Supplementary Material

Non-parametric regression analysis of diuron and gabapentin degradation in Lake Constance matrix by ozone treatment and their toxicity assessment

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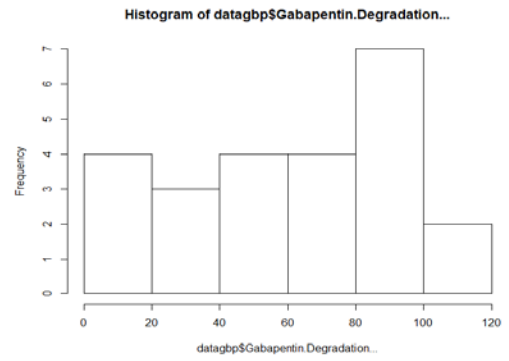
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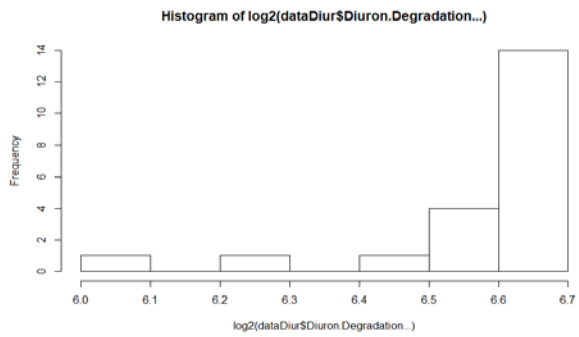[*]*Corresponding author E-mail address: jiaqian.jiang@gcu.ac.uk*
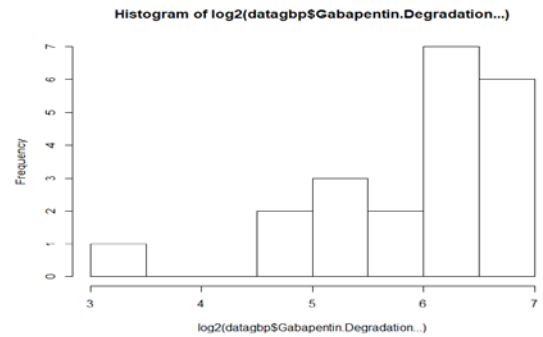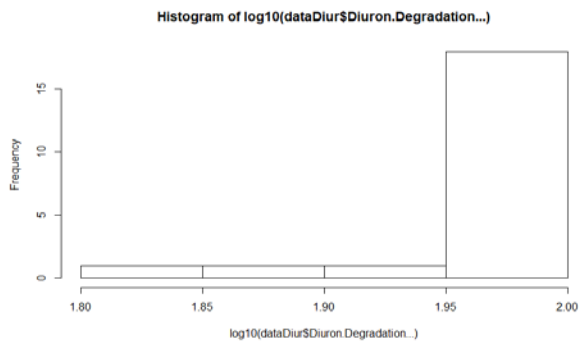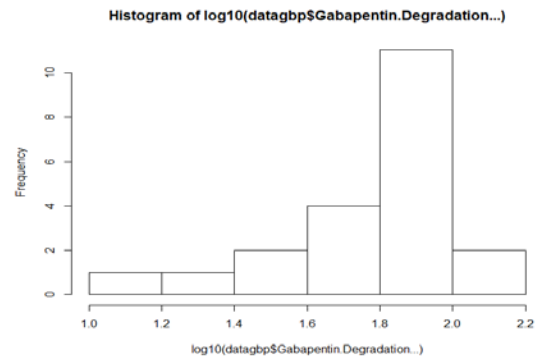
Appendix A
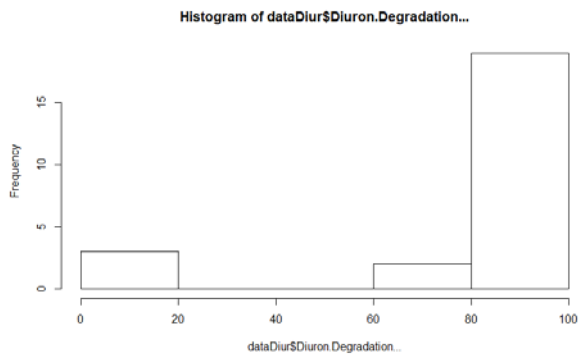
(a)

