

Statistical Analyses for Van Meter et al 2016

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Introduction

Data set, statistical analyses, graphics and inference concerning effect of organic carbon in soil on dermal bioconcentration in amphibians. Analytes include active ingredients for commonly used pesticides (atrazine, imidacloprid, fipronil, triadimenon, pendimethalin).

Computational environment

Location of this repository: https://github.com/puruckertom/VanMeteretal2016_ple_v_ols

Version and installed libraries.

```
R.Version()$version.string
```

```
## [1] "R version 3.0.2 (2013-09-25)"
```

```
Sys.info()[4]
```

```
##      nodename  
## "stp-air.local"
```

```
library(MASS)  
library(dplyr, warn.conflicts = FALSE)  
library(ggplot2)
```

Experimental data

Original file with analytical data: https://github.com/puruckertom/VanMeteretal2016_ple_v_ols/blob/master/RDATA.csv

```
#####  
#the data sets  
#####  
#everything  
frog.soil <- read.table(paste(frogsoildir,"RDATA.csv",sep=""), header = TRUE, sep = ",")  
str(frog.soil)
```

```
## 'data.frame':    264 obs. of  11 variables:  
## $ Day           : int  2 2 2 2 2 2 2 2 2 2 ...  
## $ Row           : int  1 1 3 5 6 7 1 2 2 4 ...  
## $ Column        : Factor w/ 10 levels "", "A", "B", "C",...: 2 9 4 4 7 3 3 7 10 3 ...  
## $ Pesticide     : Factor w/ 17 levels "ATZ", "ATZDEA",...: 4 4 4 4 4 4 4 4 4 4 ...  
## $ SoilType      : Factor w/ 2 levels "OLS", "PLE": 2 2 2 2 2 2 1 1 1 1 ...  
## $ BodyBurden    : num  0.337 1.227 0.701 0.367 0.352 ...  
## $ Soil          : num  22.9 39.6 19.1 16.6 28.5 ...  
## $ Weight        : num  13.18 15.87 8.39 14.54 16.43 ...  
## $ Total         : int  1 1 1 1 1 1 1 1 1 1 ...  
## $ Formulation: int  0 0 0 0 0 0 0 0 0 0 ...  
## $ Parent        : int  1 1 1 1 1 1 1 1 1 1 ...
```

Modifying data set to create factors for ANOVA, calculate BCFs and amphibian surface areas.

```
frog.soil$bowlbcbf <- frog.soil$BodyBurden/frog.soil$Soil  
frog.soil$surface_area_total <- 1.131 * frog.soil$Weight^0.579  
frog.soil$surface_area_footprint <- 0.425 * frog.soil$Weight^0.85
```

Structure of revised data set.

```
str(frog.soil)  
  
## 'data.frame':    264 obs. of  14 variables:  
## $ Day           : Factor w/ 4 levels "0","1","2","3": 3 3 3 3 3 3 3 3 3 3 ...  
## $ Row           : Factor w/ 7 levels "1","2","3","4",...: 1 1 3 5 6 7 1 2 2 4 ...  
## $ Column        : Factor w/ 10 levels "", "A", "B", "C",...: 2 9 4 4 7 3 3 7 10 3 ...  
## $ Pesticide     : Factor w/ 17 levels "ATZ", "ATZDEA",...: 4 4 4 4 4 4 4 4 4 4 ...  
## $ SoilType      : Factor w/ 2 levels "OLS", "PLE": 2 2 2 2 2 2 1 1 1 1 ...  
## $ BodyBurden    : num  0.337 1.227 0.701 0.367 0.352 ...  
## $ Soil          : num  22.9 39.6 19.1 16.6 28.5 ...  
## $ Weight        : num  13.18 15.87 8.39 14.54 16.43 ...  
## $ Total         : Factor w/ 2 levels "0","1": 2 2 2 2 2 2 2 2 2 2 ...  
## $ Formulation   : Factor w/ 2 levels "0","1": 1 1 1 1 1 1 1 1 1 1 ...  
## $ Parent        : Factor w/ 2 levels "0","1": 2 2 2 2 2 2 2 2 2 2 ...  
## $ bowlbcbf      : num  0.0147 0.031 0.0367 0.0221 0.0124 ...  
## $ surface_area_total : num  5.03 5.61 3.88 5.33 5.72 ...  
## $ surface_area_footprint: num  3.81 4.46 2.59 4.14 4.59 ...
```

Koc and organic carbon content data

Add experimental and literature Koc data to data set.

```
unique(frog.soil$Pesticide)
```

```
## [1] ATZTOT   ATZDEA   STAUGDEA ATZDIA   STAUGDIA ATZ      Imid
## [8] FipTOT   Fip      FipS     TNDTOT   TDLA      STRIKEA  TDLB
## [15] STRIKEB  TDN      Pendi
## 17 Levels: ATZ ATZDEA ATZDIA ATZTOT Fip FipS FipTOT Imid ... TNDTOT
```

```
unique(frog.soil$SoilType)
```

```
## [1] PLE OLS
## Levels: OLS PLE
```

```
Pesticide <- c("ATZTOT","FipTOT","Imid","TNDTOT","Pendi","ATZTOT","FipTOT","Imid","TNDTOT","Pendi")
expKoc <- c(2.303,4.242,2.556,3.025,6.425,2.634,2.864,3.645,3.01,1.733)
litKoc <- c(2.24,2.92,2.39,2.71,3.7,2.24,2.92,2.39,2.71,3.7)
SoilType <- c("PLE","PLE","PLE","PLE","PLE","OLS","OLS","OLS","OLS","OLS")

df.merge <- data.frame(Pesticide, expKoc, litKoc, SoilType)
#View(merge(frog.soil, df.merge, all = TRUE))
frog.soil <- (merge(frog.soil, df.merge, all = TRUE))
```

