Considerations for Development of a Total Organic Carbon Analyzer for Exploration Missions

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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

- Development phase: 2005 – 2007
- 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

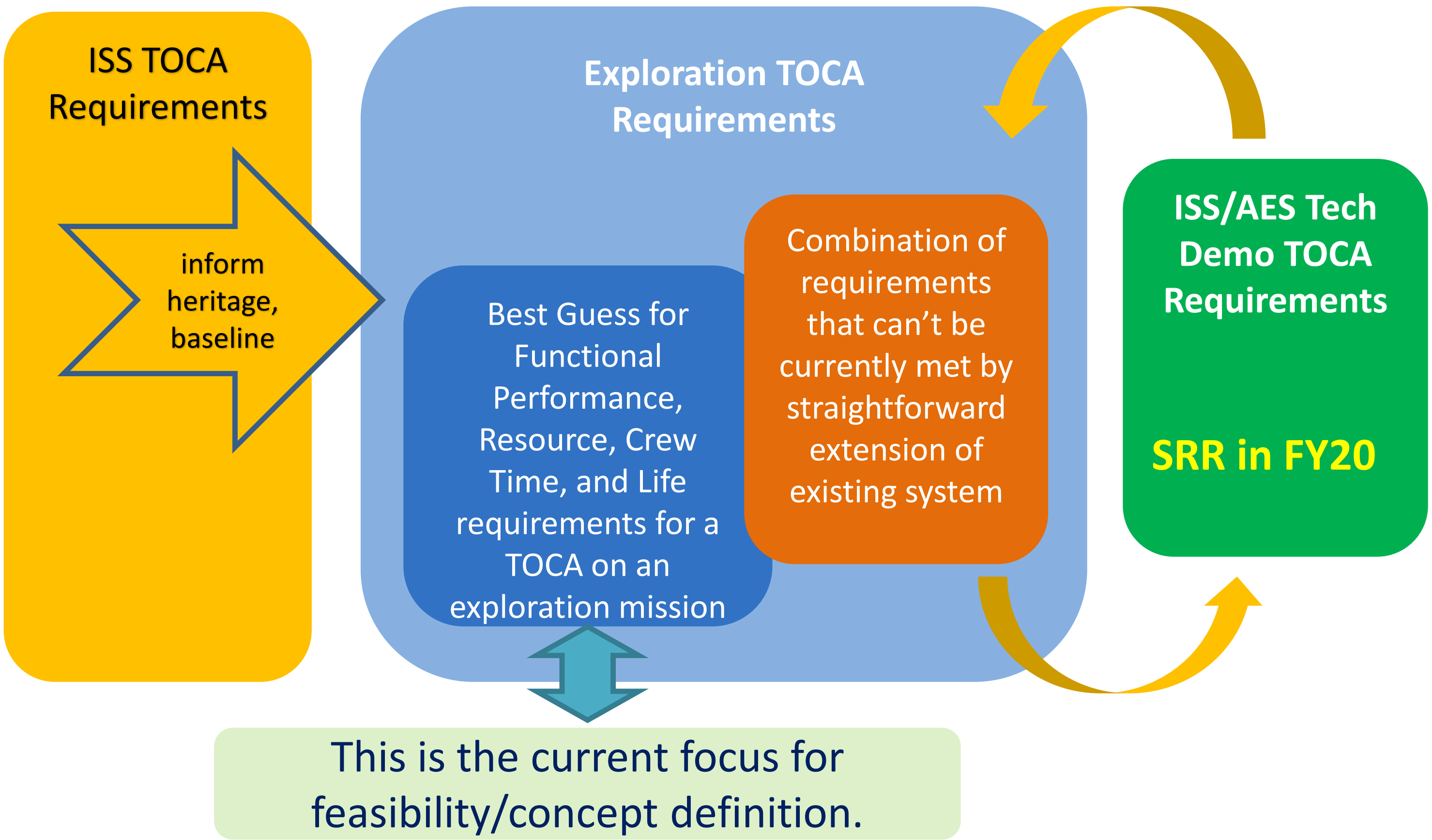
The exploration mission concept is largely undefined.

