Data Processing to Edebeli_ACP_2020

Contents

Initiate Matlab

```
% change working directory
path = matlab.desktop.editor.getActiveFilename;
[filepath,~,~] = fileparts(path);
cd(filepath);

clearvars
close all
clc
```

Load data

Data has been processed in file: 'Jacinta Snow Metamorphism Bromide Ozone/Matlab/PackedBedBrSnowOzoneExperimetns.mPackedBedBrSnowOzoneExperimetns.m'

```
load('Edebeli_ACP_2020__Data.mat')
```

Show data

Lists file names, snow sample properties, and flow settings for each data-set. See also file 'Edebeli_ACP_2020__List.dat' which holds the same information.

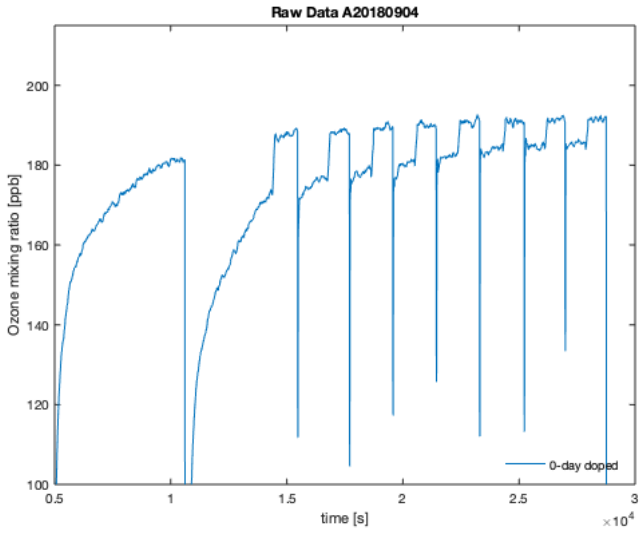
```
tmpT = struct2table(data);
disp(tmpT(:,1:8))
clearvars tmp*
```

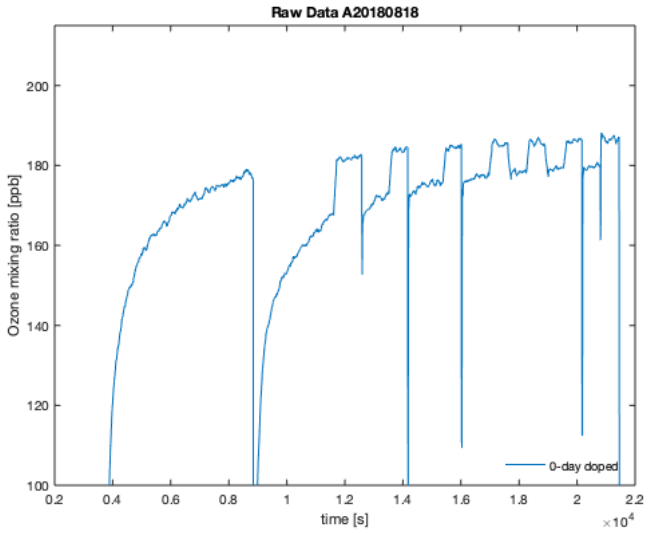
file	sample	smp_lable	totalSurfaceArea_cm2	flow_cm3_per_s	length_cm	mass_g	density
{'A20180904'}	{'0-day doped'}	{'0-1 (NaBr)'}	{[3111]}	{[6.5800]}	{[7.4000]}	{[17]}	{[0.450
{'A20180818'}	{'0-day doped'}	{'0-3 (NaBr)'}	{[2013]}	{[6.6200]}	{[5.9000]}	{[11]}	{[0.350
{'A20180716'}	{'0-day clean'}	{'0-2 (0 NaBr)'}	{[2112]}	{[6.6500]}	{[7.6000]}	{[12]}	{[0.460
{'A20180712'}	{'12-day clean'}	{'12-2 (0 NaBr)'}	{[2338]}	{[6.6300]}	{[7.6000]}	{[14]}	{[0.450
{'A20180709'}	{'12-day clean'}	{'12-1 (0 NaBr)'}	{[2839]}	{[6.5800]}	{[7.4000]}	{[17]}	{[0.350
{'A20180906'}	{'12-day doped'}	{'12-3 (NaBr)'}	{[2268]}	{[6.6000]}	{[7.4000]}	{[14]}	{[0.300
{'A20180808'}	{'Iso2_0'}	{'Iso-2 (0 NaBr)'}	{[1950]}	{[6.6833]}	{[7.6000]}	{[10]}	{[0.320
{'A20180809'}	{'Iso3_0'}	{'Iso-3 (0 NaBr)'}	{[2535]}	{[6.6417]}	{[7.6000]}	{[13]}	{[0.300
{'A20181205'}	{'Iso2_600'}	{'Iso-2 (NaBr)'}	{[2002]}	{[6.4250]}	{[7.6000]}	{[14]}	{[0.370
{'A20181206'}	{'Iso3_600'}	{'Iso-3 (NaBr)'}	{[2288]}	{[6.4250]}	{[7.4000]}	{[16]}	{[0.390
{'mean_3_4_5_7_8'}	{'0 Br'}	{'mean (0 NaBr)'}	{0×0 double}	{0×0 double}	{0×0 double}	{0×0 double}	{0×0 doub