Add organic carbon content data to dataframe.

```
# Soil Type      %OM %OC
#Plott Series    PLE 14.138 8.200
#Everbard       EC  5.448  3.160
#Orangeburg loamy-sand OLS 3.100  1.798

SoilType <- c("PLE","OLS")
OM <- c(14.138, 3.1)
OC <- c(8.2, 1.798)
df.merge2 <- data.frame(SoilType, OM, OC)
frog.soil <- (merge(frog.soil, df.merge2, all = TRUE))
```

```
str(frog.soil)
```

```
## 'data.frame':    264 obs. of  18 variables:
## $ SoilType      : Factor w/ 2 levels "OLS","PLE": 1 1 1 1 1 1 1 1 1 1 ...
## $ Pesticide     : Factor w/ 17 levels "ATZ","ATZDEA",...: 1 1 1 1 1 1 1 1 1 1 ...
## $ Day           : Factor w/ 4 levels "0","1","2","3": 3 3 3 3 3 3 3 3 3 3 ...
## $ Row           : Factor w/ 7 levels "1","2","3","4",...: 2 4 5 7 1 2 4 5 5 7 ...
## $ Column        : Factor w/ 10 levels "", "A", "B", "C",...: 10 3 9 6 6 8 10 2 8 5 ...
## $ BodyBurden    : num  0.728 0.27 0.237 1.9 0.566 ...
## $ Soil          : num  16.6 12.3 21.6 29.2 14.2 ...
## $ Weight        : num  11.1 12 17.4 11.8 11.1 ...
## $ Total         : Factor w/ 2 levels "0","1": 1 1 1 1 1 1 1 1 1 1 ...
## $ Formulation   : Factor w/ 2 levels "0","1": 1 1 1 1 2 2 2 2 2 2 ...
```

```
## $ Parent          : Factor w/ 2 levels "0","1": 2 2 2 2 2 2 2 2 2 ...
## $ bowlbcf         : num  0.044 0.022 0.011 0.065 0.0398 ...
## $ surface_area_total : num  4.57 4.76 5.91 4.71 4.55 ...
## $ surface_area_footprint: num  3.3 3.5 4.82 3.46 3.28 ...
## $ expKoc          : num  NA NA NA NA NA NA NA NA NA NA NA ...
## $ litKoc          : num  NA NA NA NA NA NA NA NA NA NA NA ...
## $ OM              : num  3.1 3.1 3.1 3.1 3.1 3.1 3.1 3.1 3.1 3.1 ...
## $ OC              : num  1.8 1.8 1.8 1.8 1.8 ...
```

