PMF runs with SoFi based on ME-2
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ACSM measures mainly ammonium nitrate, ammonium sulfate, ammonium chloride and Organic mixture ➔ Source apportionment technique
Source apportionment technique - PMF

\[ X_{\text{measured}} = \hat{X}_{\text{model}} + E_{\text{model}} \]

Bilinear model – Positive Matrix Factorization (PMF)

- The rows of the matrix F represent the factor profiles
- The columns of the matrix G represent the factor time series

Paatero and Tapper 1994
Method - PMF

Least-squares algorithm

\[ Q = \sum_{i=1}^{m} \sum_{j=1}^{n} \left( \frac{e_{ij}}{\sigma_{ij}} \right)^2 \]

- \( e_{ij} \): difference (measured – model)
- \( \sigma_{ij} \): uncertainty (measurement)

Advantages
- Values in \( G \) & \( F \) are non-negative
- Factors represent sources (POA) / aging (SOA)

Disadvantages
- Assess number of factors
- Constant factor profiles (mass spectra)
- Uncertainties are not well-known, minimal Q-value is not necessarily the best solution
  - Investigate the solution space even for slightly higher Q-values (few %)
- PMF solutions suffer from rotational ambiguity

\[ X_{\text{model}} = G \cdot F = G \cdot T \cdot T^{-1} \cdot F = G' \cdot F' \]

- Investigate the solution space

Paatero 1999, Paatero and Hopke 2008
Source apportionment technique – PMF/ME2 solver

<table>
<thead>
<tr>
<th>PMF2 solver</th>
<th>ME2 solver</th>
</tr>
</thead>
<tbody>
<tr>
<td>global rotational tool (fpeak)</td>
<td>global rotational tool (fpeak)</td>
</tr>
<tr>
<td>-</td>
<td>Individual rotational tool (fpeak)</td>
</tr>
<tr>
<td>pull towards zero (G and/or F)</td>
<td>Constraining values (G and/or F) a-value/pulling</td>
</tr>
</tbody>
</table>

**a-value approach for F**

\[ f_{p,j,\text{solution}} = f_{p,j} \pm a \cdot f_{p,j} \]
**Regular features**

- Various results plots / residual plots
- Comparison with external tracers

⇒ Validate a PMF solution

**Special features**

- ...

*Canonaco et al., 2013*
Monitor the correlation of a factor time series with external data, e.g. HOA with BC over different model runs.
Compare different model runs together
- HR data, families grouped into UMR
- Reweight based on averaged S/N ratio
- Reweight based on t-dependent S/N ratio (available with new release)
C-value approach for combined PMF data, e.g. AMS and gas-phase
C-value approach
Next release

- Fast bilinear ME-2 lane in ME-2 (Paatero)
- Restructuration of SoFi (interface and storage)
- Controlled investigation of the solution space (POA and SOA profiles)
- Propagation of the statistical uncertainty to the PMF results

⇒ Version 4.9 will cover all this…

Canonaco et al., 2013
Constant factor profile for OOA / BBOA is problematic for long-term data

Run PMF over groups of data, seasons, months, weeks

Source apportionment strategy for long-term data

- Grouped data based on daily temperature in ascending order
- Run PMF over a small window, e.g. one month (Automatic - Au)
  - HOA, COA, BBOA were always expected, constrain with the a-value
  - model 1-2 OOA factors based on mainly f44/f43 ratio
  - optimize solution based on correlation over time and diurnal cycle for:
    - HOA with NO\textsubscript{x} / BC\textsubscript{tr}, BBOA with BC\textsubscript{bb}, SV-OOA with nitrate / temperature, LV-OOA with sulfate, cooking lunch peak presence
- Shift PMF frame by a day and rerun PMF (Rolling - Ro)

AuRo – SoFi

- Same sources supposed
- Rolling window allows to dynamically adapt to changing SOA
- Small shift compared to PMF frame allows for a partial propagation of the uncertainty
ME2 interface – AuRo-SoFi result

Talk at the IAC on the 2nd of September