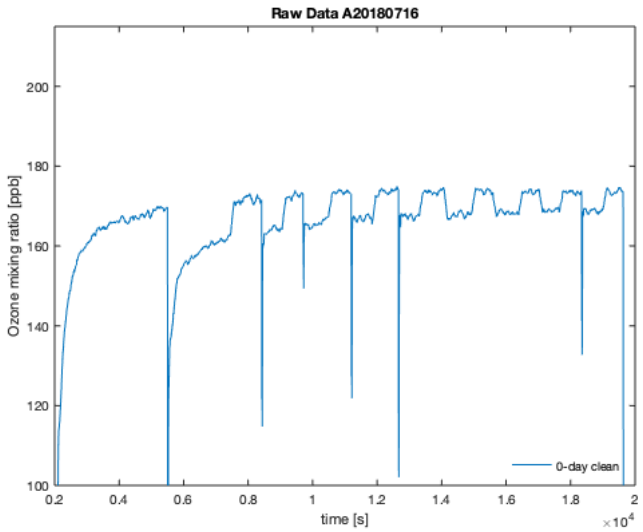
Raw data trend in ozone with time

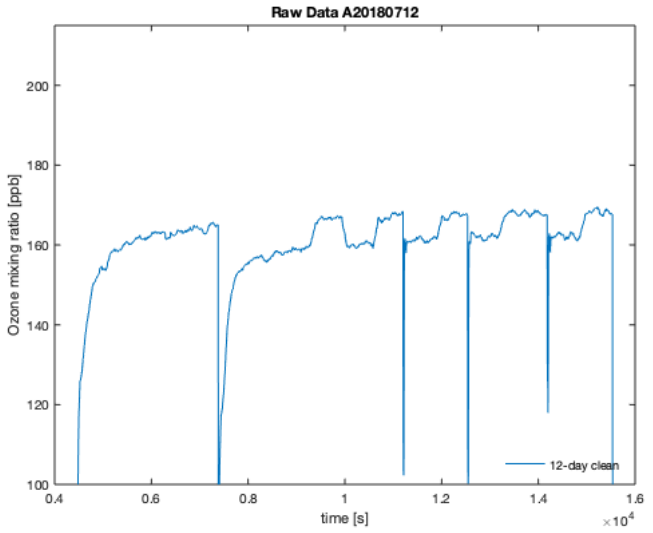
These figures show the trend of ozone mixing ratio (*O3mixingRatio_ppb*) with time (*time_s*) as measured downstream of the snow sample during the experiments. Time "0" denotes the time when data acquisition with ozone analyser was started. See also file 'Edebeli_ACP_2020__OzoneData.dat' which holds the same information.