Summary statistics

Calculate mean and standard deviations for soil and amphibian tissue residue concentrations.

```
str(frog.soil)
```

```
## 'data.frame':    264 obs. of  18 variables:
## $ SoilType       : Factor w/ 2 levels "OLS","PLE": 1 1 1 1 1 1 1 1 1 ...
## $ Pesticide      : Factor w/ 17 levels "ATZ","ATZDEA",...: 1 1 1 1 1 1 1 1 1 ...
## $ Day            : Factor w/ 4 levels "0","1","2","3": 3 3 3 3 3 3 3 3 3 ...
## $ Row            : Factor w/ 7 levels "1","2","3","4",...: 2 4 5 7 1 2 4 5 7 ...
## $ Column         : Factor w/ 10 levels "","A","B","C",...: 10 3 9 6 6 8 10 2 8 5 ...
## $ BodyBurden     : num  0.728 0.27 0.237 1.9 0.566 ...
## $ Soil           : num  16.6 12.3 21.6 29.2 14.2 ...
## $ Weight         : num  11.1 12 17.4 11.8 11.1 ...
## $ Total          : Factor w/ 2 levels "0","1": 1 1 1 1 1 1 1 1 1 ...
## $ Formulation     : Factor w/ 2 levels "0","1": 1 1 1 1 2 2 2 2 2 ...
## $ Parent         : Factor w/ 2 levels "0","1": 2 2 2 2 2 2 2 2 2 ...
## $ bowlbcf        : num  0.044 0.022 0.011 0.065 0.0398 ...
## $ surface_area_total : num  4.57 4.76 5.91 4.71 4.55 ...
## $ surface_area_footprint: num  3.3 3.5 4.82 3.46 3.28 ...
## $ expKoc         : num  NA NA NA NA NA NA NA NA NA NA NA ...
## $ litKoc         : num  NA NA NA NA NA NA NA NA NA NA NA ...
## $ OM             : num  3.1 3.1 3.1 3.1 3.1 3.1 3.1 3.1 3.1 ...
## $ OC             : num  1.8 1.8 1.8 1.8 1.8 ...
```

```
head(frog.soil)
```

```
##   SoilType Pesticide Day Row Column BodyBurden   Soil Weight Total
## 1     OLS      ATZ   2   2     I 0.7282998 16.55151 11.1447    0
## 2     OLS      ATZ   2   4     B 0.2703513 12.28110 11.9615    0
## 3     OLS      ATZ   2   5     H 0.2365494 21.60190 17.3882    0
## 4     OLS      ATZ   2   7     E 1.8995641 29.24066 11.7687    0
## 5     OLS      ATZ   2   1     E 0.5662302 14.23919 11.0822    0
## 6     OLS      ATZ   2   2     G 1.9850391 19.48325 10.0690    0
##   Formulation Parent bowlbcf surface_area_total surface_area_footprint
## 1           0      1 0.04400201          4.567885          3.299112
## 2           0      1 0.02201361          4.758833          3.503537
## 3           0      1 0.01095040          5.909763          4.815101
## 4           0      1 0.06496310          4.714269          3.455478
## 5           1      1 0.03976562          4.553036          3.283379
## 6           1      1 0.10188442          4.307167          3.026407
```

```
## expKoc litKoc OM OC
## 1 NA NA 3.1 1.798
## 2 NA NA 3.1 1.798
## 3 NA NA 3.1 1.798
## 4 NA NA 3.1 1.798
## 5 NA NA 3.1 1.798
## 6 NA NA 3.1 1.798
```

```
#View(frog.soil.total.ai)
#using dplyr
frog.soil.group <- group_by(frog.soil, Pesticide, SoilType, Formulation, Parent)
str(frog.soil.group)
```

```
## Classes 'grouped_df', 'tbl_df', 'tbl' and 'data.frame': 264 obs. of 18 variables:
## $ SoilType : Factor w/ 2 levels "OLS","PLE": 1 1 1 1 1 1 1 1 1 1 ...
## $ Pesticide : Factor w/ 17 levels "ATZ","ATZDEA",...: 1 1 1 1 1 1 1 1 1 1 ...
## $ Day : Factor w/ 4 levels "0","1","2","3": 3 3 3 3 3 3 3 3 3 3 ...
## $ Row : Factor w/ 7 levels "1","2","3","4",...: 2 4 5 7 1 2 4 5 5 7 ...
## $ Column : Factor w/ 10 levels "", "A", "B", "C",...: 10 3 9 6 6 8 10 2 8 5 ...
## $ BodyBurden : num 0.728 0.27 0.237 1.9 0.566 ...
## $ Soil : num 16.6 12.3 21.6 29.2 14.2 ...
## $ Weight : num 11.1 12 17.4 11.8 11.1 ...
## $ Total : Factor w/ 2 levels "0","1": 1 1 1 1 1 1 1 1 1 1 ...
## $ Formulation : Factor w/ 2 levels "0","1": 1 1 1 1 2 2 2 2 2 2 ...
## $ Parent : Factor w/ 2 levels "0","1": 2 2 2 2 2 2 2 2 2 2 ...
## $ bowlbcf : num 0.044 0.022 0.011 0.065 0.0398 ...
## $ surface_area_total : num 4.57 4.76 5.91 4.71 4.55 ...
## $ surface_area_footprint: num 3.3 3.5 4.82 3.46 3.28 ...
## $ expKoc : num NA NA NA NA NA NA NA NA NA ...
## $ litKoc : num NA NA NA NA NA NA NA NA NA ...
## $ OM : num 3.1 3.1 3.1 3.1 3.1 3.1 3.1 3.1 3.1 ...
## $ OC : num 1.8 1.8 1.8 1.8 1.8 ...
## - attr(*, "vars")=List of 4
## ..$ : symbol Pesticide
## ..$ : symbol SoilType
## ..$ : symbol Formulation
## ..$ : symbol Parent
## - attr(*, "drop")= logi TRUE
## - attr(*, "indices")=List of 44
## ..$ : int 0 1 2 3 10 11
## ..$ : int 4 5 6 7 8 9
## ..$ : int 136 146 151 156 158 161
## ..$ : int 135 140 144 145 153 183
## ..$ : int 24 25 26 27 28 29
## ..$ : int 137 138 148 149 169 170
## ..$ : int 36 37 38 39 40 41
## ..$ : int 139 143 204 205 206 207
## ..$ : int 16 17 18 19 48 49
## ..$ : int 12 13 14 15 50 51
## ..$ : int 155 180 181 182 185 197
## ..$ : int 133 134 150 157 160 165
## ..$ : int 32 33 34 35 76 77
## ..$ : int 162 163 166 196 200 201
## ..$ : int 44 45 46 47 88 89
```

```

## ..$ : int 132 141 142 171 211 223
## ..$ : int 20 21 56 57 58 59
## ..$ : int 186 187 195 209 224 225
## ..$ : int 30 31 55 69 72 73
## ..$ : int 159 167 168 184 210 222
## ..$ : int 42 43 67 68 71 85
## ..$ : int 86 87 90 91 102 116
## ..$ : int 147 152 172 173 176 177
## ..$ : int 178 179 220 221 235 236
## ..$ : int 54 64 65 66 95 96
## ..$ : int 154 164 192 193 194 208
## ..$ : int 78 79 94 103 108 113
## ..$ : int 202 203 244 245 246 247
## ..$ : int 52 53 101 122 124 125
## ..$ : int 174 175 216 217 218 219
## ..$ : int 22 23 60 61 92 104
## ..$ : int 188 189 190 191 226 227
## ..$ : int 74 75 109 112 123 130
## ..$ : int 198 199 240 241 242 243
## ..$ : int 107 110 118 121 128 131
## ..$ : int 212 213 214 215 250 251
## ..$ : int 83 84 97 98 99 100
## ..$ : int 62 63 80 81 93 114
## ..$ : int 228 229 230 231 232 233
## ..$ : int 234 237 238 239 248 249
## ..$ : int 106 111 115 119 120 129
## ..$ : int 70 82 105 117 126 127
## ..$ : int 252 255 256 257 258 259
## ..$ : int 253 254 260 261 262 263
## - attr(*, "group_sizes")= int 6 6 6 6 6 6 6 6 6 6 ...
## - attr(*, "biggest_group_size")= int 6
## - attr(*, "labels")='data.frame': 44 obs. of 4 variables:
## ..$ Pesticide : Factor w/ 17 levels "ATZ","ATZDEA",...: 1 1 1 1 2 2 3 3 4 4 ...
## ..$ SoilType : Factor w/ 2 levels "OLS","PLE": 1 1 2 2 1 2 1 2 1 1 ...
## ..$ Formulation: Factor w/ 2 levels "0","1": 1 2 1 2 1 1 1 1 1 2 ...
## ..$ Parent : Factor w/ 2 levels "0","1": 2 2 2 2 1 1 1 1 2 2 ...
## ..- attr(*, "vars")=List of 4
## .. ..$ : symbol Pesticide
## .. ..$ : symbol SoilType
## .. ..$ : symbol Formulation
## .. ..$ : symbol Parent

