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FINAL REPORT

# Abiotic Trichloroethylene (and Carbon Tetrachloride) Reduction by Meta-Stable Mineral Phases

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The objective of this project was to examine the formation of meta-stable reactive species under realistic groundwater scenarios, including the addition of precursor materials that have been reported to enhance abiotic degradation (e.g., magnetite, sulfate, ferrous iron, lactate). By conducting a matrix of experiments varying carbon source (lactate), carbonate concentration, magnetite mineral addition, as well as aqueous ferrous iron and sulfate addition, it was hoped that the factors controlling abiotic degradation could be isolated and quantified.

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# 1. Abstract


## Introduction and Objectives

The development of chemically-reducing conditions in the subsurface is an important strategy for in situ restoration of groundwater contaminated by chlorinated solvents. This can be accomplished by emplacement of reducing materials (e.g., ZVI, edible oil) or active pumping of reductants (e.g., sulfate, nano-minerals, labile carbon source). For actively pumped restoration activities, there is significant uncertainty regarding how long the enhanced reduction will persist once the site has been returned to more-passive conditions (i.e., active-to-passive transition). If, during active treatment, a reservoir of reactive reduced species is produced (e.g., precipitation of reactive minerals), then those minerals may continue to reduce contaminants well after active treatment has ended. However, if the reactive species are short-lived, then the ongoing effect on groundwater restoration may limited.

The objective of this project was to examine the formation of meta-stable reactive species under realistic groundwater scenarios, including the addition of precursor materials that have been reported to enhance abiotic degradation (e.g., magnetite, sulfate, ferrous iron, lactate). By conducting a matrix of experiments varying carbon source (lactate), carbonate concentration, magnetite mineral addition, as well as aqueous ferrous iron and sulfate addition, it was hoped that the factors controlling abiotic degradation could be isolated and quantified.

## Technical Approach

The matrix of experiments was conducted in large sand columns, which were initially allowed to run for a period of several months to establish steady-state conditions. Then a cocktail of chlorinated compounds was continuously injected for a period of approximately two weeks to develop a steady-state concentration profile within the column. At the end of that period, the concentrations of each of the chlorinated compounds was analyzed in water samples from along the length of the column. Column flow was then stopped to simulate the end of active pumping, and samples were periodically collected over a period of 3 months.

## Results

TCE showed a consistent degradation rate for nearly all conditions tested, with the exception of the column where no carbon source (no lactate) was added. CT degradation was observed at more-or-less consistent rates in 4 of 6 columns. The two columns showing lower rates were the column without lactate (NL) and the column without carbonate addition (NC). The latter had a low pH (~3.5), which was eventually increased to 7.2 using PIPES buffer). When the pH was increased in the NC column, the CT rate increased by an order of magnitude, but was still an order of magnitude less than the four columns with both lactate and carbonate. For both TCE and CT, an important result is that biologically-active conditions were critical for creating an environment in which abiotic degradation could occur.

## Benefits

This project was to undertaken to develop a data set for use in a concurrent larger-scale project (ER20-1357). The data set was also used to evaluate a decision tree approach to identify which subsurface conditions resulted in enhanced and sustained degradation of contaminants

# 2. Executive Summary

## Introduction

An important strategy for in situ restoration of groundwater contaminated by chlorinated solvents is the active development of reducing conditions to enhance dechlorination via biotic or abiotic means. This can be accomplished by emplacement of reducing materials (e.g., ZVI, edible oil) or active pumping of reductants (e.g., sulfate, nano-minerals, labile carbon source). For actively pumped restoration, there is significant uncertainty regarding how long the enhanced reduction will persist once the site has been returned to more-passive conditions (i.e., active-to-passive transition). If, during active treatment, a reservoir of reactive reduced species is produced (e.g., precipitation of reactive minerals), then those minerals may continue to reduce contaminants well after active treatment has ended. However, if the reactive species are short-lived, then the ongoing effect on groundwater restoration may limited.

## Objectives

The primary objective of the project was to examine if reactive dechlorination conditions formed under a range of realistic groundwater flow scenarios, including the addition of precursor materials that have been reported to enhance abiotic degradation (e.g., magnetite, sulfate, ferrous iron, lactate). By conducting a matrix of experiments varying carbon source (lactate), carbonate concentration, magnetite mineral addition, as well as aqueous ferrous iron and sulfate addition, it was hoped that the factors controlling degradation could be isolated and quantified.

A second objective was to develop a "decision tree" to assess which conditions were most effective for abiotic degradation following transition to passive groundwater flow conditions (i.e., which amendments led to the highest rates of sustained reduction of chlorinated contaminants.)

## Technical Approach

A matrix of experiments was conducted in large sand columns through which simulated groundwater was pumped. The columns, with groundwater flowing at ~10 cm/day, were allowed to run for a period of several months to establish steady-state conditions for each of the scenarios to be tested. Then a cocktail of chlorinated compounds (TCE, CT and 1,2,3-trichloropropane [TCP]) was continuously injected for a period of approximately two weeks to develop a steady-state concentration profile within the column. In these experiments the TCP was used as a conservative tracer, since it has proven to be very resistant to reduction under a wide variety of conditions. At the end of the contaminant injection period, the concentrations of each of the chlorinated compounds was analyzed in water samples from along the length of the column. Those concentrations became the initial conditions for follow-on experiments in which column flow was stopped to simulate the end of active pumping. During the stopped-flow period, samples were periodically collected from each of ports along the columns that had been sampled under flowing conditions. These experiments persisted for a period of ~3 months. During the project these "flowing-followed-by-stopped flow" experiments were conducted twice for each column over a 2-year period.

## Results and Discussion

Under flowing conditions (i.e., during the development of a steady-state concentration profile in the columns) TCE showed a consistent degradation rate for nearly all conditions tested, with the exception of the case where no carbon source (lactate) was added. Interestingly, no TCE degradation products were observed (e.g., DCE, VC, acetylene, ethane, ethane), except acetylene was observed in the case where no carbonate was added and the resulting pH was very low (~3.5). Even in that case, when the pH was increased in the column using PIPES buffer, TCE degradation persisted at more-or-less the same rate, but there was no longer acetylene accumulation. In these experiments, the use of TCP as a conservative tracer allowed us to demonstrate that volatilization or other losses were not occurring during the experiments.

CT degradation was observed at more-or-less consistent rates in 4 of 6 columns under flowing conditions. The two columns showing lower rates were the column without lactate (NL) and the column without carbonate addition (NC). For the NL column, CT degradation rates were lower by about a factor of three from the flowing case. The NC column showed a CT degradation rate about an order of magnitude lower during both sampling rounds.

Under non-flowing conditions, degradation rates for TCE dropped by about an order of magnitude relative to the flowing cases. For CT, the degradation rates were approximately the same as under flowing conditions for 4 of the 6 columns. For the NL column, CT degradation rates were somewhat complicated. In the first sampling round, when the pH was ~3.5, the rate was approximately 50 times slower than under flowing conditions. When the pH was increased during the second round, the CT rate increased to a value that was comparable to the rate during flowing conditions for that column, but which was still an order of magnitude less than the four columns receiving both lactate and carbonate.

The observed products from CT degradation included carbon monoxide (CO), chloroform (CF), and carbon disulfide (CS2), and were consistent for published data on abiotic CT degradation. The mass balance based on these products was in the range 25-55%.

Ferrous iron concentrations [Fe2+] generally decreased over the course of two years of column operation. During stopped-flow periods, there was accumulation of ferrous iron, which decreased when flow was re-initiated. However, [Fe2+] generally did not appear to correlate with degradation rates. In one column, ferrous iron was added at the ~100 uM (~5 mg/L) level, but it did not significantly affect either TCE or CT degradation rates.

For four of the six columns tested, lactate degradation occurred along the full length of the column with a first-order half-life on the order of 2-5 days. Based on the primary reaction products, propionate and acetate, the primary pathway for lactate degradation appears to have been fermentation.

It was anticipated that the addition of sulfate, and the observed production of iron sulfide precipitates in the column, would lead to increased degradation rates in sulfate column (S2) relative to an identical column without sulfate (M2). While there may have been a slightly higher rates in the sulfate column, they were not significantly different.

## Summary and Conclusions

The data from these experiments suggests, not surprisingly, that a labile carbon source probably represents the single most important factor controlling chlorinated solvent degradation for the

systems studied here. This is likely the case for three reasons: 1) the carbon represents an energy source for active microbial communities; 2) it facilitates the biological removal of any available oxygen in the system through aerobic microbial reactions; and 3) the ongoing microbial reactions likely result in the production of more-reduced surfaces (possibly including the production of reactive phases) which support abiotic reduction.

Very low pH values also impacted reduction rates. Given that carbonate is a ubiquitous component of groundwater, and pH values are more-commonly circumneutral, systems without carbonate are likely to be unusual in natural settings.

The presence of the mineral magnetite is considered by some to be an important contributor to abiotic natural attenuation. Likewise, the in situ formation of iron sulfides is often considered indicative of a site where abiotic degradation is likely. In these experiments, neither magnetite added to some of the columns, nor iron sulfide formed in one of the columns had a significant effect on either TCE of CT degradation rates.

Ferrous iron is also widely considered to be an important component for abiotic reduction. In these columns initially there was significant dissolved ferrous iron coming from the silica sand used in the columns. Over the course of the experiments the ferrous iron in solution decreased significantly, and by the conclusions of the experiments there was essentially no [Fe2+] in solution. However, the degradation rates for both TCE and CT did not decrease significantly during that time, and in fact generally increased slightly.

One of the goals of this project has been to development a decision tree to explore the factors controlling degradation under groundwater conditions. However, the results of these experiments do not lend themselves will to a decision tree approach. For TCE, degradation rates were consistent across all conditions tested, with the exception of lactate addition. For CT, both lactate addition and carbonate addition had a significant impact on degradation rate, and for CT a decision tree was constructed. It was anticipated that the effects of sulfate and magnetite additions would also impact degradation rates; however, that proved not to be the case, and as a consequence they did not contribute to the decision tree.

A second goal of the project was to examine the impacts of changes in groundwater flow on degradation rates. In this case, significant reductions in TCE degradation rate were observed when flow was stopped. Significantly less reduction was observed for CT in most columns; however, the NL and NC columns showed nearly a 2-order of magnitude reduction in CT rate during stopped flow. The reduction in observed rate during stopped flow has potentially-significant implications for in situ restoration of groundwater following the transition from active to passive site management. However, differences in the behavior of TCE and CT during the transition in the columns suggest that behavior is complicated and that more than one mechanism might be in effect.

## Implications for Future Research and Benefits

As mentioned above, the data generated in this project are being used to inform a companion project (ER20-1357). This has taken place throughout the lifetime of the two projects via joint team meetings. A focus of the companion project is the examination of the rates of dechlorination due to specific mineral phases, and the intent is that the combined projects will provide a clearer picture of the complicated suite of biotic and abiotic processes contributing to chlorinated solvent degradation in the subsurface.

# 3. Objectives

The primary objectives of this project was to develop a data set that could be used in a companion project (ER20-1357) to build a reactive transport model that effectively addressed the contribution of abiotic reduction of chlorinated solvents. To accomplish this, a matrix of realistic groundwater scenarios was tested, including the addition of materials that have been reported to enhance abiotic degradation (e.g., magnetite, sulfate, ferrous iron, lactate). By conducting a matrix of experiments varying carbon source (lactate), carbonate concentration, magnetite mineral addition, as well as aqueous ferrous iron and sulfate addition, it was hoped that the factors controlling degradation could be isolated and quantified.

# 4. Background

## Problem statement

An important strategy for in situ restoration of groundwater contaminated by chlorinated solvents is the active development of reducing conditions to enhance dechlorination via biotic or abiotic means. This can be accomplished by emplacement of reducing materials (e.g., ZVI, edible oil) or active pumping of reductants (e.g., sulfate, nano-materials, labile carbon source)

For the actively pumped restoration activities, there is significant uncertainty regarding how long the enhanced reduction will persist once the site has been returned to more-passive conditions (i.e., active-to-passive transition). If, during active treatment, a reservoir of reactive reduced species is produced (e.g., precipitation of reactive minerals), then the potential exists that those minerals will continue to reduce contaminants well after active treatment has ended. However, if the reactive species are short-lived, then the impact on groundwater restoration may be short-lived as well.

## Choice of chlorinated compounds for the study

Both trichloroethene (TCE) and carbon tetrachloride (CT) are important groundwater contaminants. In addition, their degradation pathways have been extensively studied under a wide range of biotic and abiotic conditions. We have previously used both compounds in batch and columns studies (Johnson and Tratnyek, 2020)

TCE is known to degrade by abiotic pathways (e.g., Butler and Hayes (1999), Culpepper et al. (2018), Hyun and Hayes 2009, Lee and Batchelor (2004). Shao and Butler (2009) reported that CT degradation occurred primarily by abiotic pathways. A large number of other researchers, including Amonette et al. (2000), Danielson and Hayes (2004), Devlin and Muller (1999), Elsner et al. (2004) Kenneke and Weber (2009) have looked at abiotic CT degradation under a variety of conditions.

The data for both TCE and CT degradation in the presence of a variety of mineral phases (e.g., FeS, $FeS_2$, zero-valent iron, magnetite, green rust) have been summarized by He et al. (2015). These references have been used to develop the simple sequential first order reaction schemes that are presented below.

# 5. Materials and Methods

## Experimental approach

The range of experimental conditions used in these column experiments (i.e., addition of magnetite, Fe2+, lactate, sulfate, carbonate) are shown in matrix form in Table 1. Each of the columns was allowed to run for a period of several months to establish steady-state conditions (this was achieved for some, but not all parameters). The next step was to continuously inject a cocktail of chlorinated compounds (TCE, CT and 1,2,3-trichloropropane, TCP) for a period of approximately two weeks to develop a steady-state concentration profile within the column. At the end of that period, the concentrations of each of the chlorinated compounds was analyzed in water collected from a series of sampling points along the length of the column.

*Table 1. Matrix of column conditions used the experiments*

| Name / Added | magnetite | sulfate | carbonate | lactate | $Fe^{2+}$ |
|---|---|---|---|---|---|
| NM | | | X | X | |
| NMFe | | | X | X | X |
| M2 | X | | X | X | |
| S2 | X | X | X | X | |
| NL | X | | X | | |
| NC | X | | | X | |

(Note: A seventh column was initially used; however, the conditions tested (no lactate, Fe2+ addition) resulted in the precipitation of iron at the inlet to the column and it plugged.)

## Modeling of TCE and CT Degradation

The analytical data from the flowing and non-flowing experiments examined here were modeled using the following first-order rate expressions:

$$d[TCE]/dt = -kTCE*[TCE] \quad \text{[Eqn 1]}$$
$$d[Acet]/dt = kTCE*yAcet*[TCE]-kAcet*[Acet] \quad \text{[Eqn 2]}$$
$$d[CT]/dt = -kCT*[CT] \quad \text{[Eqn 3]}$$
$$d[CF]/dt = kCT*yCF*[CT]-kCF*[CF] \quad \text{[Eqn 4]}$$
$$d[CS2]/dt = -kCT*yCS2*[CT]-kCS2*[CS2] \quad \text{[Eqn 5]}$$

where:

[TCE] = trichloroethene concentration
[Acet] = acetylene concentration
[CT] = carbon tetrachloride concentration

[CF] = chloroform concentration
[CS2] = carbon disulfide concentration
kTCE =total TCE degradation rate constant
kAcet =acetylene degradation rate constant
kCT = carbon tetrachloride degradation rate constant
kCF = chloroform degradation rate constant
kCS2 = carbon disulfide degradation rate constant
yAcet = acetylene yield from TCE degradation
yCF = chloroform yield from CT degradation
yCS2 = carbon disulfide yield from CT degradation

## Lactate Metabolism

In these experiments, lactate was used as the carbon source. Under anoxic conditions it undergoes a fermentation reaction defined by Eqn 6. The propionate produced by this reaction can react to form acetate, with the production of 3 moles of hydrogen. The hydrogen produced by this reaction can be used by a wide variety of anaerobic organisms. Eqn 7 is energetically unfavorable and relies on the consumption of hydrogen to facilitate the production of acetate (i.e., a community of hydrogen utilizers is needed to facilitate this reaction.)

$$3\ CH_3CHOHCOO^- \rightarrow CH_3COO^- + 2CH_3CH_2COO^- + CO_2 + H_2O \qquad \text{[Eqn 6]}$$

$$CH_3CH_2COO^- + 3\ H_2O \leftrightarrow CH_3COO^- + H^+ + 3\ H_2 + HCO_3^- \qquad \text{[Eqn 7]}$$

## Column setup

Figure 1 shows the basic layout of the column systems. Briefly, water containing lactate and/or carbonate flows by gravity from a carboy through a sparging tower to remove all dissolved oxygen. The water is then pumped through the column in an up-flow configuration. Effluent from the column flows to a container mounted on an electronic balance. Output from the balance goes to a computer which both measures the accumulation of flow in the container and controls operation of the pump in order to stop flow if problems with the column (e.g., leaks or overflows) are detected by deviation in the rate of accumulation of water in the container.

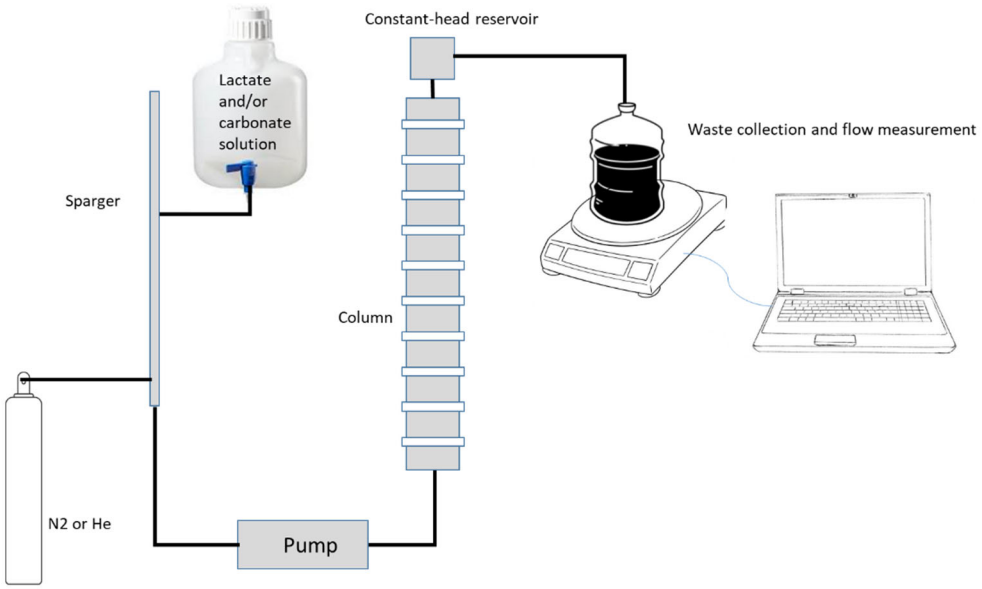


*Figure 1. Basic layout of the column experiments.*

Figure 2 shows the modification of the basic flow system used to deliver sulfate to the column. In this case, a concentrated sulfate solution is pumped from a reservoir at a slow rate (~2% of total flow).

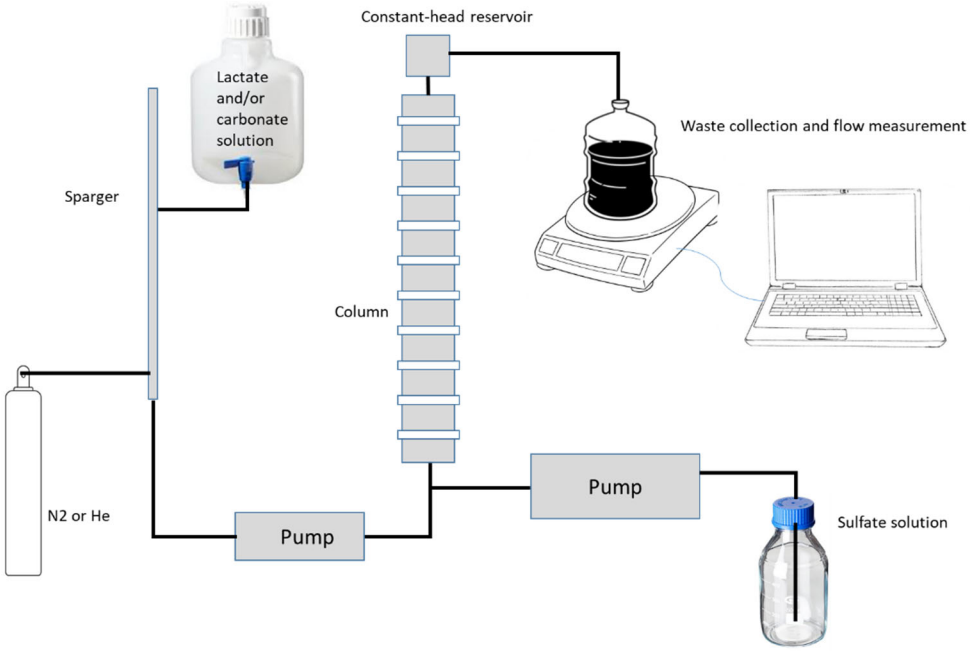


*Figure 2. Flow system used for injection of sulfate into the column.*

Figure 3 shows modification to the basic flow system for the injection of reactive species, including ferrous iron and volatile chlorinated compounds. This modification is necessary because a significant fraction of these compounds are lost in the pump head. For ferrous iron injection, the [Fe2+] concentration in the reservoir is maintained by regular injection of a ferrous iron stock solution into the bottle. In addition, a quantity of zero-valent iron was placed in the reservoir to act as an oxygen scavenger.

For injection of the volatile chlorinated compounds (TCE, CT and TCP), a non-aqueous phase containing all three chemicals is maintained in the reservoir and the reservoir was continuously stirred to maintain a uniform concentration throughout the bottle. As shown in the figure, water flowing into the reservoir is directed to the bottom of the reservoir and withdrawn from the top. There is no gaseous headspace either the [Fe2+] or chlorinated solvents bottles.

Each of the 10 white rings on the column contains a sampling port.

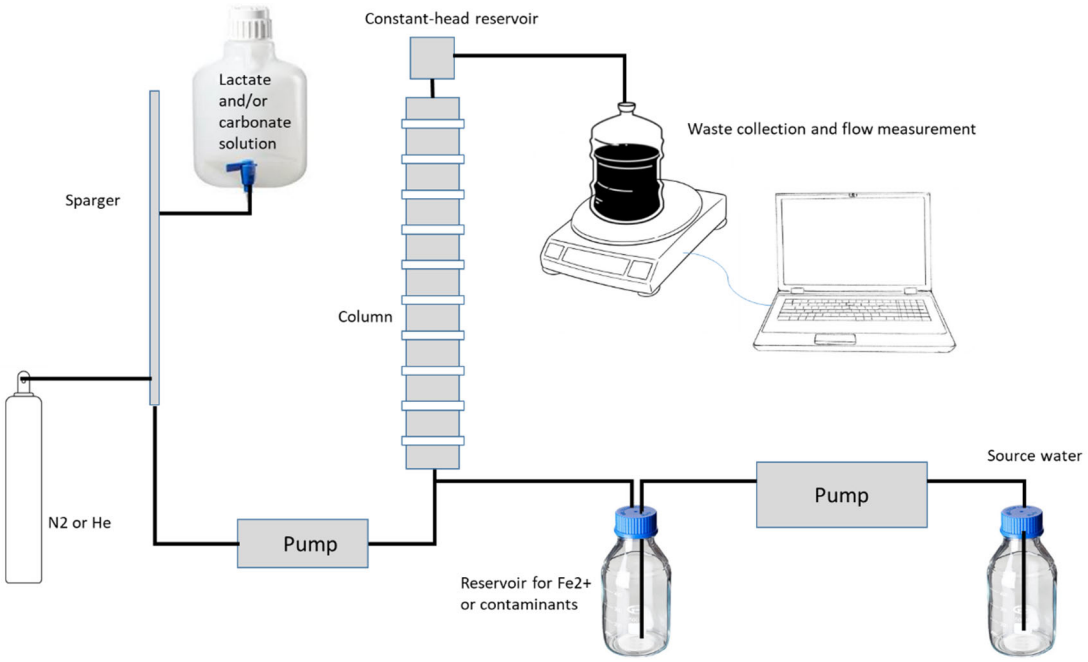


*Figure 3. Flow system used for the injection of ferrous iron and chlorinated compounds.*

The photograph in Figure 4 shows a general overview of all the components of the flow systems. The carboys are located in the upper portion of the photograph. Water collection containers and analytical balances for each column and the computer control system are on the lower shelf behind the columns

Pumps necessary for each configuration (basic flow, sulfate injection, ferrous iron injection, chlorinated solvent injection) are on the lab bench behind and alongside the columns.

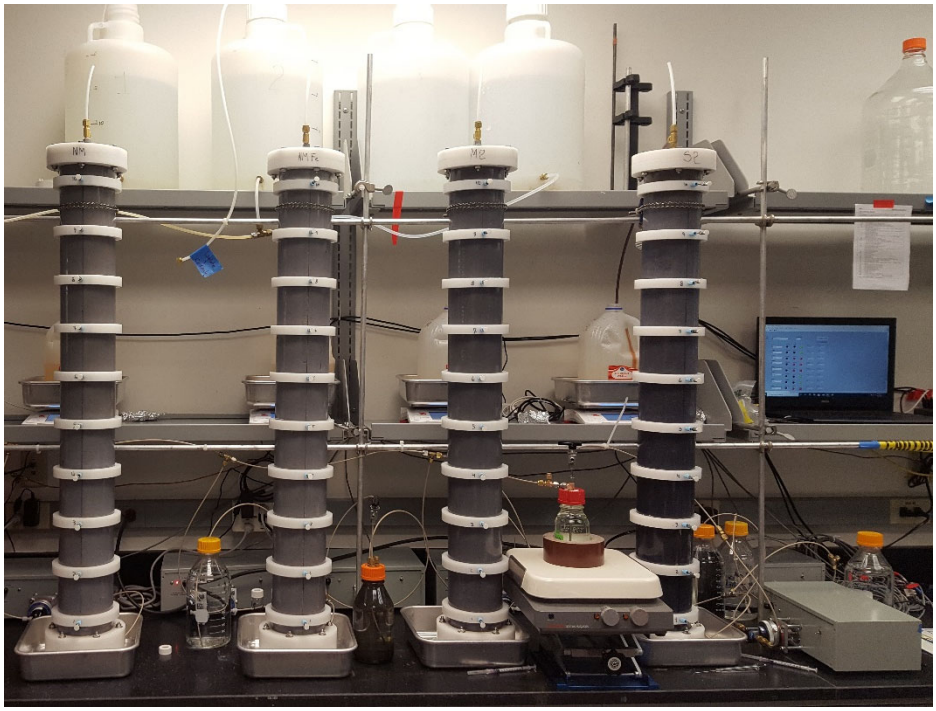

*Figure 4. Overview photograph of the columns.*

Figure 5 shows a close-up of the different injection configurations used in the experiments.

