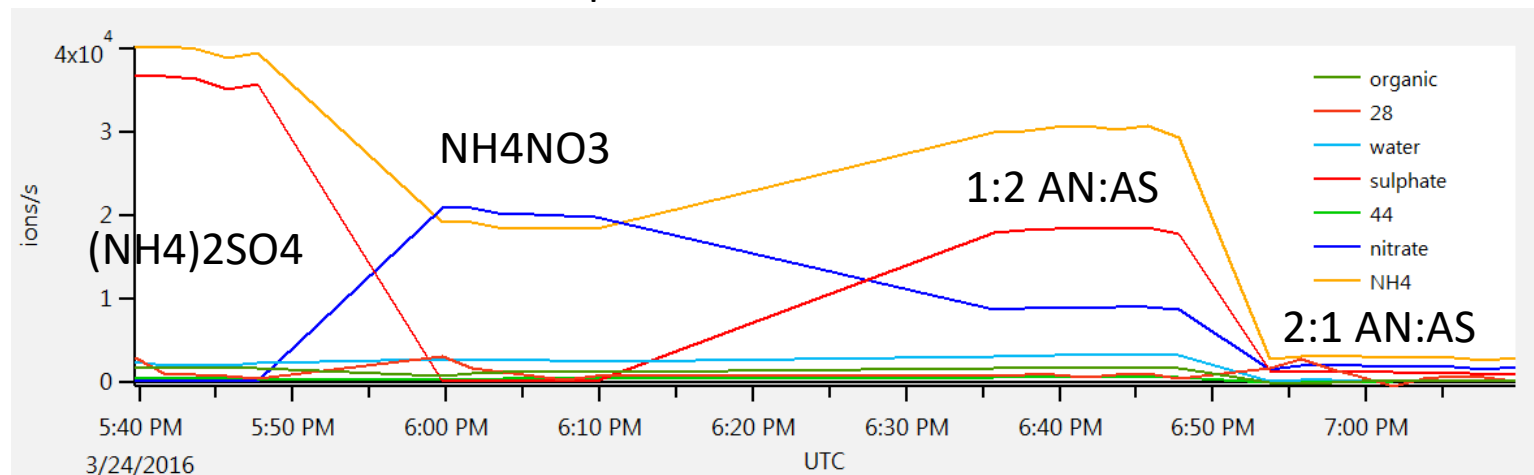Comment on mixture calibrations
AMS Users Meeting 10/22/2016
Leah Williams

ToF-ACSM-010 Paris intercomparison March 2016
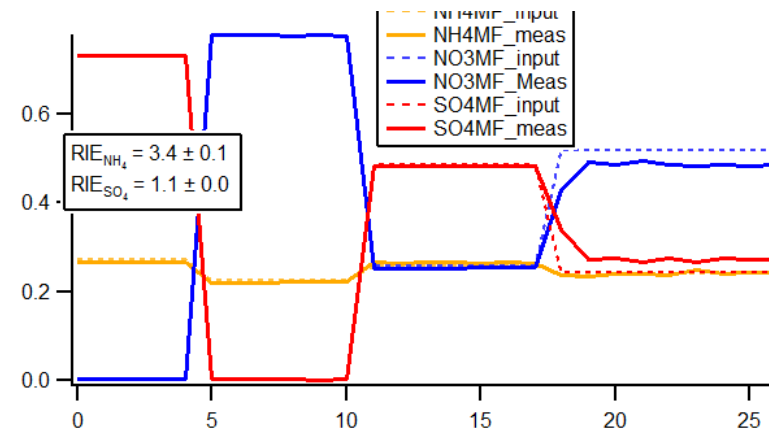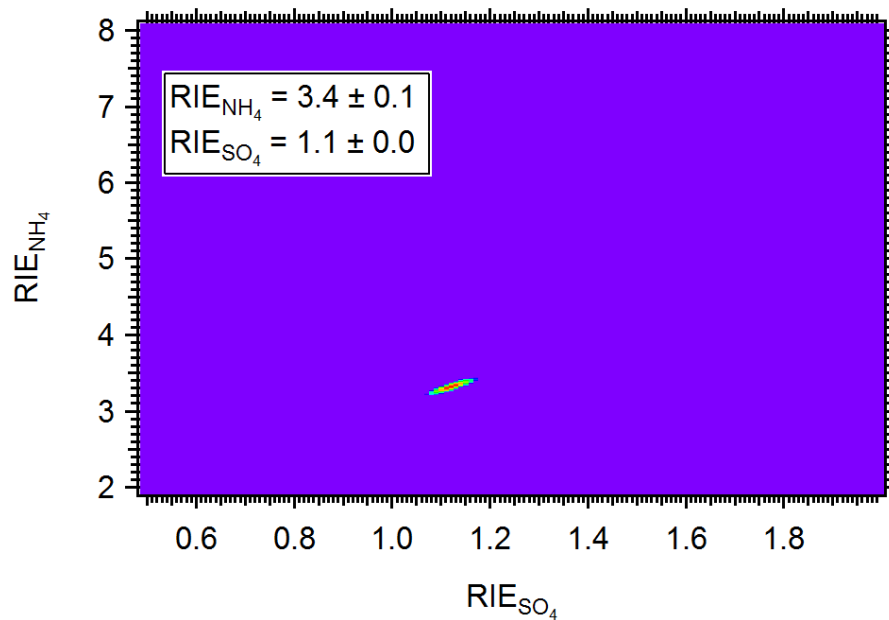