(d)

(b)

(e)

(c)

(f)

Figure S1. Degradation data distribution (a-c) diuron and, (d-f) gabapentin

Appendix B

Algorithm

Kruskal Wallis test

Kruskal-Wallis rank sum test

data: dataDiur #Diuron degradation

Kruskal-Wallis chi-squared = 35.697, df = 2, p-value = 1.772e-08

> kruskal.test(datagbp)

Kruskal-Wallis rank sum test

data: datagbp #Gabapentin degradation

Kruskal-Wallis chi-squared = 33.15, df = 2, p-value = 6.331e-08

> summary(dataDiur)

Reaction.time..min. Ozone..mg.l.   Diuron.Degradation...

Min.   : 0.0   Min. :0.0600 Min.   : 0.00

1st Qu.: 4.0   1st Qu.:0.1525   1st Qu.: 91.54

Median :17.5   Median :0.3200 Median : 98.63

Mean :19.5   Mean :0.3762 Mean   : 83.46

3rd Qu.:32.5   3rd Qu.:0.5325   3rd Qu.:100.00

Max. :45.0   Max. :1.0100 Max. :100.00

> summary(datagbp)

Reaction.time..min. Ozone..mg.l.   Gabapentin.Degradation...

Min.   : 0.0   Min. :0.0600 Min.   : 0.00

1st Qu.: 4.0   1st Qu.:0.0800   1st Qu.: 34.76

Median :17.5   Median :0.1050 Median : 66.59

Mean :19.5   Mean :0.2267 Mean   : 59.44

3rd Qu.:32.5   3rd Qu.:0.2350   3rd Qu.: 89.32

Max. :45.0   Max. :0.9100 Max. :100.27

Poisson without interaction

DImodelglm=glm(Diuron_Degradation~Ozone+Reaction_time,data=dataDi,family   =
"poisson")

GAmodelglm=glm(Gabapentin_Degradation~Ozone+Reaction_time,data=dataGaba,famil
y= "poisson")

Poisson with interaction

DImodelglmin=glm(Diuron_Degradation~Ozone*Reaction_time,data=dataDi,family = "poisson")

GAmodelglmin=glm(Gabapentin_Degradation~Ozone*Reaction_time,data=dataGaba,family= "poisson")

Gaussian without interaction

DImodelglmgaus=glm (Diuron_Degradation~Ozone+Reaction_time,

data=dataDi,family = "gaussian")

GAmodelglmgaus=glm(Gabapentin_Degradation~Ozone+Reaction_time,data=dataGaba,family= "gaussian")

Gaussian with interaction

DImodelglmin=glm(Diuron_Degradation~Ozone*Reaction_time,data=dataDi,family = "poisson")

GAmodelglmgausin=glm(Gabapentin_Degradation~Ozone*Reaction_time,data=dataGaba ,family= "gaussian")

Appendix C

GLM Poisson distribution output

Table S1

Poisson GLM regression analysis for diuron degradation results after ozonation treatment (without interaction)

Estimate	Coefficients	Std. Error	z value	Pr(>|z|)	Significant
Intercept	4.46	0.05	89.94	<2e-16	Yes
Ozone	-0.89	0.09	-9.74	<2e-16	Yes
Reaction time	0.01	0.00	8.89	<2e-16	Yes

Table S2

Poisson GLM regression analysis for diuron degradation results after ozonation treatment (with interaction)

Estimate	Coefficients	Std. Error	z value	Pr(>|z|)	Significant
Intercept	4.98	0.07	74.03	< 2e-16	Yes
Ozone	-2.31	0.18	-13.08	< 2e-16	Yes
Reaction time	-0.01	0.00	-3.84	0.000126	Yes
Ozone× Reaction time	0.06	0.01	10.42	< 2e-16	Yes