```

```
frog.soil.group
```

```

## Source: local data frame [264 x 18]
## Groups: Pesticide, SoilType, Formulation, Parent
##

```

	SoilType	Pesticide	Day	Row	Column	BodyBurden	Soil	Weight	Total
## 1	OLS	ATZ	2	2	I	0.7282998	16.551513	11.1447	0
## 2	OLS	ATZ	2	4	B	0.2703513	12.281098	11.9615	0
## 3	OLS	ATZ	2	5	H	0.2365494	21.601898	17.3882	0
## 4	OLS	ATZ	2	7	E	1.8995641	29.240663	11.7687	0
## 5	OLS	ATZ	2	1	E	0.5662302	14.239191	11.0822	0
## 6	OLS	ATZ	2	2	G	1.9850391	19.483245	10.0690	0

```
## 7      OLS      ATZ      2      4      I 0.2670444 18.094682 11.0174      0
## 8      OLS      ATZ      2      5      A 0.2356130 18.492963 12.3638      0
## 9      OLS      ATZ      2      5      G 0.3124082  7.940987 10.1878      0
## 10     OLS      ATZ      2      7      D 0.2438387 16.933410 11.5272      0
## ..      ...      ...      ...      ...      ...      ...      ...      ...
## Variables not shown: Formulation (fctr), Parent (fctr), bowlbcf (dbl),
##   surface_area_total (dbl), surface_area_footprint (dbl), expKoc (dbl),
##   litKoc (dbl), OM (dbl), OC (dbl)
```

```
frog.soil.means <- summarise(frog.soil.group,
  count = n(),
  FrogMean = mean(BodyBurden),
  FrogSD = sd(BodyBurden),
  SoilMean = mean(Soil),
  SoilSD = sd(Soil)
)
frog.soil.means
```

```
## Source: local data frame [44 x 9]
## Groups: Pesticide, SoilType, Formulation
##
##   Pesticide SoilType Formulation Parent count  FrogMean  FrogSD
## 1      ATZ      OLS           0      1      6 0.81375385 0.654947835
## 2      ATZ      OLS           1      1      6 0.60169561 0.688861900
## 3      ATZ      PLE           0      1      6 0.43815022 0.230781640
## 4      ATZ      PLE           1      1      6 0.52394830 0.336497915
## 5  ATZDEA      OLS           0      0      6 0.56841980 0.853934956
## 6  ATZDEA      PLE           0      0      6 0.11582458 0.098357479
## 7  ATZDIA      OLS           0      0      6 0.56823951 0.846310211
## 8  ATZDIA      PLE           0      0      6 0.07990814 0.074451822
## 9  ATZTOT      OLS           0      1      6 1.95041316 2.301128614
## 10 ATZTOT      OLS           1      1      6 0.82672856 0.663118510
## 11 ATZTOT      PLE           0      1      6 0.63388293 0.354753198
## 12 ATZTOT      PLE           1      1      6 0.69718557 0.337418123
## 13      Fip      OLS           0      1      6 0.09692212 0.050364156
## 14      Fip      PLE           0      1      6 0.05474889 0.033710850
## 15      FipS      OLS           0      0      6 0.06154416 0.031688542
## 16      FipS      PLE           0      0      6 0.03365841 0.025023420
## 17  FipTOT      OLS           0      1      6 0.15846628 0.078824431
## 18  FipTOT      PLE           0      1      6 0.08840730 0.055028527
## 19      Imid      OLS           0      1      6 0.03531090 0.021642805
## 20      Imid      PLE           0      1      6 0.04027054 0.025656606
## 21      Pendi      OLS           0      1      6 3.69828962 2.012556828
## 22      Pendi      OLS           1      1      6 1.73652917 1.007560748
## 23      Pendi      PLE           0      1      6 2.94789191 1.421463716
## 24      Pendi      PLE           1      1      6 3.03225651 1.606078090
## 25  STAUGDEA      OLS           1      0      6 0.09659701 0.065142138
## 26  STAUGDEA      PLE           1      0      6 0.09044778 0.036584069
## 27  STAUGDIA      OLS           1      0      6 0.12843594 0.118047484
## 28  STAUGDIA      PLE           1      0      6 0.08278948 0.026913238
## 29  STRIKEA      OLS           1      0      6 0.04013783 0.057736717
## 30  STRIKEA      PLE           1      0      6 0.01052381 0.021706468
## 31  STRIKEB      OLS           1      0      6 0.08923070 0.102226784
## 32  STRIKEB      PLE           1      0      6 0.03710196 0.041024425
```

```
## 33      TDLA      OLS          0      0      6 0.07845052 0.046822014
## 34      TDLA      PLE          0      0      6 0.02754424 0.041536786
## 35      TDLB      OLS          0      0      6 0.16031762 0.070661612
## 36      TDLB      PLE          0      0      6 0.08023899 0.054961891
## 37      TDN       OLS          0      1      6 0.08926025 0.042368742
## 38      TDN       OLS          1      1      6 0.05391972 0.007921897
## 39      TDN       PLE          0      1      6 0.07315779 0.031544457
## 40      TDN       PLE          1      1      6 0.05642193 0.024150822
## 41      TNDTOT    OLS          0      1      6 0.32802839 0.107117899
## 42      TNDTOT    OLS          1      1      6 0.18390695 0.153054256
## 43      TNDTOT    PLE          0      1      6 0.18201386 0.124224013
## 44      TNDTOT    PLE          1      1      6 0.11034839 0.063776177
## Variables not shown: SoilMean (dbl), SoilSD (dbl)
```

```
#View(frog.soil.means)
```

```
#Merge means and other statistics back into larger file.
frog.soil <- merge(frog.soil,frog.soil.means)
```

```
#treatment bcf
```

```
frog.soil$treatbcf <- frog.soil$BodyBurden/frog.soil$SoilMean
```