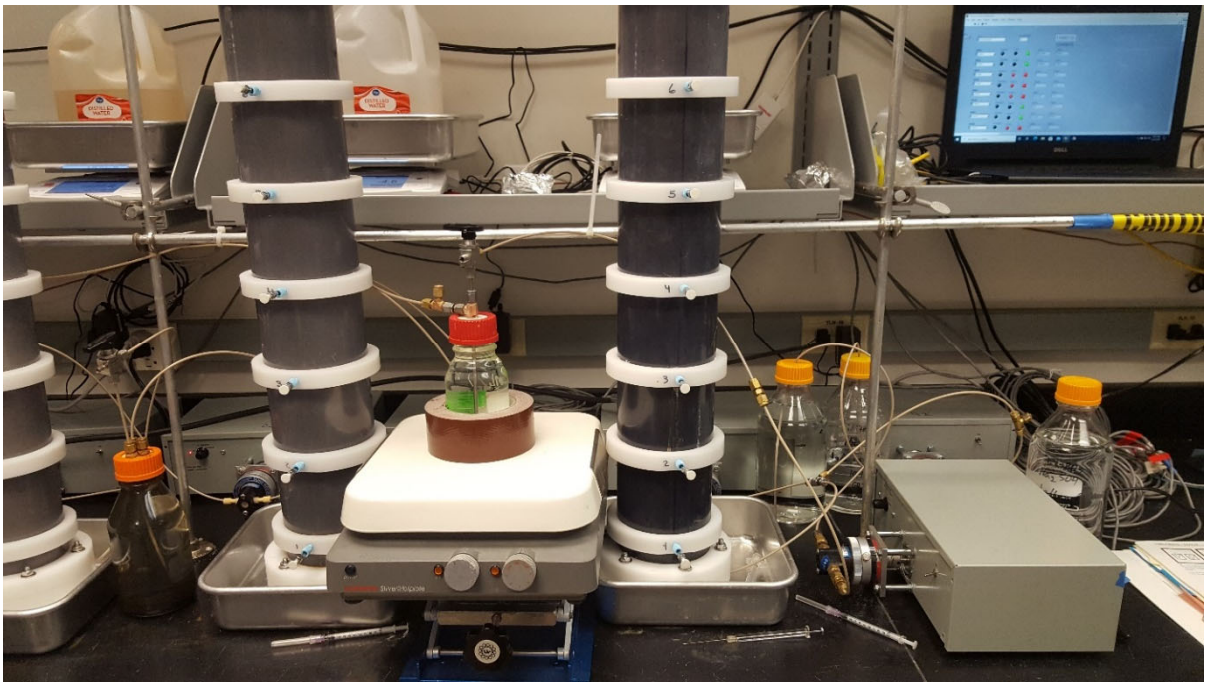

*Figure 5. Photograph showing detail of the injection system configurations*

The bottle in the lower right of Figure 5 contains ferrous iron and zero-valent iron. The bottle in the center on the stir plate contains the non-aqueous phase liquid mixture of TCE, CT, and TCP. The bottle on the far right is the sulfate stock solution and the bottles to the left of that are the sulfate injection source and the feed water for the chlorinated solvent injection pump.

*Figure 6. Close-up photograph of the sparging tower.*

Figure 6 shows a close-up photograph of the sparging tower used to remove oxygen from the feed water. Both nitrogen and helium were used as the sparge gas.

## Column operation

For all columns a nominal pumping rate of 0.5 mL per minute was maintained using the main ceramic piston pump for each column. Other injection pumps (for sulfate, ferrous iron and chlorinated solvents) were maintained at approximately 0.01 mL/min.

The dimensions of the columns were ~100 cm in length and 10 cm in diameter. This results in a total volume of approximately 8000 $cm^3$. The porosity of the columns was approximately 0.4, for a total pore volume of ~3200 $cm^3$. The daily flow was approximately 720 mL, which gives a residence time of approximately 4.5 days.

*Table 2. Nominal influent concentrations.*

| Influent species | Concentration |
|---|---|
| Lactate | 0.5 mM |
| Bicarbonate | 1 mM |
| pH | 7.2 |
| Sulfate | 0.2 mM |
| Ferrous iron | 0.15 mM |
| TCE | 1.35 µM |
| CT | 0.75 µM |
| TCP | 4.60 µM |
| PIPES Buffer | 10 mM |

Measurement of flow through each column was accomplished by measuring the increase in mass of water collected from each column. Effluent from each column flowed into a 4-L container resting on an analytical balance. The analytical balance regularly sent the total mass of water to an attached computer controlled by Labview™ software. The rate of change of water mass gives a direct measure of flow rate. If a decrease in the rate of water accumulation was detected in any of the columns, the computer has the ability to turn off individual pumps associated with each column.

## Contaminant Degradation Experiments

Near the middle of the project period, and again near the end of the project, experiments were conducted in which chlorinated compounds were continuously injected along with the groundwater into each column. Typically, this would occur for a period of a few weeks, during which samples were collected and analyzed, as discussed below.

When a quasi-steady state concentration distribution had been achieved, column flow was stopped and a regular sampling regimen was initiated. Samples collected immediately after flow stoppage were used as the "time zero" concentrations for each port. Sampling under stopped-flow conditions persisted for a period of approximately 1500 hours (~60 days).

## Column Sampling and Analysis

Each column has 10 sampling ports spaced equidistant down the column. Each sampling post consists of a 16-gage stainless steel hypodermic needle sealed into the wall of the column. The inlet to the needle is screened and positioned near the center of the column. The needle is sealed at the outside of the column with a ferrule and nut (Upchurch Scientific). The hub of the needle is sealed with a Luer plug, which is temporarily removed during sampling.

During sampling, approximately 0.5 mL is allowed to flow out of the needle before a syringe is placed on the needle to extract the sample. A range of water chemistry measurements are routinely made on water samples collected from the column. These include ferrous iron, sulfate, sulfide, and pH.

**Ferrous iron**

A one- or two-milliliter sample was collected for ferrous iron analysis (depending on expected concentration). Each sample was analyzed spectrophotometrically using the Hach™ ferrous iron method (Method 8146). In all cases, samples were filtered through a 0.45 µm filter prior to analysis.

**Sulfate**

A 10-milliliter sample was collected for sulfate analysis. Each sample was analyzed spectrophotometrically using the Hach™ sulfate method (Method 8051). In all cases, samples were filtered prior to analysis.

**Sulfide**

A two- or five-milliliter sample was collected for sulfide analysis (depending on expected concentration). Each sample was analyzed spectrophotometrically using the Hach™ sulfide method (Method 8131). In all cases, samples were filtered prior to analysis.

**pH**

Approximately seven milliliters were collected for pH analysis. Each sample was analyzed with a Vernier combination pH electrode connected to an Orion 720A meter. The electrode was calibrated daily with two standards of pH 7.0 and 10.0.

**Lactate**

Liquid samples (1 mL) were passed through 0.2 µm filters and organic acids (lactate, acetate, propionate, and butyrate) were analyzed by ion chromatography (Dionex ICS-2100), consisting of an AS-11 column (250 × 4 mm) with an AG11 guard column.

**DNA concentrations**

Water samples for DNA analysis were collected and immediately frozen at -80C. For analysis the samples thawed and filtered to collect DNA. DNA was extracted from liquid column samples (2 mL) using a modified protocol involving the Qiagen PowerWater Sterivex kit. Sequencing of 16S rRNA gene amplicons from column DNA extract was performed externally at MR DNA (Shallowwater, TX).

**Chlorinated compounds and degradation products**

Contaminants (TCE and CT) and possible relevant degradation products are listed below in Table 3.

*Table 3. List of target analytes for the GC/MSD/FID analyses*

| MSD | FID |
|---|---|
| Carbon disulfide | Carbon Monoxide |
| Vinyl chloride | Carbon Dioxide |
| cis-1,2-DCE | Methane |
| trans-1,2-DCE | Ethane |
| 1,1,2-Trichloroethene | Ethene |
| Carbon tetrachloride | Acetylene |
| Chloroform | |
| Dichloromethane | |

As part of the analysis of each sampling event, an external standard composed of all of the compounds listed in Table 3 was prepared from an aqueous stock solution and two gas mixtures. The external standard included 1,2,3-trichloropropane, the internal standard included in each of the column experiments.

Each batch of headspace samples included a blank and the external standard and, typically, five samples from one column. The samples were analyzed on a custom-designed automated headspace analyzer composed of an Agilent 6890 GC, and Agilent 6971A MSD, and a PAL robotic auto-sampler. The flow diagram for the analysis system is shown in Figure 7.

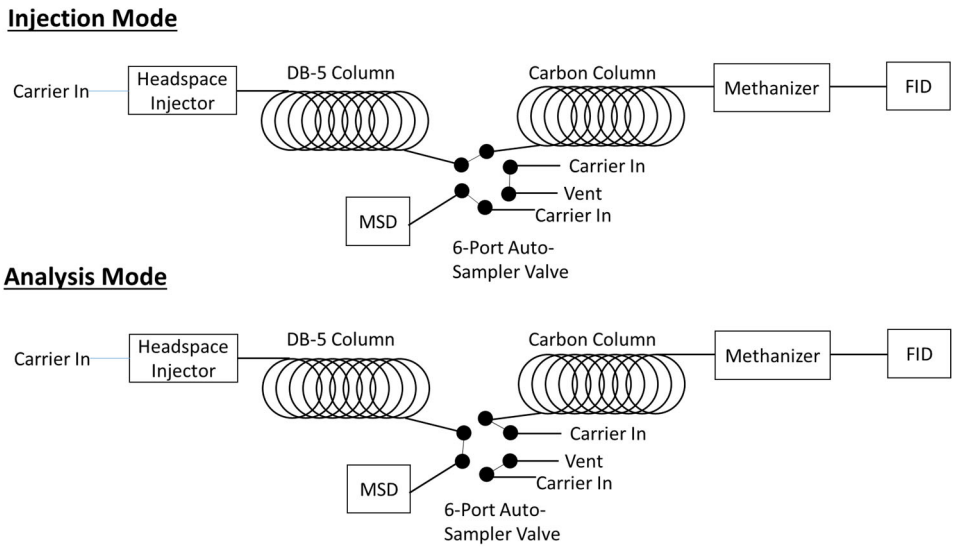


*Figure 7. Schematic flow diagram for the GC/MSD/FID system.*

# 6. Results

All of the analytical data collected in this project are located in the appendices at the end of the report and graphical summaries of those data are presented in this section. The results reported here include ferrous iron, sulfate/sulfide, pH, lactate and its degradation products, and chlorinated compounds and their degradation products.

## Ferrous Iron Concentrations

Timeseries results for ferrous iron concentrations in each of the six columns is shown in Figures 8-10

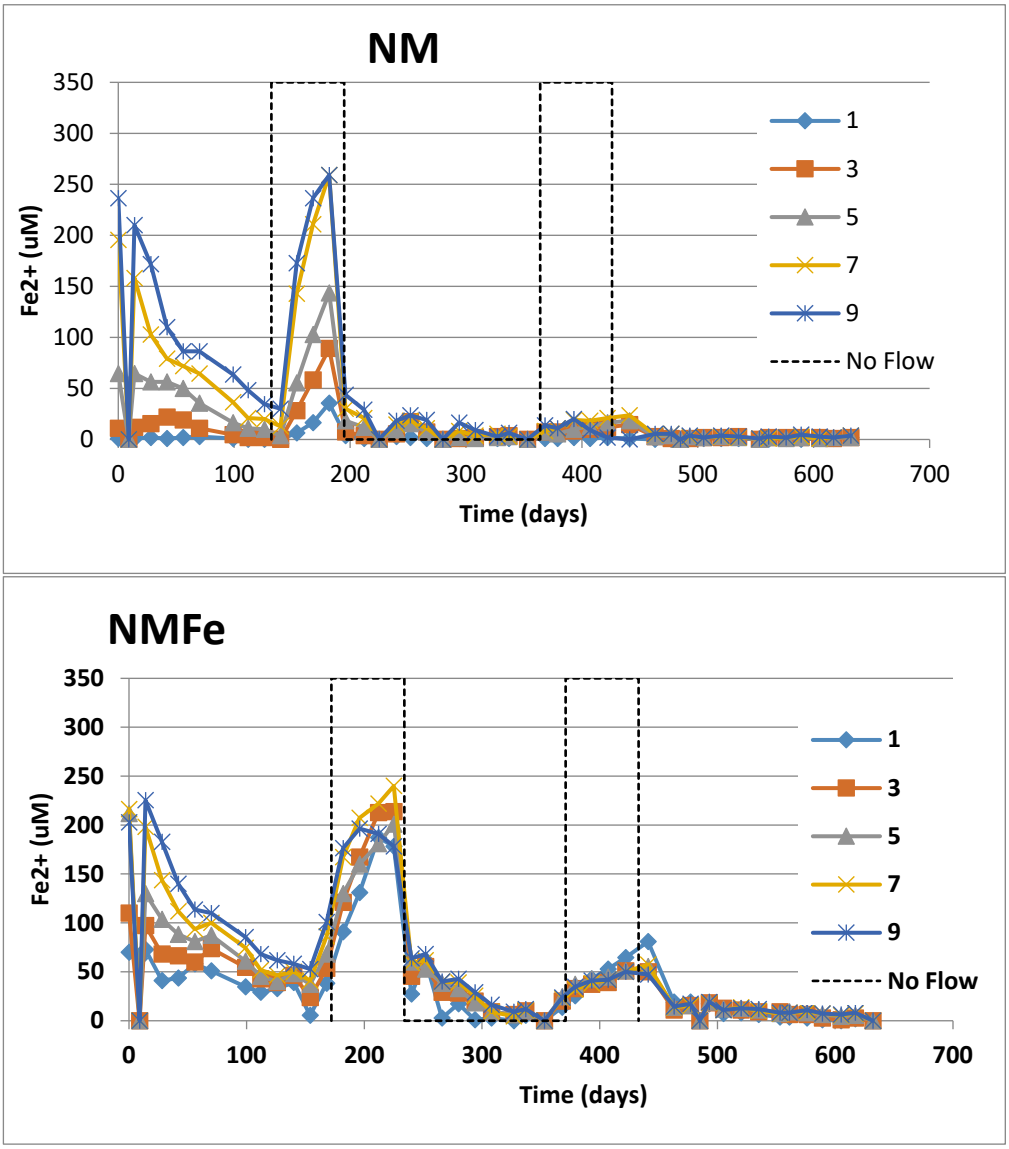


*Figure 8. Measured ferrous iron concentrations in columns NM and NMFe.*

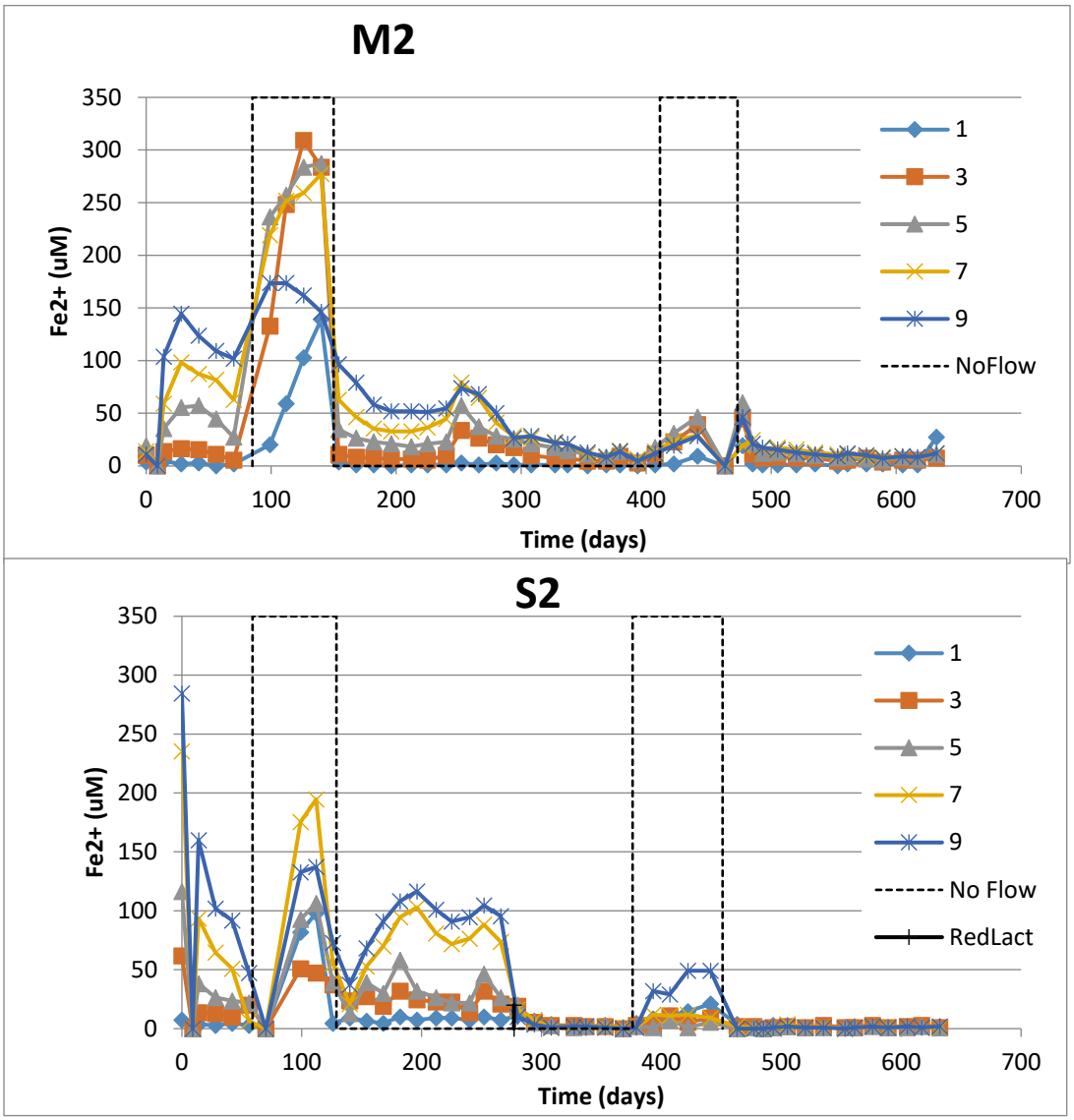


*Figure 9. Measured ferrous iron concentrations in columns M2 and S2.*

In all cases except the NL column, initial ferrous concentrations throughout much of the columns were initially in the 100-300 µM range. Influent concentrations were generally low, except in the case where ferrous iron was added to the column (NMFe, Figure 8)

Ferrous iron concentrations in the NL column were generally below detection limits. This is likely because there was no biological activity in the column and, as a consequence, conditions were not reducing enough

In all cases except NL, when flow was stopped (times between pairs of dashed vertical lines), the ferrous iron concentration rose over time and then dropped again when flow resumed.

As discussed briefly below, at day 275 the pH of the influent water for column NC was buffered and the column pH went from ~3 to ~7. As a result, the ferrous iron concentrations in this column dropped below detection limits and stayed low for the remainder of the experiment.

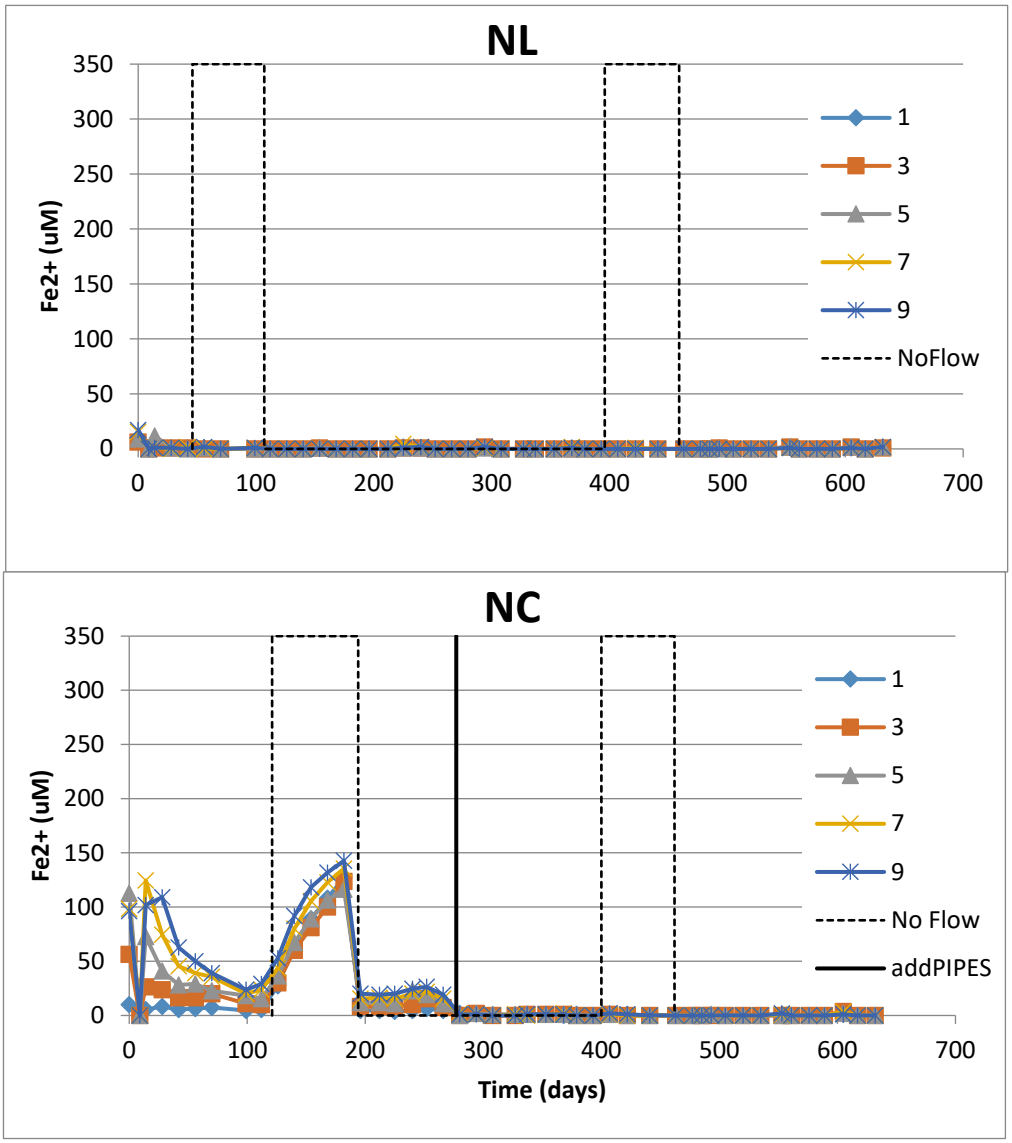


*Figure 10. Measured ferrous iron concentrations in columns NL and NC*

## Sulfate and Sulfide Concentrations

As shown in Figure 11, in general terms, sulfate entering the S2 column was consumed during the ~5 days of transport across the column. There was some variation in the rate, depending on the specific timeframe (i.e., at later times the rate of sulfate reduction increased in the column)

Correspondingly, there was detectable sulfide in aqueous samples that corresponds to about 20% of the total sulfate added to the column (i.e., ~80% appears to have precipitated and been retained on the column.) This was supported by the growth of visible black precipitate down the column over time.

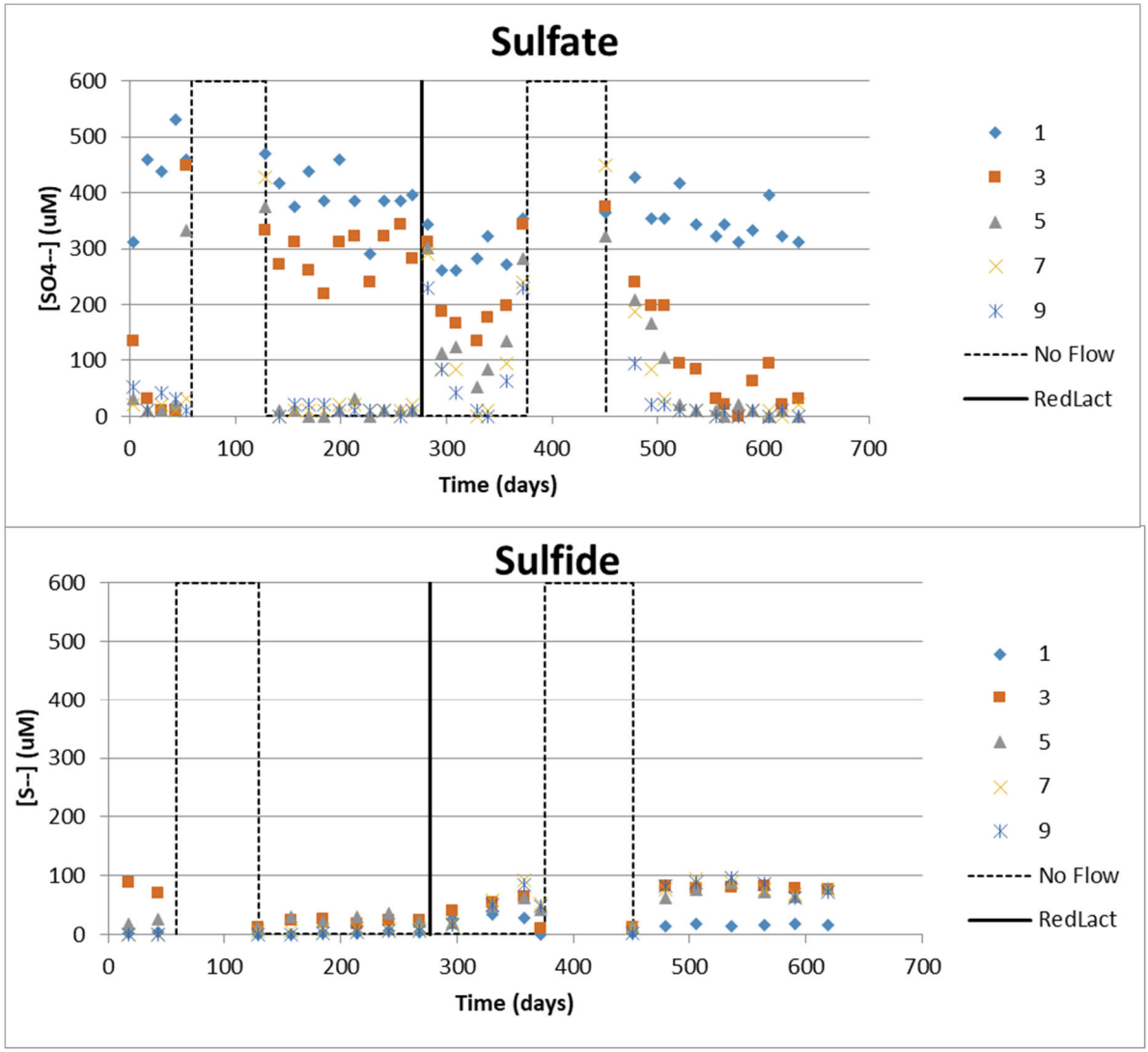


*Figure 11. Measured concentrations of sulfate and sulfide in column S2.*

## pH Data

All of the pH data for the experiments is found in Appendix E. For the NM, NMFe, M2 and S2 columns, the pH time-series data are relatively consistent. For those columns, Port 1 was slightly higher pH than the other ports. This is likely due to different reactions occurring at the entrance to the column (e.g., any oxygen in the influent would have been quickly consumed in this region, where as the rest of the length of the column was strictly anaerobic.) In general, the pH dropped slightly over the duration of the experiments. This could have resulted from changes in experimental procedure, although the reason for the drop is not clear.

