1 Procedures

All the procedures shown here are available on the server of the multiphase chemistry group of Paul-Scherrer Institute (PSI), under the following paths:

1. /Volumes/5505/People/David_Tschan/SOPs/experimental_procedures/01_SOA_Production.pdf
2. /Volumes/5505/People/David_Tschan/SOPs/experimental_procedures/02a_TOC_Glassware_Cleaning.pdf
3. /Volumes/5505/People/David_Tschan/SOPs/experimental_procedures/02b_TOC_Filter_Extraction.pdf
4. /Volumes/5505/People/David_Tschan/SOPs/experimental_procedures/02c_TOC_Measurements.pdf
5. /Volumes/5505/People/David_Tschan/SOPs/experimental_procedures/03_Solution_Preparation.pdf
6. /Volumes/5505/People/David_Tschan/SOPs/experimental_procedures/04a_CWFTR_full_experimental_day.pdf
7. /Volumes/5505/People/David_Tschan/SOPs/experimental_procedures/04b_CWFTR_half_experimental_day_part_A.pdf
8. /Volumes/5505/People/David_Tschan/SOPs/experimental_procedures/04c_CWFTR_half_experimental_day_part_B.pdf
9. /Volumes/5505/People/David_Tschan/SOPs/experimental_procedures/05_BTOF_Data_Analysis.pdf

The procedures are included below in the same order as listed above:

SOP: SOA Production

Version	4
Date	03. September 2026
Authors	David Tschan
Experiment Time	4 h

Metadata			Set	Exp
Date				
Amb. Cond.	Time	Unit	Value	Device
p_{amb}				
T_{amb}				

Documentation

☐ Raw file ID: _____

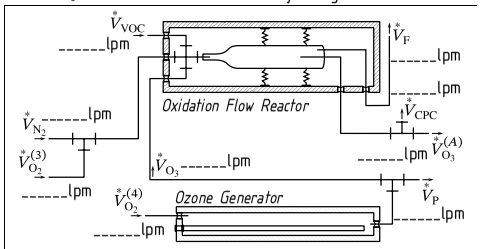
☐ Filter ID: _____

Exp. Cond. ☐ Filter in: _____

☐ Filter out: _____

AIM File Settings ☐ L: 93.5 cm ☐ r_i: 0.937 cm ☐ r_o: 1.961 cm ☐ Aerosol density: 1.2 g cm^{-3}

☐ CPC model: 3775 low
☐ Classifier model: 3080
☐ DMA: custom
☐ HV polarity: negative
☐ DMA flow rate (sheath): 3 L min^{-1}
☐ DMA flow rate (aerosol): 0.3 L min^{-1}
☐ Impactor type: none
☐ Scan time (up): 150 s
☐ Scan time (down): 30 s



Time	*Step*	*Description*	*Execute shaded cells at the same time*
		Check exhaust lines.	
		Ensure 3 way valve of O_3 analyser is open to ambient lab air.	
		Switch on O_3 analyser.	
		Ensure CPC has sufficient butanol level.	
		Ensure CPC inlet valve is set to sampling ambient air.	
		Switch on CPC so that it can warm up.	
		Check that all lines are well-connected.	*Turning on Gas Flow:* *2. Set Setpoint*
		Set flows except VOC flow (leave this at 0):	*1. Turn on Flow Valve* *3. Turn on pressure valve*

Flows to be set:				*Flows automatic:*
V_{N2}	$V_{O2}^{(3)}$	V_{VOC}	$V_{O2}^{(4)}$	V_P: 2.2 L min^{-1}
N_2 Input (Air)	O_2 Input (Air)	N_2 Input (VOC)	O_2 Input (O3)	V_{O3}: 0.8 L min^{-1}
L min^{-1}	L min^{-1}	L min^{-1}	L min^{-1}	V_{CPC}: 0.3 L min^{-1}
3.95	**1.05**	**0.00**	**3.00**	$V_{O3}^{(A)}$: ~ 1 L min^{-1}

		Ensure VOC inlet valve is closed.	
		Switch on excess O_3 pump (under O_3 generator).	
		Ensure OFR outlet valve is set to let flow pass to the O_3 analyser.	
		Ensure valve positions is such that O_3 monitor is sampling system air.	
	A	Connect O_3 analyser with Lab Computer (COM 9), start recording of O_3 analyser.	
		If needed: Take out old filter, wrap it in tin foil and label it with filter ID.	

B	Put in today's new filter with ID: _____.	
	Ensure HV is off.	
	Set valves such that SMPS flow is through DMA (close bypass valves & open DMA valves).	
	Open neutraliser valve.	
	Switch on CPC pump.	
	Switch CPC inlet valve to system air.	
	Open SMPS.vi in LabView. Ensure sheath flow is at 3 L min^{-1} (decrease and increase again).	
C	Open Aerosol Instrument Manager (AIM) and create a new file with settings as above.	
	Do not forget to hit « Set to max range ».	
	Check that all valves are in the correct positions and all flows are set correctly.	
	Start recording in AIM. After ~ 10 seconds, switch on HV source with « Programming » on.	
	Turn on O_3 generator. Let O_3 equilibrate for 45 min (15 samples).	
	Open VOC inlet valve @ _____ s after onset of sample _____.	
	Turn on VOC flow at V_{VOC} = 0.04 L min^{-1} @ onset of sample _____. Let system run 1 h (20 samples).	
	Turn off VOC flow, i.e. back to V_{VOC} = 0.00 L min^{-1} @ onset of sample _____.	
	Close VOC inlet valve Let system equilibrate for 30 min (10 samples), _____ s after sample onset.	
	Turn off O_3 generator. Let system equilibrate for 45 min (15 samples) @ onset of sample _____.	
	Stop recording in AIM.	
	Stop recording O_3 analyser.	
	Switch off HV source.	
	Remove filter holder, close ends with Swagelok caps.	
	Take out filter, wrap it in tin foil and label it with filter ID, date, VOC and investigator name.	
	Close filter holder again.	

