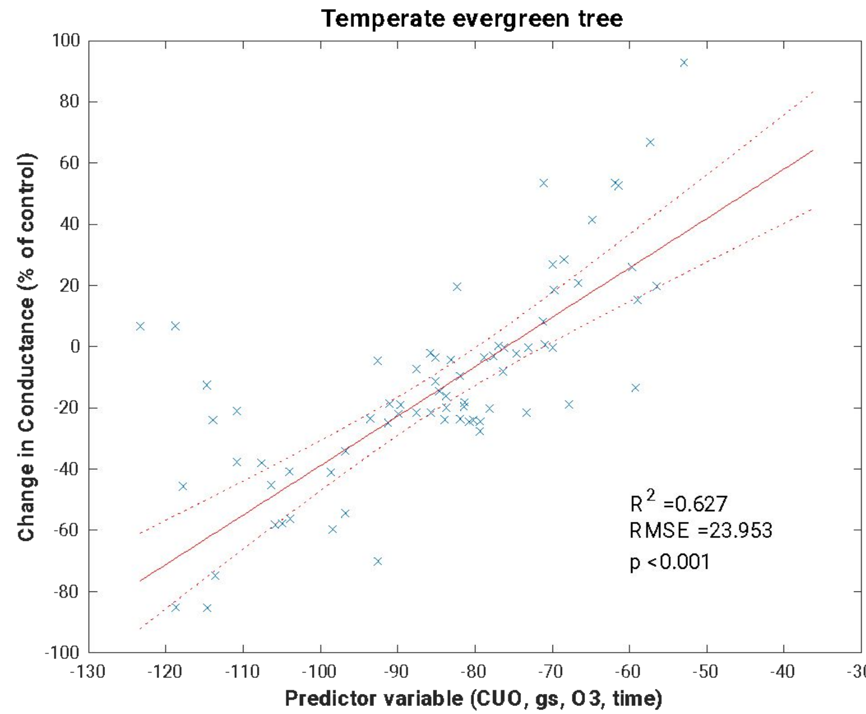



```
Linear regression model (robust fit):
    y ~ 1 + x1 + x2 + x3 + x4

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
```

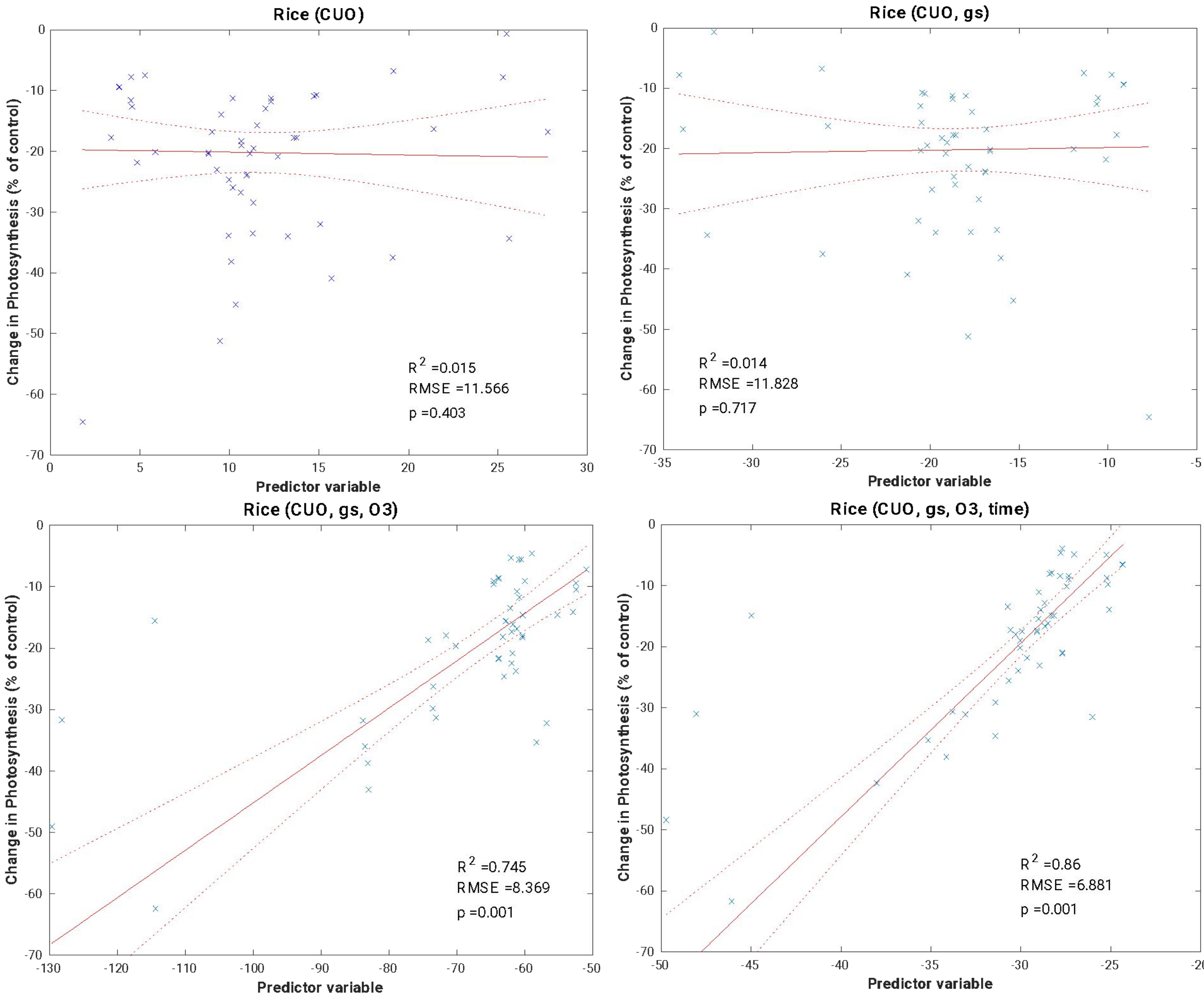


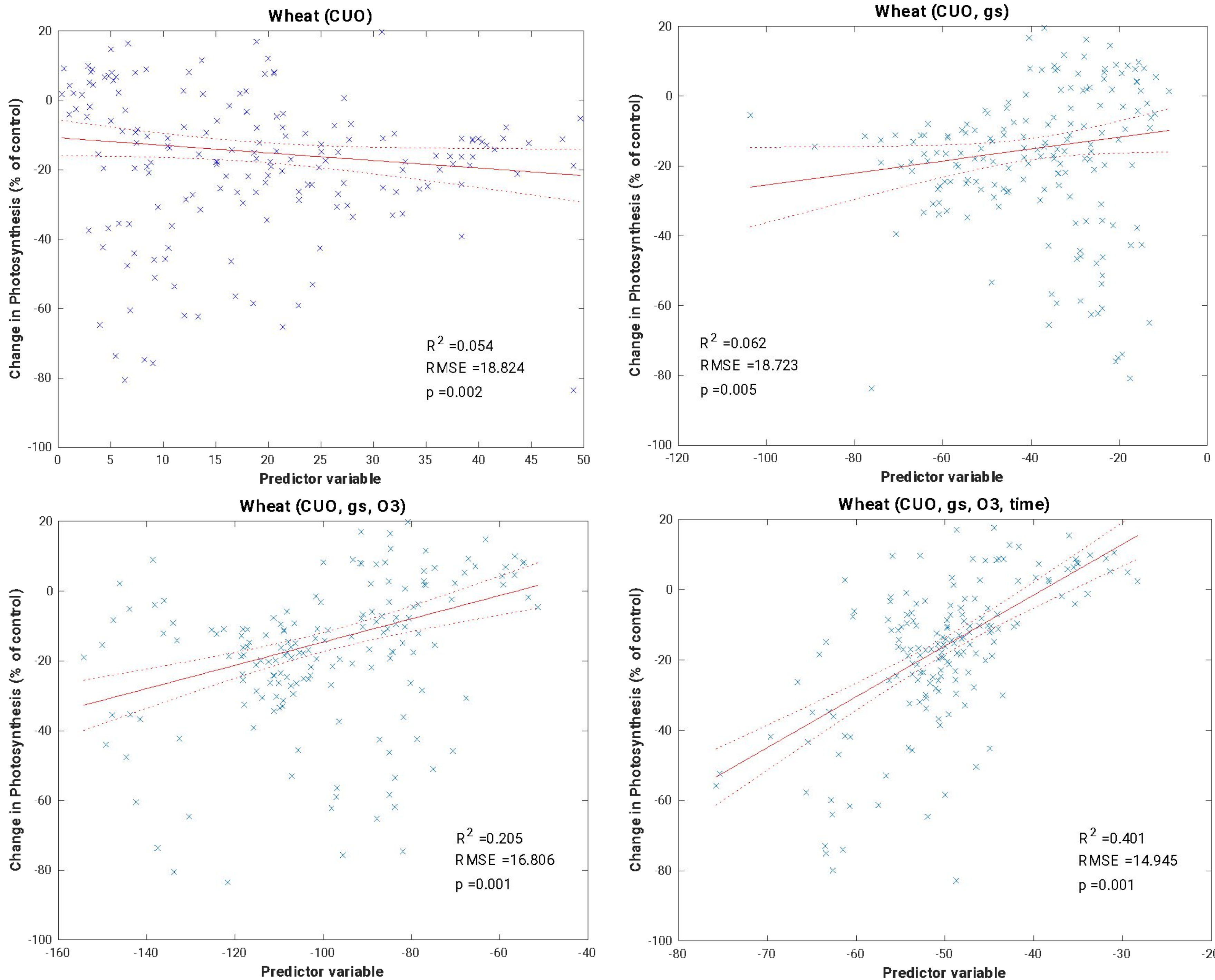

```
Linear regression model (robust fit):
    y ~ 1 + x1 + x2 + x3 + x4

Estimated Coefficients:
                   Estimate        SE          tStat        pValue
                  __________    _________    _______    __________