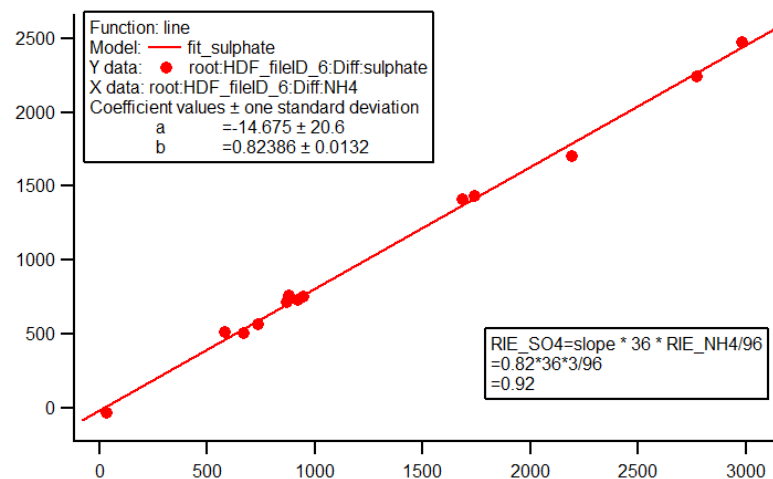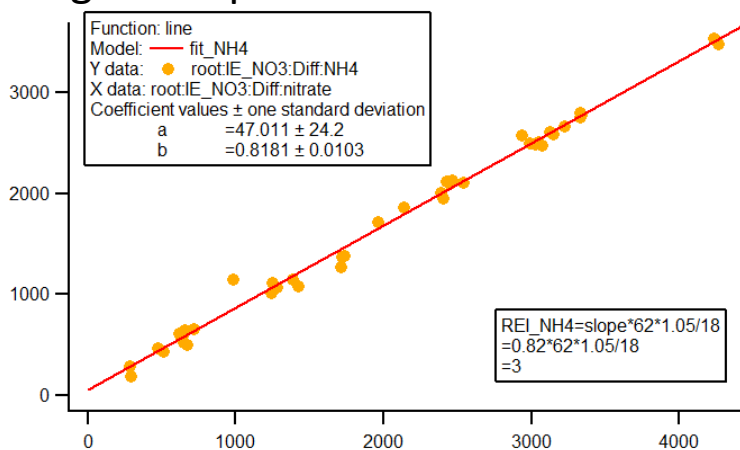$$NH_{4\,Meas}(RIE_{NH_4}) = Sig_{NH_4}/(IE_{NO_3} * RIE_{NH_4} * flowrate)$$

(Eq. 7a)

$$NH_{4\,Pred}(RIE_{NH_4}, RIE_{SO_4}) = \frac{Sig_{NO_3}}{IE_{NO_3}*1.05*flowrate} * \frac{18}{62} + \frac{Sig_{SO_4}}{IE_{NO_3}*RIE_{SO_4}*flowrate} * \frac{36}{96}$$

(Eq. 7b)

