Contents

```
%
%Script to read and process runs from the Perkin Elmer CHN 2400
%   element analyzer. The code calculates C & N content on sample
%   filter replicates
clear
close all

% Data info

cruise = 'I6SP';   %enter here cruise or campaign code

airs=5; % Number of air blanks run at the begining of run prep
```

Open Data File that contains analysis report from CHN instrument

```
filename = uigetfile('/Users/joaquin/Documents/CVO/Lab stuff/POC/Runs/*.csv',...
    'Select CHN run file');

fid = fopen(filename);

C_text = textscan(fid, '%s', 11, 'delimiter', ',');

C_data = textscan(fid, '%s %f %f %s %f %f %f %f %f %f %f','delimiter',',');

fclose(fid);
```

Assign variable names to data columns

```
        names = C_text{1};

        id          = C_data{1};
        seq         = C_data{2};
        weight      = C_data{3};
        time        = C_data{4};
        carbon      = C_data{5};
        hydrogen    = C_data{6};
        nitrogen    = C_data{7};
        zr          = C_data{8};
        cr          = C_data{9};
        hr          = C_data{10};
        nr          = C_data{11};
```

Indexing

```
    %Find index for each type of run (i.e., K factors, blanks,...
    %    ref material, filter blanks, sample, etc

K1s     = find((strcmp(id,'K1')==1));       %index of K factors calibration ...
                                                %runs (i.e., acetanilide cal runs)
blanks  = find((strcmp(id,'BLANK')==1));    %index of analytical cal blanks
f_blks  = find((strcmp(id,'TEST')==1));     %index of filter, "method blanks"
buff    = find((strcmp(id,'BUFF')==1));     %index of Buffalo River sediment runs
ace     = find((strcmp(id,'ACE')==1));      %index of acetanilide check standards

cals    = [K1s; blanks];                    %index of cal runs
stds    = [buff; ace];                      %index of standard & check runs

    length_run  = size(id,1);
    run         = 1:length_run;

samples         = setdiff(run, [cals; stds; f_blks]);  %index of sample runs

non_cal         = setdiff(run, cals);
```

Instrument signals for each element

```
    %Carbon                     %   Carbon signal [i.e., C read (cr)-N read (nr)]
        %Blanks
    CBs=cr(blanks)-nr(blanks);  %   C blanks

    CB=mean(CBs(1:end-airs));   %   Mean C blanks, except air blanks
                                %   (run report runs chron. bottom to top)

    CS = (cr - nr)-CB;          %   Carbon signals (i.e. C read - N read)

     %Nitrogen                  %   Nitrogen signal [i.e., N read (nr)-zero read (zr)]
        %Blanks
    NBs=nr(blanks)-zr(blanks);  %   N blanks
```

```
   NB=mean(NBs(1:end-airs));   %  Mean N blanks, except air blanks

   NS = (nr - zr)-NB;          %  Nitrogen signals (i.e. N read - zero read)
```