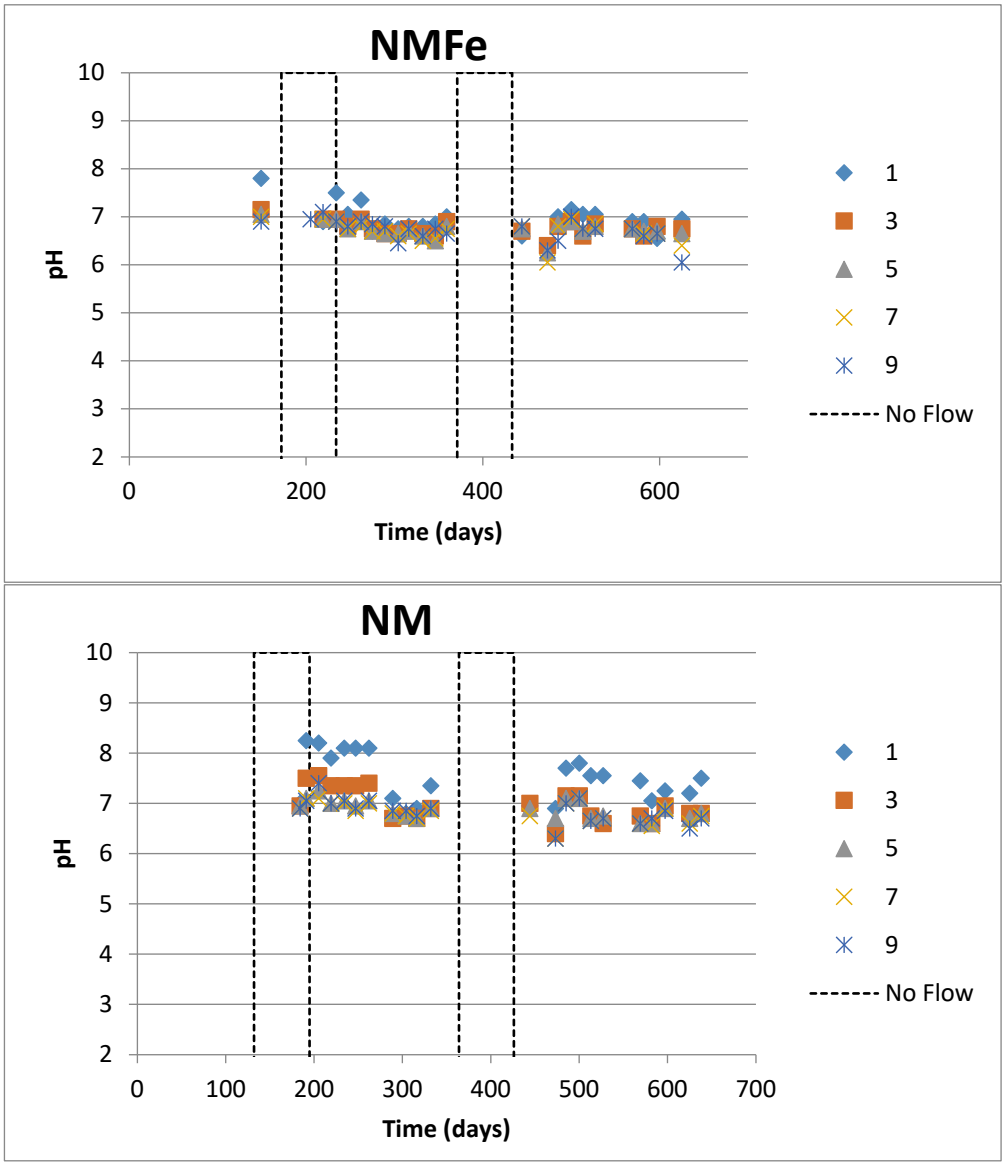


*Figure 12. Measured pH in columns NM and NMFe.*

The data from four of the columns (NM, NMFe, M2, and S2) indicate that carbonate provided adequate buffering capacity for the system. For the no lactate column (NL, Figure 14), the pH is higher than was expected, and the reason for this is unclear..

The column without carbonate (NC, Figure 14) had a very low pH during the first half of the experimental period. At day 275 the system was buffered with PIPES buffer for the remainder of the experiments.

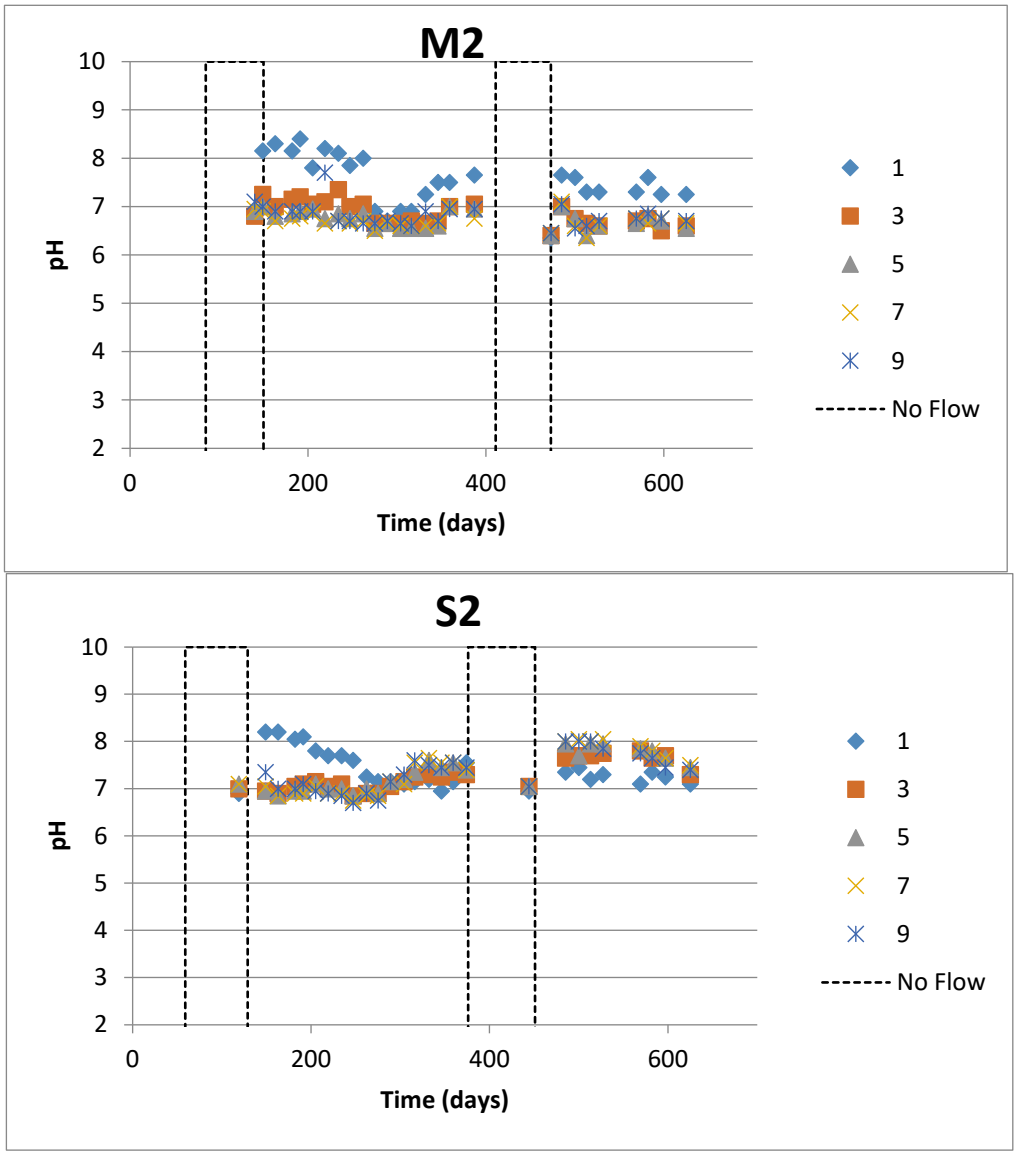


*Figure 13 . Measured pH in columns M2 and S2.*

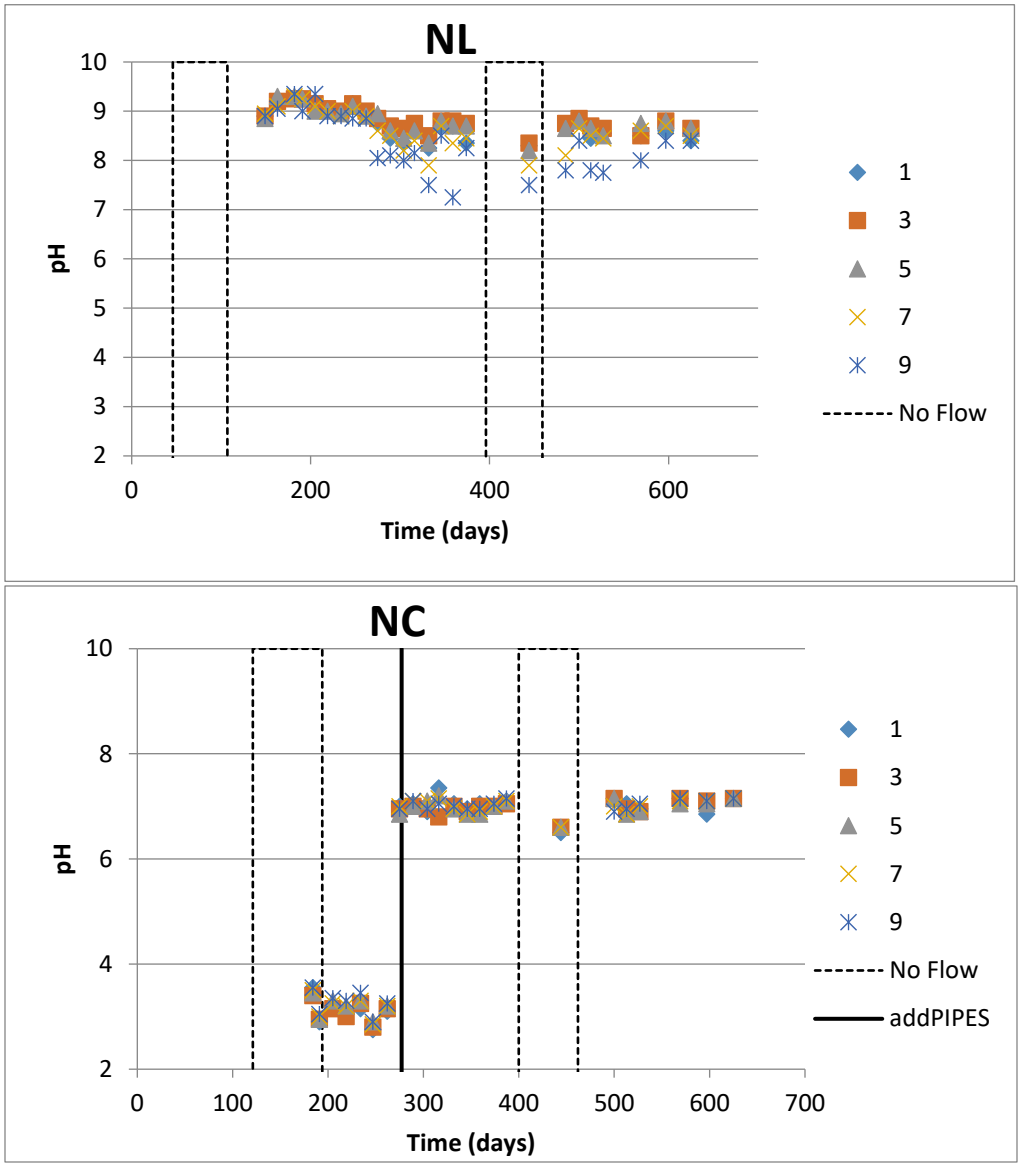


*Figure 14. . Measured pH in columns NL and NC.*

## Lactate and other Volatile Fatty Acid Concentrations

All of the volatile fatty acid data are found in Appendix F. Following the first round of stopped-flow sampling (~day 250), the columns (except NMFe) were sampled for lactate and other volatile fatty acid concentrations and the data are shown in Figures 15-17.

Degradation rates are fairly consistent along the lengths of columns NM, M2 and S2, with the majority of the lactate being degraded during the ~5 days of transport across the column.

The NL column data (Figure 17) show no VFAs, as expected, because no lactate was added. The NC column shows no degradation of lactate, nor accumulation of reaction products. Presumably this is due to the initial low pH of the column. (pH ~ 3 at the time when sampling was conducted).

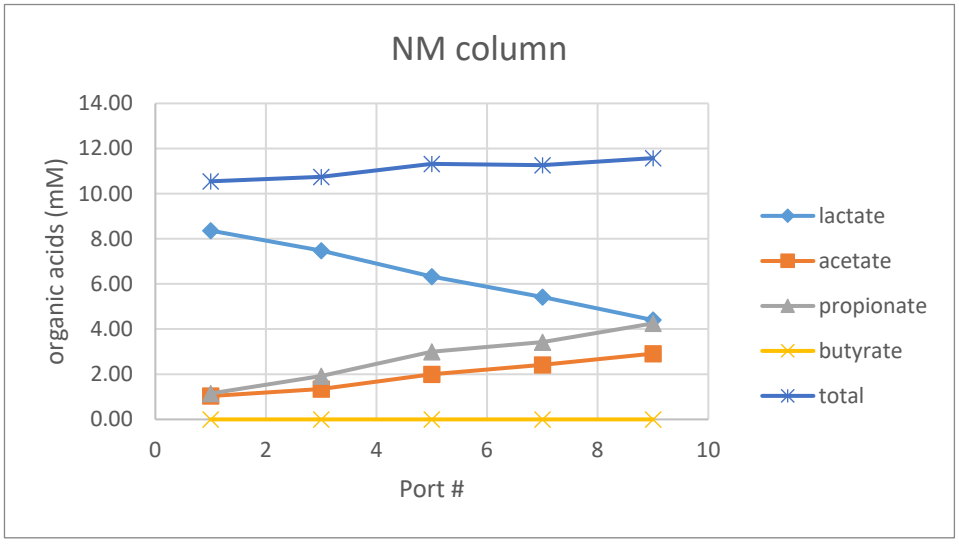


*Figure 15. Volatile fatty acid concentrations in the NM column.*

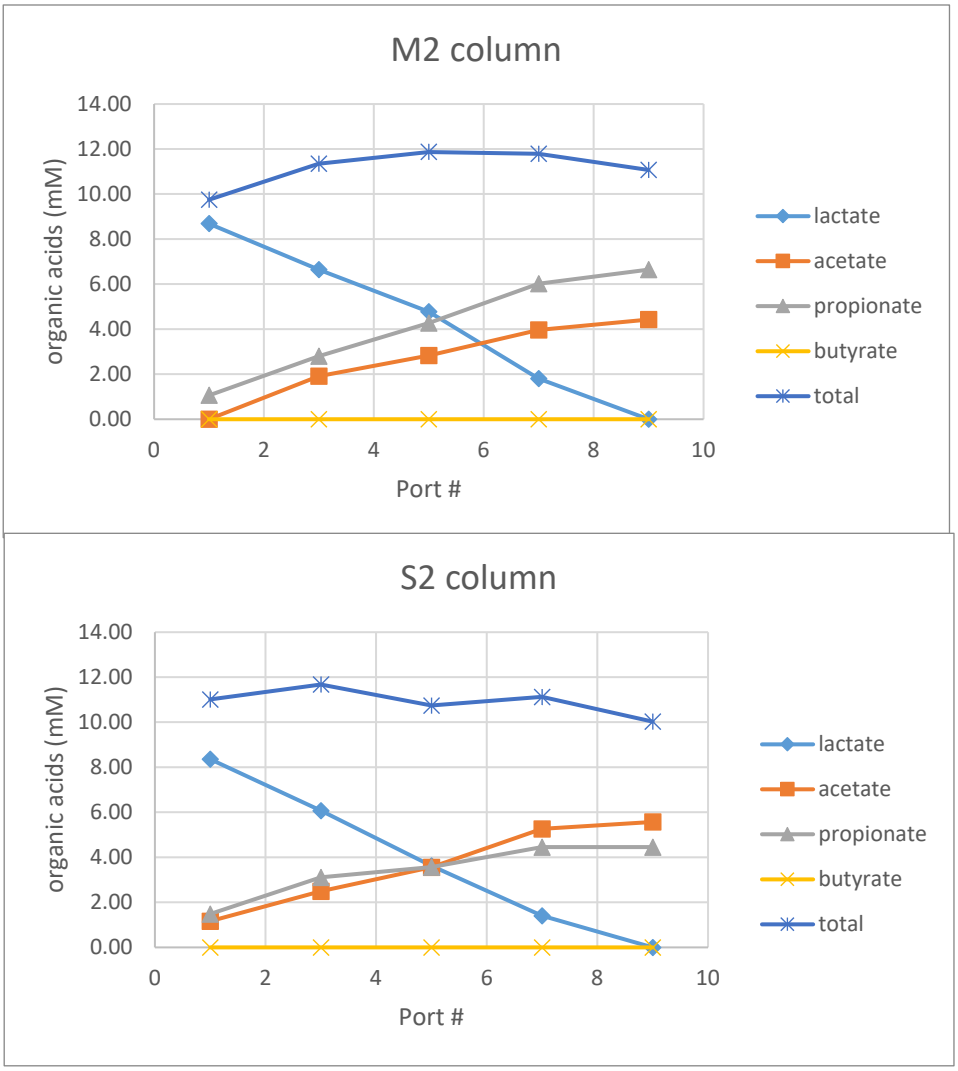


*Figure 16. Measured volatile fatty acid concentrations in columns M2 and S2.*

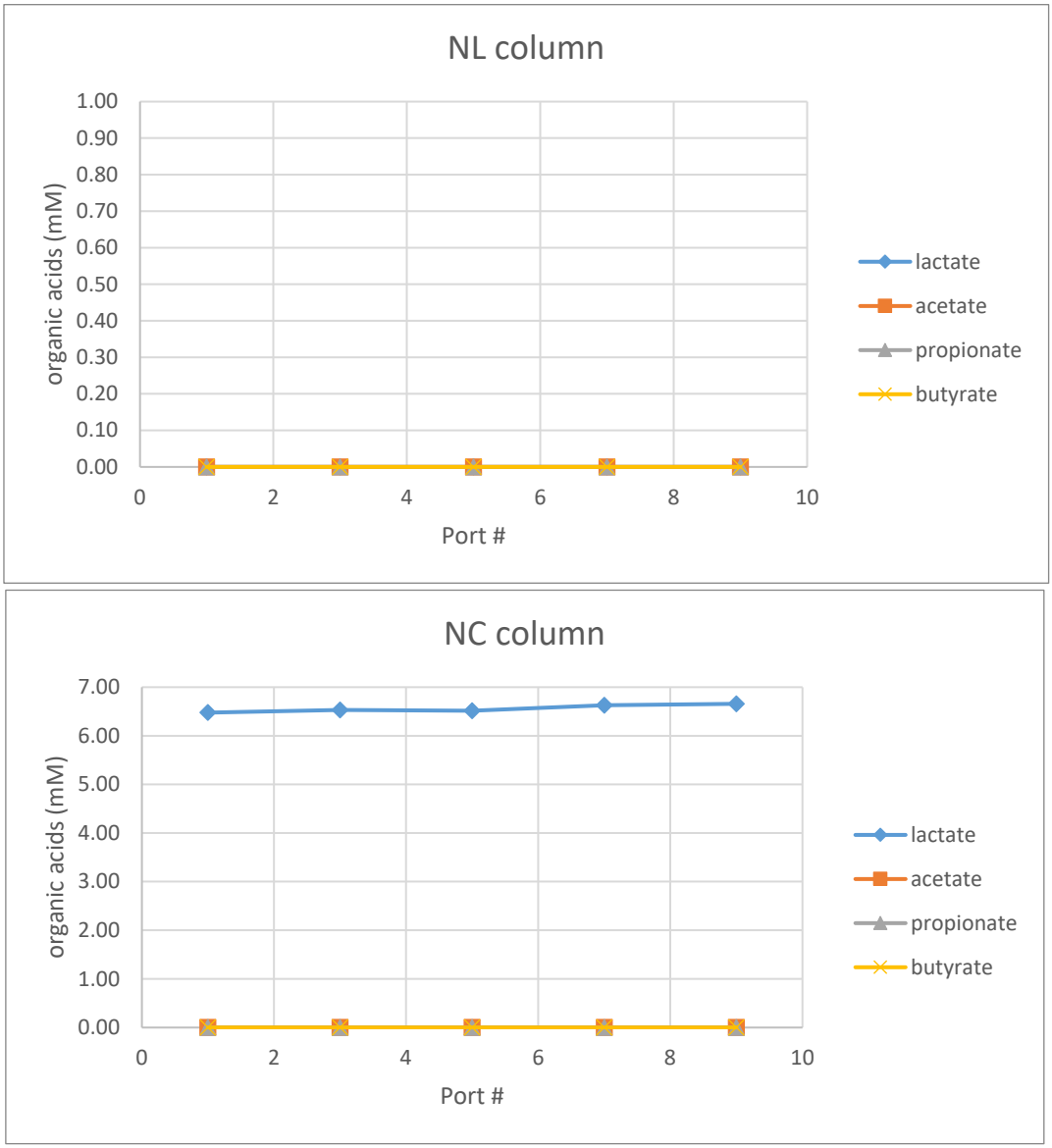


*Figure 17. Measured volatile fatty acid concentrations in columns NL and NC.*

## Chlorinated compound degradation under flowing conditions

As described in the experimental section, during two intervals for each column contaminants were continuously injected for approximately an approximate two-week period to establish steady concentrations at each sampled port along the column. At the conclusion of that period flow through the column was stopped and samples from each port were analyzed and used to determine the overall degradation rate constant for TCE and CT during flowing conditions.

The analytical data for TCE and CT for each column are located in Appendices G and H.

Examples of the data are shown as points in Figure 18 (Port 1 data from the M2 and S2 columns). Dashed lines in these figures are modeling results, which are discussed in Section 4, below.

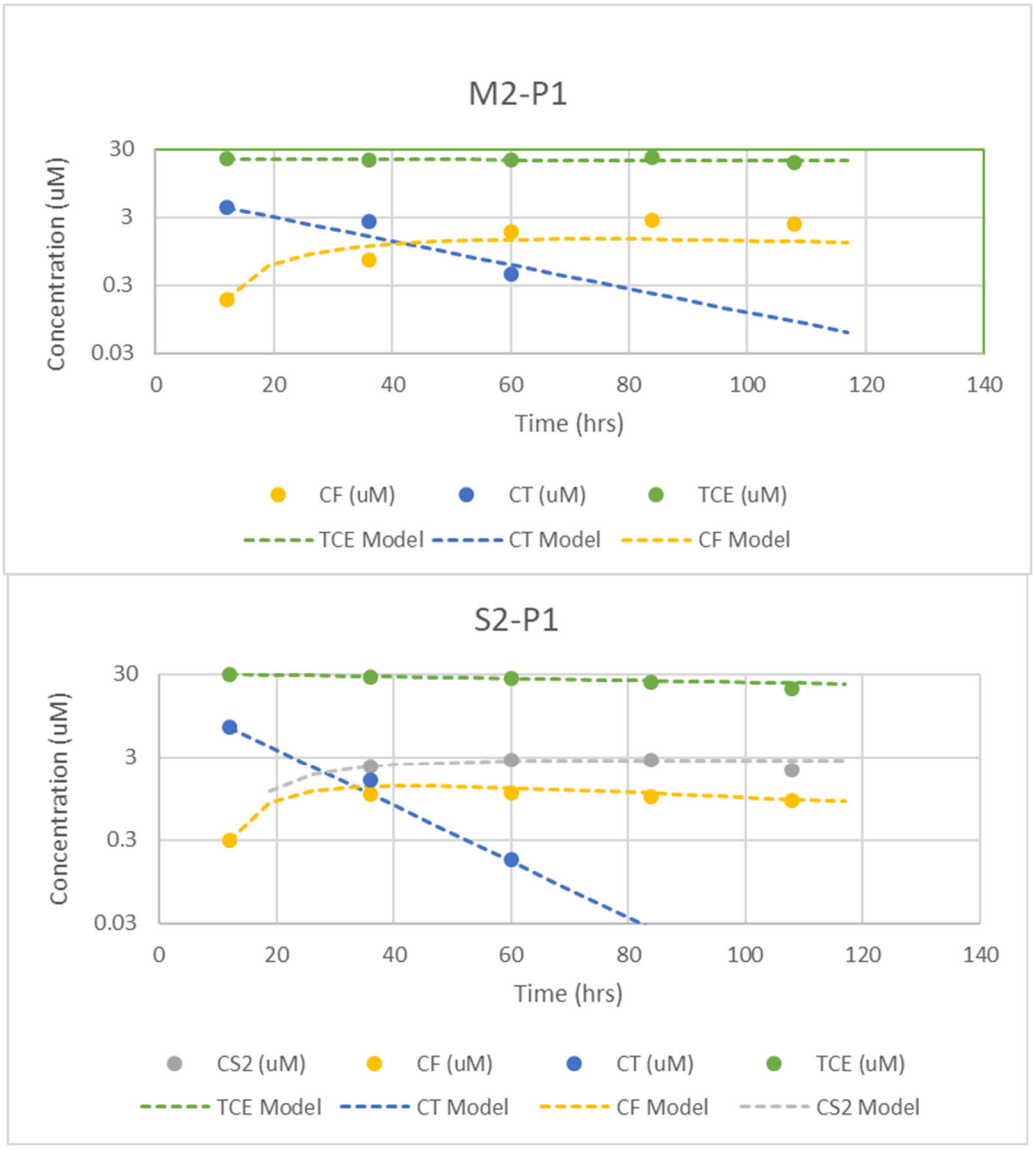


*Figure 18. Measured chlorinated compound and degradation product concentrations in columns M2 and S2.*

## Chlorinated compound degradation under stopped-flow conditions

Once the concentration profiles in a column had stabilized under flowing conditions, flow in that column was stopped and the column was periodically samples over the next ~60 days (~1500 hours). Example data, again from Port 1 on columns M2 and S2, are shown in Figure 19. All of the analytical data for the stopped-flow experiments are listed in Appendices E and F.