Setup of the complete main data set frog.soil.

```
dim(frog.soil)
```

```
## [1] 264 24
```

```
str(frog.soil)
```

```
## 'data.frame': 264 obs. of 24 variables:
## $ SoilType : Factor w/ 2 levels "OLS","PLE": 1 1 1 1 1 1 1 1 1 1 ...
## $ Pesticide : Factor w/ 17 levels "ATZ","ATZDEA",...: 1 1 1 1 1 1 1 1 1 1 ...
## $ Formulation : Factor w/ 2 levels "0","1": 1 1 1 1 1 2 2 2 2 ...
## $ Parent : Factor w/ 2 levels "0","1": 2 2 2 2 2 2 2 2 2 2 ...
## $ Day : Factor w/ 4 levels "0","1","2","3": 3 3 3 3 3 3 3 3 3 3 ...
## $ Row : Factor w/ 7 levels "1","2","3","4",...: 2 4 5 7 1 2 1 2 5 7 ...
## $ Column : Factor w/ 10 levels "", "A", "B", "C",...: 10 3 9 6 3 7 6 8 8 5 ...
## $ BodyBurden : num 0.728 0.27 0.237 1.9 0.472 ...
## $ Soil : num 16.6 12.3 21.6 29.2 29.7 ...
## $ Weight : num 11.14 11.96 17.39 11.77 9.56 ...
## $ Total : Factor w/ 2 levels "0","1": 1 1 1 1 1 1 1 1 1 1 ...
## $ bowlbcf : num 0.044 0.022 0.011 0.065 0.0159 ...
## $ surface_area_total : num 4.57 4.76 5.91 4.71 4.18 ...
## $ surface_area_footprint: num 3.3 3.5 4.82 3.46 2.9 ...
## $ expKoc : num NA NA NA NA NA NA NA NA NA NA ...
## $ litKoc : num NA NA NA NA NA NA NA NA NA NA ...
## $ OM : num 3.1 3.1 3.1 3.1 3.1 3.1 3.1 3.1 3.1 ...
## $ OC : num 1.8 1.8 1.8 1.8 1.8 ...
## $ count : int 6 6 6 6 6 6 6 6 6 ...
## $ FrogMean : num 0.814 0.814 0.814 0.814 0.814 ...
## $ FrogSD : num 0.655 0.655 0.655 0.655 0.655 ...
```



```
## $ SoilMean          : num  21.2 21.2 21.2 21.2 21.2 ...
## $ SoilSD            : num   7.08 7.08 7.08 7.08 7.08 ...
## $ treatbcf          : num   0.0344 0.0128 0.0112 0.0897 0.0223 ...
```

Subset data

Eliminate data that will not be used for this analysis and manuscript. Keep only total pesticide results and only for active ingredients, metabolites and formulations dropped.

```
## [1] 96 24
```

```
## [1] "SoilType"          "Pesticide"
## [3] "Formulation"       "Parent"
## [5] "Day"              "Row"
## [7] "Column"           "BodyBurden"
## [9] "Soil"             "Weight"
## [11] "Total"            "bowlbcf"
## [13] "surface_area_total" "surface_area_footprint"
## [15] "expKoc"           "litKoc"
## [17] "OM"              "OC"
## [19] "count"           "FrogMean"
## [21] "FrogSD"          "SoilMean"
## [23] "SoilSD"          "treatbcf"
```

```
## [1] 60 24
```

```
## [1] "SoilType"          "Pesticide"
## [3] "Formulation"       "Parent"
## [5] "Day"              "Row"
## [7] "Column"           "BodyBurden"
## [9] "Soil"             "Weight"
## [11] "Total"            "bowlbcf"
## [13] "surface_area_total" "surface_area_footprint"
## [15] "expKoc"           "litKoc"
## [17] "OM"              "OC"
## [19] "count"           "FrogMean"
## [21] "FrogSD"          "SoilMean"
## [23] "SoilSD"          "treatbcf"
```

Statistical analyses

Analysis of total analyte active ingredients concentration data set. Previously, two alternative methods for calculating bioconcentration factors were used: dividing the amphibian tissue residue concentration of each bowl by the soil concentration within that bowl (bowlbcfs) and also dividing the amphibian tissue residue concentration of each bowl by the mean of all the bowls within the treatment (treatbcfs).

A paired comparison design is implemented to examine the impacts of soil type and surface area. The paired comparison design is essentially a randomized block design where the blocking variable (pesticides) has size 2 and is therefore treated as a nuisance variable. This controls for the large variation in treatment application rates and uptake across the different pesticides tested. The paired comparison design on the bowl bcf finds soil type significant, but not amphibian surface area.