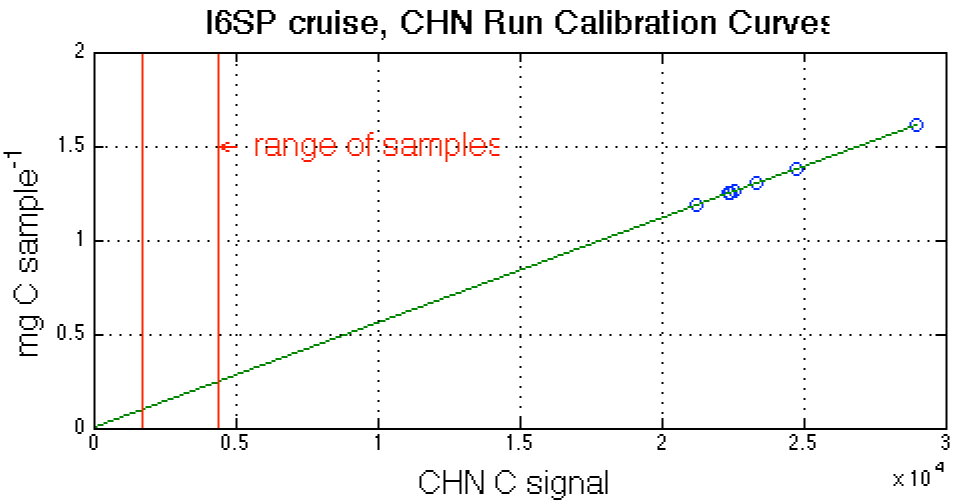
Run calibration curves

Carbon -- Amount of C in mg for K1 (acetanilide) runs

```
   K1_C   = (71.09/100).*weight(K1s); %mg C per K1 run

   % Linear regression of K1_C as a f(x) of C signal, CS.

x = CS(K1s);
y = K1_C;

   xx = union(0,x);

   C_model = polyfit(x,y,1);     %Ace std C vs C signal linear fit
   z = polyval(C_model,xx);
```

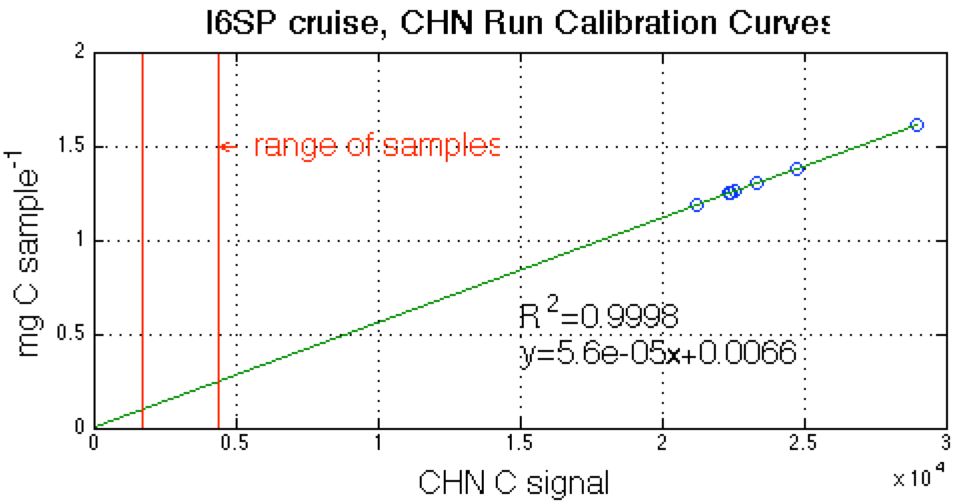
Plot Carbon Calibration curve

```
   f = figure('Position',[2000 1000 550 550]);
   subplot(2,1,1);
   plot(x,K1_C,'o')
       grid on
       hold on

      title([cruise ' cruise, CHN Run Calibration Curves'], 'FontSize', 17);

   plot(x,y,'o', xx,z ,'-')
       ylabel('mg C sample^{-1}','FontSize',16)
       xlabel('CHN C signal', 'FontSize', 16)

       aa=get(gca,'xlim');
       bb=get(gca,'ylim');

       vline([max(CS(samples)), min(CS(samples))],'r')  %vert red lines
                                                        %enclose sample
                                                        %range
       text(max(CS(samples)),bb(2)*.75,'\leftarrow  range of samples',...
           'color','r','FontSize', 16)
```



C regression statistics

```
    X =[ones(size(x,1),1) x];
    [b,bint,r,rint,stats] = regress(y,X);

    % Display R^2 & regression eq on cal curve plot
    text(aa(2)*.5,bb(2)*.3,['R^{2}=' num2str(stats(1),4)],'fontsize',16)
    text(aa(2)*.5,bb(2)*.2,['y=' num2str(b(2),2) 'x+' num2str(b(1),2)],'fontsize',16)

hold off
```