☐ *If proceeding to next filter*	*Time*	☐ *If shutting down instrument*
Export data (dN/dlogD, comma, col., all chnls., raw data)		Measure V_F through filter exhaust line (DryCal) (increase V_{N2} by 0.04, measure, decrease to 3.95)
Set up new protocol		Directly
Do step *A*.		Set CPC inlet valve to sample ambient air.
Do step *B*.		Open DMA bypass-, close flow- and neutraliser valves.
Resume protocol from step *C*.		Switch off SMPS pump.
Put filter in freezer if needed.		Set O_3 analyser valve to ambient air.
Export data as above.		Close valve from system to O_3 analyser.
Load data onto server.		Switch off excess O_3 pump.
		Close O_2 flows.
Turning off gas flows:		Close N_2 flows.
1. *Turn off flow valve*		Switch off O_3 analyser.
2. *Turn off pressure valve.*		Switch off CPC.
3. *Wait until flow is 0.*		Close SMPS.vi software
4. *Set setpoint to 0.*		Export dN/dlogD, comma, col., all chnls., raw data.
		Close AIM software.
		Load data onto server.
		Put labelled filters into zipbag in freezer.

SOP: TOC / NPOC / IC Measurement

Version	2
Date	03. September 2026
Authors	David Tschan
Experiment Time	

Materials from Lab 202	*Usage*	*Quantity*	*Cleaning Procedure*
Filter, thawed from freezer for at least 5 min	Extraction	1	–
Teflon knife	Extraction	1	Rinse in MQ (6x), dry with KimTech
Tweezers (steel)	Extraction	1	Rinse in MQ (6x), dry with KimTech
Beaker 100 mL	Extraction	1	Rinse in MQ (6x), dry outside with KimTech
Long vial + cap (for filter extraction)	Extraction	1	Vial: Rinse in MQ (6x). Cap: Sonicate overnight.
Bottle + Cap (for keeping filter extract)	Extraction	variable	Bottle: Rinse in MQ (6x). Cap: Sonicate overnight.
Pipette 10 mL	Extraction	1	–
Pipette tip 10 mL	Extraction	1	–
Syringe 10 mL	Extraction	1	–
Syringe tip filter (Nylon filter 0.45 µm pores)	Extraction	1	–
Pipette 1 mL	Dilution	1	–
Pipette tip 1 mL	Dilution	variable	–
Short vial (TOC autosampler)	Measurement	variable	Rinse in MQ (6x). Do not take wet ones.
Erlenmayer flask 250 mL	Calibration	Variable	Rinse in MQ (6x).
Beaker 250 mL	Waste	1	Rinse in MQ (1x).

1. Cleaning Procedure for glassware of Lab U202

Cleaning bottles (! when running NPOC on the cleaned bottles, remember which bottle is in which vial !)

- ☐ 1. Rinse bottle edge under MQ
- ☐ 2. Fill bottle, shake it, drain it. Repeat 6 times.
- ☐ 3. Fill bottle and put filled bottle in intermediate rack.
- ☐ 4. Measure NPOC of MQ in bottle using clean autosampler tube. If NPOC ≥ 0.1 g / L, repeat the cleaning.

Cleaning autosampler tubes

- ☐ 1. Rinse autosampler tube edge under MQ
- ☐ 2. Fill and drain. Repeat 6 times.
- ☐ 3. Put autosampler tube upside down into the rack. Opening downwards = clean. Opening upwards = dirty.

Table of cleaned bottles

Row	*Bottle*	*Label*	*Cleaning Date*	*Sample Table*	*NPOC (g / L)*	*Verdict*
1						
2						
3						
4						
5						
6						
7						
8						
9						
10						
11						
12						
13						
14						
15						

2. Extracting Filter

Required time ~ 1 h.

Materials ☐ Filter (1x) ☐ Teflon knife (1x) ☐ Tweezers (steel) (1x) ☐ Beaker 100 mL (1x) ☐ Long vial + Cap (1x) ☐ Bottle + Cap (variable) ☐ Pipette 10 mL ☐ Pipette tip 10 mL ☐ Syringe 10 mL ☐ Syringe tip filter

Preliminaries Clean Teflon scissors, tweezers, beaker 100 mL, long vial + cap, bottle + cap according to cleaning procedure. For caps: take fresh caps from the tray with proper ones.

Steps

- ☐ 1. Prepare working area with KimTech and tin foil so that it is clean.
- ☐ 2. Get MQ in a beaker 100 mL (fill it to ~100 mL).
- ☐ 3. Put long vial into rack and open it.
- ☐ 4. Cut filter into small (≤ 1 cm^2) pieces using Teflon knife. Put the pieces into the long vial (using tin foil and/or tweezers).
- ☐ 5. Pipette in 10 mL MQ with appropriate pipette into long vial. Close long vial.
- ☐ 6. Sonicate long vial for 20 min at 30 °C. Ensure sonicator has sufficient water in its bath. If needed: refill bath with MQ before sonication.
- ☐ 7. While long vial sonicates:
  - ☐ a. Prepare glass bottle etiquettes.
  - ☐ b. Rinse the syringe with the filter on 6 times. Take care to always completely remove the syringe stencil (lay it down on clean area). Pipette in 10 mL MQ with 10 mL-pipette from the top.
- ☐ 8. Vortex the long vial for 1 min.
- ☐ 9. Put the long vial into the rack and prepare the first bottle.
- ☐ 10. Filter the extract from the long vial into the first bottle through the syringe. Label this bottle with « c_1 » The volume of this solution is likely slightly less than 10 mL (losses through filter).
- ☐ 11. First dilution step:
  - ☐ a. Prepare bottle 2 by labeling it with « 0.1 c_1 » and opening it.
  - ☐ b. Pipette 1 mL from Bottle 1 into Bottle 2 with 1 mL-pipette.
  - ☐ c. Close bottle 1.
  - ☐ d. Pipette in 9 mL of MQ into bottle 2.
  - ☐ e. Close bottle 2.