Table S3

Poisson GLM regression analysis for gabapentin degradation results after ozonation treatment (without interaction)

Estimate	Coefficients	Std. Error	z value	Pr(>|z|)	Significant
Intercept	3.92	0.07	55.29	<2e-16	Yes
Ozone	-2.63	0.26	-9.98	<2e-16	Yes
Reaction time	0.02	0.00	13.37	<2e-16	Yes

Table S4

Poisson GLM regression analysis for gabapentin degradation results after ozonation treatment (with interaction)

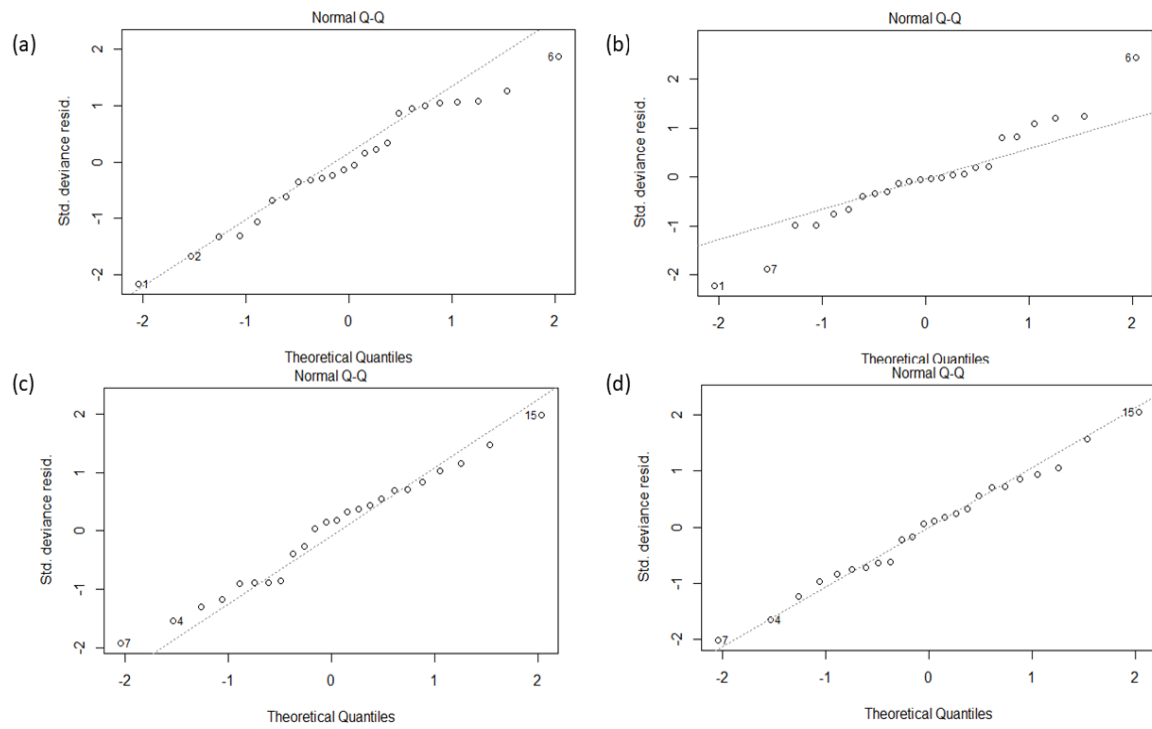| Estimate	Coefficients	Std. Error	z value	Pr(>|z|)	Significant
Intercept	4.08	0.08	48.90	< 2e-16	Yes
Ozone	-3.23	0.33	-9.74	< 2e-16	Yes
Reaction time	0.01	0.00	2.84	0.00457	Yes
Ozone× Reaction time	0.08	0.02	3.81	0.00014	Yes

Appendix D

Figure S2. Gaussian model residuals plot (a) Diuron without process variables interaction, (b) Diuron with process variables interaction, (c) Gabapentin without process variables interaction, (d) Gabapentin with process variables interaction