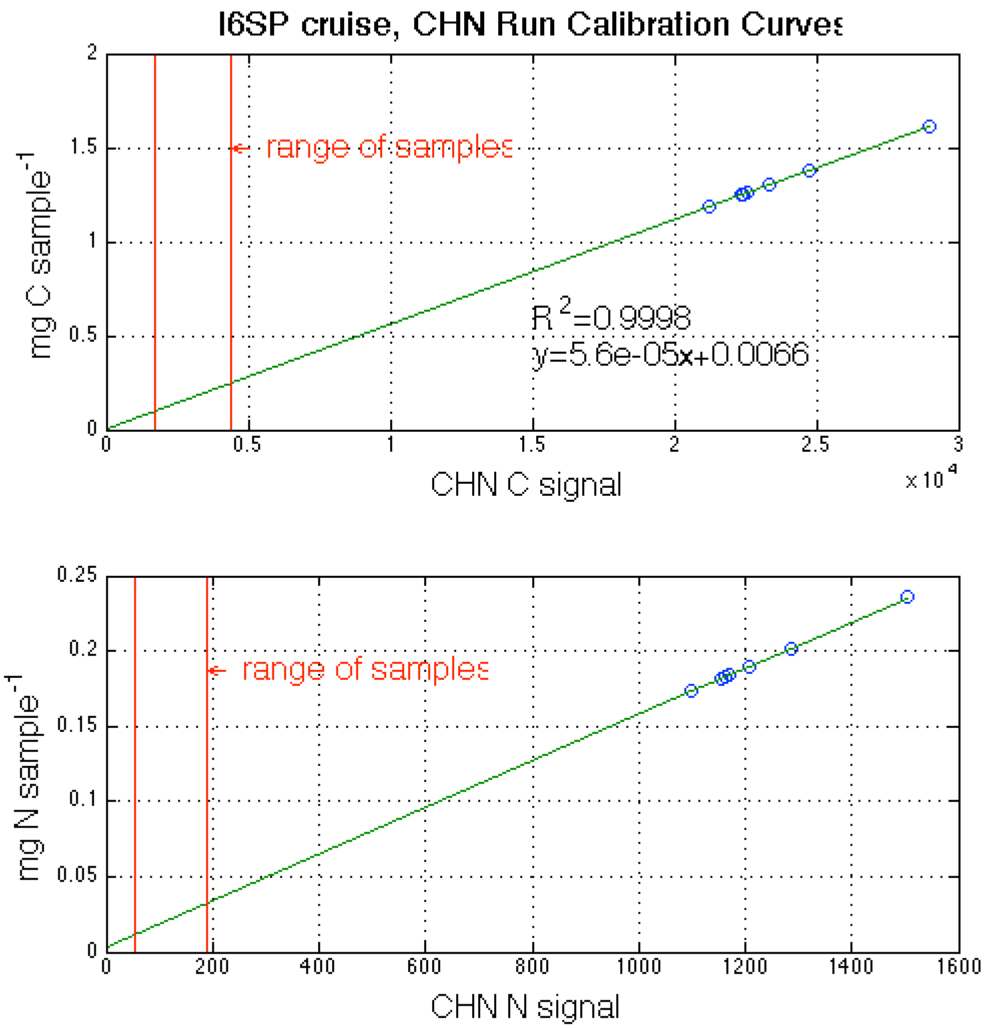


Nitrogen -- Amount of C in mg for K1 runs

```
    K1_N   = (10.36/100).*weight(K1s); %mg N per K1 run

    % Linear regression of K1_N as a f(x) of N signal, NS.

 x = NS(K1s);
 y = K1_N;
```