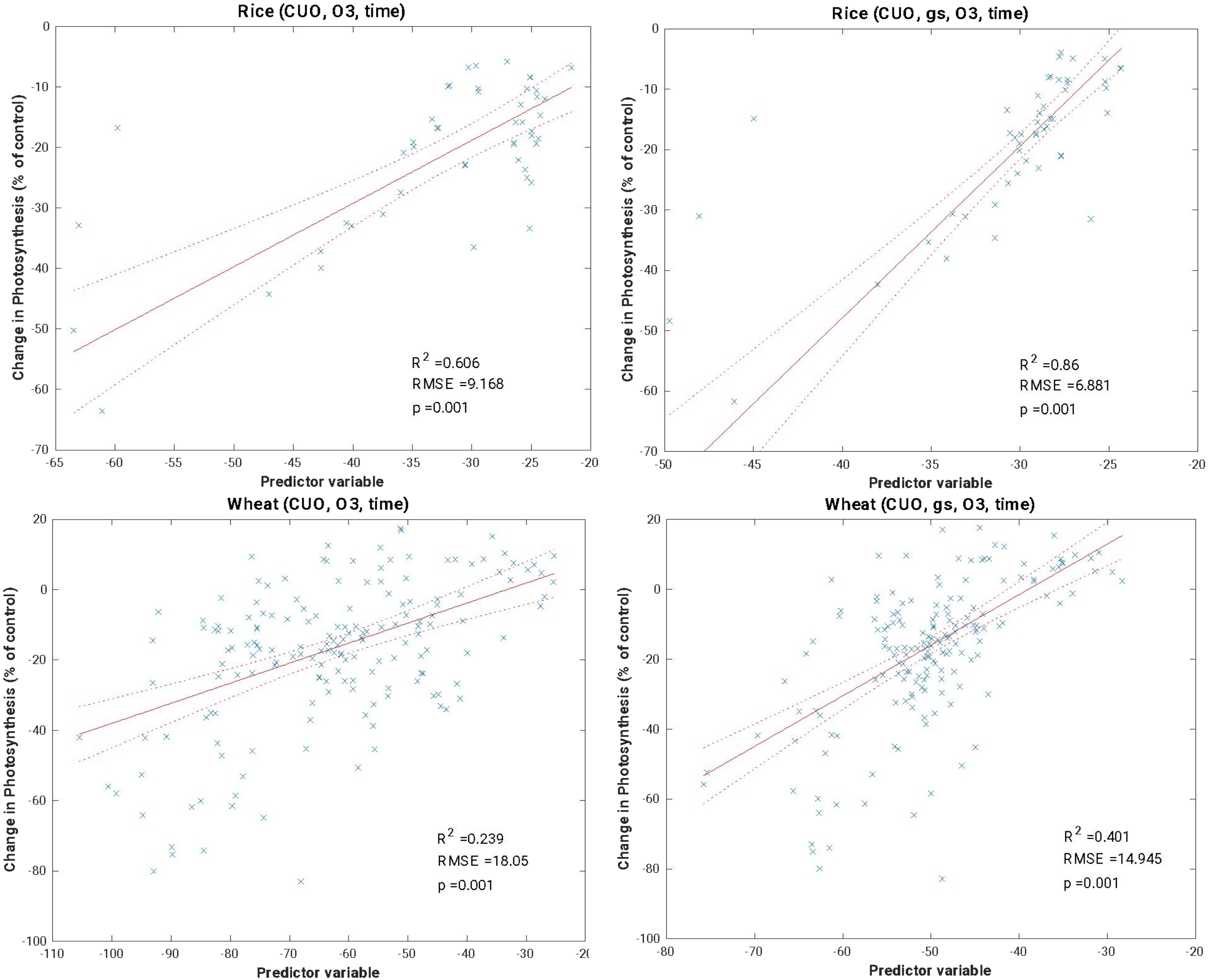
    (Intercept)       122.64       20.046     6.1179     4.647e-08
    x1               0.69696      0.08989     7.7535    4.7888e-11
    x2              -0.43097     0.045616    -9.4479    3.5107e-14
    x3                -1.391       0.2501    -5.5618    4.4192e-07
    x4            -0.0093298    0.0020015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


Rice (CUO)