Once again, the dashed lines in the figures represent modeling results, and first-order rate data for the stopped-flow experiments are found in Section 4, below.

In all cases except one, no TCE degradation products were observed. The exception was the no carbonate case when the pH was very low (~3). Our interpretation of this result is that the TCE reduction pathway is entirely through acetylene and, in most cases, the acetylene degradation rate was greater than the rate for acetylene formation and, as a consequence, there was no net acetylene accumulation.

CT shows a typical degradation pattern with production of CF, and CS2, depending on the conditions. There is also some data indicating CO production. However, the rate of CO disappearance, and the detection limit for CO make it difficult to estimate rates from these data.

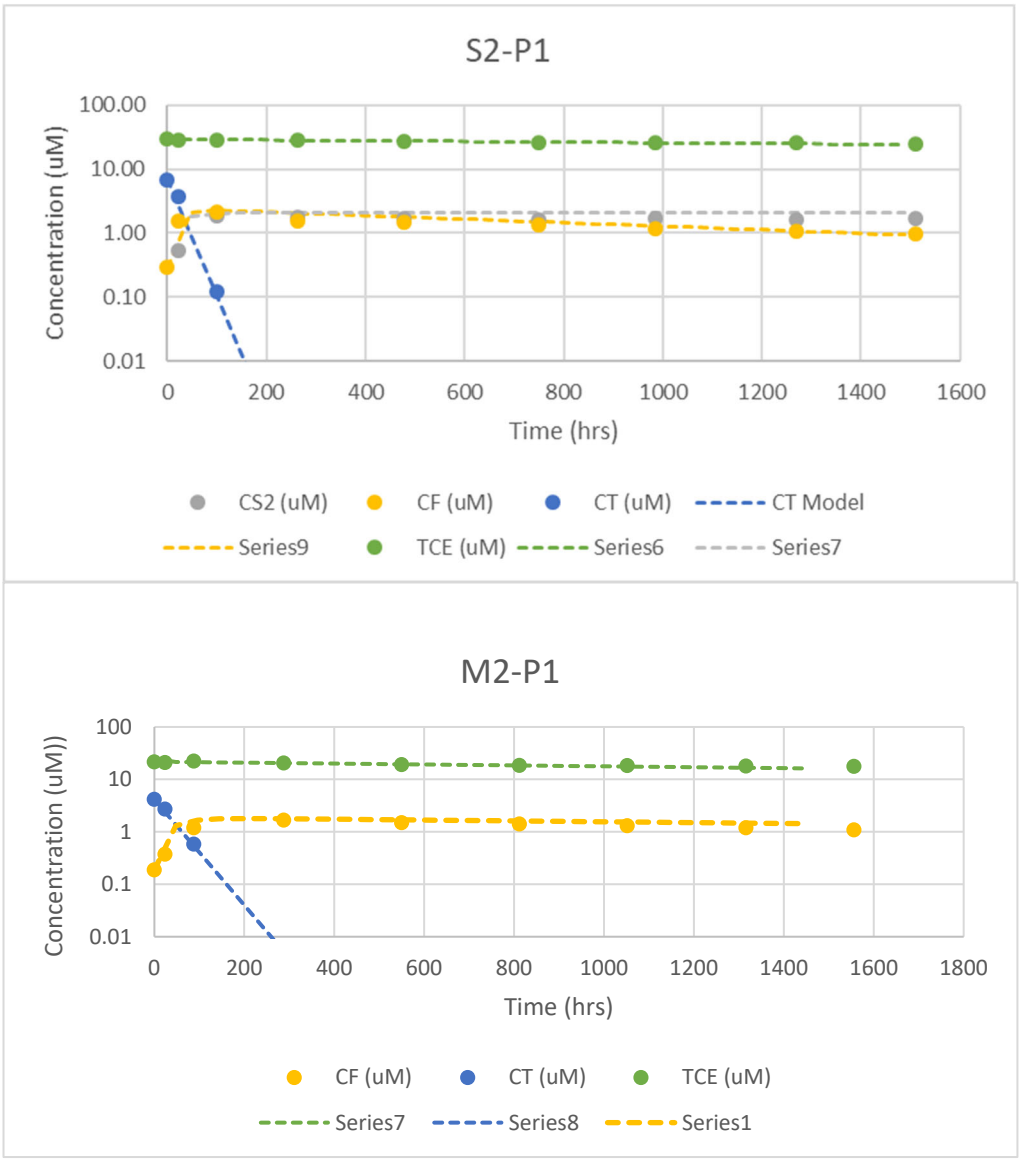


*Figure 19. Measured chlorinated solvent and degradation product concentrations in columns M2 and S2 under non-flowing conditions.*

## Measured DNA in water samples

At the same time that samples were collected for volatile fatty acid analysis, samples were collected for total DNA analysis. The data in Figure 20 show DNA concentrations for 5 of the columns (NMFe was not available at the time of sampling).

Most noticeable is that neither the NC or NL columns have any measureable DNA concentrations. The NL column result is not surprising in that there was no carbon source in the column to facilitate cell growth. The data from the NC column are consistent with the measured VFA data, which showed no lactate degradation or product formation. Presumably, this was due to the relatively low pH of the column water (due to lack of buffering at that point in time.)

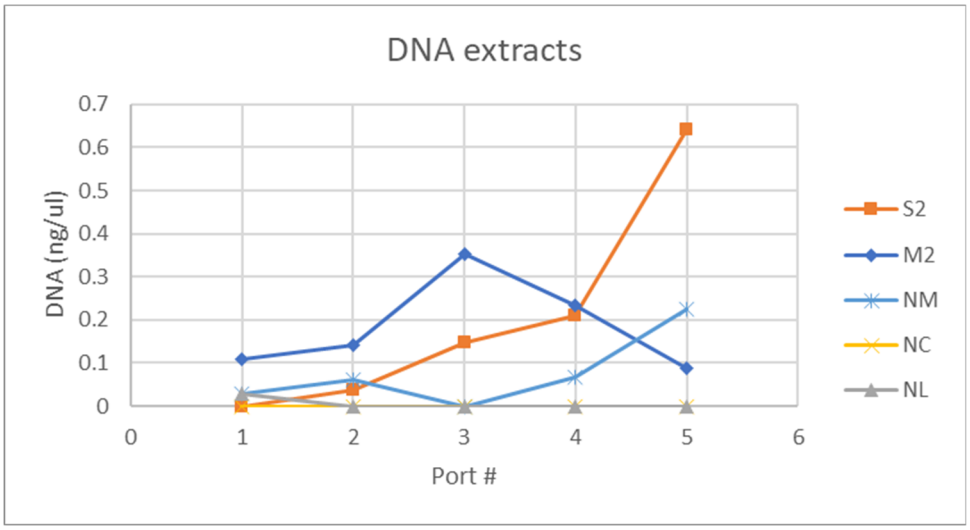


*Figure 20. Measured DNA concentrations (ng/uL)*

# 7. Modeling of Chlorinated Compound Degradation

The measured concentration data in Appendices E and F were fit using Equations 1-5, above, and an explicit finite difference scheme. Examples of the models for ports from two of the columns (M2 and S2) under flowing conditions are shown as dashed lines in Figure 18, above. Similarly, model results under stopped conditions are shown in Figure 19.

## Modeling of Chlorinated Compound Degradation under Flowing Conditions

The observed first-order degradation rate constants ($hr^{-1}$) for each column for each injection round is shown in Table 4.

*Table 4. Observed first-order rate constants for TCE and CT in all columns for the two sampling rounds.*

| Column | Round 1 | | Round 2 | |
|---|---|---|---|---|
| | kTCE* | kCT | kTCE | kCT |
| NM | 0.004 | 0.018 | 0.001 | 0.012 |
| NMFe | 0.002 | 0.06 | 0.002 | 0.02 |
| M2 | 0.002 | 0.02 | 0.001 | 0.03 |
| S2 | 0.002 | 0.03 | 0.001 | 0.02 |
| NL | 0.002 | 0.003 | BDL*** | BDL |
| NC | 0.005** | 0.002** | 0.002 | 0.002 |

* Rate in units of $hr^{-1}$

** pH~3.5 during Round 1, pH~7.2 during Round 2

*** BDL = below detection limit (column residence time only 4.5 days)

For all columns to which lactate was added, the degradation rate for TCE was relatively consistent (0.002 – 0.005 $hr^{-1}$). For those same columns the degradation rate for CT was again relatively consistent (0.02-0.06 hr-1) with the exception of the no carbonate (NC) column, in which the degradation rate was an order of magnitude lower.

The most dramatic difference among all of the columns was that the no lactate (NL) column showed no measureable degradation rate for either TCE of CT during the second round of sampling. There are a number of possible reasons why this could be the case, including the lack of biological activity in the column and the disappearance of some reactive material, present at the beginning of the experiment (e.g., Fe2+). However, the data collected in this project are not able to resolve this issue.

## Modeling of Chlorinated Compound Degradation under Stopped-Flow Conditions

Rate constant data under stopped flow conditions for CT and TCE are shown in Table 5.
TCE rates for both sampling rounds are in the range of 0.0003-0.00035 $hr^{-1}$ except for the case where there is no lactate. These are roughly an order of magnitude lower than for the flowing case.

Unlike the TCE cases, CT rates for column NM, NMFe, M2 and S2 are all similar to the rates under flowing conditions. For the NL column, non-zero rates were observed; however, they were 10-50 times smaller than for the other columns.

During round 2, the CT degradation rates for the NL column were consistently 3 to 6 times higher than for round 1, but they were still less than NM NMFe, M2, and S2.

For the NC column the observed rate for CT was far below the other lactate-containing columns. This is likely due to the lower pH. However, this effect is significantly different than was observed for TCE in the same column. The volatile fatty acid data suggest that there was no measurable lactate degradation (i.e., no biological reaction) at the low pH (~3.5) of the NC column.

Table 5. Modeled first-order rate constant data ($hr^{-1}$) for all ports on all columns under stopped-flow conditions.

| Column-Port | Round 1 | | | Round 2 | | |
|---|---|---|---|---|---|---|
| | kTCE | kAcet | kCT | kTCE | kAcet | kCT |
| NM-P1 | 0.00015 | ND* | 0.015 | 0.00003 | ND | 0.025 |
| NM-P3 | 0.00018 | ND | 0.04 | 0.00013 | ND | 0.05 |
| NM-P5 | 0.00013 | ND | ND | 0.00005 | ND | 0.05 |
| NM-P7 | 0.00025 | ND | ND | 0.00007 | ND | 0.01 |
| NM-P9 | 0.00035 | ND | ND | 0.0007 | ND | ND |
| | | | | | | |
| NMFe-P1 | 0.00013 | ND | 0.05 | 0.00017 | ND | 0.014 |
| NMFe-P3 | 0.00013 | ND | ND | 0.00013 | ND | 0.0085 |
| NMFe-P5 | 0.00013 | ND | ND | 0.0002 | ND | 0.03 |
| NMFe-P7 | 0.0002 | ND | ND | 0.0003 | ND | 0.03 |
| NMFe-P9 | 0.00025 | ND | ND | 0.0005 | ND | ND |
| | | | | | | |
| M2-P1 | 0.00013 | ND | 0.04 | 0.00025 | ND | 0.02 |
| M2-P3 | 0.00013 | ND | ND | 0.00013 | ND | ND |
| M2-P5 | 0.00013 | ND | ND | 0.00025 | ND | ND |
| M2-P7 | 0.00013 | ND | ND | 0.0002 | ND | ND |
| M2-P9 | 0.0002 | ND | ND | 0.0005 | ND | ND |
| | | | | | | |
| S2-P1 | 0.00013 | ND | 0.05 | 0.00018 | ND | 0.02 |
| S2-P3 | 0.00013 | ND | 0.05 | 0.00013 | ND | 0.03 |
| S2-P5 | 0.00013 | ND | ND | 0.00018 | ND | 0.05 |
| S2-P7 | 0.00013 | ND | ND | 0.00022 | ND | ND |
| S2-P9 | 0.00025 | ND | ND | 0.0009 | ND | ND |
| | | | | | | |
| NL-P1 | BDL** | ND | 0.0024 | 0.00015 | ND | 0.0009 |
| NL-P3 | BDL | ND | 0.0012 | 0.00013 | ND | 0.0007 |
| NL-P5 | BDL | ND | 0.0009 | 0.00013 | ND | 0.0008 |
| NL-P7 | 0.0001 | ND | 0.0008 | 0.00013 | ND | 0.0009 |
| NL-P9 | 0.00013 | ND | 0.0007 | 0.00028 | ND | 0.0009 |
| | | | | | | |
| NC-P1 | 0.0001 | 0.0008 | 0.00005 | 0.0003 | ND | 0.0015 |
| NC-P3 | 0.00013 | 0.0015 | 0.00005 | 0.00013 | ND | 0.0012 |
| NC-P5 | 0.00013 | 0.0016 | 0.00005 | 0.00018 | ND | 0.0012 |
| NC-P7 | 0.00015 | 0.0008 | 0.00005 | 0.00013 | ND | 0.0013 |
| NC-P9 | 0.00013 | 0.004 | 0.00005 | 0.0003 | ND | 0.0015 |

*ND = No acetylene/carbon tetrachloride detected, therefore no rate could be determined.

**BDL – Below detection limit

## Modeling Mass Balance

The modeled rate constants for CT were used in Equations 1-5 to estimate mass balances for CT and degradation products under stopped-flow conditions. Examples of those simulations are showing in Figure 21. The data suggest that the yield of CF in the two columns shown in the figure are comparable, as is the rate of CF degradation. The S2 column shows a significant yield of CS2, as would be anticipated based on the observed sulfide concentrations in the column.

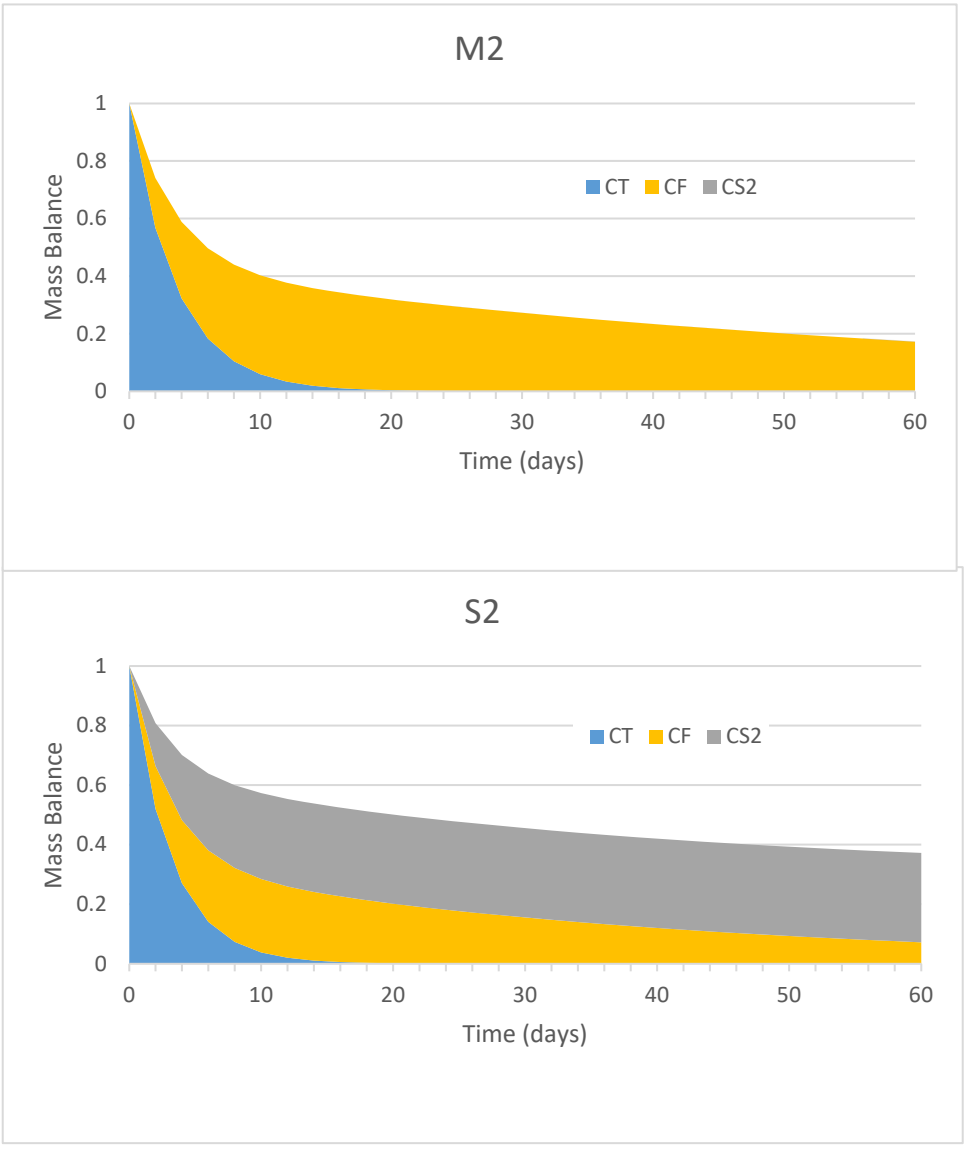


*Figure 21. Modelled mass balance of CT, CF and CS2 during stopped flow in columns M2 and S2.*

# 8. Discussion

An objective of this project has been to identify the conditions under which chlorinated compounds are degraded via abiotic pathways. Given the relatively ubiquitous nature of the TCE degradation, this has been less successful than anticipated. However, there are a number of observations that can be made with regard to both flowing and stopped-flow conditions and specific column conditions.

## Effects of different column conditions

**Magnetite addition.** The two columns to which magnetite was not added (NM and NMFe) had degradation rates for CT and TCE that were similar to the columns to which magnetite was added. This suggests that, in these experiments, the presence of magnetite did not contribute significantly to abiotic degradation. It is important to note that this does not preclude a potential role for high-surface-area magnetite formed in situ playing a significant role. However, there is no evidence in the columns tested here that magnetite was formed or contributed to abiotic degradation

**Sulfate addition**. Sulfate addition in these experiments had little effect on the overall rate of TCE or CT reduction. However, it did have a significant effect on products from CT degradation (i.e., carbon disulfide was a significant product in the S2 column. The S2 column also showed visual signs of black mineral precipitation (presumably mackinawite, pyrite, or other iron sulfide minerals).

**Lactate addition**. The lactate data are difficult to interpret. This is largely the case because TCE degradation rates were relatively consistent across all column conditions. The one exception to this is stopped-flow data for the column without lactate. There appears to be relatively little TCE degradation during the first round of sampling; however, the degradation rate in the second round increased and approached the rate for the columns in which lactate was being consumed.

For CT in the absence of lactate, the degradation rate dropped by more than an order of magnitude when compared to the columns with lactate. This was the case for both flowing and non-flowing conditions. The CT results are consistent with biotic metabolism being the driver for the system (either biotic or biologically-mediated abiotic mechanisms).

Based on the pattern of volatile fatty acid degradation products, fermentation is the primary pathway for lactate (i.e., the sum of propionate and acetate production equals the loss of lactate.) There are a variety of pathways reported in the literature that could directly couple biological reactions (e.g., extracellular processes, co-metabolism) to chlorinated compound reduction. However, it is also likely/possible that there are indirect effects of lactate-driven biological reactions (e.g., respiration activities eliminating traces of oxygen, mineral reduction/precipitation)

**Carbonate buffer addition**. In the absence of carbonate (NC column) the pH dropped to ~3.5. This resulted in a very low CT degradation rate. At the same time, the TCE degradation rate was relatively unchanged (slightly increased). Of particular note is that this was the only case in which any TCE degradation product was observed. In this case, acetylene production was observed both in the flowing column experiments and in the stopped-flow experiments.

**PIPES buffer**. For the NC column, after the first sampling event the decision was made to add PIPES buffer to control the pH near 7.2. The effect of this can be seen in Figure 14. On effect of this is that the ferrous iron concentration dropped below detection limits for the remainder of the experiment (Figure 10). The increase in pH also resulted in a 20-30 fold increase in CT

degradation rate. However, the CT rate still remained about an order of magnitude below the columns in which lactate was being metabolized.

## Chlorinated Compound Degradation Products

**Lack of TCE degradation products**. One of the surprising results of these experiments has been that, in all cases except one, TCE degradation products were not observed. (As discussed above, the exception was the NC case when the pH was very low). Our interpretation is that the pathway for TCE degradation is all through acetylene and that the acetylene is rapidly degraded, except in the very low pH case.

**CT degradation patterns**. CT shows a typical degradation pattern with production of CO, CF, and CS2, depending on the conditions. In these experiments, CO only tended to accumulate during flowing conditions, and even then was somewhat intermittent. (We have consistently observed CO production in other similar experiments). As expected, CS2 was only produced in significant quantities in the column to which sulfate was continuously added.

## Effect of extended operation

**Time-series ferrous iron data**. In all cases except the NL column (where no ferrous iron was ever present) there is a decrease in ferrous iron concentrations in the pore water over time. This is believed to be the case because the reservoir of labile iron, originally in the sand at the beginning of the experiments, was depleted over time. However, as the TCE and CT rate data in Table 4 indicate, those decreases in ferrous iron did not have a significant impact on either TCE or CT degradation rates.

The data in Figure 9 indicate that aqueous ferrous iron concentrations increased during non-flowing conditions, even when concentrations dropped below the detection limit during adjacent flowing conditions. This suggests that there was likely some ongoing production of [Fe2+]; however, the data collected does not allow estimation of a rate. For the S2 column, significant darkening of the sand grains was observed over time, which was likely due to the formation of iron sulfides (at least initially FeS). This process appeared to continue throughout the duration of the experiments and again suggests that [Fe2+] production was ongoing.

**Time-series sulfate and sulfide data**. As the data in Figure 11 indicate, sulfate was consistently metabolized in the first half of the column. When lactate concentration was reduced (~day 250), metabolism was disrupted, but eventually returned and ultimately increased in rate near the end of the experiments (i.e., by day 550 nearly all of the sulfate had disappeared by port 3.)

The dissolved sulfide concentrations (Figure 11) increased during the latter portions of the experiment, suggesting a reduction in iron sulfide precipitation, which is consistent with decreases in observed [Fe2+]. As mentioned above, the sulfide data suggest that ~80% of the sulfur introduced into the column as sulfate was removed from the water during transport through the column. It has been suggested that fresh precipitation of iron sulfides is an important contributor to abiotic chlorinated compound degradation. However, data from the column experiments conducted here suggest that it was not a dominant factor.

**Time-series pH data**.

With the exception of the low-pH case, there was relatively little of note with regard to the time-series pH data. The low pH in the NC column definitely had an impact on column behavior; however, even when the pH of that column was buffered, there was no apparent increase in

biological activity over time. This suggests that the extended low pH conditions likely had a detrimental effect on the microbial activity of that column.

## Changes in TCE and CT degradation rates over time.

**Under flowing conditions**, the TCE degradation rates were generally a factor of 2-3 lower under flowing conditions that directly preceded the second round of stopped-flow sampling compared to the first (i.e., samples collected immediately after shutdown of the column for the second time). However, it is generally not possible to say with confidence what the factors were that contributed to this change (e.g., decreased [Fe2+], effects of first stopped flow period). An exception to this was the NC column, which showed a 3X increase during the later sampling. This is likely due to the change in pH between the two sampling events (i.e., due to buffering prior to the second stopped-flow period.)

For CT, the degradation rates were generally similar for the two sampling rounds under flowing conditions. An interesting exception for both TCE and CT was that there was no measurable reactivity for either compound during the second flowing experiment for the NL column. The reason for this is not known, but it is possible that variations in injection concentrations leading up to the sampling event could have inadvertently contributed to this result.

**Under non-flowing conditions**, the TCE degradation rate dropped about an order of magnitude from the flowing case, but was surprisingly similar across all columns and both sampling events. The one exception to this is the NL column during the first sampling round. Ports 1,3 and 5 do not show any TCE degradation over ~1500 hours. Ports 7 and 9 show reactivity similar to that observed in the other columns. Interestingly, in the second round of sampling, all of the ports for the NL column showed rates similar to the other columns.

As mentioned previously, acetylene was observed in only one column (NC) and only during the first sampling event (when pH was low). Our working hypothesis is that the acetylene degradation rate was slower under these conditions, so there was an opportunity for it to accumulate.

For CT, unlike TCE, the observed rates under non-flowing conditions were similar to those during flowing conditions. The exceptions to these were the NL and NC columns, where the rates were significantly slower. A common element for these two columns is that there was no lactate metabolism in either case (NL because there was no lactate present, NC because it was not degraded.) It is also true that for both these cases there was no measured microbial biomass in water samples collected from the columns.

The observed CT degradation rates in the second round of non-flowing experiments were similar, but a bit slower, than the rates from the first round. The exception here is the NC column, which had significantly higher rates during the second, higher pH case.

## Implications for Active to Passive Transitions

An important goal for this project was to complete a systematic evaluation of column conditions that would allow a decision tree framework to be developed that would be useful for assessing active to passive transitions in groundwater remediation. While the systematic evaluation was completed successfully, the set of experimental conditions tested did not yield an experimental data set that would allow a working decision tree to be developed. For TCE, in particular, disappearance rates were surprisingly consistent across all experimental conditions.

For CT, the decision tree approach is a bit more useful (Figure 22). In this case, the metabolism of lactate had a strong impact on CT degradation (i.e., the NL column and the NC column under low pH conditions). The presence of added magnetite did not have any significant impact on rate, nor did the addition or concentration of ferrous iron. (It should be noted that an early column without lactate, but with added ferrous iron, failed because the conditions in the column were not sufficiently reducing to prevent precipitation of the iron and plugging the column.)

The addition of sulfate to the S2 column produced a different reaction products for CT (i.e., CS2), but did not significantly increase the overall CT degradation rate.

For the NC column, the very low pH made a significant difference in rate of CT degradation. (However, the conditions tested are not likely to occur in nature because of the ubiquitous presence of carbonate in natural systems.)