  This amounts to a tenfold decrease of SOA extract concentration in bottle 2 compared to bottle 1.
- ☐ 12. Repeat step 11 until desired dilution has been reached. From the last bottle, pipette out 1 mL into the waste so that all samples have 9 mL.
- ☐ 13. If planning to do both TOC and NPOC analysis.
  - ☐ a. Pipette in 9 mL of MQ into each bottle to double the volume (and half the concentration).
- ☐ 14. Put filled and labelled bottles into the fridge in the lab upstairs.
- ☐ 15. Clean Teflon knife, beaker 100 mL and long vial.
- ☐ 16. Put cap of long vial into a beaker for overnight sonication (sonicate only once there are several dirty caps).

3. Measuring TOC / NPOC / IC

Measurement:	Method:	☐ TOC ☐ NPOC ☐ IC
	Date:	☐ ____ / ____ / ________

Important Comments

☐ 1. If filter was created using procedure « SOP: SOA Production », expected SOA content is ~ 5 mg.

☐ 2. Ideally, sample NPOB/TOC is analysed right after extraction to minimise the wall- and other losses

☐ 3. Do not use wet autosampler vials when to run calibration curves and concentration measurements (risk of diluting the samples and obtaining faulty results.

Legend

TOC: Total organic carbon, including volatile organics (accuracy is within 10 ppm)

NPOB: Non-purgeable organic carbon (accuracy is within 2 ppm)

IC: Inorganic carbon (accuracy not known)

TC: Total carbon (accuracy not known), TC = TOC + IC

Steps

☐ 1. Empty waste water of TOC analyser into sink.

☐ 2. Change water of the tree containers of TOC analyser. Care should be taken so that the tubes do not come into contact with the table upon removal from the bottles (i.e. put a piece of KimTech/paper in between). Take extra care when changing the water of the water container inside the TOC analyser.

- ☐ a. Rinse containers with MQ (3x)
- ☐ b. Refill them with MQ
- ☐ c. Reinstall them

☐ 3. Switch on the TOC analyser so that it can heat up (combustion chamber needs to heat up to 680 °C).

☐ 4. TOC / NPOC Calibration (both calibrations use the same sample):

- ☐ a. In an Erlenmayer flask 250 mL, prepare a 2 ppm TOC solution
  - ☐ i.
- ☐ b. In an Erlenmayer flask 250 mL, prepare a 10 ppm TOC solution
  - ☐ i.

☐ 5. IC Calibration:

- ☐ a. In an Erlenmayer flask 250 mL, prepare a 2 ppm IC solution
  - ☐ i.
- ☐ b. In an Erlenmayer flask 10 mL, prepare a 10 ppm IC solution
  - ☐ i.

☐ 6. Prepare the short vials for 8-point calibration at dilutions:

☐ 7. 1 (10 ppm)

☐ 8. 2 (5 ppm)

☐ 9. 4 (2.5 ppm)

☐ 10. 10 (1 ppm)

☐ 11. 20 (0.5 ppm)

☐ 12. 40 (0.25 ppm)

☐ 13. 100 (0.1 ppm)

☐ 14. 200 (0.05 ppm)

☐ 15. Load the autosampler and set up the measurement

☐ 16.

☐ 17. Important to note down: filter name/number; dilution factor; probably 1 000 for all filters; instrument settings (although this can be checked)

☐ 18. Prepare working area with KimTech and tin foil so that it is clean.

☐ 19.

Overview over prepared samples:

Row	*Date*	*Bottle*	*Label*	*Filter*	*Base Extract*	*Dilution*	*NPOC*	*TOC*	*IC*	*TC*
1										
2										
3										
4										
5										
6										
7										
8										
9										
10										
11										
12										

SOP: TOC Filter Extraction

Version	1
Date	09. September 2026
Authors	David Tschan
Experiment Time	~1 h

Required time ~ 1 h.

Materials ☐ Filter (1x) ☐ Teflon knife (1x) ☐ Tweezers (steel) (1x) ☐ Beaker 100 mL (1x) ☐ Long vial + Cap (1x) ☐ Bottle + Cap (variable) ☐ Pipette 10 mL ☐ Pipette tip 10 mL ☐ Syringe 10 mL ☐ Syringe tip filter

Preliminaries Clean Teflon scissors, tweezers, beaker 100 mL, long vial + cap, bottle + cap according to cleaning procedure. For caps: take fresh caps from the tray with proper ones.

Steps

☐ 1. Prepare working area with KimTech and tin foil so that it is clean.

☐ 2. Get MQ in a beaker 100 mL (fill it to ~100 mL).

☐ 3. Put long vial into rack and open it.

☐ 4. Cut filter into small (≤ 1 cm^2) pieces using Teflon knife. Put the pieces into the long vial (using tin foil and/or tweezers).

☐ 5. Pipette in 10 mL MQ with appropriate pipette into long vial. Close long vial.

☐ 6. Sonicate long vial for 20 min at 30 °C. Ensure sonicator has sufficient water in its bath. If needed: refill bath with MQ before sonication.

☐ 7. While long vial sonicates:

- ☐ a. Prepare glass bottle etiquettes.
- ☐ b. Rinse the syringe with the filter on 6 times. Take care to always completely remove the syringe stencil (lay it down on clean area). Pipette in 10 mL MQ with 10 mL-pipette from the top.

☐ 8. Vortex the long vial for 1 min.

☐ 9. Put the long vial into the rack and prepare the first bottle.

☐ 10. Filter the extract from the long vial into the first bottle through the syringe. Label this bottle with « c_1 » The volume of this solution is likely slightly less than 10 mL (losses through filter).

☐ 11. First dilution step:

- ☐ a. Prepare bottle 2 by labeling it with « 0.1 c_1 » and opening it.
- ☐ b. Pipette 1 mL from Bottle 1 into Bottle 2 with 1 mL-pipette.
- ☐ c. Close bottle 1.
- ☐ d. Pipette in 9 mL of MQ into bottle 2.
- ☐ e. Close bottle 2.

This amounts to a tenfold decrease of SOA extract concentration in bottle 2 compared to bottle 1.