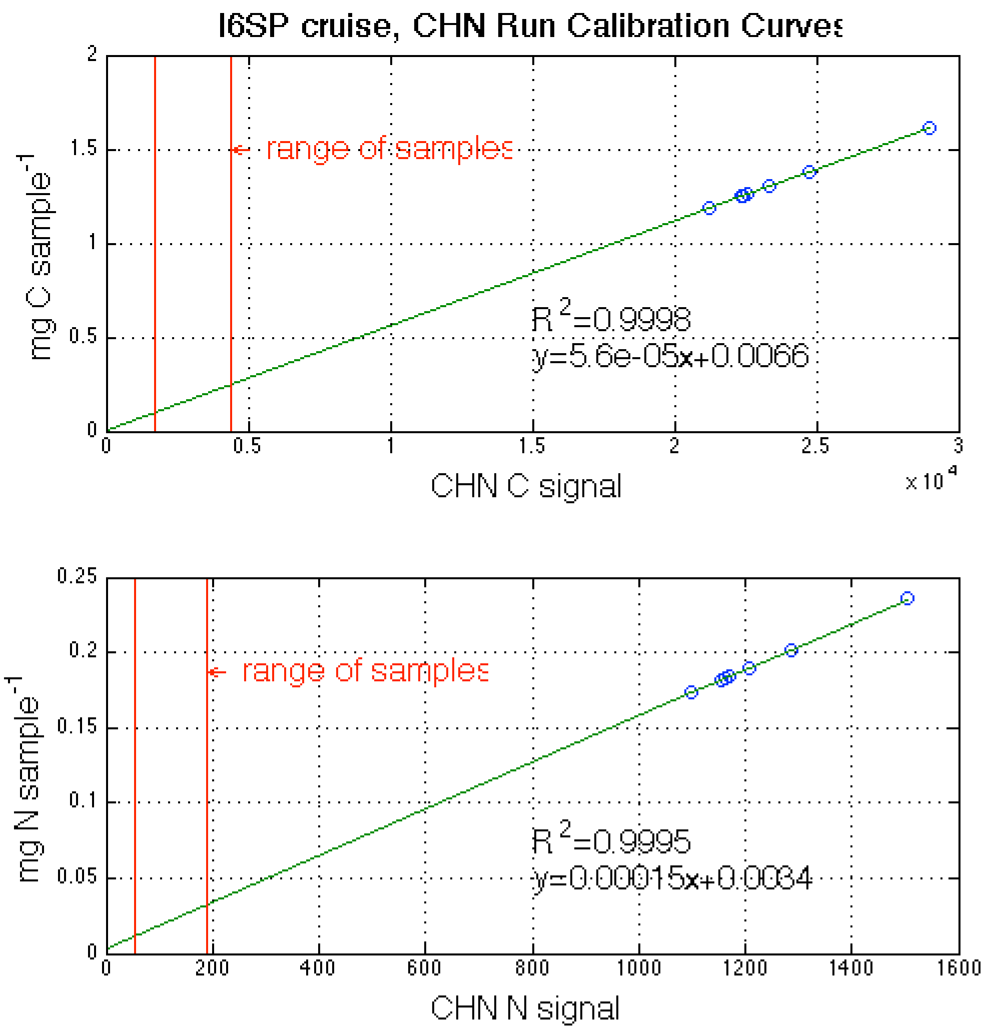
Linear regression of std_N as a f(x) of NR signal

```
 nx = NS(K1s);
 ny = K1_N;

    nxx = union(0,nx);

    N_model = polyfit(nx,ny,1);
    nz = polyval(N_model,nxx);
    subplot(2,1,2);
    plot(nx,K1_N,'o')
        grid on
        hold on

    plot(nx,ny,'o', nxx,nz ,'-')
        ylabel('mg N sample^{-1}','FontSize',16)
        xlabel('CHN N signal', 'FontSize', 16)

        aa=get(gca,'xlim');
        bb=get(gca,'ylim');

 vline([max(NS(samples)), min(NS(samples))],'r')          %vert red lines
                                                           %enclose sample
                                                           %range
     text(max(NS(samples)),bb(2)*.75,'\leftarrow  range of samples',...
            'color','r','FontSize', 16)
```



N regression statistics

```
    NX =[ones(size(x,1),1) nx];
    [n_b,n_bint,n_r,n_rint,n_stats] = regress(ny,NX);

    % Display R^2 & regression eq on cal curve plot
   text(aa(2)*.5,bb(2)*.3,['R^{2}=' num2str(n_stats(1),4)],'fontsize',16)
   text(aa(2)*.5,bb(2)*.2,['y=' num2str(n_b(2),2) 'x+' num2str(n_b(1),2)],'fontsize',16)

hold off
```



C and N (in mg) in filter samples and filter blanks

```
mgC = polyval(C_model,CS(samples));      %C in samples, mg, not corrected for filter blank
    mgC_b = polyval(C_model,CS(f_blks)); %C in filter blank
```

Blank corrections

```
  if(mean(mgC_b)>0)                        % C filter blank correction if > 0
```

```
                                          % if blank < 0, left uncorrected
   corr_C  = mgC-mean(mgC_b); disp('C filter blanks > 0, correction applied')
    else
    corr_C = mgC; disp('C filter blanks < 0, no correction applied')
  end
```

```
C filter blanks > 0, correction applied
```

