Considerations for Development of a Total Organic Carbon Analyzer for Exploration Missions
ICES Paper 2018-185

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Project Background

- TOCA is water monitoring technology critical to health and safety monitoring for regen water.
- There are gaps in the State-of-Art ISS TOCA versus exploration mission architectures/requirement, e.g., size, mass, consumables, sampling
- ECLSS community agrees an exploration-class TOCA is needed – development effort added to water monitoring roadmap.
- AES miniTOCA Project intends to advance the technology readiness of an exploration-forward TOCA system through:
  - Phase 0 - Technology Feasibility
  - Phase 1 – Ground Demonstration Prototype
  - Phase 2 – Flight Technology Demonstration (*if valued*)
TOCA History: How did we get here?

PCWQM – SS Freedom Process Control Water Quality Monitor
ISS TOCA1 – crit 3, for Russian and stored water analysis
  ➢ Shuttle DTO, 1999
  ➢ ISS operation: 2001-2002
  ➢ Project cancelled during post-Columbia return-to-flight
ISS TOCA2 – crit 1SR, required with U.S. Segment Regen ECLSS
  ➢ Certification phase: 2008
  ➢ ISS operation: 2008-present
TOCA for exploration missions
  ➢ FY17 trade study started on mini-TOCA
  ➢ FY18 trade study, technology evaluation and testing
Mission Concept

The exploration mission concept is largely undefined.
- Mars transit
- Lunar surface
- Orbital outpost

Commonality is that they are NOT low-earth orbit.
- Premium on low launch mass
- Infrequent resupply capability
  - drives high reliability, low maintenance, long life
Deriving Driving Requirements for an Exploration-Class TOCA

ISS TOCA Requirements

inform heritage, baseline

Exploration TOCA Requirements

Best Guess for Functional Performance, Resource, Crew Time, and Life requirements for a TOCA on an exploration mission

Combination of requirements that can’t be currently met by straightforward extension of existing system

ISS/AES Tech Demo TOCA Requirements

SRR in FY20

This is the current focus for feasibility/concept definition.

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## Exploration TOCA Design Goals – Functional Performance

<table>
<thead>
<tr>
<th>Title</th>
<th>ISS Requirement</th>
<th>New TOCA Goal</th>
<th>Source/Rationale</th>
</tr>
</thead>
<tbody>
<tr>
<td>Accuracy</td>
<td>+/- 25%</td>
<td>+/- 25%</td>
<td>ISS precedent</td>
</tr>
<tr>
<td>Precision</td>
<td>+/- 25%</td>
<td>+/- 10%</td>
<td>Provide reliable trending of data.</td>
</tr>
<tr>
<td>Range [see next slide]</td>
<td>1 – 25 mg/L TOC</td>
<td>1 - 10 mg/L TOC Challenge: 0.25 - 10mg/L TOC</td>
<td>Exceeds detection of potability limit (5 mg/L)</td>
</tr>
</tbody>
</table>
TOCA History:
Total inorganic /organic carbon (TIC/TOC) measurements from multiple water sources

Water Sources:
- WPA
- Shuttle
- SRV-K
- SVO-ZV
- JAXA/HTV
- ESA/ATV
- Rodnik

1 based on ISS TOCA results
2 based on ground testing

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Exploration TOCA Design Goals – Functional Performance

**Water Sample Composition:**

<table>
<thead>
<tr>
<th>Title</th>
<th>ISS Requirement</th>
<th>New TOCA Goal</th>
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</tr>
</thead>
<tbody>
<tr>
<td>TIC content</td>
<td>up to 15mg/L TIC</td>
<td>up to 5mg/L TIC</td>
<td>No minerals added in regen water. Equilibrium of CO2 in air @ 2mmHg to water=\textasciitilde4.5\text{ppm}_\text{CO}_2.</td>
</tr>
<tr>
<td>Conductivity</td>
<td>N/A</td>
<td>&lt;10\mu S/cm</td>
<td>Water processor specification</td>
</tr>
<tr>
<td>pH</td>
<td>N/A</td>
<td>pH 4.5 – 9</td>
<td>HSIR, MPCV70024, section 3.2.2.1 \textit{Note: TOCA may eliminate acidification if sample pH is &lt;8 with no buffering capacity.}</td>
</tr>
<tr>
<td>Free gas</td>
<td>5%</td>
<td>0.1%</td>
<td>NASA-STD-3001 (although HSIR states 5%)</td>
</tr>
</tbody>
</table>

**Note:** Water composition may interfere with the analysis using certain technologies.
# Exploration TOCA Design Goals – Resource Allocation