☐ 12. Repeat step 11 until desired dilution has been reached. From the last bottle, pipette out 1 mL into the waste so that all samples have 9 mL.

☐ 13. If planning to do both TOC and NPOC analysis.

- ☐ a. Pipette in 9 mL of MQ into each bottle to double the volume (and half the concentration).

☐ 14. Put filled and labelled bottles into the fridge in the lab upstairs.

☐ 15. Clean Teflon knife, beaker 100 mL and long vial.

☐ 16. Put cap of long vial into a beaker for overnight sonication (sonicate only once there are several dirty caps).

☐ TOC Measurement
☐ TOC Calibration (see above) ☐ TOC Calibration used from: ___ / ___ / _____

☐ TOC: Dilution: _____
Added Volumes:
V_{H2O} = _____ mL
$V_{_____}$ = _____ mL
Vol. (mL): _____
Label: _____ = _____
SOA conc. estimate:
_____ ≈ _____ mg / L

☐ TOC: Dilution: _____
Added Volumes:
V_{H2O} = _____ mL
$V_{_____}$ = _____ mL
Vol. (mL): _____
Label: _____ = _____
SOA conc. estimate:
_____ ≈ _____ mg / L

☐ NPOC Measurement
☐ NPOC Calibration (see above) ☐ NPOC Calibration used from ___ / ___ / _____

☐ NPOC: Dilution: _____
Added Volumes:
V_{H2O} = _____ mL
$V_{_____}$ = _____ mL
Vol. (mL): _____
Label: _____ = _____
SOA conc. estimate:
_____ ≈ _____ mg / L

☐ NPOC: Dilution: _____
Added Volumes:
V_{H2O} = _____ mL
$V_{_____}$ = _____ mL
Vol. (mL): _____
Label: _____ = _____
SOA conc. estimate:
_____ ≈ _____ mg / L

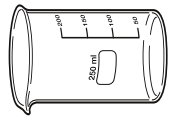
☐ IC Measurement
☐ IC Calibration (see above) ☐ IC Calibration used from ___ / ___ / _____

☐ IC: Dilution: _____
Added Volumes:
V_{H2O} = _____ mL
$V_{_____}$ = _____ mL
Vol. (mL): _____
Label: _____ = _____
SOA conc. estimate:
_____ ≈ _____ mg / L

☐ IC: Dilution: _____
Added Volumes:
V_{H2O} = _____ mL
$V_{_____}$ = _____ mL
Vol. (mL): _____
Label: _____ = _____
SOA conc. estimate:
_____ ≈ _____ mg / L



Initial Extract
Vol. (mL): _____
Label: _____
SMPS SOA conc.:
_____ ≈ _____ mg / L



Required volume of MQ:
_____ mL

SOP: TOC / NPOC / IC Measurement

Version	2
Date	03. September 2026
Authors	David Tschan
Experiment Time	

Materials from Lab 202	*Usage*	*Quantity*	*Cleaning Procedure*
Filter, thawed from freezer for at least 5 min	Extraction	1	–
Teflon knife	Extraction	1	Rinse in MQ (6x), dry with KimTech
Tweezers (steel)	Extraction	1	Rinse in MQ (6x), dry with KimTech
Beaker 100 mL	Extraction	1	Rinse in MQ (6x), dry outside with KimTech
Long vial + cap (for filter extraction)	Extraction	1	Vial: Rinse in MQ (6x). Cap: Sonicate overnight.
Bottle + Cap (for keeping filter extract)	Extraction	variable	Bottle: Rinse in MQ (6x). Cap: Sonicate overnight.
Pipette 10 mL	Extraction	1	–
Pipette tip 10 mL	Extraction	1	–
Syringe 10 mL	Extraction	1	–
Syringe tip filter (Nylon filter 0.45 µm pores)	Extraction	1	–
Pipette 1 mL	Dilution	1	–
Pipette tip 1 mL	Dilution	variable	–
Short vial (TOC autosampler)	Measurement	variable	Rinse in MQ (6x). Do not take wet ones.
Erlenmayer flask 250 mL	Calibration	Variable	Rinse in MQ (6x).
Beaker 250 mL	Waste	1	Rinse in MQ (1x).

1. Cleaning Procedure for glassware of Lab U202

Cleaning bottles (! when running NPOC on the cleaned bottles, remember which bottle is in which vial !)

- ☐ 1. Rinse bottle edge under MQ
- ☐ 2. Fill bottle, shake it, drain it. Repeat 6 times.
- ☐ 3. Fill bottle and put filled bottle in intermediate rack.
- ☐ 4. Measure NPOC of MQ in bottle using clean autosampler tube. If NPOC ≥ 0.1 g / L, repeat the cleaning.

Cleaning autosampler tubes

- ☐ 1. Rinse autosampler tube edge under MQ
- ☐ 2. Fill and drain. Repeat 6 times.
- ☐ 3. Put autosampler tube upside down into the rack. Opening downwards = clean. Opening upwards = dirty.

Table of cleaned bottles

Row	*Bottle*	*Label*	*Cleaning Date*	*Sample Table*	*NPOC (g / L)*	*Verdict*
1						
2						
3						
4						
5						
6						
7						
8						
9						
10						
11						
12						
13						
14						
15						

2. Extracting Filter

Required time ~ 1 h.

Materials ☐ Filter (1x) ☐ Teflon knife (1x) ☐ Tweezers (steel) (1x) ☐ Beaker 100 mL (1x) ☐ Long vial + Cap (1x) ☐ Bottle + Cap (variable) ☐ Pipette 10 mL ☐ Pipette tip 10 mL ☐ Syringe 10 mL ☐ Syringe tip filter

Preliminaries Clean Teflon scissors, tweezers, beaker 100 mL, long vial + cap, bottle + cap according to cleaning procedure. For caps: take fresh caps from the tray with proper ones.