- 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



Exploration TOCA Design Goals – Functional Performance

Title	ISS Requirement	New TOCA Goal	Source/Rationale
Accuracy	+/- 25%	+/- 25%	ISS precedent
Precision	+/- 25%	+/- 10%	Provide reliable trending of data.
Range [see next slide]	1 – 25 mg/L TOC	1 - 10 mg/L TOC Challenge: 0.25 - 10mg/L TOC	Exceeds detection of potability limit (5 mg/L)

TOCA History:

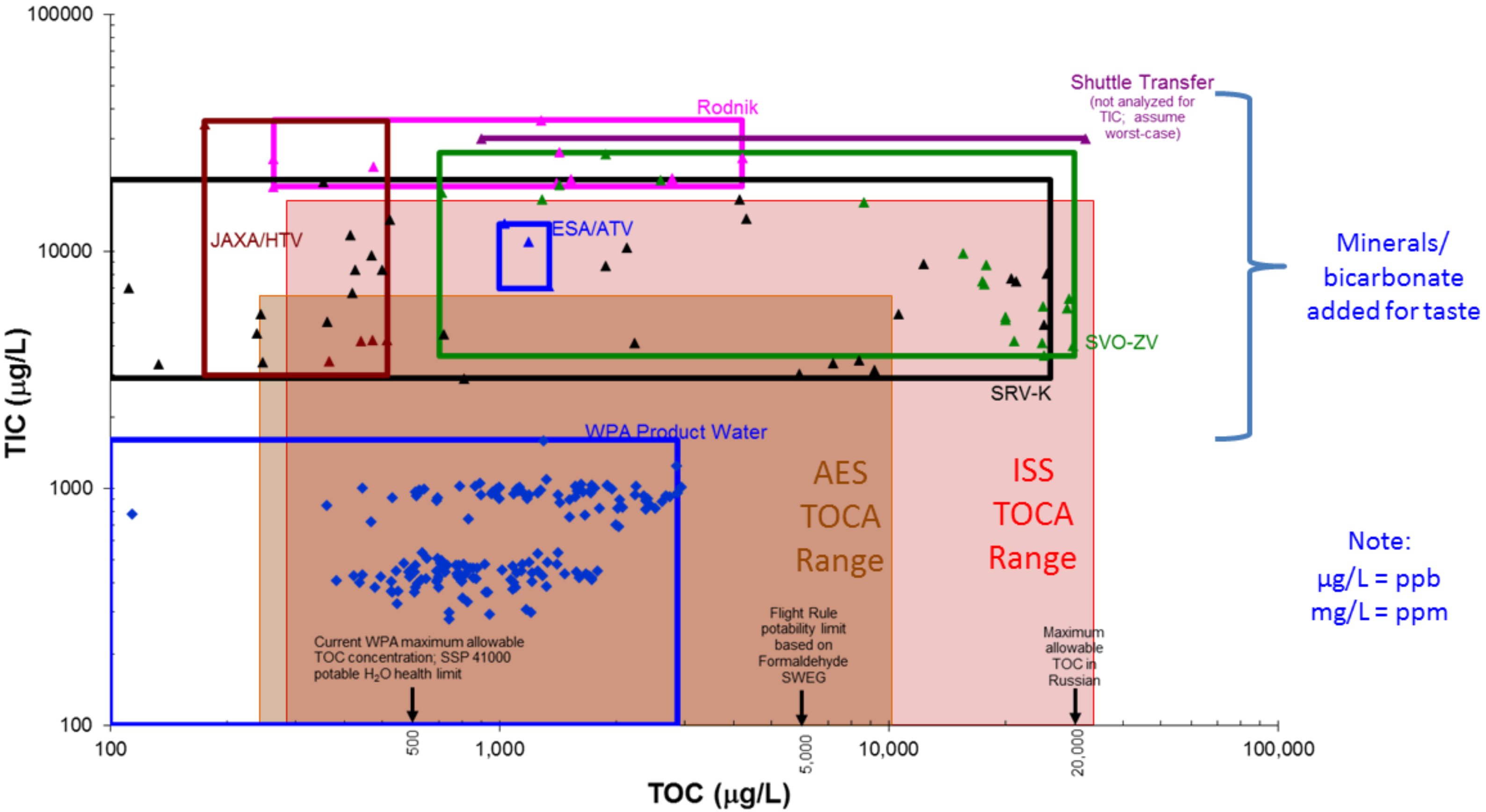
Total inorganic /organic carbon (TIC/TOC) measurements from multiple water sources

Water Sources:

- WPA[1]
- Shuttle[2]
- SRV-K[2]
- SVO-ZV[2]
- JAXA/HTV[2]
- ESA/ATV[2]
- Rodnik [2]