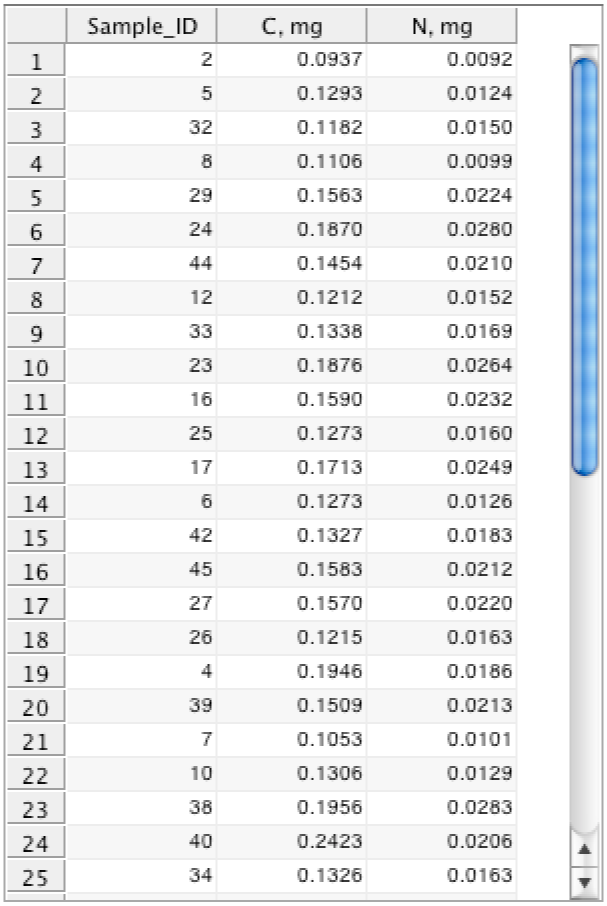
Nitrogen

```
mgN = polyval(N_model,NS(samples));       % N in samples, mg, not corrected for filter blank
    mgN_b = polyval(N_model,NS(f_blks)); % N in filter blanks

    if(mean(mgN_b)>0)                    % N filter blank correction if > 0
   corr_N  = mgN-mean(mgN_b); disp('N filter blanks > 0, correction applied')
    else
    corr_N = mgN; disp('N filter blanks < 0, no correction applied')
  end
%
```

```
N filter blanks > 0, correction applied
```

Analysis Report with filter blank-corrected results for C & N

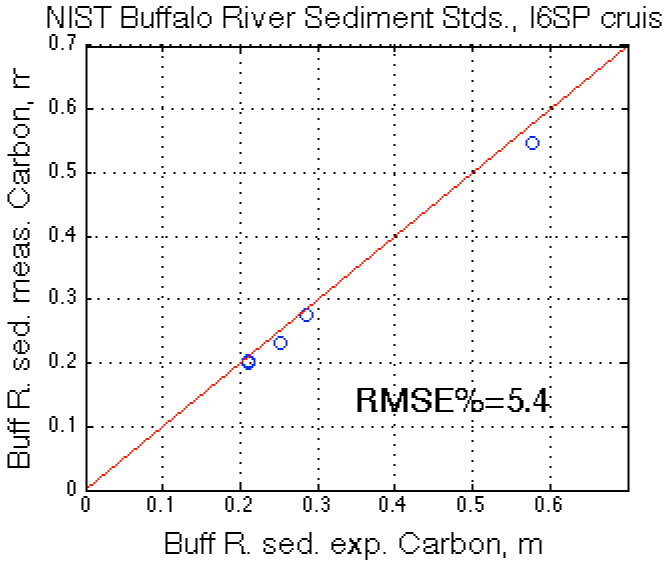
```
rep = [str2double(id(samples)),corr_C, corr_N];

    f = figure('Position',[1370 85 320 450]);
    cnames = {'Sample_ID','C, mg','N, mg'};
    t = uitable;
    set(t,'Data',rep,'ColumnName',cnames,'Position',[10 0 300 450])

dlmwrite ([cruise '_CHN_run_report_V2'], rep)   % Writes report file with sample ID...
                                                % mg C and mg N for each
                                                % sample run
```