We evaluate 3 different paired comparison designs: with bowlbcfs, where each frog tissue concentration is divided by its soil concentration, mean bcf (treatbcf), where each frog tissue concentration is divided by the mean of the soil concentrations for that treatment, and by body.burden where soil concentration is used as an additional covariate instead of in the divisor.

```
##              Df Sum Sq Mean Sq F value    Pr(>F)
## Pesticide      4  0.8852  0.22130   16.231 5.76e-10 ***
## SoilType       1  0.0262  0.02617    1.919   0.169
## Formulation    1  0.0300  0.03000    2.200   0.142
## surface_area_total 1  0.0062  0.00615    0.451   0.504
## expKoc         1  0.0005  0.00051    0.038   0.847
## Residuals     87  1.1862  0.01363
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
##              Df Sum Sq Mean Sq F value    Pr(>F)
## Pesticide      4  0.6790  0.16975   23.153 4.73e-13 ***
## SoilType       1  0.0131  0.01306    1.781   0.186
## Formulation    1  0.0145  0.01451    1.979   0.163
## surface_area_total 1  0.0146  0.01459    1.990   0.162
## expKoc         1  0.0077  0.00772    1.053   0.308
## Residuals     87  0.6379  0.00733
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

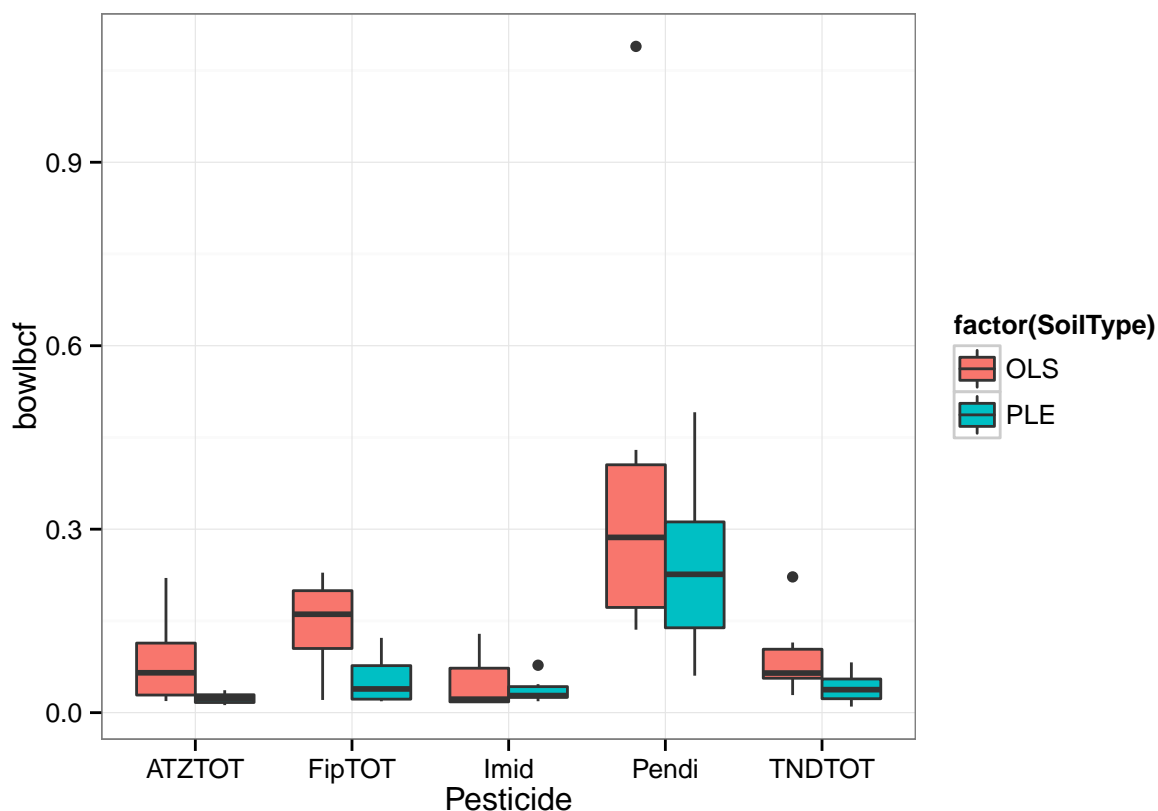
Bowl bcf results and figure.

```
# is imidacloprid being factored in correctly for the aov
bowlbcf.total.ai.aov <- aov(bowlbcf ~ Pesticide + SoilType + surface_area_total + expKoc,
                             data = frog.soil.total.ai)
summary(bowlbcf.total.ai.aov)
```

```
##              Df Sum Sq Mean Sq F value    Pr(>F)
## Pesticide      4  0.6372  0.15929    9.456 8.03e-06 ***
## SoilType       1  0.0821  0.08211    4.875   0.0317 *
## surface_area_total 1  0.0015  0.00154    0.091   0.7638
## expKoc         1  0.0304  0.03035    1.802   0.1853
## Residuals     52  0.8759  0.01684
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

This figure based on bowlbcfs is not used in the manuscript.

```
qplot(Pesticide, bowlbcf, fill=factor(SoilType), data=frog.soil.total.ai, geom="boxplot", position="dodge")
```



Treatment bcf results and figure. These analysis of variance results and the figure are used in the Van Meter at al. document. Context for interpretation - http://www.bodowinter.com/tutorial/bw_anova_general.pdf