Microbial activity was important for CT degradation in most, if not all, cases. This could be the case either because there was direct or co-metabolic biodegradation of the CT or because it helped to ensure anoxic conditions, and likely led to the production of reactive species.

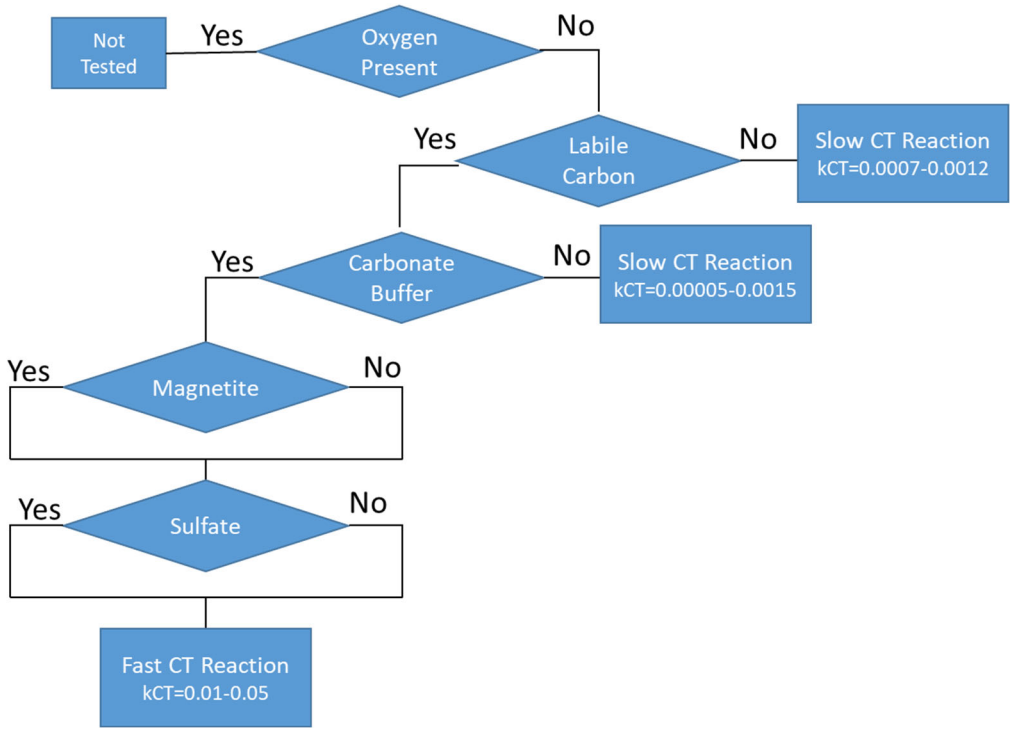


*Figure 22. Decision tree for CT degradation under various conditions.*

# 9. Conclusions and Implications

TCE degradation appeared to be quite rapid under flowing groundwater conditions with the addition of a labile carbon source. Given that few TCE degradation products were observed (i.e.., only acetylene and only under the low pH condition), it is difficult to discuss the specific degradation pathway. However, the lack of chlorinated degradation products is generally interpreted as indicating an abiotic pathway. And, modeling of the available acetylene data suggest that its rate of degradation is sufficiently fast to prevent accumulation (except in the low-pH case).

When groundwater flow was stopped, the rate of TCE degradation slowed by an order of magnitude. The most likely explanation for this is that the labile carbon source (lactate) was consumed within a few days and, as a consequence, microbial activity slowed. This is supported by the lactate degradation data, where a half-life in all of the carbonate buffered columns was on the order of 2-5 days under flowing conditions.)

In contrast to TCE, CT reduction rates generally did not decrease under no-flow conditions. This suggest a pathway for CT reduction that was less dependent on short-lived reactants actively produced in conjunction with lactate metabolism. In contrast, this result may suggest that somewhat longer-lived reactive species (e.g., mineral phases) could have played a significant role for CT

Microbiology likely had several important roles in the columns containing lactate. These include: 1) removal of residual oxygen from the influent groundwater; 2) reduction of mineral surfaces present in the column; and 3) production of reactive species.

The experiments described here are relevant for examining active to passive transition. In these experiments, flowing conditions represent the sustained delivery of materials to a treatment zone such as might be the case during active remediation. In the flowing groundwater case, the different ports on the column can be used to follow a parcel of amended groundwater as it moves through a treatment zone. When the flow in the column is stopped, the flux of additives into the treatment zone, obviously, stops. In this context it is useful to think about sequential sampling of stopped-flow conditions in the column as representing time-series analysis of a specific parcel of water within the treatment zone under conditions of natural (i.e., not further amended or pumped) groundwater flow.

Fermentation was the dominant biological process in the columns. This is likely to be the case whenever a significant carbon source is added to the subsurface. As discussed above, the reaction of propionate to acetate yields molecular hydrogen, which can be used by a wide variety of microorganisms, including dehalogenators, to reduce chlorinated compounds. These reactions may also produce extracellular biomolecules or other reactive species which can directly, or indirectly, result in chlorinated compound degradation.

An important conclusion from these experiments is that the addition of magnetite (or ferrous iron) and sulfate did not significantly impact reaction rates. Given the abundance of literature on the potential roles of magnetite and FeS on abiotic reduction, this is somewhat surprising. However, it may also be the case that the relatively organic-rich conditions in the columns overwhelmed the effects of the mineral phases

An important, if not surprising, conclusion is that addition of a carbon source was the main factor impacting contaminant degradation. The microbial metabolism facilitated by the carbon made the

columns more reducing (e.g., by removing all oxygen) and likely provided species that facilitated abiotic reactions (i.e., biologically-mediated abiotic degradation – BMAD).

# 10. Recommendations

## Follow-On Experiments

These experiments were designed to provide preliminary data to be used in the follow-on project (ER20-1357). The conclusions from these experiments can be extended by completing some additional, complimentary experiments. These include:

1. Conduct a more-detailed characterization of the microbial population. This could include a more-quantitative assessment of the different categories of microorganisms.
2. Conduct batch experiments using materials from one or more of the columns. This could include manipulation of geochemical conditions to examine their effects on reactivity.
3. Use of "Min-Trap" columns on the effluent of one or more columns and use the materials from those columns in batch reactivity experiments.
4. Temporary removal of lactate from the influent of one or more columns to observe the effects on degradation rates.

## Closing note on Reduction Potential

Reduction potential data were not collected during these column studies. This is, in part, due to challenges in making accurate measurements of reduction potential without access to solid-phase materials (which were not convenient to collect from the columns). As a separate set of experiments in our laboratory, platinum and glassy carbon electrodes were emplaced into a column such that they were in close physical proximity to the solid phase materials. These electrodes were monitored over periods of months and a relatively consistent pattern emerged. Generally speaking, the reduction potential measured with the platinum electrode was initially lower than that of the glassy carbon electrode. However, over periods of a week or two, the reduction potentials of both electrodes tended to drop significantly, and ended up below -700mV relative to the silver-silver chloride reverence electrode used for both working electrodes. Our interpretation of these data are that, initially, the platinum electrode was influenced by the presence of molecular hydrogen, leading to its lower value. However, over time, as both electrodes dropped in value, it is believed that microbial growth (or possibly precipitation) directly on the electrodes let do readings that more-accurately reflect the conditions experienced in biologically-active systems. As a test of this hypothesis, the electrodes were occasionally either removed and cleaned, or rotated in place to remove materials accumulated on the surface of the electrode. This resulted in initially less-negative potentials, which again returned to the lower values over time. One interpretation of these results is that biologically-associated micro-environments may have significantly lower reduction potentials in biologically active systems than are reflected in bulk water samples coming from monitoring wells.

# 11. References


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# 12. Appendices

## Appendix A - Acronyms

BDL – below detection limit (changes in concentrations were too small to allow a rate determination)

BMAD - biologically-mediated abiotic degradation

CF – chloroform

CO – carbon monoxide

CT – Carbon tetrachloride

DCE – dichloroethene

DCM – dichloromethane

DNA - Deoxyribonucleic acid

FID – Flame Ionization Detector

GCMS – Gas chromatograph, mass spectroscopy

MSD - Mass Spectrometric Detector

ND – no acetylene/carbon tetrachloride detected

TCE – trichloroethene

TCP – 1,2,3-trichloropropene

VC – vinyl chloride

VFA – Volatile Fatty Acids

Column Names:

NM – No Magnetite

NMFe – No Magnetite, Iron Added

M2 – Magnetite 2

S2 – Sulfate 2

NL – No Lactate

NLFe – No Lactate, Iron Added

NC – No Carbonate

## Appendix B. Ferrous Iron Data (μM)

| Date | NM | | | | | NMFe | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | 1 | 3 | 5 | 7 | 9 | 1 | 3 | 5 | 7 | 9 |
| 7/6/2020 | 0.91 | 10.91 | 64.55 | 195.45 | 236.36 | 70.00 | 110.00 | 211.82 | 216.36 | 202.73 |
| 7/15/2020 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 63.64 | 0.00 | 0.00 | 0.00 | 0.00 |
| 7/20/2020 | 0.91 | 11.82 | 64.55 | 158.18 | 210.00 | 72.73 | 97.27 | 130.00 | 198.18 | 225.45 |
| 8/3/2020 | 1.82 | 15.45 | 56.36 | 102.73 | 171.82 | 40.91 | 68.18 | 103.64 | 143.64 | 182.73 |
| 8/17/2020 | 0.91 | 21.82 | 56.36 | 79.09 | 110.00 | 43.64 | 66.36 | 88.18 | 111.82 | 140.00 |
| 8/31/2020 | 1.82 | 19.09 | 50.00 | 71.82 | 86.36 | 58.18 | 60.00 | 80.91 | 93.64 | 113.64 |
| 9/14/2020 | 2.73 | 10.91 | 35.45 | 64.55 | 86.36 | 50.91 | 73.64 | 87.27 | 100.00 | 110.00 |
| 10/13/2020 | 0.91 | 4.55 | 16.36 | 36.36 | 63.64 | 34.55 | 54.55 | 60.91 | 74.55 | 85.45 |
| 10/26/2020 | 0.00 | 1.82 | 10.91 | 20.91 | 48.18 | 29.09 | 42.73 | 45.45 | 51.82 | 68.18 |
| 11/9/2020 | 0.00 | 1.82 | 10.00 | 20.00 | 34.55 | 32.73 | 39.09 | 40.00 | 46.36 | 61.82 |
| 11/23/2020 | 0.00 | 0.00 | 3.64 | 12.73 | 30.00 | 39.09 | 46.36 | 48.18 | 50.00 | 58.18 |
| 12/7/2020 | 6.36 | 28.18 | 55.45 | 142.73 | 172.73 | 5.45 | 23.64 | 37.27 | 40.91 | 52.73 |
| 12/21/2020 | 16.36 | 58.18 | 102.73 | 210.91 | 236.36 | 38.18 | 53.64 | 68.18 | 86.36 | 100.91 |
| 1/4/2021 | 35.45 | 89.09 | 143.64 | 259.09 | 259.09 | 90.91 | 120.91 | 130.00 | 167.27 | 176.36 |
| 1/18/2021 | 3.64 | 7.27 | 18.18 | 30.00 | 43.64 | 130.91 | 167.27 | 160.00 | 207.27 | 196.36 |
| 2/3/2021 | 0.91 | 3.64 | 11.82 | 20.91 | 29.09 | 187.27 | 212.73 | 180.91 | 221.82 | 190.91 |
| 2/16/2021 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 178.18 | 213.64 | 200.91 | 240.00 | 178.18 |
| 3/3/2021 | 2.73 | 5.45 | 9.09 | 14.55 | 18.18 | 27.27 | 45.45 | 60.00 | 59.09 | 63.64 |
| 3/15/2021 | 1.82 | 17.27 | 15.45 | 18.18 | 23.64 | 61.82 | 55.45 | 52.73 | 61.82 | 68.18 |
| 3/29/2021 | 0.91 | 7.27 | 7.27 | 10.91 | 19.09 | 2.73 | 29.09 | 38.18 | 40.00 | 40.00 |
| 4/12/2021 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 17.27 | 28.18 | 32.73 | 39.09 | 42.73 |
| 4/26/2021 | 0.91 | 0.91 | 1.82 | 8.18 | 16.36 | 0.91 | 20.00 | 18.18 | 25.45 | 29.09 |
| 5/10/2021 | 1.82 | 1.82 | 0.91 | 3.64 | 9.09 | 2.73 | 9.09 | 9.09 | 9.09 | 16.36 |
| 5/29/2021 | 0.91 | 2.73 | 1.82 | 5.45 | 2.73 | 0.00 | 6.36 | 6.36 | 4.55 | 9.09 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 6/8/2021 | 0.91 | 3.64 | 2.73 | 2.73 | 6.36 | 5.45 | 10.00 | 10.00 | 10.91 | 11.82 |
| 6/24/2021 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 7/9/2021 | 0.91 | 7.27 | 7.27 | 8.18 | 13.64 | 13.64 | 20.00 | 24.55 | 22.73 | 23.64 |
| 7/20/2021 | 0.91 | 7.27 | 5.45 | 10.91 | 10.91 | 25.45 | 32.73 | 37.27 | 31.82 | 34.55 |
| 8/3/2021 | 1.82 | 8.18 | 10.00 | 19.09 | 20.00 | 42.73 | 37.27 | 42.73 | 38.18 | 40.91 |
| 8/17/2021 | 0.91 | 10.00 | 12.73 | 18.18 | 9.09 | 52.73 | 39.09 | 44.55 | 41.82 | 41.82 |
| 9/1/2021 | 1.82 | 11.82 | 16.36 | 20.91 | 1.82 | 64.55 | 50.91 | 50.91 | 50.00 | 50.00 |
| 9/20/2021 | 0.91 | 14.55 | 18.18 | 23.64 | 0.00 | 80.91 | 50.00 | 55.45 | 57.27 | 47.27 |
| 10/12/2021 | 0.00 | 2.73 | 2.73 | 4.55 | 5.45 | 19.09 | 10.91 | 13.64 | 13.64 | 14.55 |
| 10/26/2021 | 0.00 | 0.91 | 3.64 | 5.45 | 5.45 | 19.09 | 15.45 | 15.45 | 15.45 | 17.27 |
| 11/3/2021 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 11/11/2021 | 0.91 | 0.91 | 2.73 | 2.73 | 3.64 | 17.27 | 18.18 | 19.09 | 18.18 | 19.09 |
| 11/23/2021 | 0.91 | 1.82 | 1.82 | 1.82 | 1.82 | 7.27 | 12.73 | 11.82 | 10.91 | 10.91 |
| 12/8/2021 | 0.91 | 1.82 | 2.73 | 2.73 | 3.64 | 8.18 | 10.91 | 12.73 | 13.64 | 12.73 |
| 12/23/2021 | 0.91 | 2.73 | 1.82 | 1.82 | 2.73 | 6.36 | 9.09 | 10.91 | 10.00 | 11.82 |
| 1/10/2022 | 0.00 | 0.00 | 0.00 | 0.91 | 0.91 | 3.64 | 9.09 | 7.27 | 7.27 | 8.18 |
| 1/18/2022 | 0.00 | 1.82 | 1.82 | 0.91 | 2.73 | 3.64 | 6.36 | 9.09 | 8.18 | 8.18 |
| 2/2/2022 | 0.91 | 1.82 | 0.91 | 1.82 | 1.82 | 2.73 | 6.36 | 8.18 | 9.09 | 10.91 |
| 2/15/2022 | 0.00 | 1.82 | 1.82 | 2.73 | 4.55 | 0.91 | 2.73 | 6.36 | 7.27 | 7.27 |
| 3/3/2022 | 0.91 | 1.82 | 0.91 | 0.91 | 2.73 | 0.00 | 0.91 | 4.55 | 5.45 | 6.36 |
| 3/15/2022 | 0.91 | 0.91 | 1.82 | 1.82 | 1.82 | 1.82 | 2.73 | 5.45 | 7.27 | 8.18 |
| 3/30/2022 | 1.82 | 1.82 | 1.82 | 3.64 | 3.64 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |

| Date | M2 | | | | | S2 | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | 1 | 3 | 5 | 7 | 9 | 1 | 3 | 5 | 7 | 9 |
| 7/6/2020 | 3.64 | 10.00 | 19.09 | 13.64 | 10.91 | 7.27 | 61.82 | 116.36 | 235.45 | 284.55 |
| 7/15/2020 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 7/20/2020 | 4.55 | 13.64 | 35.45 | 59.09 | 103.64 | 3.64 | 13.64 | 38.18 | 93.64 | 160.00 |
| 8/3/2020 | 1.82 | 16.36 | 55.45 | 98.18 | 144.55 | 2.73 | 12.73 | 26.36 | 64.55 | 101.82 |
| 8/17/2020 | 2.73 | 15.45 | 57.27 | 87.27 | 123.64 | 4.55 | 10.00 | 23.64 | 50.91 | 91.82 |
| 8/31/2020 | 0.00 | 10.91 | 44.55 | 81.82 | 109.09 | 2.73 | 20.00 | 21.82 | 6.36 | 47.27 |
| 9/14/2020 | 1.82 | 5.45 | 27.27 | 62.73 | 101.82 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 10/13/2020 | 20.00 | 132.73 | 236.36 | 219.09 | 173.64 | 81.82 | 50.91 | 92.73 | 175.45 | 132.73 |
| 10/26/2020 | 59.09 | 248.18 | 257.00 | 251.82 | 173.64 | 98.18 | 47.27 | 106.36 | 194.55 | 137.27 |
| 11/9/2020 | 102.73 | 309.09 | 283.64 | 259.09 | 161.82 | 4.55 | 37.27 | 39.09 | 55.45 | 72.73 |
| 11/23/2020 | 139.09 | 283.64 | 287.27 | 277.27 | 146.36 | 9.09 | 23.64 | 12.73 | 20.91 | 37.27 |
| 12/7/2020 | 3.64 | 10.91 | 34.55 | 62.73 | 96.36 | 6.36 | 27.27 | 39.09 | 52.73 | 68.18 |
| 12/21/2020 | 0.91 | 8.18 | 26.36 | 46.36 | 79.09 | 4.55 | 19.09 | 30.00 | 70.00 | 90.91 |
| 1/4/2021 | 0.91 | 7.27 | 22.73 | 35.45 | 58.18 | 10.00 | 31.82 | 58.18 | 94.55 | 108.18 |
| 1/18/2021 | 0.00 | 6.36 | 20.91 | 32.73 | 51.82 | 7.27 | 24.55 | 31.82 | 102.73 | 116.36 |
| 2/3/2021 | 0.91 | 6.36 | 18.18 | 32.73 | 51.82 | 9.09 | 22.73 | 26.36 | 80.91 | 100.91 |
| 2/16/2021 | 0.91 | 5.45 | 20.91 | 36.36 | 50.91 | 9.09 | 22.73 | 21.82 | 71.82 | 90.91 |
| 3/3/2021 | 0.91 | 10.00 | 22.73 | 44.55 | 54.55 | 7.27 | 13.64 | 21.82 | 76.36 | 94.55 |
| 3/15/2021 | 2.73 | 33.64 | 57.27 | 79.09 | 73.64 | 10.00 | 31.82 | 46.36 | 88.18 | 104.55 |
| 3/29/2021 | 0.91 | 26.36 | 37.27 | 64.55 | 68.18 | 7.27 | 20.91 | 26.36 | 73.64 | 95.45 |
| 4/12/2021 | 2.73 | 20.00 | 28.18 | 40.91 | 50.00 | 10.91 | 19.09 | 20.00 | 16.36 | 10.00 |
| 4/26/2021 | 0.91 | 17.27 | 25.45 | 28.18 | 26.36 | 6.36 | 5.45 | 5.45 | 7.27 | 3.64 |
| 5/10/2021 | 0.91 | 10.00 | 20.91 | 26.36 | 28.18 | 3.64 | 2.73 | 2.73 | 0.91 | 0.91 |
| 5/29/2021 | 0.91 | 7.27 | 17.27 | 22.73 | 21.82 | 0.91 | 2.73 | 0.91 | 1.82 | 1.82 |
| 6/8/2021 | 0.91 | 7.27 | 14.55 | 20.91 | 20.91 | 0.91 | 1.82 | 1.82 | 1.82 | 1.82 |
| 6/24/2021 | 0.00 | 4.55 | 10.91 | 10.91 | 12.73 | 2.73 | 1.82 | 2.73 | 1.82 | 0.91 |
| 7/9/2021 | 0.91 | 4.55 | 8.18 | 9.09 | 8.18 | 0.91 | 0.00 | 0.00 | 0.91 | 0.00 |
| 7/20/2021 | 0.91 | 9.09 | 13.64 | 14.55 | 13.64 | 4.55 | 2.73 | 1.82 | 0.91 | 0.91 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 8/3/2021 | 0.00 | 2.73 | 5.45 | 6.36 | 4.55 | 8.18 | 2.73 | 0.91 | 11.82 | 31.82 |
| 8/17/2021 | 0.91 | 10.91 | 17.27 | 13.64 | 11.82 | 10.91 | 10.91 | 7.27 | 10.91 | 29.09 |
| 9/1/2021 | 1.82 | 22.73 | 30.91 | 23.64 | 19.09 | 14.55 | 5.45 | 0.91 | 11.82 | 49.09 |
| 9/20/2021 | 9.09 | 39.09 | 46.36 | 29.09 | 28.18 | 20.91 | 9.09 | 5.45 | 9.09 | 49.09 |
| 10/12/2021 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 3.64 | 1.82 | 0.00 | 1.82 | 0.00 |
| 10/26/2021 | 19.09 | 44.55 | 60.00 | 19.09 | 46.36 | 1.82 | 1.82 | 0.91 | 0.91 | 0.00 |
| 11/3/2021 | 1.82 | 10.91 | 20.91 | 24.55 | 20.91 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 11/11/2021 | 0.91 | 7.27 | 11.82 | 16.36 | 17.27 | 2.73 | 0.91 | 0.91 | 0.91 | 0.91 |
| 11/23/2021 | 0.91 | 8.18 | 12.73 | 17.27 | 15.45 | 2.73 | 1.82 | 1.82 | 3.64 | 1.82 |
| 12/8/2021 | 0.91 | 7.27 | 11.82 | 15.45 | 12.73 | 0.91 | 0.91 | 0.91 | 0.91 | 0.91 |
| 12/23/2021 | 1.82 | 7.27 | 10.00 | 12.73 | 10.91 | 0.91 | 2.73 | 0.91 | 1.82 | 0.91 |
| 1/10/2022 | 0.00 | 4.55 | 7.27 | 10.91 | 9.09 | 0.91 | 0.91 | 0.91 | 0.00 | 0.00 |
| 1/18/2022 | 1.82 | 5.45 | 8.18 | 10.91 | 11.82 | 1.82 | 0.91 | 0.91 | 0.91 | 0.91 |
| 2/2/2022 | 1.82 | 7.27 | 6.36 | 8.18 | 10.00 | 1.82 | 2.73 | 1.82 | 1.82 | 1.82 |
| 2/15/2022 | 1.82 | 3.64 | 5.45 | 8.18 | 7.27 | 0.91 | 0.91 | 0.91 | 1.82 | 0.91 |
| 3/3/2022 | 0.91 | 5.45 | 8.18 | 9.09 | 9.09 | 1.82 | 1.82 | 0.91 | 1.82 | 1.82 |
| 3/15/2022 | 0.91 | 5.45 | 6.36 | 8.18 | 8.18 | 1.82 | 2.73 | 1.82 | 0.91 | 0.91 |
| 3/30/2022 | 27.27 | 7.27 | 10.91 | 11.82 | 11.82 | 1.82 | 0.91 | 0.91 | 0.91 | 1.82 |

| Date | NL | | | | | nv | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | 1 | 3 | 5 | 7 | 9 | 1 | 3 | 5 | 7 | 9 |
| 7/6/2020 | 10.00 | 6.36 | 9.09 | 15.45 | 17.27 | 10.00 | 56.36 | 112.73 | 98.18 | 96.36 |
| 7/15/2020 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 7/20/2020 | 6.36 | 0.91 | 11.82 | 0.91 | 0.91 | 5.45 | 26.36 | 72.73 | 124.55 | 101.82 |
| 8/3/2020 | 0.91 | 0.91 | 0.91 | 0.00 | 0.91 | 8.18 | 23.64 | 40.91 | 74.55 | 109.09 |
| 8/17/2020 | 0.91 | 0.91 | 0.00 | 1.82 | 0.00 | 5.45 | 16.36 | 28.18 | 45.45 | 62.73 |
| 8/31/2020 | 0.91 | 0.00 | 0.91 | 0.00 | 1.82 | 6.36 | 16.36 | 29.09 | 39.09 | 50.00 |
| 9/14/2020 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 7.27 | 20.00 | 22.73 | 35.45 | 39.09 |
| 10/13/2020 | 0.00 | 0.00 | 0.00 | 0.91 | 0.91 | 4.55 | 10.91 | 18.18 | 20.00 | 23.64 |
| 10/26/2020 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 5.45 | 10.00 | 15.45 | 23.64 | 29.09 |
| 11/9/2020 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 27.27 | 30.00 | 36.36 | 43.64 | 52.73 |
| 11/23/2020 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 65.45 | 60.00 | 67.27 | 80.00 | 91.82 |
| 12/7/2020 | 0.91 | 0.91 | 0.91 | 0.00 | 0.00 | 89.09 | 80.91 | 89.09 | 105.45 | 118.18 |
| 12/21/2020 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 108.18 | 100.00 | 106.36 | 122.73 | 131.82 |
| 1/4/2021 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 127.27 | 123.64 | 116.36 | 135.45 | 142.73 |
| 1/18/2021 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 4.55 | 8.18 | 11.82 | 15.45 | 20.00 |
| 2/3/2021 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 4.55 | 8.18 | 11.82 | 16.36 | 19.09 |
| 2/16/2021 | 1.82 | 0.91 | 0.91 | 4.55 | 0.91 | 3.64 | 8.18 | 10.91 | 15.45 | 20.00 |
| 3/3/2021 | 0.91 | 0.91 | 0.91 | 1.82 | 1.82 | 4.55 | 10.00 | 22.73 | 20.00 | 24.55 |
| 3/15/2021 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 6.36 | 15.45 | 19.09 | 21.82 | 26.36 |
| 3/29/2021 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 4.55 | 7.27 | 10.91 | 15.45 | 19.09 |
| 4/12/2021 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 1.82 | 0.00 | 0.00 | 1.82 | 0.91 |
| 4/26/2021 | 0.91 | 1.82 | 0.91 | 0.91 | 1.82 | 1.82 | 1.82 | 1.82 | 0.91 | 0.91 |
| 5/10/2021 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.91 | 0.00 | 0.00 |
| 5/29/2021 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.91 | 0.91 | 0.00 |
| 6/8/2021 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.91 | 0.91 | 0.91 | 0.00 | 0.91 |
| 6/24/2021 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.91 | 0.91 | 0.91 | 0.91 | 0.91 |
| 7/9/2021 | 0.91 | 0.00 | 0.00 | 1.82 | 0.91 | 0.00 | 0.91 | 0.91 | 1.82 | 0.91 |
| 7/20/2021 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.91 | 0.00 | 0.00 | 0.00 | 0.00 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 8/3/2021 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 8/17/2021 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.91 | 0.91 | 0.91 | 0.91 | 1.82 |
| 9/1/2021 | 0.00 | 0.00 | 0.00 | 0.91 | 0.00 | 0.91 | 0.00 | 0.00 | 0.00 | 0.91 |
| 9/20/2021 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 10/12/2021 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 10/26/2021 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 11/3/2021 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 11/11/2021 | 0.91 | 0.91 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.91 | 0.00 | 0.00 |
| 11/23/2021 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 12/8/2021 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 12/23/2021 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 1/10/2022 | 1.82 | 1.82 | 1.82 | 0.91 | 0.91 | 0.91 | 0.00 | 0.00 | 0.91 | 1.82 |
| 1/18/2022 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 2/2/2022 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 2/15/2022 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 3/3/2022 | 0.91 | 1.82 | 1.82 | 0.91 | 0.91 | 0.91 | 3.64 | 1.82 | 3.64 | 0.91 |
| 3/15/2022 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 3/30/2022 | 1.82 | 0.91 | 1.82 | 1.82 | 1.82 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |