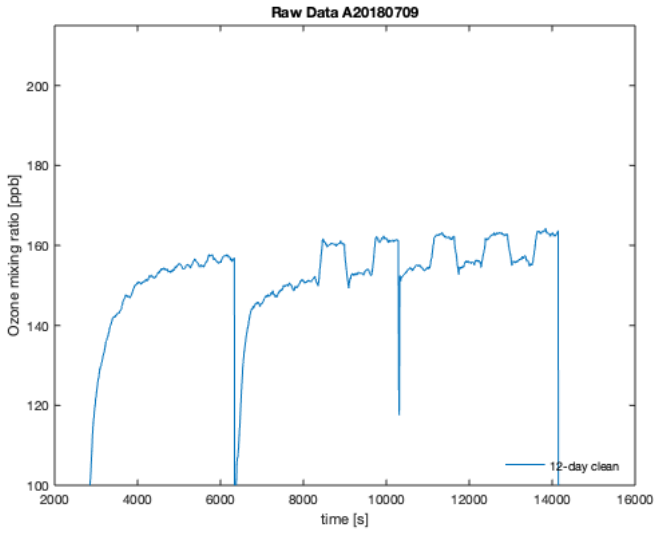
```
for iDataCurve = 1:10
    figure('Name',data(iDataCurve).file)
    plot(data(iDataCurve).time_s, data(iDataCurve).O3mixingRatio_ppb,'DisplayName',data(iDataCurve).sample);
    ylabel('Ozone mixing ratio [ppb]');
    xlabel('time [s]');
    title(['Raw Data ' data(iDataCurve).file])
    ylim([100 215]);
    legend
    legend('boxoff')
    legend( 'interpreter','none','Location','SouthEast')
end
clearvars -except data
```