Change in Photosynthesis (% of control)
Predictor variable
R 2 =0.015
RMSE =11.566
p =0.403
Rice (CUO, gs)
Change in Photosynthesis (% of control)
Predictor variable
R 2 =0.014
RMSE =11.828
p =0.717
Rice (CUO, gs, O3)
Change in Photosynthesis (% of control)
Predictor variable
R 2 =0.745
RMSE =8.369
p =0.001
Rice (CUO, gs, O3, time)
Change in Photosynthesis (% of control)
Predictor variable
R 2 =0.86
RMSE =6.881
p =0.001

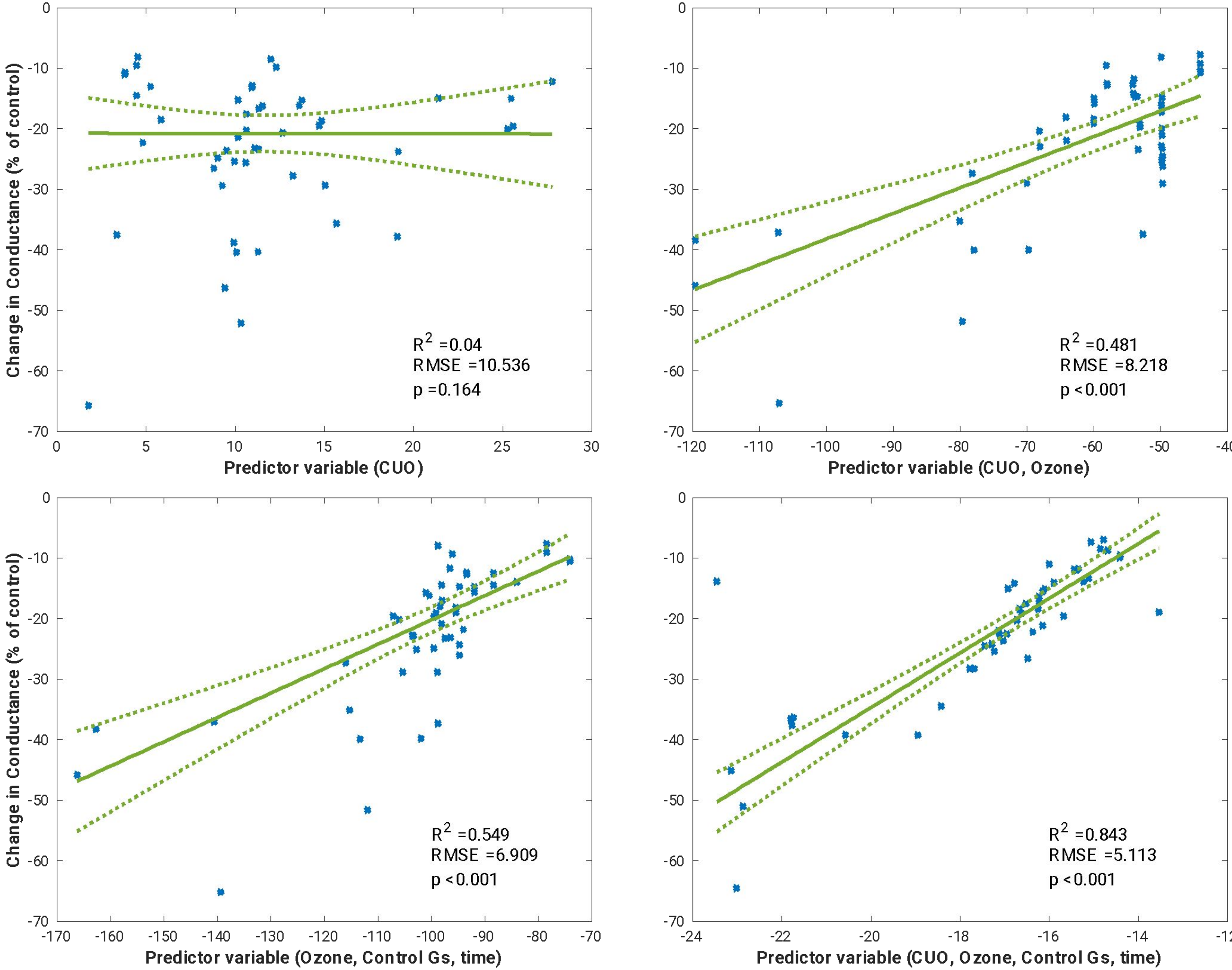


Wheat (CUO)
Change in Photosynthesis (% of control)
Predictor variable
R2 =0.054
RMSE =18.824
p =0.002
Wheat (CUO, gs)
Change in Photosynthesis (% of control)
Predictor variable
R2 =0.062
RMSE =18.723
p =0.005
Wheat (CUO, gs, O3)
Change in Photosynthesis (% of control)
Predictor variable
R2 =0.205
RMSE =16.806
p =0.001
Wheat (CUO, gs, O3, time)
Change in Photosynthesis (% of control)
Predictor variable
R2 =0.401
RMSE =14.945
p =0.001



Rice (CUO, O3, time)
Change in Photosynthesis (% of control)
Predictor variable
R 2 =0.606
RMSE =9.168
p =0.001
Rice (CUO, gs, O3, time)
Change in Photosynthesis (% of control)
Predictor variable
R 2 =0.86
RMSE =6.881
p =0.001
Wheat (CUO, O3, time)
Change in Photosynthesis (% of control)
Predictor variable
R 2 =0.239
RMSE =18.05
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

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



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