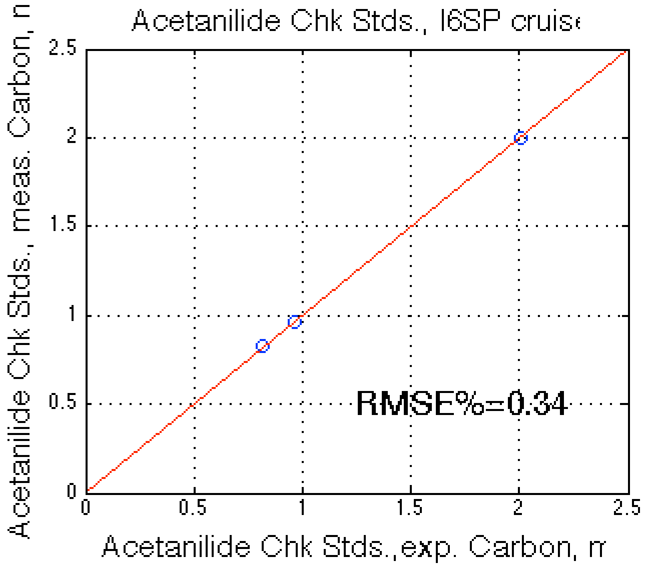


	Sample_ID	C, mg	N, mg
1	2	0.0937	0.0092
2	5	0.1293	0.0124
3	32	0.1182	0.0150
4	8	0.1106	0.0099
5	29	0.1563	0.0224
6	24	0.1870	0.0280
7	44	0.1454	0.0210
8	12	0.1212	0.0152
9	33	0.1338	0.0169
10	23	0.1876	0.0264
11	16	0.1590	0.0232
12	25	0.1273	0.0160
13	17	0.1713	0.0249
14	6	0.1273	0.0126
15	42	0.1327	0.0183
16	45	0.1583	0.0212
17	27	0.1570	0.0220
18	26	0.1215	0.0163
19	4	0.1946	0.0186
20	39	0.1509	0.0213
21	7	0.1053	0.0101
22	10	0.1306	0.0129
23	38	0.1956	0.0283
24	40	0.2423	0.0206
25	34	0.1326	0.0163

QA/QC

```
% Carbon percent error based on Buffallo River runs
    %NIST certified C % content in Buff R. sed. is 3.51%

%Buffalo River Sediment Ref stds
mgC_buff=polyval(C_model,CS(buff)); % measured C in Buff stds

mgC_buff_t=.0351*weight(buff);              % expected C in Buff stds

%ACE check stds
mgC_ace=polyval(C_model,CS(ace));     % measured C in ACE chk stds

mgC_ace_t=.7109*weight(ace);              % expected C in ACE chk stds


figure('Position',[2000 100 350 650]);

subplot(2,1,1)

plot(mgC_buff_t,mgC_buff,'o')
    grid on
    hold on

   a=max(get(gca,'xlim'));
     set(gca,'xlim',[0 a]);
     set(gca,'ylim',[0 a]);
    line([0 a],[0 a],'color','r')

    xlabel('Buff R. sed. exp. Carbon, mg','fontsize',15)
     ylabel('Buff R. sed. meas. Carbon, mg','fontsize',15)

     error=errperf(mgC_buff_t,mgC_buff,'rmspe');

     text(a*.5,a*.2,['RMSE%=' num2str(error,2)],'fontsize',17)

     title(['NIST Buffalo River Sediment Stds., ' cruise ' cruise'],...
         'fontsize',15)

subplot(2,1,2)


plot(mgC_ace_t,mgC_ace,'o')
    grid on
    hold on

   a=max(get(gca,'xlim'));
     set(gca,'xlim',[0 a]);
     set(gca,'ylim',[0 a]);
    line([0 a],[0 a],'color','r')

    xlabel('Acetanilide Chk Stds.,exp. Carbon, mg','fontsize',15)
     ylabel('Acetanilide Chk Stds., meas. Carbon, mg','fontsize',15)

     error=errperf(mgC_ace_t,mgC_ace,'rmspe');

     text(a*.5,a*.2,['RMSE%=' num2str(error,2)],'fontsize',17)

     title(['Acetanilide Chk Stds., ' cruise ' cruise'],...
         'fontsize',15)
     hold off
```





Published with MATLAB® 7.14