[1]based on ISS TOCA results

[2]based on ground testing



Exploration TOCA Design Goals – Functional Performance

- **<u>Water Sample Composition:</u>**

Title	ISS Requirement	New TOCA Goal	Source/Rationale
TIC content	up to 15mg/L TIC	up to 5mg/L TIC	No minerals added in regen water. Equilibrium of CO2 in air @ 2mmHg to water=~4.5ppm$_{CO2}$.
Conductivity	N/A	<10µS/cm	Water processor specification Not an HSIR or medical requirement
pH	N/A	pH 4.5 – 9	HSIR, MPCV70024, section 3.2.2.1 Note: TOCA may eliminate acidification if sample pH is <8 with no buffering capacity.
Free gas	5%	0.1%	NASA-STD-3001 (although HSIR states 5%)

Note: Water composition may interfere with the analysis using certain technologies.

Exploration TOCA Design Goals – Resource Allocation

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

Exploration TOCA Design Goals – Crew Time Allocation

Title	ISS Requirement	New TOCA Goal	Source/Rationale
Analysis Time	190 mins	12 hours GOAL: less than 190 mins	No hard requirement. GOAL = less than ISS TOCA
★ Analysis Frequency / yr.	N/A	60 analyses / year	Allows > weekly analyses per ops concept
Crew Time for Analysis	< 15 mins / analysis	< 15 mins / analysis	No more crew time than ISS TOCA. Goal for inline, automated sampling. [1]
Crew Time for Maintenance	< 8 hrs / year	< 8 hrs / year	Includes consumable replacements and calibration.

[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

Title	ISS Requirement	New TOCA Goal	Source/Rationale
TOCA Lifetime	5 years with maintenance	10 years with maintenance	Match the entire life of TBD habitat to eliminate resupply costs. (Device life = ground assembly/certification + mission life)
TOCA Cycle Life	1200 analyses with maintenance	600 analyses with maintenance	60 samples/year x 10 years
Component Shelf Life	1 year	> 3 years	assumes a minimum resupply frequency for maintenance components every 2 years.

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: 1st 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.

ISS TOCA2
Developed 2005-2008
1st unit ops 2009-2013
2nd unit ops 2013-current

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

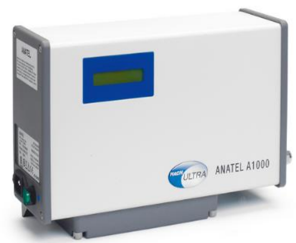
1. **Size is still too large**
2. **1 year life due to persulfate**
3. **Tox 2 hazardous chemicals**

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 of non-carbon conductivity interferences.
- Non-spaceflight reliability and safety.



Hach A1000

Millipore A10 TOC monitor

OI /Xylem Aurora UV Combustion or UV Persulfate / NDIR

Sievers M9

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.