$$\chi^2(RIE_{NH_4}, RIE_{SO_4}) = \sum_i \left(\frac{NH_{4\,Meas,i} - NH_{4\,Pred,i}}{\sqrt{0.10*NH_{4\,Pred,i}}}\right)^2$$
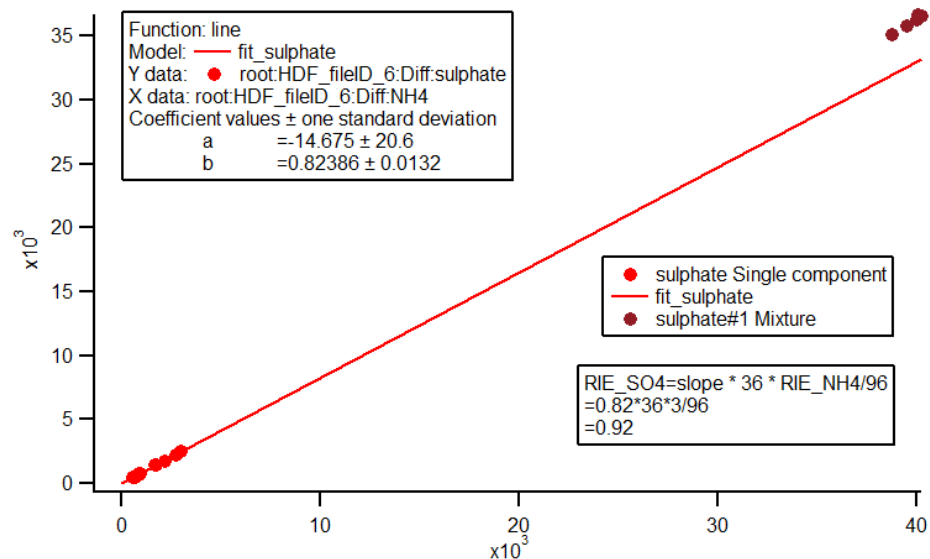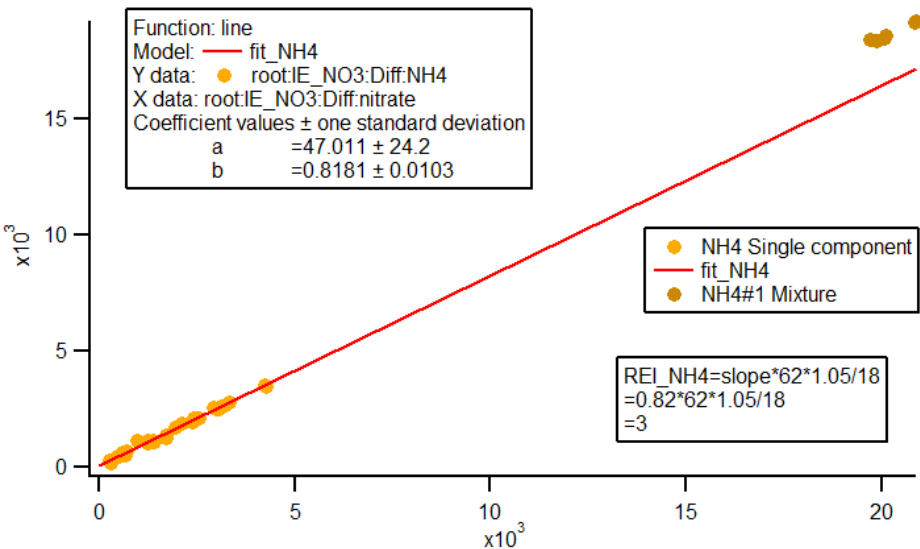
(Eq. 7c)

INERIS ToF-ACSM-010 MixCal, Mixture

$RIE_{NH_4} = 3.4 \pm 0.1$
$RIE_{SO_4} = 1.1 \pm 0.0$

$RIE_{NH_4} = 3.4 \pm 0.1$
$RIE_{SO_4} = 1.1 \pm 0.0$

Legend:
- NH4MF_input
- NH4MF_meas
- NO3MF_input
- NO3MF_Meas
- SO4MF_input
- SO4MF_meas

Single Component RIE calibrations

Function: line
Model: fit_NH4
Y data: root:IE_NO3:Diff:NH4
X data: root:IE_NO3:Diff:nitrate
Coefficient values ± one standard deviation
a   =47.011 ± 24.2
b   =0.8181 ± 0.0103

REI_NH4=slope*62*1.05/18
=0.82*62*1.05/18
=3

Function: line
Model: fit_sulphate
Y data: root:HDF_fileID_6:Diff:sulphate
X data: root:HDF_fileID_6:Diff:NH4
Coefficient values ± one standard deviation
a   =-14.675 ± 20.6
b   =0.82386 ± 0.0132

RIE_SO4=slope * 36 * RIE_NH4/96
=0.82*36*3/96
=0.92

INERIS ToF-ACSM-010 MixCal, Mixture, standard frag table

Mixture concentrations were very high compared to single component concentrations. This seems to have biased NH4 high relative to NO3, and SO4 high relative to NH4. Explains why mixture analysis is yielding higher RIE_NH4 and RIE_SO4 than single component analysis.

Recommendations
- If you want to do a mixture calibration, use solution concentrations close to what is encountered in ambient.
- Clean atomizer carefully between solutions.
- Do multiple particle concentrations for each solution.