Biomass Burning

(*high loading*)

Frag Table Modifications

Amber M. Ortega

J-Group

Data from FLAME-3
Biomass Burning
*(high loading)*

Frag Table Modifications

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Data from FLAME-3

Outline
- Sampling Conditions
- Frag Panel
- Interference
- Frag Table Rebuilding
- Improvements
Biomass Burning Study
• FLAME-3 at Fire Sciences Lab in Missoula, MT

High Loadings
• Up to 1000+ µg/m³
• Scanning to m/z 500
• W-mode

Applicability
• Organic to inorganic ratio >> Ambient
• Flying in BB plumes
• Sources: Diesel exhaust, burns
• Chamber studies

Goal
• Use UMR data for quick analysis
• Avoiding full details of PIKA
• Or UMR-only Data
Standard Frag SQUIRREL

Frag Table Modifications & Checks v1.50

All plots except SO4 Fragments are colored by time.

In addition to plots in this panel, users should make average mass spectra and time series plots of filter periods to ensure all m/z aerosol loadings are ~ zero.

Suppl. plots of surface ionization for K.

Suppl. plots of H2O coefficients at 16,17
Standard Frag SQUIRREL

In addition to plots in this panel, users should make average mass spectra and time series plots of filter periods to ensure all m/z aerosol loadings are ~ zero.
Standard Frag SQUIRREL

![Graph showing correlation between SO4 µg/m³ and Org µg/m³]
Standard Frag SQUIRREL

Graphs showing ion rate and signal Hz over time with dates and times from 8:30 to 11:00 on 9/22/2009.
Standard Frag SQUIRREL

<table>
<thead>
<tr>
<th>m/z</th>
<th>frag_organic</th>
<th>frag_sulphate</th>
<th>frag_SO3</th>
</tr>
</thead>
<tbody>
<tr>
<td>18</td>
<td>0.225*frag_organic[44]</td>
<td>frag_SO3[18]</td>
<td>0.67<em>frag_SO3[54], 0.67</em>frag_SO3[48]</td>
</tr>
</tbody>
</table>

Ion rate (Hz)

![Graph with m/z and ion rate data](image)

PIKA SO₄

SQUIRREL SO₄

![Graph with signal Hz over time](image)

Date and Time

9/22/2009 8:30 to 11:00
<table>
<thead>
<tr>
<th>m/z</th>
<th>frag_organic</th>
<th>frag_sulphate</th>
<th>frag_SO3</th>
</tr>
</thead>
<tbody>
<tr>
<td>63</td>
<td>63,-frag_nitrate63</td>
<td></td>
<td></td>
</tr>
<tr>
<td>64</td>
<td>0.5<em>frag_organic[50],0.5</em>frag_organic[78]</td>
<td>frag_SO3[64],frag_H2SO4[64]</td>
<td>64,-frag_organic[64],-frag_H2SO4[64]</td>
</tr>
<tr>
<td>65</td>
<td>0.5<em>frag_organic[51],0.5</em>frag_organic[79]</td>
<td>frag_SO3[65],frag_H2SO4[65]</td>
<td>0.00868*frag_SO3[64]</td>
</tr>
<tr>
<td>66</td>
<td>66,-frag_sulphate66</td>
<td>frag_SO3[66],frag_H2SO4[66]</td>
<td>0.0482*frag_SO3[64]</td>
</tr>
</tbody>
</table>

**Standard Frag SQ**

- All +12279.18
- Org +8270.94
- SO₄ +15.90

**SQ est. Org mz64 = 38.53**
**PK actual Org mz64 = 18.22**

**m/z 64: SO₂⁺**

**m/z 50: C₄H₂⁺**

**m/z 78: C₆H₆⁺**

**PIKA**
m/z 48: SO⁺

m/z 64: SO₂⁺

m/z 80: SO₃⁺

m/z 81: HSO₃⁺

m/z 98: H₂SO₄⁺
Org at m/z 48(C₄⁺) = 0.032*Ave (m/z 47 and m/z 49)
m/z 64($\text{SO}_2^+$) = 1.14*m/z 48($\text{SO}^+$)