Assessment of ISS and Current Commercial Technologies: Summary

- 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

2018

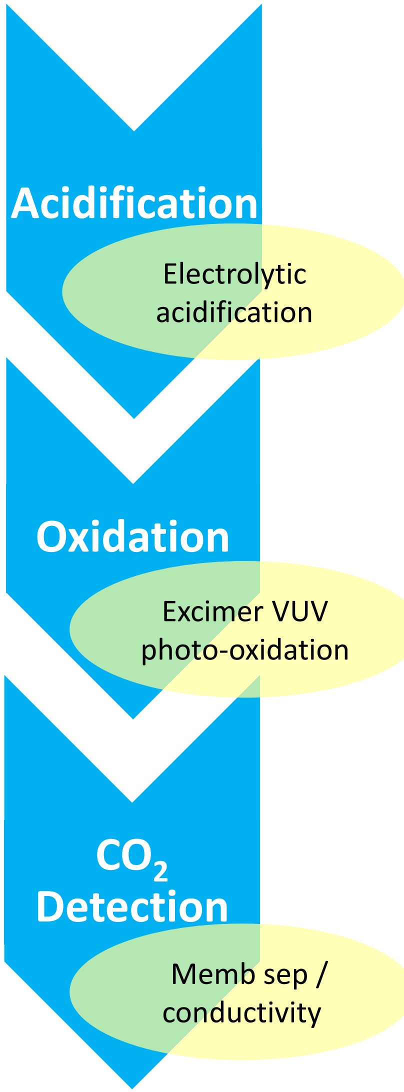
2019

2020

Technology Matrix Highlights

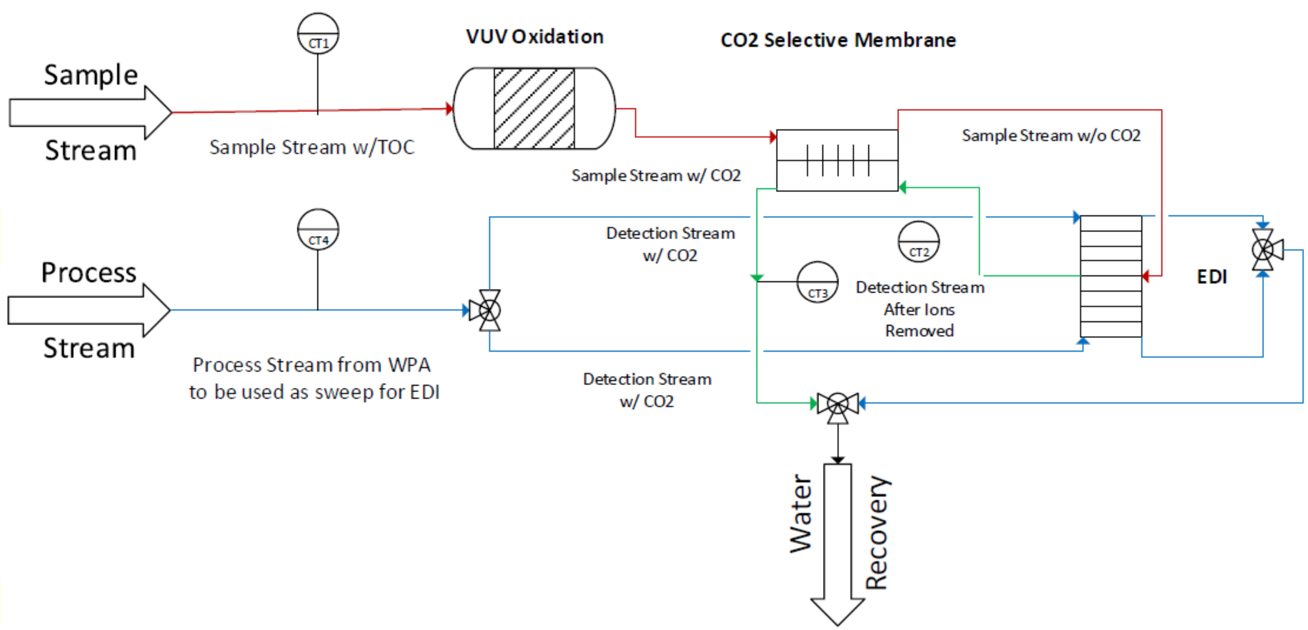
Acidification	Oxidation	CO2 Detection
Electrolytic anion removal	Mercury UV	Membrane conductivity (aq)
Electrolytic protonation	Excimer UV (172nm)	Raman spectroscopy (aq)
Electrochemical generation from salt	LED UV / catalyst	Laser Spectroscopy (aq) (absorbance or acoustic)
Chemical reagent	Combustion (catalytic 450-850C)	NDIR (gas)
	Boron-doped diamond electrochemical	Laser Spectroscopy (gas)
	Ozone	Methanizer/Flame Ionization (gas)
	Chemical reagent	UV/Vis spectroscopy (aq)
		Pulsed discharge detector (gas)
		Thermal conductivity (gas)