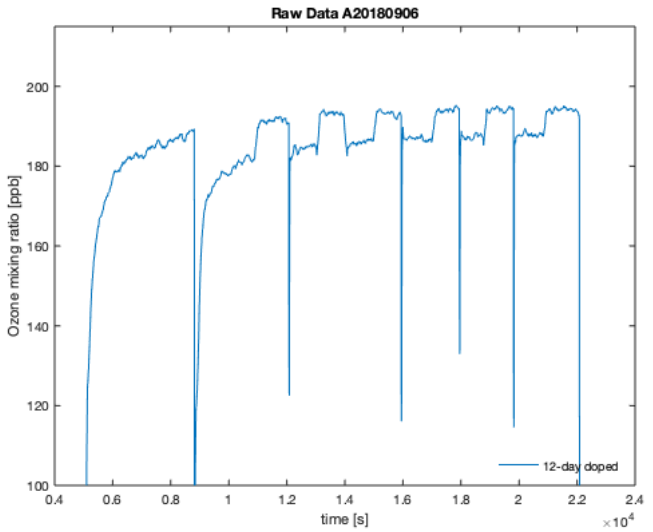

Raw Data A20180904
Ozone mixing ratio [ppb]
time [s]
×10^4
0-day doped

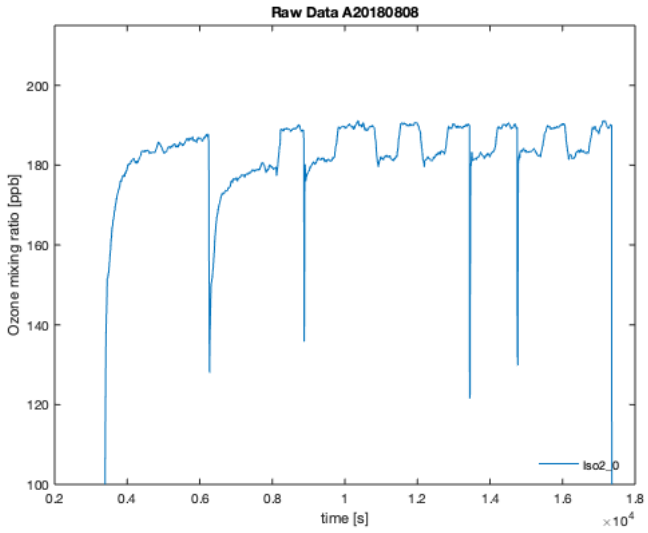

Raw Data A20180818
Ozone mixing ratio [ppb]
time [s]
×10^4
0-day doped

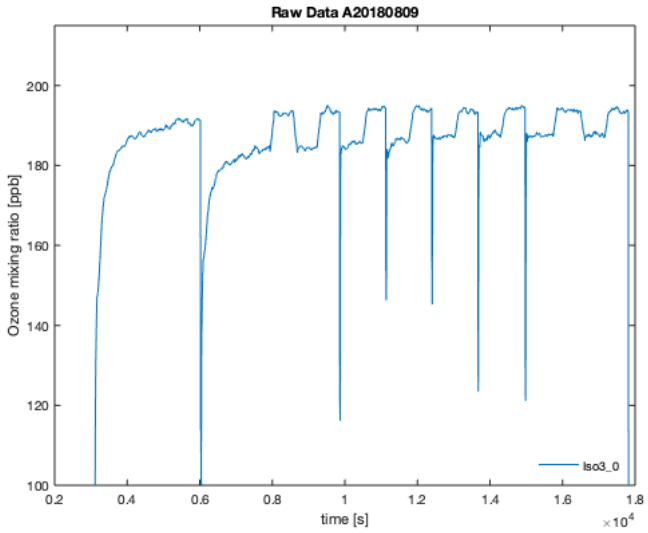

Raw Data A20180716
Ozone mixing ratio [ppb]
time [s]
×10^4
0-day clean

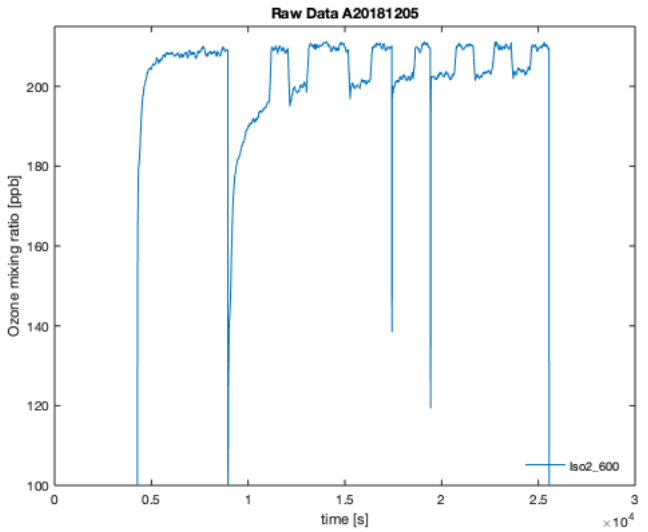

Raw Data A20180712
Ozone mixing ratio [ppb]
time [s]
12-day clean

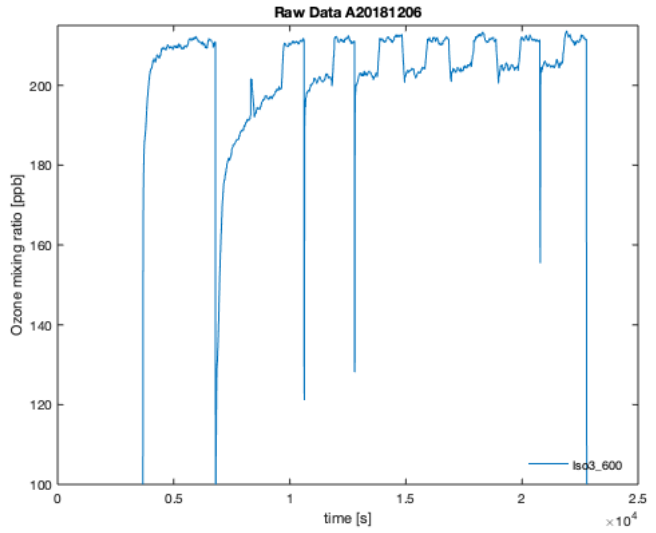

Raw Data A20180709
Ozone mixing ratio [ppb]
time [s]
12-day clean


Raw Data A20180906
Ozone mixing ratio [ppb]
time [s]
12-day doped


Raw Data A20180808
Ozone mixing ratio [ppb]
time [s]
×10^4
Iso2_0


Raw Data A20180809
Ozone mixing ratio [ppb]
time [s]
×10^4
Iso3_0

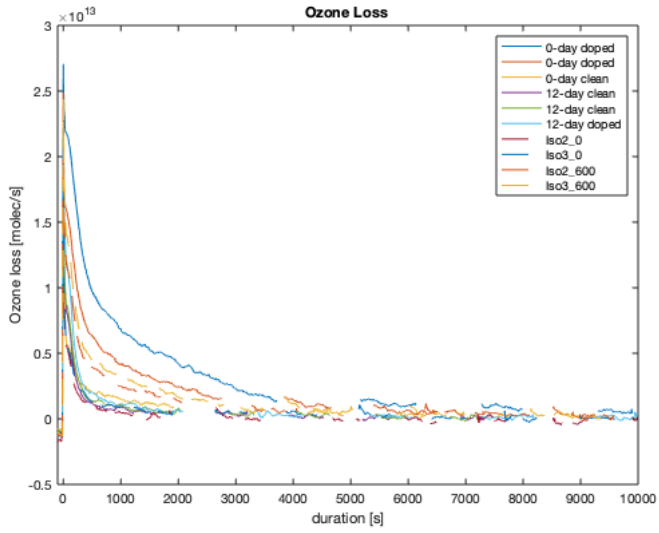

Raw Data A20181205
Ozone mixing ratio [ppb]
time [s]
×10^4
Iso2_600



Ozone loss in molec/s

These figures show the ozone (*nOzone_molec_per_s*) loss for each experiment with duration of ozone exposure (*duration_s*) of ozone exposure, as derived from the ozone trends shown above. Time "0" denotes the time when the carrier gas with ozone was passed via the snow sample. See also file 'Edebeli_ACP_2020__OzoneData.dat' which holds the same information.

```
figure('Name','O3 loss in molec/s')
tmp_color = colormap(lines(10));
for iFile = 1:10