Steps

- ☐ 1. Prepare working area with KimTech and tin foil so that it is clean.
- ☐ 2. Get MQ in a beaker 100 mL (fill it to ~100 mL).
- ☐ 3. Put long vial into rack and open it.
- ☐ 4. Cut filter into small (≤ 1 cm^2) pieces using Teflon knife. Put the pieces into the long vial (using tin foil and/or tweezers).
- ☐ 5. Pipette in 10 mL MQ with appropriate pipette into long vial. Close long vial.
- ☐ 6. Sonicate long vial for 20 min at 30 °C. Ensure sonicator has sufficient water in its bath. If needed: refill bath with MQ before sonication.
- ☐ 7. While long vial sonicates:
  - ☐ a. Prepare glass bottle etiquettes.
  - ☐ b. Rinse the syringe with the filter on 6 times. Take care to always completely remove the syringe stencil (lay it down on clean area). Pipette in 10 mL MQ with 10 mL-pipette from the top.
- ☐ 8. Vortex the long vial for 1 min.
- ☐ 9. Put the long vial into the rack and prepare the first bottle.
- ☐ 10. Filter the extract from the long vial into the first bottle through the syringe. Label this bottle with « c_1 » The volume of this solution is likely slightly less than 10 mL (losses through filter).
- ☐ 11. First dilution step:
  - ☐ a. Prepare bottle 2 by labeling it with « 0.1 c_1 » and opening it.
  - ☐ b. Pipette 1 mL from Bottle 1 into Bottle 2 with 1 mL-pipette.
  - ☐ c. Close bottle 1.
  - ☐ d. Pipette in 9 mL of MQ into bottle 2.
  - ☐ e. Close bottle 2.

  This amounts to a tenfold decrease of SOA extract concentration in bottle 2 compared to bottle 1.
- ☐ 12. Repeat step 11 until desired dilution has been reached. From the last bottle, pipette out 1 mL into the waste so that all samples have 9 mL.
- ☐ 13. If planning to do both TOC and NPOC analysis.
  - ☐ a. Pipette in 9 mL of MQ into each bottle to double the volume (and half the concentration).
- ☐ 14. Put filled and labelled bottles into the fridge in the lab upstairs.
- ☐ 15. Clean Teflon knife, beaker 100 mL and long vial.
- ☐ 16. Put cap of long vial into a beaker for overnight sonication (sonicate only once there are several dirty caps).

3. Measuring TOC / NPOC / IC

Measurement:	Method:	☐ TOC ☐ NPOC ☐ IC
	Date:	☐ ____ / ____ / ________

Important Comments

☐ 1. If filter was created using procedure « SOP: SOA Production », expected SOA content is ~ 5 mg.

☐ 2. Ideally, sample NPOB/TOC is analysed right after extraction to minimise the wall- and other losses

☐ 3. Do not use wet autosampler vials when to run calibration curves and concentration measurements (risk of diluting the samples and obtaining faulty results.

Legend

TOC: Total organic carbon, including volatile organics (accuracy is within 10 ppm)

NPOB: Non-purgeable organic carbon (accuracy is within 2 ppm)

IC: Inorganic carbon (accuracy not known)

TC: Total carbon (accuracy not known), TC = TOC + IC

Steps

☐ 1. Empty waste water of TOC analyser into sink.

☐ 2. Change water of the tree containers of TOC analyser. Care should be taken so that the tubes do not come into contact with the table upon removal from the bottles (i.e. put a piece of KimTech/paper in between). Take extra care when changing the water of the water container inside the TOC analyser.

- ☐ a. Rinse containers with MQ (3x)
- ☐ b. Refill them with MQ
- ☐ c. Reinstall them

☐ 3. Switch on the TOC analyser so that it can heat up (combustion chamber needs to heat up to 680 °C).

☐ 4. TOC / NPOC Calibration (both calibrations use the same sample):

- ☐ a. In an Erlenmayer flask 250 mL, prepare a 2 ppm TOC solution
  - ☐ i.
- ☐ b. In an Erlenmayer flask 250 mL, prepare a 10 ppm TOC solution
  - ☐ i.

☐ 5. IC Calibration:

- ☐ a. In an Erlenmayer flask 250 mL, prepare a 2 ppm IC solution
  - ☐ i.
- ☐ b. In an Erlenmayer flask 10 mL, prepare a 10 ppm IC solution
  - ☐ i.

☐ 6. Prepare the short vials for 8-point calibration at dilutions:

☐ 7. 1 (10 ppm)

☐ 8. 2 (5 ppm)

☐ 9. 4 (2.5 ppm)

☐ 10. 10 (1 ppm)

☐ 11. 20 (0.5 ppm)

☐ 12. 40 (0.25 ppm)

☐ 13. 100 (0.1 ppm)

☐ 14. 200 (0.05 ppm)

☐ 15. Load the autosampler and set up the measurement

☐ 16.

☐ 17. Important to note down: filter name/number; dilution factor; probably 1 000 for all filters; instrument settings (although this can be checked)

☐ 18. Prepare working area with KimTech and tin foil so that it is clean.

☐ 19.

Overview over prepared samples:

Row	*Date*	*Bottle*	*Label*	*Filter*	*Base Extract*	*Dilution*	*NPOC*	*TOC*	*IC*	*TC*
1										
2										
3										
4										
5										
6										
7										
8										
9										
10										
11										
12										

SOP: Title

Version	Number
Date	31. August 2026
Authors	David Tschan

1. Section

1. Step

SOP: CWFTR Full Experiment Day

Version	2
Date	03. September 2026
Authors	David Tschan
Experiment Time	~ 7 h

Metadata

Date Set Exp

Tube

Sample ☐ Old. ☐ New ☐ ID:_____

☐ Smpl. Doc ☐ pH:_____ ☐ Device:_____

MQ ☐ Date

☐ New ☐ Resistance MΩ•cm

☐ Old ☐ TOC ppb

Ambient Conditions

	t (HH/MM)	Val. / Unit	Device
p_{amb}			
T_{amb}			

Positions

	Time t (HH / MM)	Value (mL / min)
0 – Inlet		
1 – After humidifier		
2 – After reac. (BP)		
2 – After reac. (tube)		
3 – After dilution		
4 – Before stack (BP)		
4 – Before stack (tube)		
5 – Exhaust (BP)		