Technology Architectures: ED / UV / MC

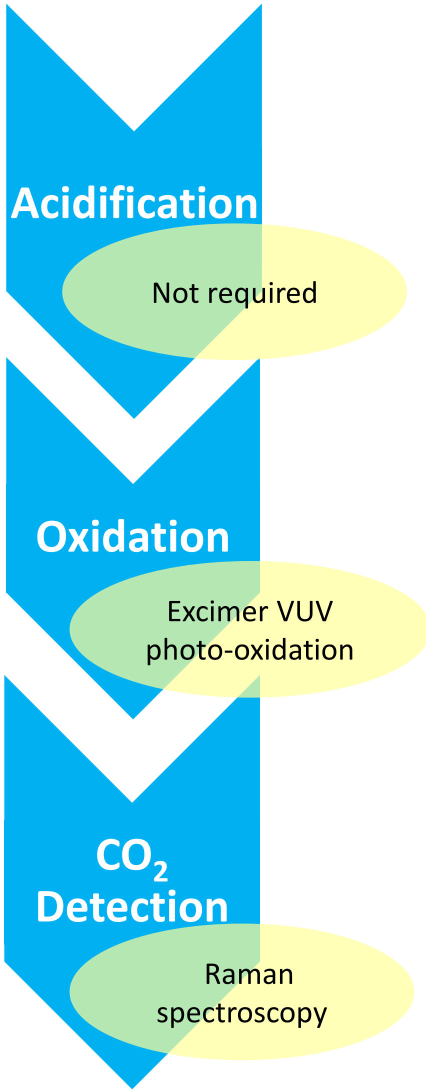


Advantages:

- 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.

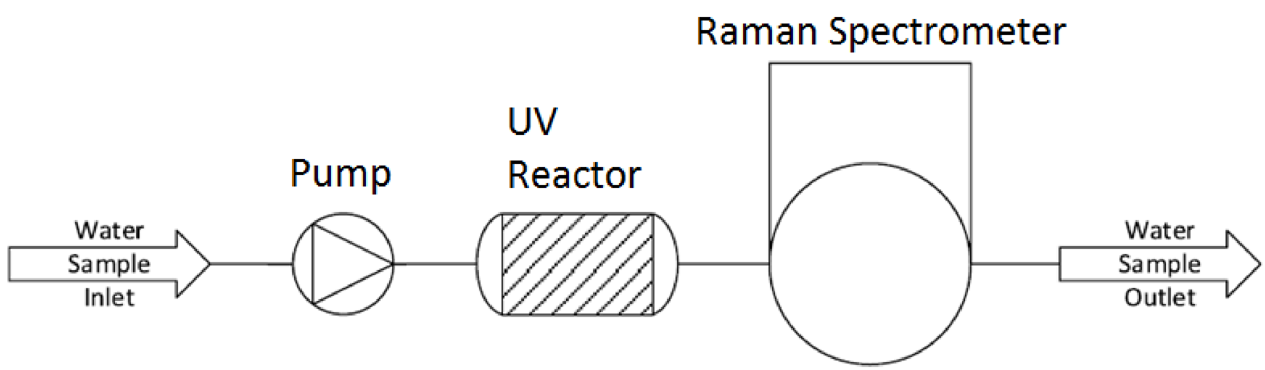


Technology Architectures: UV/Raman

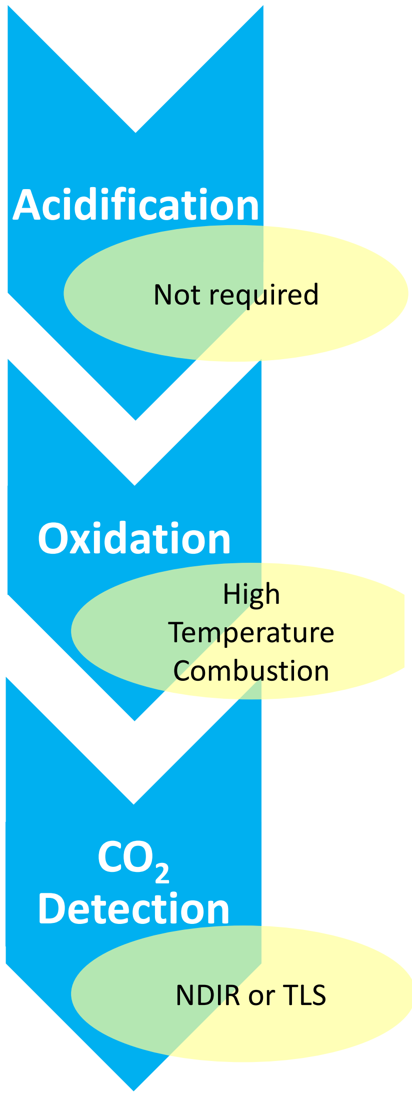


Advantages:

- 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.