<table>
<thead>
<tr>
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<th>ISS Requirement</th>
<th>New TOCA Goal</th>
<th>Source/Rationale</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume</td>
<td>4160 in(^3) (actual)</td>
<td>&lt; 1200 in(^3)</td>
<td>Notional reduction. Balancing achievable with return on development investment.</td>
</tr>
<tr>
<td>Device Weight</td>
<td>80 lbs (actual)</td>
<td>&lt; 25 lbs</td>
<td>Notional reduction. Balancing achievable with return on development investment.</td>
</tr>
<tr>
<td>System Weight per 5-year ops</td>
<td>N/A</td>
<td>&lt;35lbs</td>
<td>Includes device plus all consumables and unreclaimed water consumption</td>
</tr>
<tr>
<td>Power Consumption</td>
<td>&lt; 175 W avg.</td>
<td>&lt; 175 W avg.</td>
<td>ISS precedent. AES vehicles will have reduced power availability than ISS.</td>
</tr>
<tr>
<td></td>
<td>&lt; 225 W peak</td>
<td>&lt; 225 W peak</td>
<td></td>
</tr>
<tr>
<td>Sample Size</td>
<td>&lt; 150mL</td>
<td>&lt; 150mL</td>
<td>Any water returned to the water balance does not count against the requirement.</td>
</tr>
<tr>
<td>Supply Gases</td>
<td>N2</td>
<td>N2 or O2 are acceptable</td>
<td>Compressed N2 and O2 can be utilized if favorable to overall design trades. Supplied H2 is not available.</td>
</tr>
</tbody>
</table>

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## Exploration TOCA Design Goals – Crew Time Allocation

<table>
<thead>
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<th>ISS Requirement</th>
<th>New TOCA Goal</th>
<th>Source/Rationale</th>
</tr>
</thead>
<tbody>
<tr>
<td>Analysis Time</td>
<td>190 mins</td>
<td>12 hours</td>
<td>No hard requirement. GOAL = less than ISS TOCA</td>
</tr>
<tr>
<td></td>
<td></td>
<td>GOAL: less than 190 mins</td>
<td></td>
</tr>
<tr>
<td>Analysis Frequency / yr.</td>
<td>N/A</td>
<td>60 analyses / year</td>
<td>Allows &gt; weekly analyses per ops concept</td>
</tr>
<tr>
<td>Crew Time for Analysis</td>
<td>&lt; 15 mins / analysis</td>
<td>&lt; 15 mins / analysis</td>
<td>No more crew time than ISS TOCA. Goal for inline, automated sampling.</td>
</tr>
<tr>
<td>Crew Time for Maintenance</td>
<td>&lt; 8 hrs / year</td>
<td>&lt; 8 hrs / year</td>
<td>Includes consumable replacements and calibration.</td>
</tr>
</tbody>
</table>

1. Automated sampling should be traded with size, complexity. The current assumption is that automation reduces size due to large size of crewed interfaces.

**Forward Work:** Combine total resource and crew time into equivalent system mass calculation for future evaluation.
## Exploration TOCA Design Goals – Life

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<th>New TOCA Goal</th>
<th>Source/Rationale</th>
</tr>
</thead>
<tbody>
<tr>
<td>TOCA Lifetime</td>
<td>5 years with maintenance</td>
<td>10 years with maintenance</td>
<td>Match the entire life of TBD habitat to eliminate resupply costs. (Device life = ground assembly/certification + mission life)</td>
</tr>
<tr>
<td>TOCA Cycle Life</td>
<td>1200 analyses with maintenance</td>
<td>600 analyses with maintenance</td>
<td>60 samples/year x 10 years</td>
</tr>
<tr>
<td>Component Shelf Life</td>
<td>1 year</td>
<td>&gt; 3 years</td>
<td>assumes a minimum resupply frequency for maintenance components every 2 years.</td>
</tr>
</tbody>
</table>
Feasibility Studies

Potential sources for exploration TOCA technology include:

- Current ISS TOCA
- Original Crit3 ISS TOCA
- Commercial TOC analyzers (i.e. modify and fly)
- SBIR spaceflight TOC analyzer prototypes
- Future new development options
Why not use the ISS TOCA?

Size of existing TOCA cannot be reduced dramatically unless the electrochemical oxidizer is redesigned due to flow rates required

**Advantages**
- Proven environmental compatibility, range, accuracy, reliability, safety.
- Detection range: 0 – 25ppm TOC;
- Accuracy: +/- 25%; Reliability: >4.5 years of operation on ISS
- Maintenance: 1\textsuperscript{st} maintenance and calibration occurred after 3.5 years (238 samples)

**Disadvantages**
- 80 lbs, 22 x 16 x 12 inches
- Not packaged for “in-line” potable water monitoring.
- Requires resupply and consumable replacement: manual waste water bag replacement every 6 samples; acidic buffer container replacement every 7 month or 46 samples.
TOCA1 technology is also a possibility...