Documentation

☐ Excel Protocol Created Excel ☐ Protocol Completed

Sample Composition

Component	Name	ID (SA)	c_{sample} (M)	c_{film} (M)
FS				
PS				
IS				

Sample Preparation FS: PS: IS:

Required Mass (g)

Actual Mass (g)

Flow (mL / min)

N_2 Dilution

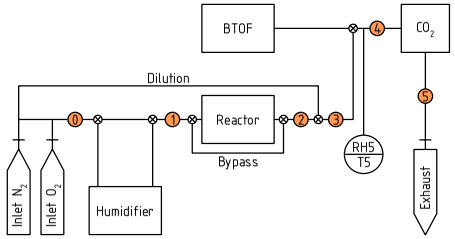
N_2

O_2

Light Light On Light Off

Flow Stch. N_2

O_2



Time	*Description*
	Create Excel Protocol.
	BTOF to ready mode (carefully follow instructions in BTOF_Notes.txt).
	Check water level in CWFTR humidifier bath. If needed: refill using De-Ion and big plastic flask.
	Check water level in CFWTR humidifier cell. If needed: refill using MQ.
	Check water level of coating bubbler. If needed: refill using MQ.
	Set Flows.
	Turn on N_2 valve.
	Turn on O_2 valve.
	Turn on Teledyne CO_2.
	Turning On Gas Flows:
	1. Set Setpoint.
	2. Turn on Flow Valve.
	3. Turn on Pressure Valve.
	Turn on cooling system of CWFTR (check fittings carefully so no silicone oil spills).
	Tube cleaned. Or: tube cleaned on: ___/___/_____. Dry tube with Ar. Remove sticker and add here.
	Start Teledyne CO2 and start recording (do this now – device needs to warm up).

	Start recording RH5 / T5.
	Flow through humidifier (expectation: jump of RH).
	Flow measurements.
	Measure p_{amb} / T_{amb} (use DryCal for p_{amb} and T5 for T_{amb}).
	Slightly coat tube with MQ, then put it in the CWFTR (Pipette in a little MQ).
	Flow to tube.
	Flow measurements with flow through tube.
	Flow back to bypass.
	Take out tube.
	Rinse tube tips and flow jacks with MQ 3 times.
	Connect BTOF.
	Start BTOF recording (ensure correct sequencing service is used).
	Open coating valve flow. $RH_{100\%}$ flow: _____, $RH_{0\%}$ flow: _____ at ____/_____.
	Lights On.
	Start coating. Measure sample pH using strip. pH: _____. Coating process should take ~1h.
	Stop coating when everything looks homogeneous and no movement can be detected by eye anymore.
	Lights Off.
	Check RH5 sensor.
	Rub outside of tube using a paper with acetone to remove sticker marks.
	Tube in reactor.
	Flow through tube. Let equilibrate 1h.
	Measure pH (not using strip). pH: _____.
	Lights on. Measurement time 2h.
	Lights off. Wait 1h to let products flow away.
	Stop BTOF recording.
	Screenshot of BTOF, upload to obsidian and store in folder.
	Flow through bypass.
	Open BTOF to ambient air.
	Stop Teledyne CO_2 recording.
	Stop RH5 / T5 recording.
	If BTOF is not needed anytime soon: BTOF to sleep (carefully read instructions in BTOF_Notes.txt).
	Take out tube and put a new sticker on it. Was the coating homogeneous? _____.
	Bypass humidifier.
	Turn off cooling.
	Turn off Teledyne CO_2.
	Set Flows or turn off gas flows.
	Clean tubes, other glassware and instruments.
	Fill in Excel protocol.
	Turning off gas flows:
	1. Turn off flow valve.
	2. Turn off pressure valve.
	3. Wait until flow is 0.
	4. Set setpoint to 0.

SOP: CWFTR Half Experimental Day – Part A

Version	2
Date	03. September 2026
Authors	David Tschan
Experiment Time	~ 5 h (overlaps ~2 h with part B)

Metadata

Date Set Exp

Part B

Tube

Sample ☐ Old. ☐ New ☐ ID:_____

☐ Smpl. Doc ☐ pH:_____ ☐ Device:_____

MQ ☐ Date

☐ New ☐ Resistance MΩ•cm

☐ Old ☐ TOC ppb

Ambient Conditions

	t (HH/MM)	Val. / Unit	Device
p_{amb}			
T_{amb}			

Positions

	Time t (HH / MM)	Value (mL / min)
0 – Inlet		
1 – After humidifier		
2 – After reac. (BP)		
2 – After reac. (tube)		
3 – After dilution		
4 – Before stack (BP)		
4 – Before stack (tube)		
5 – Exhaust (BP)		

Documentation

☐ Excel Protocol Created Excel ☐ Protocol Completed

Sample Composition

Component	Name	ID (SA)	c_{sample} (M)	c_{film} (M)
FS				
PS				
IS				

Sample Preparation FS: PS: IS:

Required Mass (g)

Actual Mass (g)

Flow (mL / min)

N_2 Dilution

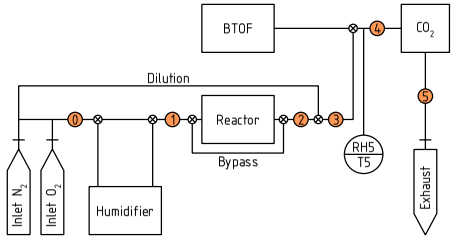
N_2

O_2

Light Light On Light Off

Flow Stch. N_2

O_2



Time	*Description*
	Create Excel Protocol.
	BTOF to ready mode (carefully follow instructions in BTOF_Notes.txt).
	Check water level in CWFTR humidifier bath. If needed: refill using De-Ion and big plastic flask.
	Check water level in CFWTR humidifier cell. If needed: refill using MQ.
	Check water level of coating bubbler. If needed: refill using MQ.
	Set Flows.
	Turn on N_2 valve.
	Turn on O_2 valve.
	Turn on Teledyne CO_2.
	Turning On Gas Flows:
	1. Set Setpoint.
	2. Turn on Flow Valve.
	3. Turn on Pressure Valve.
	Turn on cooling system of CWFTR (check fittings carefully so no silicone oil spills).
	Tube cleaned. Or: tube cleaned on: ___/___/_____. Dry tube with Ar. Remove sticker and add here.
	Start Teledyne CO2 and start recording (do this now – device needs to warm up).