<table>
<thead>
<tr>
<th>mz</th>
<th>frag_organic_BB</th>
<th>frag_sulphate_BB</th>
</tr>
</thead>
<tbody>
<tr>
<td>48</td>
<td>48,-frag_sulphate_BB[48]</td>
<td>0.032<em>0.5</em>frag_organic_BB[47], 0.032<em>0.5</em>frag_organic_BB[49]</td>
</tr>
<tr>
<td>64</td>
<td>64,-frag_sulphate_BB[64]</td>
<td>1.14*frag_sulphate_BB[48]</td>
</tr>
</tbody>
</table>

Different Biofuels
m/z 80(\text{SO}_3^+ \text{)} = 0.32 \times \text{m/z 48(\text{SO}^+ \text{)}}

<table>
<thead>
<tr>
<th>m/z</th>
<th>frag_organic_BB</th>
<th>frag_sulphate_BB</th>
</tr>
</thead>
<tbody>
<tr>
<td>48</td>
<td>48,-frag_sulphate_BB[48]</td>
<td>0.032<em>0.5</em>frag_organic_BB[47], 0.032<em>0.5</em>frag_organic_BB[49]</td>
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<tr>
<td>64</td>
<td>64,-frag_sulphate_BB[64]</td>
<td>1.14*frag_sulphate_BB[48]</td>
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<tr>
<td>80</td>
<td>80,-frag_sulphate_BB[80]</td>
<td>0.32*frag_sulphate_BB[48]</td>
</tr>
</tbody>
</table>
### Standard Frag Table SQUIRREL

<table>
<thead>
<tr>
<th>m/z</th>
<th>frag_organic</th>
<th>frag_sulphate</th>
<th>frag_SO3</th>
<th>frag_H2SO4</th>
</tr>
</thead>
<tbody>
<tr>
<td>48</td>
<td>0.5*frag_organic[62]</td>
<td>frag_SO3[48], frag_H2SO4[48]</td>
<td>48,-frag_organic[48],-frag_nitrate[48],-frag_H2SO4[48]</td>
<td>0.5*.93<em>frag_H2SO4[81], 0.5</em>.93*frag_H2SO4[98]</td>
</tr>
</tbody>
</table>

### Updated Frag Table SQUIRREL

<table>
<thead>
<tr>
<th>m/z</th>
<th>frag_organic_BB</th>
<th>frag_sulphate_BB</th>
</tr>
</thead>
<tbody>
<tr>
<td>48</td>
<td>0.032<em>0.5</em>frag_organic_BB[47], 0.032<em>0.5</em>frag_organic_BB[49]</td>
<td>48,-frag_organic_BB[48]</td>
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</tbody>
</table>

### Updated Batch Table SQUIRREL

<table>
<thead>
<tr>
<th>specname_list</th>
<th>spec_list</th>
<th>frag_list</th>
<th>IEfac_list</th>
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</thead>
<tbody>
<tr>
<td>Organics_OLD</td>
<td>Org_OLD</td>
<td>frag_organic</td>
<td>1.4</td>
</tr>
<tr>
<td>Organics</td>
<td>Org</td>
<td>frag_organic_BB</td>
<td>1.4</td>
</tr>
<tr>
<td>m/z</td>
<td>frag_organic_BB</td>
<td>frag_sulphate_BB</td>
<td></td>
</tr>
<tr>
<td>-----</td>
<td>----------------</td>
<td>-----------------</td>
<td></td>
</tr>
<tr>
<td>63</td>
<td>63, frag_nitrate[63]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>64</td>
<td>64, frag_sulphate_BB[64]</td>
<td>1.14*frag_sulphate_BB[48]</td>
<td></td>
</tr>
<tr>
<td>65</td>
<td>0.5<em>frag_organic_BB[51], 0.5</em>frag_organic_BB[79]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Updated Frag SQ**

- All +12279.18
- Org +8387.78
- SO\(_4\) +72.46

**m/z 48: SO\(^+\)**
Works For All Burns,
not perfect but much improved
102 nm PSL, c=4%