    h = plot(data(iFile).duration_s, data(iFile).nOzone_molec_per_s,'DisplayName',data(iFile).sample,'Color',tmp_color(iFile,:));
    if iFile >= 7
        h.LineStyle = '--';
    end
    hold on
end
ylabel('Ozone loss [molec/s]');
xlabel('duration [s]');
xlim([-100 10000]);
title('Ozone Loss ')
legend
set(legend,'Interpreter','none')
```

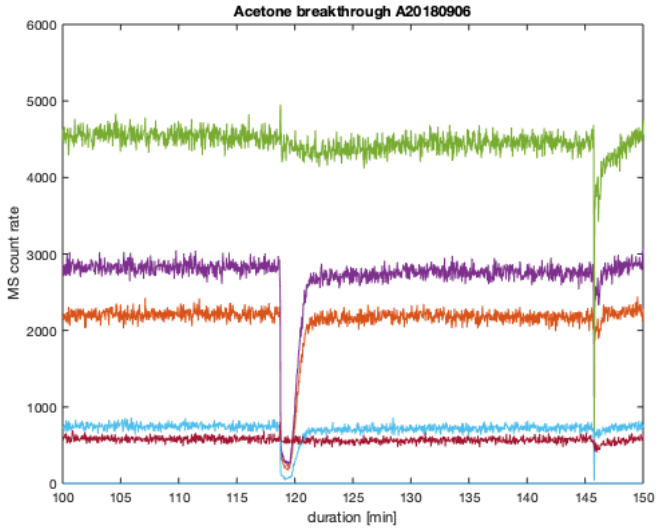


Flow tube: Acetone breakthrough

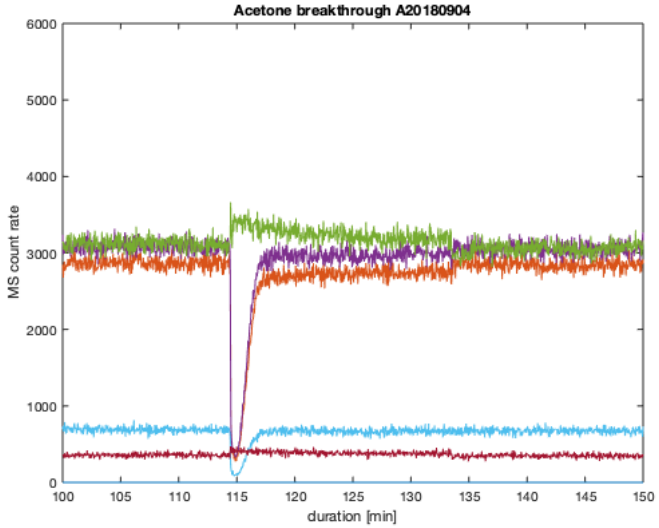
These figures show the signal intensity of the acetone-water-cluster and water-cluster (as derived by a chemical ionisation mass spectrometer) with time in the carrier gas downstream of packed bed flow tube holding the snow sample or the by-pass, respectively. Time "0" denotes the time when the mass spectrometer data acquisition was started. When the carrier gas with acetone was passed via the packed bed flow tube, that is switched from by-pass to pass the snow, acetone concentration in the carrier gas rapidly dropped due to surface adsorption and slowly recovered as the adsorption sites saturate. From this, the surface area can be obtained. See also file 'Edebeli_ACP_2020__AcetoneData.dat' which holds the same information (time_min and intensity_cps).

```
 close all
clearvars -except data

figure
plot(data(6).acetoneCims{:,10},data(6).acetoneCims{:,1:8})
ylabel('MS count rate');
```