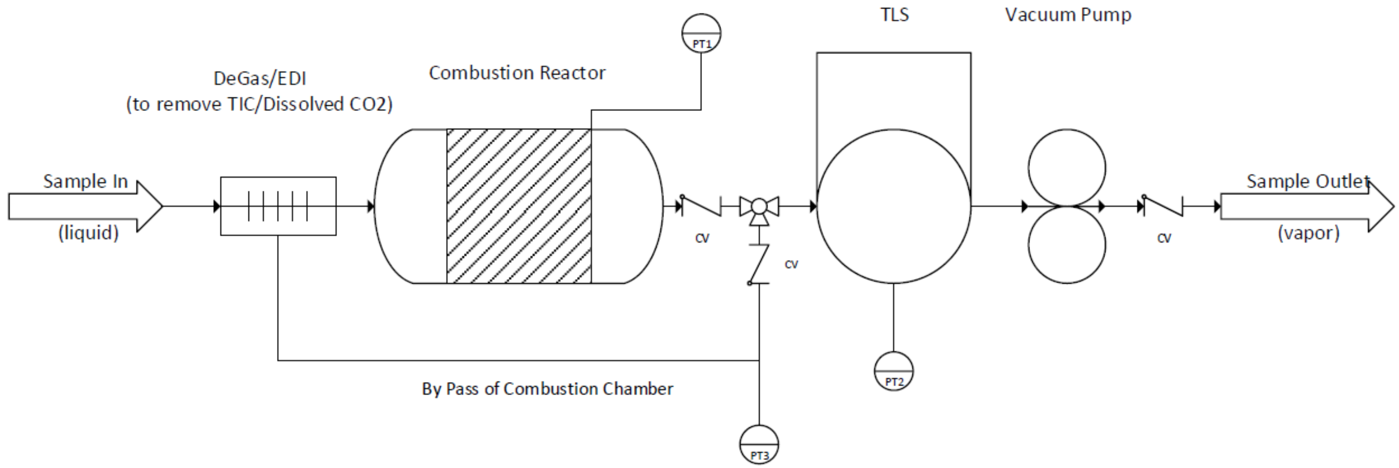


Technology Architectures: Combustion / NDIR or Combustion / TLS



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

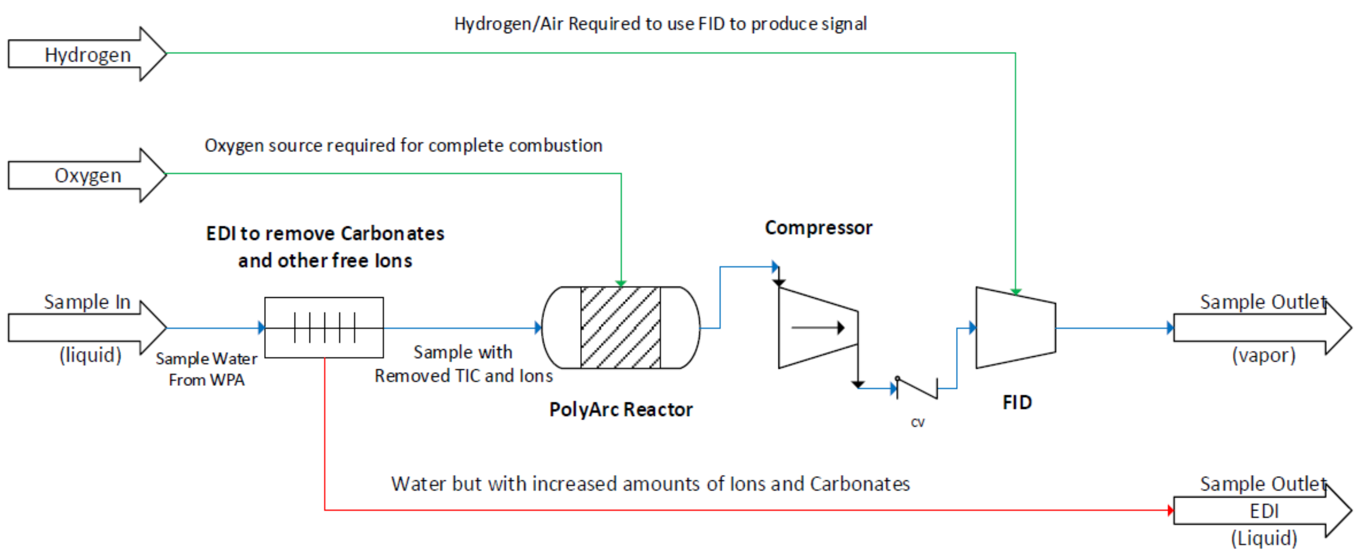
Acidification
Not required

Oxidation
High Temperature Combustion

CO_2 Detection
CH4 - Flame Ionization Detector

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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Acknowledgements

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