## Appendix C. Sulfate Data (μM)

| Date | | | S2 | | |
|---|---|---|---|---|---|
| | 1 | 3 | 5 | 7 | 9 |
| 7/9/2020 | 312.5 | 135.42 | 31.25 | 20.833 | 52.0833 |
| 7/23/2020 | 458.33 | 31.25 | 10.417 | 10.417 | 10.4167 |
| 8/5/2020 | 437.5 | 10.417 | 10.417 | 20.833 | 41.6667 |
| 8/19/2020 | 531.25 | 10.417 | 20.833 | 10.417 | 31.25 |
| 8/28/2020 | 458.33 | 447.92 | 333.33 | 31.25 | 10.4167 |
| 11/11/2020 | 468.75 | 333.33 | 375 | 427.08 | 781.25 |
| 11/25/2020 | 416.67 | 270.83 | 10.417 | 0 | 0 |
| 12/9/2020 | 375 | 312.5 | 10.417 | 10.417 | 20.8333 |
| 12/23/2020 | 437.5 | 260.42 | 0 | 10.417 | 20.8333 |
| 1/6/2021 | 385.42 | 218.75 | 0 | 10.417 | 20.8333 |
| 1/20/2021 | 458.33 | 312.5 | 10.417 | 20.833 | 10.4167 |
| 2/4/2021 | 385.42 | 322.92 | 31.25 | 20.833 | 10.4167 |
| 2/19/2021 | 291.67 | 239.58 | 0 | 10.417 | 10.4167 |
| 3/4/2021 | 385.42 | 322.92 | 10.417 | 10.417 | 10.4167 |
| 3/19/2021 | 385.42 | 343.75 | 10.417 | 10.417 | 0 |
| 3/31/2021 | 395.83 | 281.25 | 10.417 | 20.833 | 10.4167 |
| 4/14/2021 | 343.75 | 312.5 | 302.08 | 291.67 | 229.167 |
| 4/28/2021 | 260.42 | 187.5 | 114.58 | 83.333 | 83.3333 |
| 5/11/2021 | 260.42 | 166.67 | 125 | 83.333 | 41.6667 |
| 5/31/2021 | 281.25 | 135.42 | 52.083 | 0 | 10.4167 |
| 6/10/2021 | 322.92 | 177.08 | 83.333 | 10.417 | 0 |
| 6/28/2021 | 270.83 | 197.92 | 135.42 | 93.75 | 62.5 |
| 7/13/2021 | 354.17 | 343.75 | 281.25 | 239.58 | 229.167 |
| 9/30/2021 | 364.58 | 375 | 322.92 | 447.92 | 1093.75 |
| 10/27/2021 | 427.08 | 239.58 | 208.33 | 187.5 | 93.75 |
| 11/12/2021 | 354.17 | 197.92 | 166.67 | 83.333 | 20.8333 |

| | | | | | |
|---|---|---|---|---|---|
| 11/24/2021 | 354.17 | 197.92 | 104.17 | 31.25 | 20.8333 |
| 12/9/2021 | 416.67 | 93.75 | 20.833 | 10.417 | 10.4167 |
| 12/24/2021 | 343.75 | 83.333 | 10.417 | 10.417 | 10.4167 |
| 1/12/2022 | 322.92 | 31.25 | 10.417 | 0 | 0 |
| 1/20/2022 | 343.75 | 20.833 | 0 | 10.417 | 10.4167 |
| 2/3/2022 | 312.5 | 0 | 20.833 | 0 | 0 |
| 2/16/2022 | 333.33 | 62.5 | 10.417 | 10.417 | 10.4167 |
| 3/4/2022 | 395.83 | 93.75 | 0 | 10.417 | 0 |
| 3/16/2022 | 322.92 | 20.833 | 10.417 | 0 | 10.4167 |
| 3/31/2022 | 312.5 | 31.25 | 0 | 20.833 | 0 |

## Appendix D. Sulfide Data

| Date | S2 (μM) | | | | |
|---|---|---|---|---|---|
| | 1 | 3 | 5 | 7 | 9 |
| 7/24/2020 | 2.28 | 88.59 | 18.44 | 0.22 | 0.00 |
| 8/18/2020 | 4.38 | 70.31 | 26.25 | 0.88 | 0.00 |
| 11/12/2020 | 0.20 | 12.81 | 12.13 | 5.47 | 0.09 |
| 12/10/2020 | 0.31 | 25.00 | 29.31 | 6.75 | 0.06 |
| 1/7/2021 | 1.16 | 26.75 | 21.88 | 7.50 | 2.66 |
| 2/5/2021 | 2.50 | 18.88 | 30.63 | 9.13 | 3.06 |
| 3/4/2021 | 5.19 | 23.75 | 36.00 | 10.75 | 5.28 |
| 3/31/2021 | 3.75 | 23.56 | 22.25 | 9.72 | 5.28 |
| 4/28/2021 | 27.00 | 39.56 | 20.00 | 17.59 | 15.56 |
| 6/1/2021 | 33.88 | 54.69 | 48.13 | 58.28 | 51.09 |
| 6/29/2021 | 27.19 | 63.59 | 62.81 | 93.13 | 83.75 |
| 7/13/2021 | 0.84 | 10.13 | 42.03 | 53.13 | 48.59 |
| 9/30/2021 | 2.19 | 12.81 | 14.84 | 11.41 | 1.72 |
| 10/28/2021 | 13.69 | 82.19 | 62.19 | 76.88 | 82.81 |
| 11/24/2021 | 18.75 | 78.13 | 76.56 | 93.75 | 87.50 |
| 12/24/2021 | 13.13 | 80.47 | 87.50 | 88.28 | 95.94 |
| 1/21/2022 | 17.00 | 81.88 | 72.19 | 75.31 | 86.88 |
| 2/17/2022 | 17.97 | 77.34 | 64.53 | 67.50 | 61.88 |
| 3/17/2022 | 16.38 | 75.78 | 78.28 | 75.78 | 72.34 |

## Appendix E. pH Data

| Date | NM | | | | | NMFe | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | 1 | 3 | 5 | 7 | 9 | 1 | 3 | 5 | 7 | 9 |
| 7/13/20 | | | 6.90 | | | | | 7.00 | | |
| 12/2/20 | | | | | | 7.80 | 7.15 | 7.05 | 7.00 | 6.90 |
| 1/6/21 | 7.00 | 6.95 | 6.95 | 6.90 | 6.90 | | | | | |
| 1/13/21 | 8.25 | 7.50 | 7.10 | 7.10 | 7.05 | | | | | |
| 1/27/21 | 8.20 | 7.55 | 7.25 | 7.10 | 7.40 | | | | | 6.95 |
| 2/10/21 | 7.90 | 7.35 | 7.00 | 7.00 | 7.00 | 6.90 | 6.95 | 6.95 | 6.95 | 7.10 |
| 2/25/21 | 8.10 | 7.35 | 7.05 | 7.00 | 7.05 | 7.50 | 6.95 | 6.95 | 6.90 | 6.90 |
| 3/10/21 | 8.10 | 7.35 | 6.95 | 6.85 | 6.90 | 7.05 | 6.80 | 6.75 | 6.75 | 6.80 |
| 3/25/21 | 8.10 | 7.40 | 7.05 | 7.00 | 7.05 | 7.35 | 6.95 | 6.90 | 6.80 | 6.90 |
| 4/7/21 | | | | | | 6.70 | 6.75 | 6.70 | 6.70 | 6.85 |
| 4/21/21 | 7.10 | 6.70 | 6.80 | 6.80 | 6.85 | 6.85 | 6.65 | 6.65 | 6.70 | 6.80 |
| 5/6/21 | 6.80 | 6.75 | 6.75 | 6.75 | 6.85 | 6.75 | 6.65 | 6.65 | 6.60 | 6.45 |
| 5/18/21 | 6.90 | 6.70 | 6.70 | 6.70 | 6.75 | 6.80 | 6.75 | 6.70 | 6.65 | 6.75 |
| 6/3/21 | 7.35 | 6.90 | 6.90 | 6.85 | 6.90 | 6.80 | 6.65 | 6.60 | 6.50 | 6.60 |
| 6/17/21 | | | | | | 6.85 | 6.60 | 6.50 | 6.55 | 6.75 |
| 6/30/21 | | | | | | 7.00 | 6.90 | 6.80 | 6.75 | 6.65 |
| 9/23/21 | 6.95 | 7.00 | 6.90 | 6.75 | | 6.60 | 6.70 | 6.75 | 6.80 | 6.80 |
| 10/22/21 | 6.90 | 6.40 | 6.70 | 6.30 | 6.30 | 6.35 | 6.40 | 6.25 | 6.05 | 6.30 |
| 11/3/21 | 7.70 | 7.15 | 7.10 | 7.00 | 7.00 | 7.00 | 6.80 | 6.85 | 6.80 | 6.50 |
| 11/18/21 | 7.80 | 7.15 | 7.10 | 7.10 | 7.10 | 7.15 | 6.90 | 6.90 | 6.95 | 7.00 |
| 12/1/21 | 7.55 | 6.75 | 6.70 | 6.65 | 6.65 | 7.05 | 6.60 | 6.70 | 6.75 | 6.75 |
| 12/15/21 | 7.55 | 6.60 | 6.75 | 6.70 | 6.70 | 7.05 | 6.85 | 6.80 | 6.85 | 6.75 |
| 1/26/22 | 7.45 | 6.75 | 6.60 | 6.60 | 6.60 | 6.90 | 6.75 | 6.75 | 6.75 | 6.75 |
| 2/8/22 | 7.05 | 6.60 | 6.60 | 6.55 | 6.70 | 6.90 | 6.60 | 6.70 | 6.65 | 6.60 |
| 2/23/22 | 7.25 | 6.95 | 6.90 | 6.90 | 6.85 | 6.55 | 6.80 | 6.70 | 6.65 | 6.65 |
| 3/23/22 | 7.20 | 6.80 | 6.70 | 6.60 | 6.50 | 6.95 | 6.75 | 6.65 | 6.40 | 6.05 |

| Date | M2 | | | | | S2 | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | 1 | 3 | 5 | 7 | 9 | 1 | 3 | 5 | 7 | 9 |
| 7/13/20 | | | 7.30 | | | | | 7.30 | | |
| 11/2/20 | | | | | | 6.90 | 7.00 | 7.10 | 7.10 | |
| 11/23/20 | 6.90 | 6.80 | 6.90 | 6.95 | 7.10 | | | | | |
| 12/2/20 | 8.15 | 7.25 | 7.00 | 6.90 | 7.00 | 8.20 | 6.95 | 6.95 | 7.05 | 7.35 |
| 12/16/20 | 8.30 | 7.00 | 6.80 | 6.70 | 6.90 | 8.20 | 6.90 | 6.85 | 6.85 | 7.00 |
| 1/4/21 | 8.15 | 7.15 | 6.85 | 6.75 | 6.90 | 8.05 | 7.05 | 6.95 | 6.90 | 7.00 |
| 1/13/21 | 8.40 | 7.20 | 6.90 | 6.80 | 6.90 | 8.10 | 7.10 | 6.95 | 6.90 | 7.10 |
| 1/27/21 | 7.80 | 7.05 | 6.95 | 6.85 | 6.90 | 7.80 | 7.15 | 7.10 | 7.05 | 6.95 |
| 2/10/21 | 8.20 | 7.10 | 6.75 | 6.65 | 7.70 | 7.70 | 7.05 | 7.00 | 6.90 | 6.90 |
| 2/25/21 | 8.10 | 7.35 | 6.85 | 6.70 | 6.70 | 7.70 | 7.10 | 7.00 | 6.90 | 6.85 |
| 3/10/21 | 7.85 | 7.00 | 6.75 | 6.65 | 6.70 | 7.60 | 6.85 | 6.85 | 6.75 | 6.70 |
| 3/25/21 | 8.00 | 7.05 | 6.85 | 6.70 | 6.65 | 7.25 | 6.90 | 7.00 | 6.85 | 6.90 |
| 4/7/21 | 6.90 | 6.65 | 6.55 | 6.50 | 6.65 | 7.15 | 6.90 | 6.90 | 6.85 | 6.75 |
| 4/21/21 | 6.70 | 6.65 | 6.65 | 6.65 | 6.70 | 7.15 | 7.05 | 7.15 | 7.15 | 7.15 |
| 5/6/21 | 6.90 | 6.65 | 6.55 | 6.60 | 6.65 | 7.10 | 7.15 | 7.20 | 7.10 | 7.30 |
| 5/18/21 | 6.90 | 6.70 | 6.55 | 6.60 | 6.60 | 7.15 | 7.25 | 7.35 | 7.55 | 7.60 |
| 6/3/21 | 7.25 | 6.65 | 6.55 | 6.60 | 6.90 | 7.20 | 7.30 | 7.60 | 7.65 | 7.50 |
| 6/17/21 | 7.50 | 6.70 | 6.60 | 6.65 | 6.70 | 6.95 | 7.25 | 7.45 | 7.55 | 7.45 |
| 6/30/21 | 7.50 | 7.00 | 7.00 | 7.00 | 6.95 | 7.15 | 7.35 | 7.55 | 7.55 | 7.55 |
| 7/15/21 | | | | | | 7.55 | 7.30 | 7.40 | 7.40 | 7.45 |
| 7/28/21 | 7.65 | 7.05 | 6.95 | 6.75 | 6.95 | | | | | |
| 9/23/21 | | | | | | 6.95 | 7.05 | 7.05 | 7.05 | 7.05 |
| 10/22/21 | 6.35 | 6.40 | 6.40 | 6.45 | 6.45 | | | | | |
| 11/3/21 | 7.65 | 7.00 | 7.00 | 7.10 | 7.05 | 7.35 | 7.65 | 7.95 | 8.00 | 8.00 |
| 11/18/21 | 7.60 | 6.75 | 6.75 | 6.60 | 6.55 | 7.45 | 7.70 | 7.70 | 8.05 | 8.00 |
| 12/1/21 | 7.30 | 6.65 | 6.40 | 6.35 | 6.60 | 7.20 | 7.70 | 7.95 | 8.00 | 8.00 |
| 12/15/21 | 7.30 | 6.60 | 6.60 | 6.60 | 6.70 | 7.30 | 7.75 | 7.95 | 8.05 | 7.85 |
| 1/26/22 | 7.30 | 6.70 | 6.65 | 6.75 | 6.75 | 7.10 | 7.80 | 7.85 | 7.90 | 7.75 |
| 2/8/22 | 7.60 | 6.75 | 6.80 | 6.65 | 6.85 | 7.35 | 7.65 | 7.80 | 7.80 | 7.65 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 23/22 | 7.25 | 6.50 | 6.70 | 6.75 | 6.75 | 7.25 | 7.70 | 7.65 | 7.65 | 7.45 |
| 3/23/22 | 7.25 | 6.60 | 6.55 | 6.65 | 6.70 | 7.10 | 7.30 | 7.45 | 7.50 | 7.40 |
| Date | NL | | | | | NC | | | | |
| | 1 | 3 | 5 | 7 | 9 | 1 | 3 | 5 | 7 | 9 |
| 7/13/20 | | | 8.50 | | | | | 6.30 | | |
| 10/19/20 | | | | 8.70 | 8.70 | | | | | |
| 12/2/20 | 8.90 | 8.90 | 8.85 | 8.95 | 8.90 | | | | | |
| 12/16/20 | 9.20 | 9.20 | 9.30 | 9.10 | 9.05 | | | | | |
| 1/4/21 | 9.25 | 9.25 | 9.30 | 9.30 | 9.35 | | | | | |
| 1/6/21 | | | | | | 3.55 | 3.40 | 3.45 | 3.50 | 3.55 |
| 1/13/21 | 9.25 | 9.25 | 9.25 | 9.25 | 9.00 | 2.90 | 2.95 | 2.95 | 3.00 | 3.05 |
| 1/27/21 | 9.15 | 9.15 | 9.00 | 9.10 | 9.35 | 3.20 | 3.15 | 3.30 | 3.25 | 3.35 |
| 2/10/21 | 9.05 | 9.05 | 9.00 | 9.00 | 8.90 | 3.05 | 3.00 | 3.20 | 3.20 | 3.30 |
| 2/25/21 | 8.95 | 9.00 | 8.95 | 8.90 | 8.90 | 3.15 | 3.25 | 3.30 | 3.30 | 3.45 |
| 3/10/21 | 9.15 | 9.15 | 9.10 | 9.00 | 8.85 | 2.75 | 2.80 | 2.90 | 2.85 | 2.90 |
| 3/25/21 | 8.95 | 9.00 | 8.90 | 8.90 | 8.85 | 3.10 | 3.15 | 3.20 | 3.20 | 3.25 |
| 4/7/21 | 8.75 | 8.85 | 8.95 | 8.60 | 8.05 | 7.00 | 6.95 | 6.85 | 7.00 | 6.95 |
| 4/21/21 | 8.45 | 8.70 | 8.60 | 8.50 | 8.10 | 7.05 | 7.00 | 7.00 | 7.10 | 7.10 |
| 5/6/21 | 8.35 | 8.65 | 8.45 | 8.20 | 8.00 | 6.90 | 6.95 | 7.10 | 7.10 | 6.95 |
| 5/18/21 | 8.65 | 8.75 | 8.60 | 8.40 | 8.15 | 7.35 | 6.80 | 7.20 | 7.15 | 7.05 |
| 6/3/21 | 8.25 | 8.50 | 8.35 | 7.90 | 7.50 | 7.05 | 7.00 | 6.95 | 6.95 | 7.00 |
| 6/17/21 | 8.70 | 8.80 | 8.80 | 8.70 | 8.50 | 6.95 | 6.90 | 6.85 | 6.85 | 6.95 |
| 6/30/21 | 8.70 | 8.80 | 8.70 | 8.35 | 7.25 | 7.05 | 7.00 | 6.85 | 6.90 | 6.95 |
| 7/15/21 | 8.35 | 8.75 | 8.70 | 8.45 | 8.25 | 7.00 | 7.00 | 7.00 | 7.00 | 7.05 |
| 7/28/21 | | | | | | 7.10 | 7.05 | 7.10 | 7.10 | 7.15 |
| 9/23/21 | 8.30 | 8.35 | 8.20 | 7.90 | 7.50 | 6.50 | 6.60 | 6.60 | 6.60 | |
| 11/3/21 | 8.70 | 8.75 | 8.65 | 8.10 | 7.80 | | | | | |
| 11/18/21 | 8.80 | 8.85 | 8.80 | 8.65 | 8.40 | 7.15 | 7.15 | 7.15 | 7.00 | 6.90 |
| 12/1/21 | 8.45 | 8.70 | 8.65 | 8.50 | 7.80 | 7.05 | 6.95 | 6.85 | 6.85 | 6.95 |
| 12/15/21 | 8.55 | 8.65 | 8.50 | 8.45 | 7.75 | 6.95 | 6.90 | 6.90 | 7.00 | 7.05 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 1/26/22 | 8.50 | 8.50 | 8.75 | 8.60 | 8.00 | 7.15 | 7.15 | 7.05 | 7.10 | 7.15 |
| 2/23/22 | 8.60 | 8.80 | 8.80 | 8.70 | 8.40 | 6.85 | 7.10 | 7.05 | 7.10 | 7.10 |
| 3/23/22 | 8.40 | 8.65 | 8.65 | 8.50 | 8.40 | 7.15 | 7.15 | 7.15 | 7.15 | 7.15 |

## Appendix F. Volatile Fatty Acid Data (mM).

| Sample | Lactate (mM) | Acetate (mM) | Propionate (mM) | Butyrate (mM) | Total (mM) |
|---|---|---|---|---|---|
| NL-P1 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| NL-P3 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| NL-P5 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| NL-P7 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| NL-P9 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| S2-P1 | 8.36 | 1.17 | 1.49 | 0.00 | 11.01 |
| S2-P3 | 6.07 | 2.49 | 3.11 | 0.00 | 11.68 |
| S2-P5 | 3.62 | 3.56 | 3.56 | 0.00 | 10.74 |
| S2-P7 | 1.40 | 5.27 | 4.46 | 0.00 | 11.12 |
| S2-P9 | 0.00 | 5.57 | 4.46 | 0.00 | 10.03 |
| NC-P1 | 6.48 | 0.00 | 0.00 | 0.00 | 6.48 |
| NC-P3 | 6.53 | 0.00 | 0.00 | 0.00 | 6.53 |
| NC-P5 | 6.51 | 0.00 | 0.00 | 0.00 | 6.51 |
| NC-P7 | 6.63 | 0.00 | 0.00 | 0.00 | 6.63 |
| NC-P9 | 6.66 | 0.00 | 0.00 | 0.00 | 6.66 |
| M2-P1 | 8.68 | 0.00 | 1.06 | 0.00 | 9.75 |
| M2-P3 | 6.64 | 1.91 | 2.80 | 0.00 | 11.35 |
| M2-P5 | 4.77 | 2.83 | 4.27 | 0.00 | 11.87 |
| M2-P7 | 1.81 | 3.96 | 6.02 | 0.00 | 11.78 |
| M2-P9 | 0.00 | 4.43 | 6.64 | 0.00 | 11.07 |
| NM-P1 | 8.36 | 1.04 | 1.15 | 0.00 | 10.55 |
| NM-P3 | 7.48 | 1.34 | 1.92 | 0.00 | 10.74 |

| | | | | | |
|---|---|---|---|---|---|
| NM-P5 | 6.33 | 1.99 | 2.99 | 0.00 | 11.32 |
| NM-P7 | 5.42 | 2.42 | 3.42 | 0.00 | 11.26 |
| NM-P9 | 4.40 | 2.91 | 4.26 | 0.00 | 11.57 |