Designed by Sievers with Wyle/NASA

H x W x D, in. 8.9 x 19.3 x 16.3
Weight, lb. 54.1
Max. power, W 69.3 avg.; 93.2 peak
Criticality 3
Range: 0-25ppm TOC

Mission duration spec.:
- RME, days 90+ required/365 design
- ISS, mos. 12
- ISS, analyses 50 required/85 design

1. Size is still too large
2. 1 year life due to persulfate
3. Tox 2 hazardous chemicals

TOCA1 in use on ISS October 2001
Are COTS TOC Analyzers an Option?

COTS TOC analyzers generally have at least one of the problems below:

- Hazardous chemicals are used for acidification and oxidation.
- Reagentless analyzers employ mercury UV lamps.
- Reagentless analyzers are only compatible with purified water sources.
- Infrared CO2 detection requires gas-liquid separation typically employing gravity-dependent sparging.
- Conductivity-based TOC measurement requires an ultra pure water source.
- Additional CO2 separation membrane is required for conductivity detection to eliminate non-carbon conductivity interferences.
- Non-spaceflight reliability and safety.
Can we utilize previous SBIR development?

- SBIR awards have produced two prototype TOC analyzers that were developed with goals for small size, no hazardous reagents, and microgravity compatibility.
- Prototypes were delivered to NASA in 2007 and 2011.
- NASA priorities at that time did not warrant continued funding to Phase III.
- Lessons learned and design solutions from the previous SBIR prototypes may be useful and are currently being investigated.
Proposed AES TOCA requirements cannot be met directly by
- ISS TOCA2
- ISS TOCA1
- Commercial TOC analyzers
- SBIR prototype deliverables

SBIR components will require additional evaluation and testing.

Custom commercial work is costly and appears likely to lead to a “one off” device for an ISS demo, not a development of knowledge and capabilities for a sustainable flight project.

Many subsystem/component technologies within the list above are attractive.

The current focus is to evaluate available technologies for selection based on performance and cost.
Project Plan
Technology Maturation

Develop Technology Matrix
- Component Performance
- Fit with system architecture
- Availability

Investigate and Test the most favorable technologies

Downselect best technologies and integrate into system breadboard(s)

Test and select the best breadboard system

Build Prototype TOCA

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## Technology Matrix Highlights

<table>
<thead>
<tr>
<th>Acidification</th>
<th>Oxidation</th>
<th>CO2 Detection</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electrolytic anion removal</td>
<td>Mercury UV</td>
<td>Membrane conductivity (aq)</td>
</tr>
<tr>
<td>Electrolytic protonation</td>
<td>Excimer UV (172nm)</td>
<td>Raman spectroscopy (aq)</td>
</tr>
<tr>
<td>Electrochemical generation from salt</td>
<td>LED UV / catalyst</td>
<td>Laser Spectroscopy (aq) (absorbance or acoustic)</td>
</tr>
<tr>
<td>Chemical reagent</td>
<td>Combustion (catalytic 450-850C)</td>
<td>NDIR (gas)</td>
</tr>
<tr>
<td>Electrochemical generation from salt</td>
<td>Boron-doped diamond electrochemical</td>
<td>Laser Spectroscopy (gas)</td>
</tr>
<tr>
<td>Chemical reagent</td>
<td>Ozone</td>
<td>Methanizer/Flame Ionization (gas)</td>
</tr>
<tr>
<td>Chemical reagent</td>
<td>UV/Vis spectroscopy (aq)</td>
<td>Pulsed discharge detector (gas)</td>
</tr>
<tr>
<td>Chemical reagent</td>
<td>Thermal conductivity (gas)</td>
<td></td>
</tr>
</tbody>
</table>
Advantages:
- Architecture based on proven techniques performed by Sievers (now Suez) – UV oxidation with membrane/conductivity detection.
- Electrodeionization cell is added to eliminate consumable and life limited acidic reagent. Development needed.
- Excimer UV is proposed instead of mercury-based UV. Excimer lamp was utilized in the TOCA1 along with persulfate.
Technology Architectures: UV/Raman

Advantages:
- Raman has capability for direct measurement of CO2 and carbonate species in the aqueous phase which could eliminate need for acidification and membrane separation.
- Raman needs development to reach low-level sensitivity.

Acidification
- Not required

Oxidation
- Excimer VUV photo-oxidation

CO2 Detection
- Raman spectroscopy
Advantages:
• Combustion/NDIR is a common TOC analysis technique. See Shimadzu, Teledyne, OI Analytical, etc...
• Combustion allows small sample sizes and complete oxidation.
• Tunable Laser Spectrometer is less sensitive to water vapor interference than NDIR.
• pH control is not required if mineral carbonates precipitate and gaseous CO2 is measured and subtracted.
Technology Architectures: Combustion(Polyarc®) / FID

Advantages:
• Polyarc is marketed for liquid injection gas chromatography analysis and has not been applied to TOC analysis.
• Polyarc performs catalyzed combustion and methanization in one step at a lower temperature than TOC combustion chambers.
• FID is selective to methane. Insensitive to water vapor or other interferences.
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2018

2019

2020
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