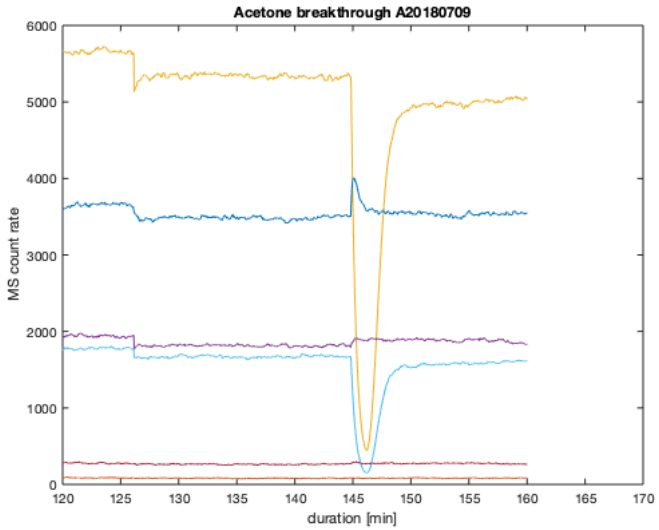
```
xlabel('duration [min]');
title(['Acetone breakthrough ' data(6).file])
ylim([0 0.6E4])
xlim([100 150])
```




```
figure
plot(data(1).acetoneCims{:,10},data(1).acetoneCims{:,1:8})
ylabel('MS count rate');
xlabel('duration [min]');
title(['Acetone breakthrough ' data(1).file])
ylim([0 0.6E4])
xlim([100 150])
```




```
figure
plot(data(5).acetoneCims{:,10},data(5).acetoneCims{:,1:8})
ylabel('MS count rate');
xlabel('duration [min]');
title(['Acetone breakthrough ' data(5).file])
ylim([0 0.6E4])
xlim([120 170])
clearvars -except data
```