## Appendix G. Chlorinated Compounds and Degradation Products Data – Round 1 (µM)

| NM-P1 | | | | | | |
|---|---|---|---|---|---|---|
| Time (hrs) | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 9.71 | 0.00 | 0.00 | 0.29 | 3.19 | 20.14 |
| 49 | 3.97 | 0.00 | 0.00 | 1.13 | 0.58 | 18.58 |
| 117 | 0.00 | 0.00 | 0.00 | 1.38 | 0.00 | 18.07 |
| 285 | 0.00 | 0.00 | 0.00 | 1.38 | 0.00 | 17.07 |
| 502 | 0.00 | 0.00 | 0.00 | 1.36 | 0.00 | 16.36 |
| 790 | 0.00 | 0.00 | 0.00 | 1.01 | 0.00 | 15.57 |
| 1030 | 0.00 | 0.00 | 0.00 | 0.95 | 0.00 | 15.32 |

| NM-P3 | | | | | | |
|---|---|---|---|---|---|---|
| Time (hrs) | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 5.90 | 0.00 | 0.00 | 0.42 | 1.67 | 16.32 |
| 49 | 4.57 | 0.00 | 0.00 | 1.19 | 0.00 | 15.03 |
| 117 | 1.73 | 0.00 | 0.00 | 1.12 | 0.00 | 14.61 |
| 285 | 0.00 | 0.00 | 0.00 | 1.08 | 0.00 | 14.17 |
| 502 | 0.00 | 0.00 | 0.00 | 0.92 | 0.00 | 13.46 |
| 790 | 0.00 | 0.00 | 0.00 | 0.78 | 0.00 | 12.68 |
| 1030 | 0.00 | 0.00 | 0.00 | 0.69 | 0.00 | 12.51 |

| NM-P5 | | | | | | |
|---|---|---|---|---|---|---|
| Time (hrs) | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 0.00 | 0.00 | 0.00 | 0.98 | 0.11 | 13.00 |
| 49 | 0.00 | 0.00 | 0.00 | 1.15 | 0.00 | 13.47 |
| 117 | 0.00 | 0.00 | 0.00 | 1.09 | 0.00 | 12.77 |
| 285 | 0.00 | 0.00 | 0.00 | 0.96 | 0.00 | 12.79 |
| 502 | 0.00 | 0.00 | 0.00 | 0.82 | 0.00 | 12.51 |
| 790 | 0.00 | 0.00 | 0.00 | 0.64 | 0.00 | 11.48 |
| 1030 | 0.00 | 0.00 | 0.00 | 0.53 | 0.00 | 10.91 |

| NM-P7 | | | | | | |
|---|---|---|---|---|---|---|
| Time (hrs) | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 0.00 | 0.00 | 0.00 | 1.17 | 0.00 | 13.13 |
| 49 | 0.00 | 0.00 | 0.00 | 1.14 | 0.00 | 12.51 |
| 117 | 0.00 | 0.00 | 0.00 | 1.09 | 0.00 | 12.61 |
| 285 | 0.00 | 0.00 | 0.00 | 0.91 | 0.00 | 11.80 |
| 502 | 0.00 | 0.00 | 0.00 | 0.81 | 0.00 | 11.26 |
| 790 | 0.00 | 0.00 | 0.00 | 0.56 | 0.00 | 10.83 |
| 1030 | 0.00 | 0.00 | 0.00 | 0.42 | 0.00 | 10.06 |

| NM-P9 | | | | | | |
|---|---|---|---|---|---|---|
| Time (hrs) | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 0.00 | 0.00 | 0.00 | 1.10 | 0.00 | 12.60 |
| 49 | 0.00 | 0.00 | 0.00 | 1.08 | 0.00 | 11.88 |
| 117 | 0.00 | 0.00 | 0.00 | 0.99 | 0.00 | 11.86 |
| 285 | 0.00 | 0.00 | 0.00 | 0.89 | 0.00 | 10.96 |
| 502 | 0.00 | 0.00 | 0.00 | 0.68 | 0.00 | 10.79 |
| 790 | 0.00 | 0.00 | 0.00 | 0.43 | 0.00 | 9.44 |
| 1030 | 0.00 | 0.00 | 0.00 | 0.32 | 0.00 | 8.48 |

| NMFe-P1 | | | | | | |
|---|---|---|---|---|---|---|
| Time (hrs) | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 6.55 | 0.00 | 0.00 | 0.26 | 0.41 | 9.42 |
| 47 | 0.00 | 0.00 | 0.00 | 0.50 | 0.00 | 9.21 |
| 142 | 0.00 | 0.00 | 0.00 | 0.46 | 0.00 | 8.88 |
| 264 | 0.00 | 0.00 | 0.00 | 0.43 | 0.00 | 8.94 |
| 503 | 0.00 | 0.00 | 0.00 | 0.40 | 0.00 | 8.42 |
| 742 | 0.00 | 0.00 | 0.00 | 0.26 | 0.00 | 8.42 |
| 982 | 1.17 | 0.00 | 0.00 | 0.01 | 0.00 | 7.70 |
| 1246 | 1.57 | 0.00 | 0.00 | 0.01 | 0.00 | 8.01 |
| 1510 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 7.92 |

| NMFe-P3 | | | | | | |
|---|---|---|---|---|---|---|
| Time (hrs) | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 1.43 | 0.00 | 0.00 | 0.61 | 0.00 | 11.23 |
| 47 | 0.00 | 0.00 | 0.00 | 0.62 | 0.00 | 10.76 |
| 142 | 0.00 | 0.00 | 0.00 | 0.55 | 0.00 | 10.46 |
| 264 | 0.00 | 0.00 | 0.00 | 0.53 | 0.00 | 10.82 |
| 503 | 0.00 | 0.00 | 0.00 | 0.46 | 0.00 | 10.13 |
| 742 | 0.00 | 0.00 | 0.00 | 0.36 | 0.00 | 10.13 |
| 982 | 0.00 | 0.00 | 0.00 | 0.24 | 0.00 | 9.40 |
| 1246 | 0.00 | 0.00 | 0.00 | 0.19 | 0.00 | 9.64 |
| 1510 | 0.00 | 0.00 | 0.00 | 0.15 | 0.00 | 9.81 |

| NMFe-P5 | | | | | | |
|---|---|---|---|---|---|---|
| Time (hrs) | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 1.02 | 0.00 | 0.00 | 0.62 | 0.00 | 11.01 |
| 47 | 0.00 | 0.00 | 0.00 | 0.62 | 0.00 | 11.32 |
| 142 | 0.00 | 0.00 | 0.00 | 0.58 | 0.00 | 11.15 |
| 264 | 0.00 | 0.00 | 0.00 | 0.53 | 0.00 | 10.97 |
| 503 | 0.00 | 0.00 | 0.00 | 0.37 | 0.00 | 10.87 |
| 742 | 0.00 | 0.00 | 0.00 | 0.27 | 0.00 | 10.02 |
| 982 | 0.00 | 0.00 | 0.00 | 0.16 | 0.00 | 9.31 |
| 1246 | 1.27 | 0.00 | 0.00 | 0.16 | 0.00 | 9.32 |
| 1510 | 0.00 | 0.00 | 0.00 | 0.09 | 0.00 | 8.89 |

| NMFe-P7 | | | | | | |
|---|---|---|---|---|---|---|
| Time (hrs) | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 0.87 | 0.00 | 0.00 | 0.70 | 0.00 | 12.01 |
| 47 | 0.00 | 0.00 | 0.00 | 0.69 | 0.00 | 12.26 |
| 142 | 0.00 | 0.00 | 0.00 | 0.61 | 0.00 | 11.80 |
| 264 | 0.00 | 0.00 | 0.00 | 0.54 | 0.00 | 11.55 |
| 503 | 0.00 | 0.00 | 0.00 | 0.22 | 0.00 | 10.84 |
| 742 | 0.00 | 0.00 | 0.00 | 0.01 | 0.00 | 10.15 |
| 982 | 0.00 | 0.00 | 0.00 | 0.11 | 0.00 | 9.44 |
| 1246 | 0.00 | 0.00 | 0.00 | 0.01 | 0.00 | 9.10 |
| 1510 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 8.76 |

| NMFe-P9 | | | | | | |
|---|---|---|---|---|---|---|
| Time (hrs) | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 0.00 | 0.00 | 0.00 | 0.63 | 0.00 | 10.22 |
| 47 | 0.00 | 0.00 | 0.00 | 0.62 | 0.00 | 10.56 |
| 142 | 0.00 | 0.00 | 0.00 | 0.60 | 0.00 | 10.35 |
| 264 | 0.00 | 0.00 | 0.00 | 0.51 | 0.00 | 10.08 |
| 503 | 0.00 | 0.00 | 0.00 | 0.17 | 0.00 | 9.21 |
| 742 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 8.62 |
| 982 | 0.00 | 0.00 | 0.00 | 0.07 | 0.00 | 7.55 |
| 1246 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 6.89 |
| 1510 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 6.69 |

| M2-P1 | | | | | | |
|---|---|---|---|---|---|---|
| Time (hrs) | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 9.40 | 0.00 | 0.00 | 0.19 | 4.15 | 21.38 |
| 24 | 6.33 | 0.00 | 0.00 | 0.37 | 2.71 | 20.80 |
| 88 | 4.13 | 0.00 | 0.14 | 1.18 | 0.58 | 22.25 |
| 288 | 0.00 | 0.00 | 0.00 | 1.66 | 0.00 | 20.40 |
| 550 | 16.50 | 0.00 | 0.00 | 1.49 | 0.00 | 19.03 |
| 812 | 0.00 | 0.00 | 0.06 | 1.41 | 0.00 | 18.39 |
| 1052 | 0.00 | 0.00 | 0.18 | 1.30 | 0.00 | 18.25 |
| 1316 | 0.00 | 0.00 | 0.33 | 1.19 | 0.00 | 17.84 |
| 1556 | 0.00 | 0.00 | 0.39 | 1.08 | 0.00 | 17.68 |

| M2-P3 | | | | | | |
|---|---|---|---|---|---|---|
| Time (hrs) | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 5.13 | 0.00 | 0.00 | 0.70 | 2.60 | 20.72 |
| 24 | 1.61 | 0.00 | 0.00 | 1.80 | 0.48 | 21.08 |
| 88 | 0.00 | 0.00 | 0.00 | 2.16 | 0.00 | 21.46 |
| 288 | 0.00 | 0.00 | 0.00 | 2.01 | 0.00 | 20.33 |
| 550 | 22.06 | 0.00 | 0.00 | 1.94 | 0.00 | 19.80 |
| 812 | 0.00 | 0.00 | 0.00 | 1.88 | 0.00 | 18.91 |
| 1052 | 0.00 | 0.00 | 0.00 | 1.78 | 0.00 | 18.74 |
| 1316 | 0.00 | 0.00 | 0.00 | 1.52 | 0.00 | 18.14 |
| 1556 | 0.00 | 0.00 | 0.00 | 1.45 | 0.00 | 18.13 |

| M2-P5 | | | | | | |
|---|---|---|---|---|---|---|
| Time (hrs) | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 0.00 | 0.00 | 0.00 | 1.86 | 0.44 | 20.77 |
| 24 | 0.00 | 0.00 | 0.00 | 2.26 | 0.00 | 21.08 |
| 88 | 1.36 | 0.00 | 0.00 | 2.14 | 0.00 | 20.00 |
| 288 | 0.00 | 0.00 | 0.00 | 1.99 | 0.00 | 18.65 |
| 550 | 18.67 | 0.00 | 0.00 | 1.94 | 0.00 | 18.70 |
| 812 | 0.00 | 0.00 | 0.00 | 1.99 | 0.00 | 18.82 |
| 1052 | 0.00 | 0.00 | 0.00 | 1.89 | 0.00 | 18.08 |
| 1316 | 0.00 | 0.00 | 0.00 | 1.70 | 0.00 | 17.86 |
| 1556 | 0.00 | 0.00 | 0.00 | 1.55 | 0.00 | 17.43 |

| M2-P7 | | | | | | |
|---|---|---|---|---|---|---|
| Time (hrs) | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 1.28 | 0.00 | 0.00 | 2.68 | 0.00 | 22.55 |
| 24 | 0.00 | 0.00 | 0.00 | 2.64 | 0.00 | 21.25 |
| 88 | 2.48 | 0.00 | 0.00 | 2.36 | 0.00 | 19.95 |
| 288 | 0.00 | 0.00 | 0.00 | 2.37 | 0.00 | 20.67 |
| 550 | 21.26 | 0.00 | 0.00 | 2.21 | 0.00 | 19.89 |
| 812 | 0.00 | 0.00 | 0.00 | 2.12 | 0.00 | 19.15 |
| 1052 | 0.00 | 0.00 | 0.00 | 2.03 | 0.00 | 18.43 |
| 1316 | 0.00 | 0.00 | 0.00 | 1.85 | 0.00 | 18.23 |
| 1556 | 0.00 | 0.00 | 0.00 | 1.72 | 0.00 | 17.39 |

| M2-P9 | | | | | | |
|---|---|---|---|---|---|---|
| Time (hrs) | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 0.00 | 0.00 | 0.00 | 2.37 | 0.00 | 19.11 |
| 24 | 0.00 | 0.00 | 0.00 | 2.34 | 0.00 | 18.52 |
| 88 | 10.81 | 0.00 | 0.00 | 2.22 | 0.00 | 18.04 |
| 288 | 0.00 | 0.00 | 0.00 | 2.19 | 0.00 | 17.90 |
| 550 | 14.09 | 0.00 | 0.00 | 1.99 | 0.00 | 16.23 |
| 812 | 0.00 | 0.00 | 0.00 | 1.96 | 0.00 | 15.95 |
| 1052 | 0.00 | 0.00 | 0.00 | 1.89 | 0.00 | 15.46 |
| 1316 | 0.00 | 0.00 | 0.00 | 1.58 | 0.00 | 12.83 |
| 1556 | 0.00 | 0.00 | 0.00 | 1.45 | 0.00 | 13.07 |

| S2-P1 | | | | | | |
|---|---|---|---|---|---|---|
| Time (hrs) | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 7.16 | 0.00 | 0.00 | 0.29 | 6.87 | 29.28 |
| 23 | 3.38 | 0.00 | 0.54 | 1.56 | 3.79 | 29.03 |
| 100 | 0.00 | 0.00 | 1.85 | 2.11 | 0.12 | 28.88 |
| 263 | 0.00 | 0.00 | 1.79 | 1.56 | 0.00 | 28.38 |
| 479 | 0.00 | 0.00 | 1.67 | 1.45 | 0.00 | 26.97 |
| 749 | 2.45 | 0.00 | 1.62 | 1.32 | 0.00 | 26.42 |
| 986 | 0.00 | 0.00 | 1.66 | 1.18 | 0.00 | 25.47 |
| 1270 | 0.00 | 0.00 | 1.63 | 1.07 | 0.00 | 25.40 |
| 1510 | 0.00 | 0.00 | 1.69 | 0.99 | 0.00 | 24.80 |

| S2-P3 | | | | | | |
|---|---|---|---|---|---|---|
| Time (hrs) | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 3.32 | 0.00 | 2.29 | 1.06 | 1.58 | 27.97 |
| 23 | 1.38 | 0.00 | 2.95 | 1.14 | 0.10 | 26.99 |
| 100 | 0.00 | 0.00 | 3.02 | 1.09 | 0.00 | 27.62 |
| 263 | 0.00 | 0.00 | 2.54 | 1.00 | 0.00 | 25.91 |
| 479 | 0.00 | 0.00 | 2.10 | 0.95 | 0.00 | 25.88 |
| 749 | 2.39 | 0.00 | 1.65 | 0.86 | 0.00 | 24.27 |
| 986 | 0.00 | 0.00 | 1.53 | 0.89 | 0.00 | 23.35 |
| 1270 | 0.00 | 0.00 | 1.26 | 0.90 | 0.00 | 23.75 |
| 1510 | 0.00 | 0.00 | 1.11 | 0.80 | 0.00 | 23.22 |

| S2-P5 | | | | | | |
|---|---|---|---|---|---|---|
| Time (hrs) | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 0.00 | 0.00 | 2.77 | 1.09 | 0.18 | 26.56 |
| 23 | 0.58 | 0.00 | 2.77 | 1.08 | 0.00 | 25.45 |
| 100 | 0.00 | 0.00 | 2.71 | 1.02 | 0.00 | 26.94 |
| 263 | 0.00 | 0.00 | 2.14 | 0.99 | 0.00 | 25.47 |
| 479 | 0.00 | 0.00 | 1.75 | 0.94 | 0.00 | 25.18 |
| 749 | 2.53 | 0.00 | 1.43 | 0.91 | 0.00 | 24.36 |
| 986 | 0.00 | 0.00 | 1.21 | 0.87 | 0.00 | 23.15 |
| 1270 | 0.00 | 0.00 | 0.93 | 0.83 | 0.00 | 23.80 |
| 1510 | 0.00 | 0.00 | 0.77 | 0.75 | 0.00 | 22.96 |

| S2-P7 | | | | | | |
|---|---|---|---|---|---|---|
| Time (hrs) | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 0.00 | 0.00 | 2.73 | 1.00 | 0.00 | 24.35 |
| 23 | 1.17 | 0.00 | 2.40 | 1.00 | 0.00 | 24.23 |
| 100 | 0.00 | 0.00 | 1.90 | 0.97 | 0.00 | 24.20 |
| 263 | 0.00 | 0.00 | 1.44 | 0.96 | 0.00 | 22.20 |
| 479 | 0.00 | 0.00 | 1.14 | 0.90 | 0.00 | 22.78 |
| 749 | 3.06 | 0.00 | 0.93 | 0.79 | 0.00 | 22.68 |
| 986 | 0.00 | 0.00 | 0.73 | 0.81 | 0.00 | 20.90 |
| 1270 | 0.00 | 0.00 | 0.48 | 0.75 | 0.00 | 20.98 |
| 1510 | 0.00 | 0.00 | 0.34 | 0.66 | 0.00 | 20.55 |

| S2-P9 | | | | | | |
|---|---|---|---|---|---|---|
| Time (hrs) | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 0.00 | 0.00 | 2.11 | 0.88 | 0.00 | 20.28 |
| 23 | 0.00 | 0.00 | 2.00 | 0.86 | 0.00 | 20.42 |
| 100 | 0.00 | 0.00 | 1.66 | 0.77 | 0.00 | 19.77 |
| 263 | 0.00 | 0.00 | 1.20 | 0.74 | 0.00 | 19.00 |
| 479 | 0.00 | 0.00 | 0.81 | 0.69 | 0.00 | 18.23 |
| 749 | 3.45 | 0.00 | 0.52 | 0.57 | 0.00 | 15.55 |
| 986 | 0.00 | 0.00 | 0.32 | 0.57 | 0.00 | 14.33 |
| 1270 | 0.00 | 0.00 | 0.19 | 0.51 | 0.00 | 15.46 |
| 1510 | 0.00 | 0.00 | 0.03 | 0.49 | 0.00 | 13.54 |

| NL-P1 | | | | | | |
|---|---|---|---|---|---|---|
| Time (hrs) | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 6.49 | 0.00 | 0.00 | 0.21 | 11.84 | 35.38 |
| 96 | 4.62 | 0.00 | 0.00 | 0.52 | 9.34 | 34.46 |
| 360 | 0.00 | 0.00 | 0.00 | 0.00 | 3.90 | 40.21 |
| 672 | 0.00 | 0.00 | 0.00 | 0.00 | 2.00 | 37.52 |
| 936 | 0.00 | 0.00 | 0.00 | 0.00 | 0.74 | 37.31 |

| NL-P3 | | | | | | |
|---|---|---|---|---|---|---|
| Time (hrs) | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 5.50 | 0.00 | 0.00 | 0.19 | 10.18 | 31.34 |
| 96 | 4.52 | 0.00 | 0.00 | 0.29 | 9.44 | 30.92 |
| 360 | 3.51 | 0.00 | 0.24 | 1.10 | 7.46 | 37.06 |
| 672 | 0.00 | 0.00 | 0.00 | 0.00 | 3.22 | 37.28 |
| 936 | 0.00 | 0.00 | 0.00 | 0.00 | 1.62 | 35.37 |

| NL-P5 | | | | | | |
|---|---|---|---|---|---|---|
| Time (hrs) | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 4.42 | 0.00 | 0.00 | 0.24 | 10.79 | 32.16 |
| 96 | 2.95 | 0.00 | 0.00 | 0.26 | 9.84 | 31.27 |
| 360 | 4.18 | 0.00 | 0.16 | 0.52 | 7.09 | 30.51 |
| 672 | 10.19 | 0.00 | 0.20 | 1.05 | 5.66 | 37.53 |
| 936 | 8.27 | 0.00 | 0.23 | 1.16 | 3.64 | 35.67 |

| NL-P7 | | | | | | |
|---|---|---|---|---|---|---|
| Time (hrs) | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 3.44 | 0.00 | 0.00 | 0.18 | 10.09 | 29.54 |
| 96 | 2.59 | 0.00 | 0.00 | 0.26 | 8.66 | 27.76 |
| 360 | 2.74 | 0.00 | 0.09 | 0.38 | 6.74 | 26.67 |
| 672 | 2.52 | 0.00 | 0.12 | 0.63 | 4.73 | 26.06 |
| 936 | 3.08 | 0.00 | 0.15 | 0.71 | 3.35 | 25.00 |
| 1229 | 7.95 | 0.00 | 0.32 | 1.18 | 4.45 | 24.63 |
| 1468 | 2.37 | 0.00 | 0.18 | 0.78 | 1.83 | 24.90 |

| NL-P9 | | | | | | |
|---|---|---|---|---|---|---|
| Time (hrs) | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 3.18 | 0.00 | 0.00 | 0.19 | 7.76 | 26.02 |
| 96 | 2.88 | 0.00 | 0.00 | 0.26 | 7.91 | 26.69 |
| 360 | 2.63 | 0.00 | 0.08 | 0.33 | 6.35 | 25.97 |
| 672 | 2.39 | 0.00 | 0.09 | 0.44 | 4.77 | 24.51 |
| 936 | 3.07 | 0.00 | 0.12 | 0.52 | 3.88 | 24.47 |
| 1229 | 4.57 | 0.00 | 0.20 | 0.51 | 2.78 | 23.25 |
| 1468 | 2.75 | 0.00 | 0.12 | 0.61 | 2.21 | 23.05 |

| NC-P1 | | | | | | |
|---|---|---|---|---|---|---|
| Time (hrs) | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 143.31 | 2.42 | 0.00 | 0.00 | 4.20 | 22.25 |
| 22 | 54.06 | 1.00 | 0.00 | 0.03 | 4.43 | 20.34 |
| 46 | 32.88 | 1.08 | 0.00 | 0.07 | 4.49 | 19.76 |
| 116 | 18.90 | 0.89 | 0.00 | 0.10 | 4.58 | 20.02 |
| 189 | 10.68 | 0.60 | 0.00 | 0.16 | 3.90 | 17.30 |
| 286 | 11.05 | 0.76 | 0.00 | 0.16 | 4.18 | 17.55 |
| 502 | 10.11 | 0.42 | 0.00 | 0.15 | 4.09 | 16.10 |
| 718 | 9.66 | 0.38 | 0.00 | 0.16 | 3.95 | 15.86 |
| 790 | 7.78 | 0.59 | 0.00 | 0.13 | 4.10 | 15.84 |
| 1054 | 7.28 | 0.29 | 0.04 | 0.12 | 3.95 | 15.59 |
| 1318 | 6.42 | 0.32 | 0.07 | 0.14 | 3.94 | 15.11 |
| 1510 | 6.80 | 0.46 | 0.10 | 0.13 | 3.91 | 15.05 |

| NC-P3 | | | | | | |
|---|---|---|---|---|---|---|
| Time (hrs) | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 17.46 | 2.58 | 0.00 | 0.00 | 3.48 | 17.83 |
| 22 | 16.79 | 1.08 | 0.00 | 0.04 | 3.63 | 16.96 |
| 46 | 13.65 | 0.61 | 0.00 | 0.07 | 3.54 | 16.68 |
| 116 | 9.86 | 0.75 | 0.00 | 0.10 | 3.35 | 15.43 |
| 189 | 9.26 | 0.57 | 0.00 | 0.12 | 3.38 | 15.33 |
| 286 | 8.68 | 0.57 | 0.00 | 0.10 | 3.48 | 15.43 |
| 502 | 7.36 | 0.78 | 0.00 | 0.08 | 3.28 | 14.48 |
| 718 | 6.50 | 0.62 | 0.00 | 0.11 | 3.26 | 13.89 |
| 790 | 6.98 | 0.43 | 0.00 | 0.07 | 3.35 | 13.48 |
| 1054 | 4.99 | 0.35 | 0.01 | 0.08 | 3.29 | 13.78 |
| 1318 | 4.98 | 0.00 | 0.03 | 0.11 | 3.27 | 13.15 |
| 1510 | 5.10 | 0.56 | 0.01 | 0.09 | 3.26 | 13.12 |

| NC-P5 | | | | | | |
|---|---|---|---|---|---|---|
| Time (hrs) | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 14.52 | 1.55 | 0.00 | 0.03 | 3.37 | 16.71 |
| 22 | 10.61 | 0.98 | 0.00 | 0.07 | 3.25 | 16.39 |
| 46 | 10.58 | 0.74 | 0.00 | 0.10 | 3.32 | 15.87 |
| 116 | 8.75 | 0.81 | 0.00 | 0.10 | 3.18 | 15.07 |
| 189 | 8.40 | 0.87 | 0.00 | 0.09 | 3.26 | 14.95 |
| 286 | 6.45 | 0.58 | 0.00 | 0.09 | 3.18 | 14.89 |
| 502 | 6.53 | 0.47 | 0.00 | 0.08 | 3.29 | 13.54 |
| 718 | 6.56 | 0.62 | 0.00 | 0.11 | 3.28 | 14.01 |
| 790 | 7.04 | 0.43 | 0.00 | 0.07 | 3.37 | 13.59 |
| 1054 | 5.26 | 0.29 | 0.00 | 0.09 | 3.23 | 13.31 |
| 1318 | 4.34 | 0.00 | 0.04 | 0.10 | 3.06 | 12.98 |
| 1510 | 5.25 | 0.57 | 0.01 | 0.08 | 3.22 | 12.71 |

| NC-P7 | | | | | | |
|---|---|---|---|---|---|---|
| Time (hrs) | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 11.75 | 1.34 | 0.00 | 0.08 | 3.19 | 15.81 |
| 22 | 9.84 | 0.88 | 0.00 | 0.07 | 3.12 | 14.92 |
| 46 | 6.70 | 0.64 | 0.00 | 0.08 | 3.00 | 14.92 |
| 116 | 6.63 | 0.82 | 0.00 | 0.06 | 2.91 | 13.87 |
| 189 | 6.11 | 0.62 | 0.00 | 0.08 | 2.92 | 13.28 |
| 286 | 5.00 | 0.50 | 0.00 | 0.08 | 2.88 | 13.14 |
| 502 | 4.95 | 0.76 | 0.00 | 0.09 | 2.94 | 12.95 |
| 718 | 5.23 | 0.65 | 0.05 | 0.10 | 2.73 | 12.15 |
| 790 | 4.39 | 0.44 | 0.00 | 0.11 | 2.85 | 11.72 |
| 1054 | 3.72 | 0.00 | 0.00 | 0.11 | 2.70 | 11.50 |
| 1318 | 3.48 | 0.00 | 0.03 | 0.11 | 2.61 | 11.24 |
| 1510 | 4.00 | 0.00 | 0.08 | 0.12 | 2.69 | 11.14 |

| NC-P9 | | | | | | |
|---|---|---|---|---|---|---|
| 0 | 0 | | | | | |
| Time (hrs) | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 8.04 | 0.90 | 0.00 | 0.08 | 2.45 | 13.01 |
| 22 | 7.18 | 0.52 | 0.00 | 0.07 | 2.40 | 12.87 |
| 46 | 5.20 | 0.78 | 0.00 | 0.07 | 2.55 | 12.66 |
| 116 | 5.99 | 0.61 | 0.00 | 0.08 | 2.36 | 11.98 |
| 189 | 4.38 | 0.67 | 0.00 | 0.08 | 2.33 | 11.19 |
| 286 | 3.84 | 0.46 | 0.00 | 0.09 | 2.37 | 11.43 |
| 502 | 4.81 | 0.77 | 0.00 | 0.06 | 2.39 | 10.59 |
| 718 | 4.44 | 0.42 | 0.02 | 0.05 | 2.21 | 10.27 |
| 790 | 2.89 | 0.31 | 0.00 | 0.07 | 2.23 | 10.27 |
| 1054 | 4.04 | 0.29 | 0.05 | 0.06 | 2.10 | 9.59 |
| 1318 | 3.40 | 0.00 | 0.15 | 0.05 | 2.00 | 8.93 |
| 1510 | 2.78 | 0.00 | 0.17 | 0.06 | 2.00 | 8.35 |