	Start recording RH5 / T5.
	Flow through humidifier (expectation: jump of RH).
	Flow measurements.
	Measure p_{amb} / T_{amb} (use DryCal for p_{amb} and T5 for T_{amb}).
	Slightly coat tube with MQ, then put it in the CWFTR (Pipette in a little MQ).
	Flow to tube.
	Flow measurements with flow through tube.
	Flow back to bypass.
	Take out tube.
	Rinse tube tips and fittings with MQ 3 times.
	Connect BTOF.
	Start BTOF recording (ensure correct sequencing service is used).
	Open coating valve flow. $RH_{100\%}$ flow: _____, $RH_{0\%}$ flow: _____ at ____/_____.
	Lights On.
	Start coating (1 mL). Measure sample pH using strip. pH: _____. Coating process should take ~1h.
	Stop coating when everything looks homogeneous and no movement can be detected by eye anymore.
	Close coating flow.
	Lights Off.
	Check RH5 sensor.
	Rub outside of tube using a paper with acetone to remove sticker marks. Mount tube fittings.
	Tube in reactor.
	Flow through tube. Let equilibrate 1h.
	Measure pH (not using strip). pH: _____.
	Lights on. Measurement time 2h.
	Rest of today's experimental protocol in part B: SET _____ / EXP _____.

SOP: CWFTR Half Experimental Day – Part B

Version	2
Date	03. September 2026
Authors	David Tschan
Experiment Time	~ 5 h (overlaps ~2 h with part A)

Metadata

Date Set Exp

Tube

Sample ☐ Old. ☐ New ☐ ID:_____

☐ Smpl. Doc ☐ pH:_____ ☐ Device:_____

MQ ☐ Date

☐ New ☐ Resistance MΩ•cm

☐ Old ☐ TOC ppb

Ambient Conditions

	t (HH/MM)	Val. / Unit	Device
p_{amb}			
T_{amb}			

Positions

	Time t (HH / MM)	Value (mL / min)
1 – After reac. (tube)		

Documentation

☐ Excel Protocol Created Excel ☐ Protocol Completed

Sample Composition

Component	Name	ID (SA)	c_{sample} (M)	c_{film} (M)
FS				
PS				
IS				

Sample Preparation FS: PS: IS:

Required Mass (g)

Actual Mass (g)

Flow (mL / min)

N_2 Dilution

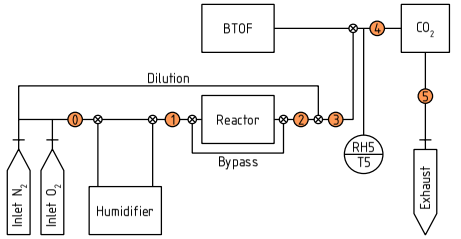
N_2

O_2

Light Light On Light Off

Flow Stch. N_2

O_2



Time	*Description*
	Create Excel Protocol for part B.
	Tube cleaned. Or: tube cleaned on: ___/___/_____. Dry tube with Ar. Remove sticker and add here.
	If using 2nd fitting pair: Rinse 3 times with MQ and put in clean area to dry.
	Open coating valve flow. $RH_{100\%}$ flow: _____, $RH_{0\%}$ flow: _____ at ____/_____.
	Start coating (1 mL). Measure sample pH using strip. pH: _____. Coating process should take ~1h.
	Stop coating when everything looks homogeneous and no movement can be detected by eye anymore.
	Close coating flow.
	Rub outside of tube using a paper with acetone to remove sticker marks.
	Cover coated tube with (fresh) tin foil and keep the wrapped & closed tube in the dark.
	Lights off (part A). Wait 1h to let products flow away.
	Stop BTOF recording (part A).
	Screenshot of BTOF (part A), upload to obsidian and store in folder.
	Flow through bypass.
	Open BTOF to ambient air.
	Stop Teledyne CO_2 recording form part A.
	Stop RH5 / T5 recording from part A.
	Flow through bypass.

Take first tube (part A) out of reactor. Pertaining experiment: SET _____ / EXP _____.

Put new sticker on tube from part A. Was the coating homogeneous? _____.

Start new recording of Teledyne CO2 (for part B here).

Start new recording of RH5 / T5 (for part B here).

Turn off O2 valve if part B is without oxygen.

Set flows.

Reconnect BTOF to system.

If using 1st (part A) pair of fittings: rinse 3 times with MQ, dry with Ar and KimTech.

Mount fittings on prepared tube for part B (under the tin foil).

Check RH5 sensor.

Tube in reactor.

Flow through tube. Let equilibrate 1h.

Measure pH (not using strip). pH: _____.

Lights on. Measurement time 2h.

Lights off. Wait 1h to let products flow away.

Stop BTOF recording.

Screenshot of BTOF, upload to obsidian and store in folder.

Flow measurement.

Measure p_{amb} / T_{amb} (use DryCal for p_{amb} and T5 for T_{amb}).

Flow through bypass.

Open BTOF to ambient air.

Stop Teledyne CO_2 recording.

Stop RH5 / T5 recording.

If BTOF is not needed anytime soon: BTOF to sleep (carefully read instructions in BTOF_Notes.txt).

Take out tube and put a new sticker on it. Was the coating homogeneous? _____.

Bypass humidifier.

Turn off cooling.

Turn off Teledyne CO_2.

Set Flows or turn off gas flows.

Clean tubes, other glassware and instruments.

Fill in Excel protocols for parts A and B.