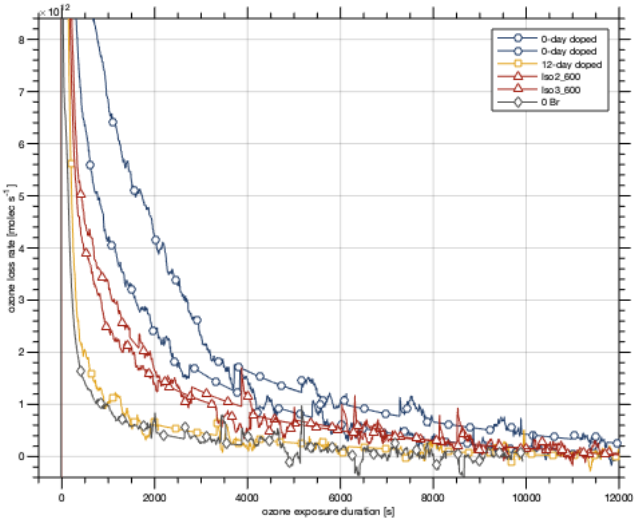


Data in Figure 1

See also file 'Edebeli_ACP_2020__Fig1Data.dat' which holds the same information.

```
close all
clearvars -except data
% Defaults for these figures
width   = 8;        % Width in cm
height = 10;        % Height in cm
alw     = 0.5;      % AxesLineWidth
fsz     = 8;        % Fontsize
lw      = 0.5;      % LineWidth
msz     = 6;        % MarkerSize
% prepare figure
set(groot,'defaultLineMarkerSize',10)
figure( 'Name', 'Figure 1');
hold on
% plot
for iFile = [1,2,6,9,10,11]
       hi(iFile)=plot(data(iFile).duration_s, data(iFile).Fig1_yData,'-o','DisplayName',data(iFile).sample,...
        'MarkerIndices',1:150:length(data(iFile).nOzone_molec_per_s),'MarkerFaceColor','white');
end

% set color, type, style of data points
hi(1).Color     =   [37/255 65/255 108/255];    % 500 ppb Br-, 0 days
hi(2).Color     =   [37/255 65/255 108/255];    % 500 ppb Br-, 0 days
hi(6).Color     =   [227/255 164/255 31/255];   % 500 ppb Br-, 12 days
hi(9).Color     =   [164/255 36/255 23/255];    % 500 ppb Br-, Iso
hi(10).Color    =   [164/255 36/255 23/255];    % 500 ppb Br-, Iso
hi(11).Color    =   [78/255 78/255 77/255];     % 0 ppb.

% set marker of data points
hi(1).Marker    =   'o';                        % 500 ppb Br-, 0 days
hi(2).Marker    =   'o';                        % 500 ppb Br-, 0 days
hi(6).Marker    =   's';                        % 500 ppb Br-, 12 days
hi(9).Marker    =   '^';                        % 500 ppb Br-, Iso
hi(10).Marker   =   '^';                        % 500 ppb Br-, Iso
hi(11).Marker   =   'diamond';                  % 0 ppb.

for i=[1,2,6,9,10,11]
    hi(i).MarkerSize   = msz;
end


% label and axes
hXLabel= xlabel('ozone exposure duration [s]');
hYLabel= ylabel('ozone loss rate [molec s^{-1}]');
ylim([-0.4E12 8.4E12])
xlim([-500 12000]);
ax=gca;
grid on
legend OFF

set( gca                       , ...
    'FontName'   , 'Helvetica Neue','FontSize'   , fsz );
set([hXLabel, hYLabel], ...
    'FontName'   , 'Helvetica Neue');
set([hXLabel, hYLabel]  , ...
    'FontSize'   , fsz          );

set(gca, ...
    'Box'         , 'on'     , ...
    'TickDir'     , 'out'     , ...
```

```
    'TickLength'  , [.02 .02] , ...
    'XMinorTick'  , 'on'      , ...
    'YMinorTick'  , 'on'      , ...
    'YGrid'       , 'on'      , ...
    'XColor'      , [0 0 0], ...
    'YColor'      , [0 0 0], ...
    'LineWidth'   , alw         );
legend('interpreter','none')
```



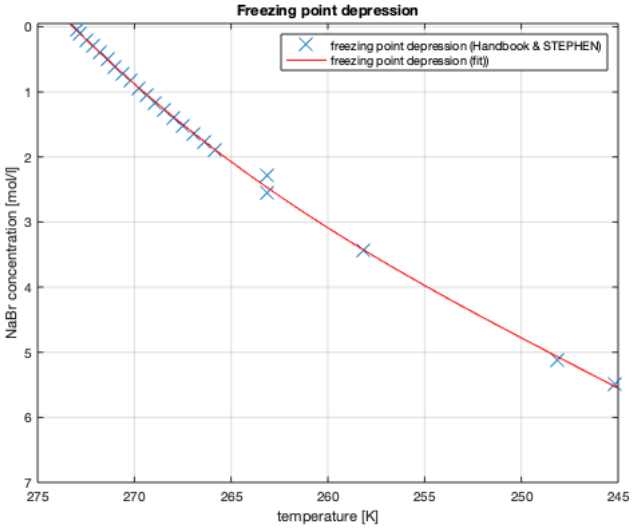
Freezing point depression data

1. The Handbook has data on concentration (molarity: moles of solute per litre of solution) vs. Freezing point depression in dC relative to pure water down to -7dC: http://hbcponline.com/faces/contents/InteractiveTable.xhtml?tableId=71