Significance of soiltype: $p = 0.00165$, $F = 10.999$, $df1 = 1$, $df2 = 53$.

```
treatbcf.total.ai.aov <- aov(treatbcf ~ Pesticide + SoilType + expKoc,
                             data = frog.soil.total.ai)
summary(treatbcf.total.ai.aov)
```

```
##           Df Sum Sq Mean Sq F value    Pr(>F)
## Pesticide   4  0.4257  0.10642   18.180 1.87e-09 ***
## SoilType    1  0.0644  0.06438   10.999  0.00165 **
## expKoc      1  0.0201  0.02012    3.438  0.06928 .
## Residuals  53  0.3102  0.00585
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

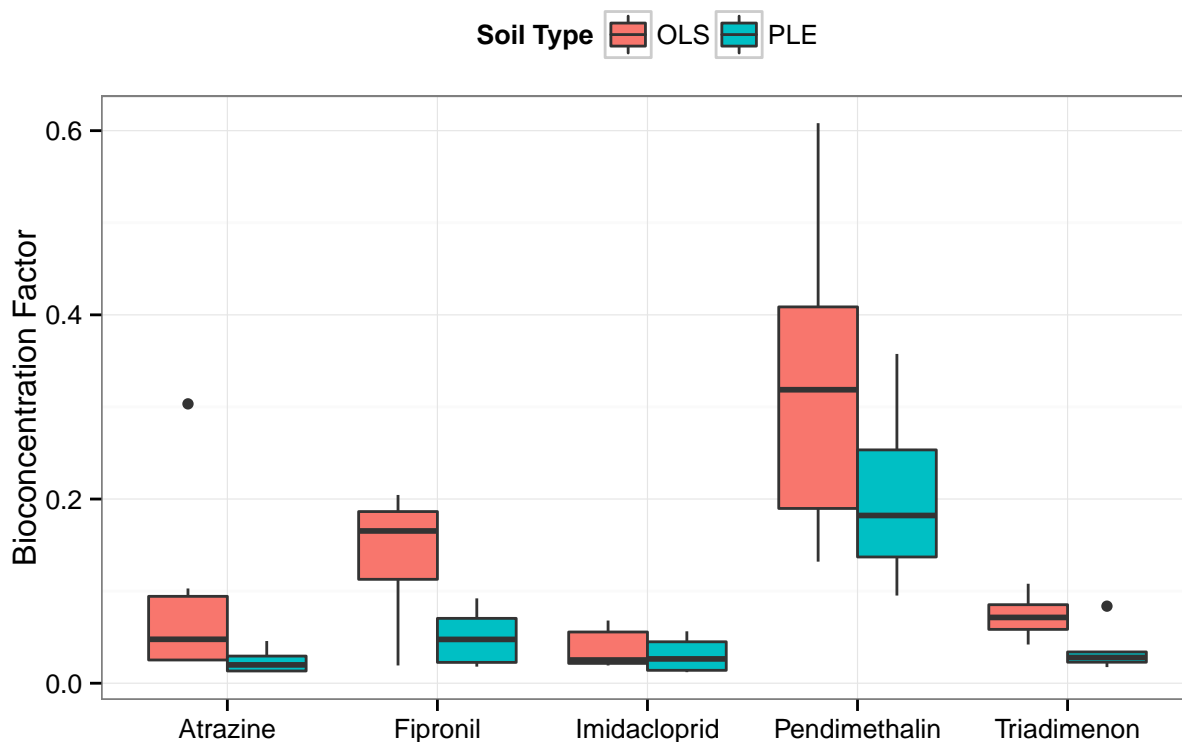
```
model.tables(treatbcf.total.ai.aov)
```

```
## Warning in replications(paste("~", xx), data = mf): non-factors ignored:
## expKoc
```

```
## Tables of effects
##
## Pesticide
```

```
## Pesticide
## ATZTOT FipTOT Imid Pendi TNDTOT
## -0.04343 -0.00611 -0.06732 0.16376 -0.04691
##
## SoilType
## SoilType
## OLS PLE
## 0.03276 -0.03276
##
## expKoc
## expKoc
## 1.733 2.303 2.556 2.634 2.864 3.01 3.025 3.645
## 0.03371 0.01133 0.01813 -0.01133 0.00399 -0.00823 0.00823 -0.01813
## 4.242 6.425
## -0.00399 -0.03371
```

```
pesticides <- c("Atrazine", "Fipronil", "Imidacloprid", "Pendimethalin", "Triadimenon")
qplot(x=Pesticide, y=treatbcf, fill=factor(SoilType), xlab="", ylab="Bioconcentration Factor",
      data=frog.soil.total.ai, geom="boxplot", position="dodge") +
  theme_bw() + scale_x_discrete(breaks=c("ATZTOT", "FipTOT", "Imid", "Pendi", "TNDTOT"), labels=
```



Generate figure as png for the manuscript.

```
#figure 1 of Van Meter et al. manuscript
#pdf(paste(frogsoildir,"rvm2016_fig1.pdf", sep=""))
png(paste(frogsoildir,"rvm2016_fig1.png", sep=""))
```

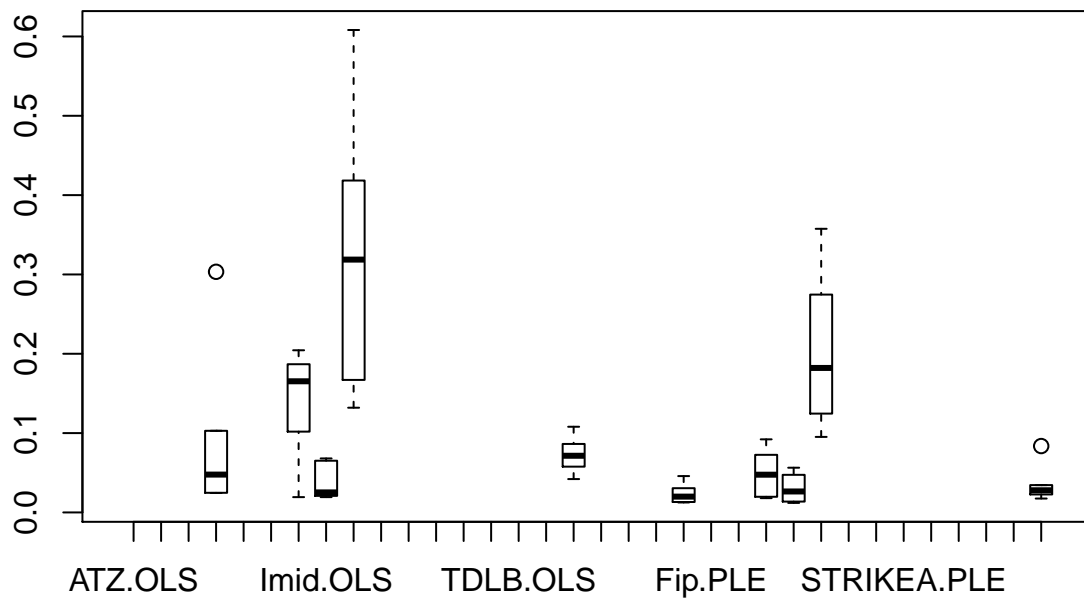
```
pesticides <- c("Atrazine", "Fipronil", "Imidacloprid", "Pendimethalin", "Triadimenon")
qplot(x=Pesticide, y=treatbcf, fill=factor(SoilType), xlab="", ylab="Bioconcentration Factor",
      data=frog.soil.total.ai, geom="boxplot", position="dodge") +
  theme_bw() + scale_x_discrete(breaks=c("ATZTOT", "FipTOT", "Imid", "Pendi", "TNDTOT"), labels:
dev.off()
```

```
## pdf
## 2
```

Some additional stuff we did not use

A figure.