Turning off gas flows:

1. *Turn off flow valve*
2. *Turn off pressure valve.*
3. *Wait until flow is 0.*
4. *Set setpoint to 0.*

SOP: BTOF Data Analysis

Version	2
Date	31. August 2026
Authors	David Tschan

1. Prerequisites

1. IGOR Pro 64-bit is available;
2. Folder ~/xTOF_fileSplitter/ is available, giving availability of:
    a. Executable xTOF_fileSplitterApp.exe;
3. Folder ~/Tofware_v4_1_1_CIMS/Tofware_v4_1_1/ is available on machine, containing:
    a. Experiment file for IGOR Pro 64-bit called Tofware_4_1_1_CIMS.pxt;
    b. Subfolder ./IPF_WORKFLOWS/ with file twV4_1_1_wkf_HRTS.ipf;
4. Mass calibration files for all reagent ions are available, named something like masscal_Iodine_DENALI2025.cal for Iodine (similar for other reagent ions);
5. BTOF output data file(s) (named something like PWB-005-2026.05.27_13h47m12s.h5 available.
6. Create a folder where you store the BTOF output data file(s), then call the files splitter to split the raw data file.

! The following steps are necessary for all the reagent ions !

2. Setting up the environment on IGOR Pro 64-bit

1. Open IGOR Pro 64-bit.
2. Open the experiment Tofware_4_1_1_CIMS.pxt and save the experiment under the name you desire in the location you desire (likely, in the same folder where there is the raw data makes sense).
3. Open **split** file(s) in batch mode by adding them to the experiment.
4. If not already available, import the workflow twV4_1_1_wkf_HRTS.ipf.
5. Save the experiment.

3. Step-by-step guideline

1. Go to Miscellaneous/Settings, make sure of the following things:
    a. Files are set up with correct UTC time.
    b. Save to p-files.
    c. Save instrument func files.
2. **Mass Calibration**: in this step we calibrate the BTOF data using certain known masses of selected calibrants.
    a. Load list of calibrates from Z:\People\David_Tschan\BTOF_analysis_IGOR\Mass_Calibration_Files. Select load just list (this avoids downstream parametrization issues).
    b. Adapt the peak search range D (smaller: more peak-specific: scroll wheel for zooming in and out) until peaks are reasonably well covered.
    c. Set fit type to Gaussian with fit equation: $p_1\sqrt{m}+p_2$. More parameters in the fit equation will increase the chances of overfitting, thereby increasing the inaccuracies outside of calibrants mass range (for a n parametric fit, we require at least n calibrant peaks).
    d. Set Fitted Coeffs to Initial Coeffs to resize the windows to the center of the peaks so that they are not missed during mass calibration.
    e. Select batch mass calibration with averaging timescale of 2 min (if it can be assumed that BTOF was in stable conditions for 2 minutes), auto improve ticked, threshold 5 ppm (BTOF is precise) max number of peaks to remove chosen such that fit equation is not under-determined (i.e. we need as many peaks as parameters).
    f. Calibrate selected files.
    g. Plot parameters (these change over time, since BTOF is drifting over time). Criteria for good mass calibration:
        i. No residuals bigger than threshold (CTRL + I to check values by drag and drop).
        ii. No flags raised.
        iii. t_ion jumps not too large, else this indicates that the existence of a double peak.

    If one of these criteria is not met, the mass calibration should be repeated (i.e. go back to the calibration of the file with the pertaining ID).
3. Define reference spectrum at the nominal mass of the reagent ion (Iodine: m/z = 127 Th). This step is to define the baseline of the instrument.
    a. Choose correct time frame by dragging a box in the upper plot that shows the offset from the mass calibration. The selected time frame should be a period of stable and high signal.
    b. Right click with the cursor and hit Place Cursor here and update MS (Marquee Spacebar).
    c. If it is good, accept, else choose another time frame and go back to step a.
4. Refine Baseline: in this step, why do we do it?
    a. Adapt the width (actual signal – instrument baseline) parameter, noise scaling and lo-pass filter parameters.
    b. If satisfied, hit save to all files and save.
5. Refine peak width and shape for average peak: in this step, why do we do this?
    a. Go to peak and remove outliers
    b. Go to tails and remove outliers
    c. If struggling, use CTRL + CLICK to show m/z to clean up more.
    d. Save (if there are several files: chose between all, one file, active)
6. Refine peak width: this step is for what? The goal here is to have high resolution.
    a. Adjust the tolerance of max ions/ex.
    b. Remove points by clicking on them until the fit looks good.
7. Do the second round of mass calibration: go to step 2. Choose the custom fit profile we created in our workflow.
    a. After the second calibration, check the spectrum of the calibrants (peak shape and -width). If this is OK, we can trust it and go on to peak fitting. Else refine.
8. Peak fitting: in this step, we identify actual molecules in the BTOF data
    a. Click HR
    b. Go to peak
    c. Select and click on composition and Isotopes
    d. If everything looks good, assign peak and go to next peak.
    e. Aids in peak fitting:
        i. Isotope ratios create characteristic spectral behavior, both in terms of relative intensity and position of peaks
        ii. H Content of organics has an upper bound (the pure hydrocarbon chain)
        iii. Nominal masses we're interested in: we have to fit them all!
    f. Finish peak list and calculate isotopes
9. Batch file export
    a. Fully constrained, subtract MS baseline, constrain isotopes, reallocate isotope signal, UMR for quick data analysis (integrated masses, same as in quick view), then execute

Commented [DT1]: Is this correct? I feel uncertain about this.

Commented [DT2]: Ideal is for instance during coating of tube, when BTOF is stable.

Commented [DT3]: I am not sure anymore...

Commented [DT4]: This is not the meaning of the width parameter, or is it?

Commented [DT5]: I am not sure

Commented [DT6]: Why is this useful?

Commented [DT7]: Again not su sure

Commented [DT8]: What does that mean?

Commented [DT9]: I noted this down but I am no longer sure what it means...

b. Export all either as csv or PMF/SoFi (for IGOR, this is a more specific type of export)