**SOP for PTR-TOF-MS: QA/QC based on fast gas standard injections**

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**First results from field deployment:**

High variability of individual retrievals shows that reproducibility of injections should be improved (possible through fine tuning the injection sequence). Nevertheless, the time series reveals drift in both, instrument sensitivity and sample flow into the instrument.

**Background (Ion chemistry):**

Proton transfer reactions (PTR) are used to calculate Volume mixing ratios (VMR):

\[ R_2H^+ + R \rightarrow RH^+ + H_2O \]  

Water clusters are formed and complicate ion chemistry in the reaction chamber because the net-reaction rate is not always close to the collisional rate:

\[ (R_2H) + R \rightarrow RH^+ + H_2O \]  
\[ (R_2H) + R \rightarrow RH^+ + (R_2H) + H \]  
\[ (R_2H) + N \rightarrow RH^+ + H_2O + N \]

Other primary ions such as O\(^{3+}\) and ND\(^{+}\) should be kept at low levels.

**Conceptual framework:**

Key features are (i) clear distinction between ion intensity (I) and ion counts (C), and (ii) exploiting the correspondence of the kinetic and calibration methods to develop QA/QC tools.

**Volume Mixing Ratio**

Calibration Method:

Kinetic method:

\[ VMR = \frac{N_j \cdot \text{Calibration factor}}{I_j} \]

\[ I_j = \frac{N_j \cdot \text{Calibration factor}}{V_j} \]

\[ N_j = \frac{x_{\text{background}} + \text{Sample}}{x_{\text{background}}} \]

\[ V_j = \frac{x_{\text{background}}}{x_{\text{background}}} \]

Methods correspond:

\[ \frac{I_{VMR}}{I_{PM}} = \frac{N_j \cdot \text{Calibration factor}}{V_j} \]

\[ X_{\text{background}} = \frac{N_j \cdot \text{Calibration factor}}{V_j} \]

\[ X_j = \frac{N_j \cdot \text{Calibration factor}}{V_j} \]

**Considerations defining a Standard Operation Protocol (SOP):**

1. Recommendations for the operation of the ion source (1), the reaction chamber (2), and the mass spectrometer (3) have been compiled.

2. Setup and operation in the field.

3. Retrieving sample gas flow into instrument.

4. Retrieving mass dependent transmission.

5. Retrieving sensitivity (S) and humidity factor (X\(_N\)).

6. Retrieving conditions in reaction chamber: E/N and I\(_37\)/I\(_19\).