2. And this work lists them down to the eutectic: H. STEPHEN and T. STEPHEN, Eds., in Binary Systems, Pergamon CY -, 1963, pp. 5?960. (page 109) https://doi.org/10.1016/B978-0-08-009923-1.50006-9

```
clearvars -except  data
% Copy of data from above sources
freezedepression_NaBr.dT    = [0.170000000000000;0.340000000000000;0.690000000000000;1.04000000000000;1.39000000000000;1.76000000000000;2.14000000000000;2.53000000000000;2.93000000000000;3.34000000000000;3.77000000000000;4.21000000000000;4.67000000000000;5.15000000000000;5.65000000000000;6.18000000000000;6.74000000000000;7.32000000000000;NaN;NaN;10;10;NaN;NaN;15;NaN;NaN;NaN;NaN;25;28];
freezedepression_NaBr.c_NaBr = [0.0490000000000000;0.0980000000000000;0.197000000000000;0.298000000000000;0.400000000000000;0.504000000000000;0.610000000000000;0.717000000000000;0.826000000000000;0.937000000000000;1.05000000000000;1.16400000000000;1.28100000000000;1.39900000000000;1.51900000000000;1.64100000000000;1.76500000000000;1.89100000000000;2.02000000000000;2.15000000000000;2.28300000000000;2.55500000000000;2.83700000000000;3.12900000000000;3.43100000000000;3.74400000000000;4.06900000000000;4.40600000000000;4.75500000000000;5.11900000000000;5.49600000000000];
[xData, yData] = prepareCurveData(273.15-freezedepression_NaBr.dT,freezedepression_NaBr.c_NaBr);
% Set up fit type and options.
ft = fittype( 'poly3' );
% Fit model to data.
[fitresult.c_freezing_NaBr, ~] = fit( xData, yData, ft );
figure('Name', 'Freezing point depression')
plot(xData,yData,'x')
xlim([245,275]);
ylim([-0.05,7]);
hold on
plot( fitresult.c_freezing_NaBr)
set(gca, 'Xdir', 'reverse')
set(gca, 'Ydir', 'reverse')
xlabel('temperature [K]');
ylabel('NaBr concentration [mol/l]');
grid on
title('Freezing point depression')
legend('freezing point depression (Handbook & STEPHEN)', 'freezing point depression (fit))')
```

```
Warning: Removing NaN and Inf from data
Warning: Equation is badly conditioned. Remove repeated data points or try
centering and scaling.
```



Liquid volume

This table shows the liquid fraction in l for -6°C and -15°C for all samples. Calculated based on total amount of bromide doped to the samples and the concentration of the brine as derived from the freezing point depression data (1.6 mol/l at -6°C and 3.4 mol/l at -15°C):

```
% at -6°C (typical for metamorphism)
temp_snow       = -6; % °C
c_liqfrac   = fitresult.c_freezing_NaBr(273.15+temp_snow); % mol/l, concentration of NaBr in liquid fraction
for iFile = [1,2,6,9,10]
    data(iFile).liqFrac_m6_l = 1./c_liqfrac .* (data(iFile).n_Bromide_molec./6.02205E23);
end
% at -15°C (typical for packed bed flow tube)
temp_snow       = -15; % °C
c_liqfrac   = fitresult.c_freezing_NaBr(273.15+temp_snow); % mol/l, concentration of NaBr in liquid fraction
for iFile = [1,2,6,9,10]
    data(iFile).liqFrac_m15_l = 1./c_liqfrac .* (data(iFile).n_Bromide_molec./6.02205E23);
end
T = struct2table(data);
T([1,2,6,9,10],{'sample','liqFrac_m6_l','liqFrac_m15_l'})
```

```
ans =

  5×3 table

        sample          liqFrac_m6_l     liqFrac_m15_l
    ________________    _____________    _____________

    {'0-day doped' }    {[6.6891e-08]}    {[3.0899e-08]}
    {'0-day doped' }    {[4.3282e-08]}    {[1.9993e-08]}
    {'12-day doped'}    {[5.5087e-08]}    {[2.5446e-08]}
    {'Iso2_600'    }    {[5.5087e-08]}    {[2.5446e-08]}
    {'Iso3_600'    }    {[6.2956e-08]}    {[2.9081e-08]}
```

```
clearvars -except data
```

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