```
boxplot(treatbcf ~ Pesticide + SoilType, data =frog.soil.total.ai)
```



We considered dropping imidacloprid for analytical reasons but it was unnecessary.

```
# more significant if imidacloprid is dropped (but not necessary)
bowlbcf.total.noimid.aov <- aov(bowlbcf ~ Pesticide + SoilType + surface_area_total,
                                data = frog.soil.total.noimid)
summary(bowlbcf.total.noimid.aov)
```

```
##          Df Sum Sq Mean Sq F value    Pr(>F)
```

```
## Pesticide          3 0.5563 0.18543    8.857 0.000115 ***
## SoilType           1 0.0961 0.09613    4.592 0.037968 *
## surface_area_total 1 0.0001 0.00013    0.006 0.936840
## Residuals         42 0.8793 0.02094
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
treatbcf.total.noimid.aov <- aov(treatbcf ~ Pesticide + SoilType + surface_area_total,
                                data = frog.soil.total.noimid)
summary(treatbcf.total.noimid.aov)
```

```
##              Df Sum Sq Mean Sq F value    Pr(>F)
## Pesticide      3  0.3577   0.11924   16.072 4.18e-07 ***
## SoilType       1  0.0771   0.07711   10.394  0.00245 **
## surface_area_total 1  0.0014   0.00142    0.192  0.66354
## Residuals     42  0.3116   0.00742
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Tukey as anova post-hoc proxy.

```
TukeyHSD(treatbcf.total.ai.aov)
```

```
## Warning in replications(paste("-", xx), data = mf): non-factors ignored:
## expKoc
```

```
## Warning in TukeyHSD.aov(treatbcf.total.ai.aov): 'which' specified some
## non-factors which will be dropped
```

```
##   Tukey multiple comparisons of means
##     95% family-wise confidence level
##
## Fit: aov(formula = treatbcf ~ Pesticide + SoilType + expKoc, data = frog.soil.total.ai)
##
## $Pesticide
##              diff              lwr              upr              p adj
## FipTOT-ATZTOT  0.037321911 -0.05088198  0.12552581  0.7542455
## Imid-ATZTOT   -0.023891382 -0.11209528  0.06431251  0.9394943
## Pendi-ATZTOT   0.207189936  0.11898604  0.29539383  0.0000002
## TNDTOT-ATZTOT -0.003481293 -0.09168519  0.08472260  0.9999639
## Imid-FipTOT   -0.061213293 -0.14941719  0.02699060  0.2996226
## Pendi-FipTOT   0.169868025  0.08166413  0.25807192  0.0000135
## TNDTOT-FipTOT -0.040803204 -0.12900710  0.04740069  0.6884923
## Pendi-Imid     0.231081318  0.14287742  0.31928521  0.0000000
## TNDTOT-Imid    0.020410089 -0.06779381  0.10861398  0.9652483
## TNDTOT-Pendi  -0.210671229 -0.29887512 -0.12246733  0.0000001
##
## $SoilType
##              diff              lwr              upr              p adj
## PLE-OLS -0.06551572 -0.1051385 -0.02589299  0.0016508
```

Bartlett's test results.

```
#Bartlett test to test the null hypothesis of equal group variances
bartlett.test(treatbcf ~ Pesticide, data =frog.soil.total.ai)
```

```
##
## Bartlett test of homogeneity of variances
##
## data: treatbcf by Pesticide
## Bartlett's K-squared = 44.5486, df = 4, p-value = 4.935e-09
```

```
#no sale! for pesticides
bartlett.test(treatbcf ~ SoilType, data = frog.soil.total.ai)
```

```
##
## Bartlett test of homogeneity of variances
##
## data: treatbcf by SoilType
## Bartlett's K-squared = 7.5497, df = 1, p-value = 0.006002
```

```
#also rejected for soil type, but not grouped by pesticide
```

Bartlett's test results.

```
#the oneway.test() applies a Welch correction for nonhomogeneity
oneway.test(treatbcf ~ Pesticide + SoilType, data =frog.soil.total.ai)
```

```
##
## One-way analysis of means (not assuming equal variances)
##
## data: treatbcf and Pesticide + SoilType
## F = 6.0442, num df = 9.000, denom df = 20.078, p-value = 0.0003999
```

Kruskal test results.

```
#nonparameteric kruskal test
kruskal.test(treatbcf ~ Pesticide, data =frog.soil.total.ai)
```

```
##
## Kruskal-Wallis rank sum test
##
## data: treatbcf by Pesticide
## Kruskal-Wallis chi-squared = 27.9798, df = 4, p-value = 1.259e-05
```

```
kruskal.test(treatbcf ~ SoilType, data =frog.soil.total.ai)
```

```
##
## Kruskal-Wallis rank sum test
##
## data: treatbcf by SoilType
## Kruskal-Wallis chi-squared = 7.0035, df = 1, p-value = 0.008135
```

We can also consider the pairwise t-test. For this we need the means of the pesticide treatments by soil for the test. Doesn't make any sense.