## Appendix H. Chlorinated Compounds and Degradation Products Data – Round 2 (µM)

| NM-P1 | | | | | | |
|---|---|---|---|---|---|---|
| Time | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 1.67 | 0.00 | 0.00 | 0.00 | 1.00 | 1.99 |
| 24 | 1.39 | 0.00 | 0.00 | 0.04 | 0.47 | 2.06 |
| 48 | 1.47 | 0.00 | 0.00 | 0.06 | 0.18 | 1.84 |
| 96 | 1.37 | 0.00 | 0.00 | 0.16 | 0.00 | 2.08 |
| 144 | 1.85 | 0.00 | 0.00 | 0.17 | 0.00 | 2.18 |
| 336 | 1.90 | 0.00 | 0.00 | 0.21 | 0.00 | 2.15 |
| 504 | 0.00 | 0.00 | 0.00 | 0.17 | 0.00 | 2.19 |
| 744 | 0.00 | 0.00 | 0.00 | 0.16 | 0.00 | 2.03 |
| 1008 | 0.00 | 0.00 | 0.00 | 0.11 | 0.00 | 2.10 |
| 1248 | 0.00 | 0.00 | 0.00 | 0.13 | 0.00 | 1.95 |
| 1488 | 0.00 | 0.00 | 0.00 | 0.07 | 0.00 | 1.89 |

| NM-P3 | | | | | | |
|---|---|---|---|---|---|---|
| Time | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 2.57 | 0.00 | 0.00 | 0.22 | 0.84 | 3.08 |
| 24 | 1.49 | 0.00 | 0.00 | 0.51 | 0.13 | 2.66 |
| 48 | 1.05 | 0.00 | 0.00 | 0.49 | 0.00 | 2.54 |
| 96 | 1.62 | 0.00 | 0.00 | 0.54 | 0.00 | 2.65 |
| 144 | 1.59 | 0.00 | 0.00 | 0.49 | 0.00 | 2.74 |
| 336 | 1.54 | 0.00 | 0.00 | 0.41 | 0.00 | 2.66 |
| 504 | 0.00 | 0.00 | 0.00 | 0.35 | 0.00 | 2.49 |
| 744 | 0.00 | 0.00 | 0.00 | 0.30 | 0.00 | 2.37 |
| 1008 | 0.00 | 0.00 | 0.00 | 0.21 | 0.00 | 2.46 |
| 1248 | 0.00 | 0.00 | 0.00 | 0.16 | 0.00 | 2.26 |
| 1488 | 0.00 | 0.00 | 0.00 | 0.12 | 0.00 | 2.11 |

| NM-P5 | | | | | | |
|---|---|---|---|---|---|---|
| Time | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 1.56 | 0.00 | 0.00 | 0.22 | 0.53 | 2.31 |
| 24 | 0.71 | 0.00 | 0.00 | 0.47 | 0.05 | 2.38 |
| 48 | 1.48 | 0.00 | 0.00 | 0.52 | 0.00 | 2.33 |
| 96 | 1.38 | 0.00 | 0.00 | 0.47 | 0.00 | 2.31 |
| 144 | 1.60 | 0.00 | 0.00 | 0.43 | 0.00 | 2.37 |
| 336 | 1.98 | 0.00 | 0.00 | 0.38 | 0.00 | 2.53 |
| 504 | 0.00 | 0.00 | 0.00 | 0.33 | 0.00 | 2.33 |
| 744 | 0.00 | 0.00 | 0.00 | 0.29 | 0.00 | 2.31 |
| 1008 | 0.00 | 0.00 | 0.00 | 0.19 | 0.00 | 2.32 |
| 1248 | 0.00 | 0.00 | 0.00 | 0.13 | 0.00 | 2.11 |
| 1488 | 0.00 | 0.00 | 0.00 | 0.08 | 0.00 | 2.11 |

| NM-P7 | | | | | | |
|---|---|---|---|---|---|---|
| Time | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 0.00 | 0.00 | 0.00 | 0.54 | 0.00 | 2.35 |
| 24 | 1.00 | 0.00 | 0.00 | 0.62 | 0.00 | 2.59 |
| 48 | 0.94 | 0.00 | 0.00 | 0.54 | 0.00 | 2.54 |
| 96 | 2.00 | 0.00 | 0.00 | 0.51 | 0.00 | 2.64 |
| 144 | 1.88 | 0.00 | 0.00 | 0.49 | 0.00 | 2.74 |
| 336 | 0.00 | 0.00 | 0.00 | 0.44 | 0.00 | 2.74 |
| 504 | 0.00 | 0.00 | 0.00 | 0.37 | 0.00 | 2.68 |
| 744 | 0.00 | 0.00 | 0.00 | 0.34 | 0.00 | 2.68 |
| 1008 | 0.00 | 0.00 | 0.00 | 0.30 | 0.00 | 2.60 |
| 1248 | 0.00 | 0.00 | 0.00 | 0.18 | 0.00 | 2.60 |
| 1488 | 0.00 | 0.00 | 0.00 | 0.17 | 0.00 | 2.14 |

| NM-P9 | | | | | | |
|---|---|---|---|---|---|---|
| Time | CO (μM) | Acet (μM) | CS2 (μM) | CF (μM) | CT (μM) | TCE (μM) |
| 0 | 2.42 | 0.00 | 0.00 | 1.36 | 0.00 | 5.17 |
| 24 | 0.00 | 0.00 | 0.00 | 0.74 | 0.00 | 3.11 |
| 48 | 2.27 | 0.00 | 0.12 | 0.63 | 0.00 | 3.05 |
| 96 | 2.11 | 0.00 | 0.00 | 0.70 | 0.00 | 3.09 |
| 144 | 1.07 | 0.00 | 0.00 | 0.65 | 0.00 | 3.39 |
| 336 | 0.00 | 0.00 | 0.00 | 0.57 | 0.00 | 3.19 |
| 504 | 0.00 | 0.00 | 0.00 | 0.51 | 0.00 | 2.65 |
| 744 | 0.00 | 0.00 | 0.00 | 0.40 | 0.00 | 2.29 |
| 1008 | 0.00 | 0.00 | 0.00 | 0.32 | 0.00 | 1.80 |
| 1248 | 0.00 | 0.00 | 0.00 | 0.23 | 0.00 | 1.53 |

| NMFe--P1 | | | | | | |
|---|---|---|---|---|---|---|
| Time | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 6.45 | 0.00 | 0.00 | 0.57 | 27.16 | 42.63 |
| 24 | 9.28 | 0.00 | 0.24 | 1.99 | 18.85 | 43.73 |
| 48 | 9.78 | 0.00 | 0.47 | 3.39 | 12.55 | 43.74 |
| 89 | 10.36 | 0.00 | 0.60 | 4.83 | 6.54 | 41.06 |
| 192 | 7.74 | 0.00 | 0.67 | 7.20 | 1.23 | 41.43 |
| 336 | 0.00 | 0.00 | 0.57 | 7.50 | 0.00 | 38.51 |
| 504 | 0.00 | 0.00 | 0.56 | 7.89 | 0.00 | 39.01 |
| 744 | 0.00 | 0.00 | 0.32 | 7.96 | 0.00 | 36.42 |
| 984 | 0.00 | 0.00 | 0.37 | 8.03 | 0.00 | 35.27 |
| 1248 | 0.00 | 0.00 | 0.26 | 8.06 | 0.00 | 34.42 |
| 1488 | 0.00 | 0.00 | 0.18 | 7.75 | 0.00 | 32.36 |

| NMFe-P3 | | | | | | |
|---|---|---|---|---|---|---|
| Time | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 7.77 | 0.00 | 0.20 | 3.01 | 13.17 | 38.72 |
| 24 | 6.06 | 0.00 | 0.35 | 6.26 | 9.33 | 37.68 |
| 48 | 4.85 | 0.00 | 0.51 | 8.60 | 5.64 | 37.09 |
| 89 | 3.80 | 0.00 | 0.45 | 10.34 | 2.77 | 36.95 |
| 192 | 2.96 | 0.00 | 0.51 | 11.73 | 0.23 | 36.54 |
| 336 | 0.00 | 0.00 | 0.30 | 11.05 | 0.00 | 34.44 |
| 504 | 0.00 | 0.00 | 0.24 | 10.90 | 0.00 | 34.35 |
| 744 | 0.00 | 0.00 | 0.07 | 10.02 | 0.00 | 32.32 |
| 984 | 0.00 | 0.00 | 0.00 | 9.62 | 0.00 | 32.05 |
| 1248 | 0.00 | 0.00 | 0.00 | 8.06 | 0.00 | 29.73 |
| 1488 | 0.00 | 0.00 | 0.00 | 8.44 | 0.00 | 32.89 |

| NMFe-P5 | | | | | | |
|---|---|---|---|---|---|---|
| Time | CO (μM) | Acet (μM) | CS2 (μM) | CF (μM) | CT (μM) | TCE (μM) |
| 0 | 2.87 | 0.00 | 0.32 | 6.72 | 4.56 | 35.07 |
| 24 | 2.64 | 0.00 | 0.41 | 11.40 | 1.84 | 34.81 |
| 48 | 4.33 | 0.00 | 0.45 | 12.37 | 0.44 | 34.29 |
| 89 | 2.21 | 0.00 | 0.45 | 13.07 | 0.05 | 34.87 |
| 192 | 0.00 | 0.00 | 0.27 | 12.57 | 0.00 | 33.28 |
| 336 | 0.00 | 0.00 | 0.50 | 11.28 | 0.00 | 30.97 |
| 504 | 0.00 | 0.00 | 0.00 | 10.61 | 0.00 | 32.04 |
| 744 | 0.00 | 0.00 | 0.00 | 9.20 | 0.00 | 29.42 |
| 984 | 0.00 | 0.00 | 0.00 | 7.64 | 0.00 | 29.28 |
| 1248 | 0.00 | 0.00 | 0.00 | 6.29 | 0.00 | 27.10 |
| 1488 | 0.00 | 0.00 | 0.00 | 5.33 | 0.00 | 25.77 |

| NMFe-P7 | | | | | | |
|---|---|---|---|---|---|---|
| Time | CO (μM) | Acet (μM) | CS2 (μM) | CF (μM) | CT (μM) | TCE (μM) |
| 0 | 1.91 | 0.00 | 0.38 | 8.25 | 5.58 | 34.38 |
| 24 | 1.89 | 0.00 | 0.48 | 13.25 | 1.51 | 35.25 |
| 48 | 2.38 | 0.00 | 0.43 | 14.27 | 0.12 | 32.22 |
| 89 | 1.25 | 0.00 | 0.31 | 14.50 | 0.00 | 34.06 |
| 192 | 0.00 | 0.00 | 0.19 | 13.43 | 0.00 | 32.64 |
| 336 | 0.00 | 0.00 | 0.64 | 11.45 | 0.00 | 29.51 |
| 504 | 0.00 | 0.00 | 0.00 | 10.74 | 0.00 | 29.88 |
| 744 | 0.00 | 0.00 | 0.00 | 8.90 | 0.00 | 25.90 |
| 984 | 0.00 | 0.00 | 0.00 | 7.20 | 0.00 | 25.24 |
| 1248 | 0.00 | 0.00 | 0.00 | 5.67 | 0.00 | 21.77 |
| 1488 | 0.00 | 0.00 | 0.00 | 4.97 | 0.00 | 21.58 |

| NMFe-P9 | | | | | | |
|---|---|---|---|---|---|---|
| 0 | 1.87 | 0.00 | 0.46 | 10.90 | 0.87 | 30.80 |
| 24 | 1.23 | 0.00 | 0.43 | 11.98 | 0.00 | 31.72 |
| 48 | 1.91 | 0.00 | 0.35 | 11.95 | 0.00 | 30.49 |
| 89 | 1.22 | 0.00 | 0.26 | 12.02 | 0.00 | 30.95 |
| 192 | 1.92 | 0.00 | 0.09 | 11.66 | 0.00 | 29.10 |
| 336 | 0.00 | 0.00 | 0.11 | 10.73 | 0.00 | 27.30 |
| 504 | 0.00 | 0.00 | 0.00 | 9.71 | 0.00 | 25.28 |
| 744 | 0.00 | 0.00 | 0.00 | 8.68 | 0.00 | 21.61 |
| 984 | 0.00 | 0.00 | 0.00 | 7.43 | 0.00 | 19.57 |
| 1248 | 0.00 | 0.00 | 0.00 | 6.34 | 0.00 | 17.55 |
| 1488 | 0.00 | 0.00 | 0.00 | 5.32 | 0.00 | 15.40 |

| M2-P1 | | | | | | |
|---|---|---|---|---|---|---|
| Time | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 4.65 | 0.00 | 0.00 | 0.00 | 3.35 | 10.19 |
| 24 | 3.02 | 0.00 | 0.00 | 0.27 | 1.47 | 8.13 |
| 48 | 1.65 | 0.00 | 0.00 | 0.53 | 0.86 | 8.32 |
| 96 | 0.00 | 0.00 | 0.00 | 0.88 | 0.19 | 7.91 |
| 170 | 0.00 | 0.00 | 0.13 | 1.26 | 0.00 | 7.71 |
| 336 | 6.04 | 0.00 | 0.00 | 1.21 | 0.00 | 7.67 |
| 504 | 0.00 | 0.00 | 0.00 | 0.96 | 0.00 | 6.15 |
| 816 | 0.00 | 0.00 | 0.00 | 0.85 | 0.00 | 6.46 |
| 1032 | 0.00 | 0.00 | 0.00 | 0.76 | 0.00 | 5.95 |
| 1296 | 0.00 | 0.00 | 0.00 | 0.61 | 0.00 | 5.89 |
| 1488 | 0.00 | 0.00 | 0.00 | 0.48 | 0.00 | 5.58 |

| M2-P3 | | | | | | |
|---|---|---|---|---|---|---|
| Time | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 24 | 1.27 | 0.00 | 0.01 | 1.52 | 0.00 | 6.86 |
| 48 | 0.00 | 0.00 | 0.01 | 1.51 | 0.00 | 6.93 |
| 96 | 0.00 | 0.00 | 0.00 | 1.49 | 0.00 | 6.65 |
| 170 | 0.00 | 0.00 | 0.01 | 1.42 | 0.00 | 6.29 |
| 336 | 4.16 | 0.00 | 0.00 | 1.28 | 0.00 | 6.14 |
| 504 | 0.00 | 0.00 | 0.00 | 1.24 | 0.00 | 6.42 |
| 816 | 0.00 | 0.00 | 0.00 | 0.91 | 0.00 | 5.57 |
| 1032 | 0.00 | 0.00 | 0.00 | 1.09 | 0.00 | 8.12 |
| 1296 | 0.00 | 0.00 | 0.00 | 0.78 | 0.00 | 6.70 |
| 1488 | 0.00 | 0.00 | 0.00 | 0.58 | 0.00 | 6.56 |

| M2-P5 | | | | | | |
|---|---|---|---|---|---|---|
| Time | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 0.00 | 0.00 | 0.00 | 1.98 | 0.39 | 9.34 |
| 24 | 0.00 | 0.00 | 0.00 | 2.00 | 0.00 | 9.04 |
| 48 | 0.00 | 0.00 | 0.00 | 1.66 | 0.00 | 7.76 |
| 96 | 0.00 | 0.00 | 0.00 | 2.01 | 0.00 | 8.66 |
| 170 | 0.00 | 0.00 | 0.00 | 1.71 | 0.00 | 7.97 |
| 336 | 6.89 | 0.00 | 0.00 | 1.45 | 0.00 | 7.51 |
| 504 | 0.00 | 0.00 | 0.00 | 1.26 | 0.00 | 7.42 |
| 816 | 0.00 | 0.00 | 0.00 | 0.86 | 0.00 | 6.63 |
| 1032 | 0.00 | 0.00 | 0.00 | 0.69 | 0.00 | 6.51 |
| 1296 | 0.00 | 0.00 | 0.00 | 0.52 | 0.00 | 6.20 |
| 1488 | 0.00 | 0.00 | 0.00 | 0.40 | 0.00 | 5.77 |

| M2-P7 | | | | | | |
|---|---|---|---|---|---|---|
| Time | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 0.00 | 0.00 | 0.00 | 1.73 | 0.00 | 7.87 |
| 24 | 0.00 | 0.00 | 0.00 | 1.68 | 0.00 | 7.78 |
| 48 | 0.00 | 0.00 | 0.00 | 1.69 | 0.00 | 7.96 |
| 96 | 0.00 | 0.00 | 0.00 | 1.57 | 0.00 | 7.06 |
| 170 | 0.00 | 0.00 | 0.00 | 1.26 | 0.00 | 6.48 |
| 336 | 3.90 | 0.00 | 0.00 | 1.19 | 0.00 | 6.58 |
| 504 | 0.00 | 0.00 | 0.00 | 1.05 | 0.00 | 6.02 |
| 816 | 0.00 | 0.00 | 0.00 | 0.74 | 0.00 | 5.90 |
| 1032 | 0.00 | 0.00 | 0.00 | 0.57 | 0.00 | 5.42 |
| 1296 | 0.00 | 0.00 | 0.00 | 0.42 | 0.00 | 5.24 |
| 1488 | 0.00 | 0.00 | 0.00 | 0.31 | 0.00 | 7.96 |

| M2-P9 | | | | | | |
|---|---|---|---|---|---|---|
| Time | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 0.00 | 0.00 | 0.00 | 1.38 | 0.00 | 6.41 |
| 24 | 0.00 | 0.00 | 0.00 | 1.31 | 0.00 | 6.05 |
| 48 | 0.00 | 0.00 | 0.00 | 1.31 | 0.00 | 6.15 |
| 96 | 0.00 | 0.00 | 0.00 | 1.19 | 0.00 | 5.83 |
| 170 | 0.00 | 0.00 | 0.00 | 1.18 | 0.00 | 5.71 |
| 336 | 0.00 | 0.00 | 0.00 | 0.89 | 0.00 | 5.45 |
| 504 | 0.00 | 0.00 | 0.00 | 0.80 | 0.00 | 4.76 |
| 816 | 0.00 | 0.00 | 0.00 | 0.59 | 0.00 | 4.51 |
| 1032 | 0.00 | 0.00 | 0.00 | 0.42 | 0.00 | 4.13 |
| 1296 | 0.00 | 0.00 | 0.00 | 0.35 | 0.00 | 3.22 |
| 1488 | 0.00 | 0.00 | 0.00 | 0.24 | 0.00 | 3.16 |

| S2-P1 | | | | | | |
|---|---|---|---|---|---|---|
| Time | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 3 | 1.99 | 0.00 | 1.14 | 0.34 | 26.02 | 32.09 |
| 22 | 0.97 | 0.00 | 5.87 | 1.58 | 15.35 | 31.92 |
| 43 | 0.00 | 0.00 | 10.39 | 2.57 | 8.53 | 32.73 |
| 91 | 0.00 | 0.00 | 13.46 | 3.15 | 0.96 | 32.16 |
| 163 | 0.00 | 0.00 | 11.65 | 2.98 | 0.00 | 30.86 |
| 307 | 0.00 | 0.00 | 10.16 | 3.04 | 0.00 | 30.65 |
| 502 | 0.00 | 0.00 | 9.17 | 3.18 | 0.00 | 31.13 |
| 767 | 0.00 | 0.00 | 6.93 | 2.59 | 0.00 | 27.32 |
| 1003 | 0.00 | 0.00 | 6.35 | 2.54 | 0.00 | 26.76 |
| 1316 | 0.00 | 0.00 | 5.43 | 2.35 | 0.00 | 25.55 |
| 1555 | 0.00 | 0.00 | 6.30 | 2.68 | 0.00 | 32.40 |

| S2-P3 | | | | | | |
|---|---|---|---|---|---|---|
| Time | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 3 | 2.04 | 0.00 | 7.99 | 2.00 | 13.90 | 32.86 |
| 22 | 0.00 | 0.00 | 11.69 | 2.53 | 4.23 | 32.35 |
| 43 | 0.00 | 0.00 | 14.01 | 2.85 | 0.88 | 33.28 |
| 91 | 0.00 | 0.00 | 14.54 | 2.96 | 0.00 | 34.04 |
| 163 | 0.00 | 0.00 | 13.20 | 2.79 | 0.00 | 32.32 |
| 307 | 0.00 | 0.00 | 11.91 | 2.69 | 0.00 | 31.85 |
| 502 | 0.00 | 0.00 | 10.36 | 2.55 | 0.00 | 30.24 |
| 767 | 0.00 | 0.00 | 8.21 | 2.34 | 0.00 | 28.70 |
| 1003 | 0.00 | 0.00 | 7.75 | 2.26 | 0.00 | 29.21 |
| 1316 | 0.00 | 0.00 | 6.66 | 2.11 | 0.00 | 26.53 |
| 1555 | 0.00 | 0.00 | 5.85 | 1.91 | 0.00 | 24.76 |

| S2-P5 | | | | | | |
|---|---|---|---|---|---|---|
| Time | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 3 | 1.86 | 0.00 | 11.84 | 2.56 | 2.42 | 29.70 |
| 22 | 0.00 | 0.00 | 12.13 | 2.62 | 0.00 | 29.88 |
| 43 | 0.00 | 0.00 | 12.09 | 2.60 | 0.00 | 30.12 |
| 91 | 0.00 | 0.00 | 11.64 | 2.53 | 0.00 | 30.12 |
| 163 | 0.00 | 0.00 | 11.16 | 2.47 | 0.00 | 29.97 |
| 307 | 0.00 | 0.00 | 9.51 | 2.37 | 0.00 | 28.88 |
| 502 | 0.00 | 0.00 | 8.56 | 2.37 | 0.00 | 28.40 |
| 767 | 0.00 | 0.00 | 6.61 | 2.07 | 0.00 | 25.62 |
| 1003 | 0.00 | 0.00 | 6.16 | 2.01 | 0.00 | 25.29 |
| 1316 | 0.00 | 0.00 | 5.05 | 1.80 | 0.00 | 23.45 |
| 1555 | 0.00 | 0.00 | 4.61 | 1.64 | 0.00 | 21.64 |

| S2-P7 | | | | | | |
|---|---|---|---|---|---|---|
| Time | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 3 | 0.00 | 0.00 | 13.17 | 2.73 | 0.00 | 27.68 |
| 22 | 0.00 | 0.00 | 10.94 | 2.42 | 0.00 | 27.96 |
| 43 | 0.00 | 0.00 | 11.00 | 2.45 | 0.00 | 28.48 |
| 91 | 0.00 | 0.00 | 10.85 | 2.47 | 0.00 | 29.70 |
| 163 | 0.00 | 0.00 | 9.59 | 2.44 | 0.00 | 28.00 |
| 307 | 0.00 | 0.00 | 7.55 | 2.23 | 0.00 | 25.88 |
| 502 | 0.00 | 0.00 | 6.82 | 2.21 | 0.00 | 25.51 |
| 767 | 0.00 | 0.00 | 5.24 | 1.86 | 0.00 | 23.55 |
| 1316 | 0.00 | 0.00 | 3.72 | 1.62 | 0.00 | 20.53 |
| 1555 | 0.00 | 0.00 | 2.73 | 1.42 | 0.00 | 17.31 |

| S2-P9 | | | | | | |
|---|---|---|---|---|---|---|
| Time | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 3 | 0.00 | 0.00 | 10.54 | 2.42 | 0.00 | 25.22 |
| 22 | 0.00 | 0.00 | 9.23 | 2.23 | 0.00 | 25.27 |
| 43 | 0.00 | 0.00 | 9.25 | 2.24 | 0.00 | 24.91 |
| 91 | 0.00 | 0.00 | 8.71 | 2.23 | 0.00 | 25.63 |
| 163 | 0.00 | 0.00 | 7.70 | 2.19 | 0.00 | 24.00 |
| 307 | 0.00 | 0.00 | 5.55 | 1.98 | 0.00 | 19.89 |
| 502 | 0.00 | 0.00 | 1.94 | 1.80 | 0.00 | 17.29 |
| 767 | 0.00 | 0.00 | 0.69 | 1.22 | 0.00 | 12.46 |
| 1316 | 0.00 | 0.00 | 0.00 | 0.82 | 0.00 | 8.05 |
| 1555 | 0.00 | 0.00 | 0.00 | 0.72 | 0.00 | 7.80 |

| NL-P1 | | | | | | |
|---|---|---|---|---|---|---|
| Time | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 0.88 | 0.00 | 0.00 | 0.00 | 6.71 | 10.52 |
| 24 | 1.00 | 0.00 | 0.00 | 0.01 | 6.72 | 10.48 |
| 48 | 0.00 | 0.00 | 0.00 | 0.05 | 6.11 | 10.10 |
| 96 | 0.00 | 0.00 | 0.00 | 0.09 | 6.22 | 10.58 |
| 168 | 0.00 | 0.00 | 0.00 | 0.13 | 5.79 | 10.38 |
| 336 | 0.00 | 0.00 | 0.03 | 0.20 | 4.60 | 9.79 |
| 504 | 0.00 | 0.00 | 0.08 | 0.24 | 4.00 | 9.58 |
| 744 | 2.65 | 0.00 | 0.15 | 0.33 | 3.17 | 9.54 |
| 1153 | 0.00 | 0.00 | 0.20 | 0.39 | 2.05 | 8.71 |
| 1344 | 0.00 | 0.00 | 0.16 | 0.36 | 1.49 | 8.05 |
| 1512 | 5.94 | 0.00 | 0.28 | 0.45 | 1.24 | 7.87 |

| NL-P3 | | | | | | |
|---|---|---|---|---|---|---|
| Time | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 0.94 | 0.00 | 0.00 | 0.00 | 7.50 | 11.49 |
| 24 | 0.92 | 0.00 | 0.00 | 0.02 | 7.04 | 10.52 |
| 48 | 0.00 | 0.00 | 0.00 | 0.04 | 7.30 | 11.43 |
| 96 | 0.00 | 0.00 | 0.00 | 0.11 | 9.14 | 14.91 |
| 168 | 0.00 | 0.00 | 0.00 | 0.11 | 6.62 | 11.20 |
| 336 | 0.00 | 0.00 | 0.00 | 0.14 | 5.95 | 10.97 |
| 504 | 0.00 | 0.00 | 0.05 | 0.17 | 5.11 | 10.55 |
| 744 | 5.02 | 0.00 | 0.07 | 0.27 | 4.62 | 10.42 |
| 1153 | 0.00 | 0.00 | 0.05 | 0.30 | 3.31 | 9.59 |
| 1344 | 0.00 | 0.00 | 0.08 | 0.29 | 2.64 | 8.58 |
| 1512 | 2.00 | 0.00 | 0.03 | 0.25 | 1.82 | 6.56 |

| NL-P5 | | | | | | |
|---|---|---|---|---|---|---|
| Time | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 0.00 | 0.00 | 0.00 | 0.00 | 7.04 | 10.78 |
| 24 | 0.00 | 0.00 | 0.00 | 0.03 | 7.10 | 10.57 |
| 48 | 0.00 | 0.00 | 0.00 | 0.04 | 6.93 | 10.60 |
| 96 | 0.00 | 0.00 | 0.00 | 0.08 | 6.65 | 10.82 |
| 168 | 0.00 | 0.00 | 0.01 | 0.13 | 6.61 | 11.42 |
| 336 | 0.00 | 0.00 | 0.00 | 0.21 | 5.40 | 10.29 |
| 504 | 0.00 | 0.00 | 0.09 | 0.29 | 4.65 | 10.40 |
| 744 | 0.00 | 0.00 | 0.04 | 0.34 | 3.84 | 10.14 |
| 1153 | 0.00 | 0.00 | 0.07 | 0.41 | 2.63 | 9.47 |
| 1344 | 0.00 | 0.00 | 0.12 | 0.38 | 1.93 | 8.57 |
| 1512 | 3.20 | 0.00 | 0.08 | 0.40 | 1.81 | 8.73 |

| NL-P7 | | | | | | |
|---|---|---|---|---|---|---|
| Time | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 0.00 | 0.00 | 0.00 | 0.00 | 6.50 | 9.87 |
| 24 | 1.90 | 0.00 | 0.00 | 0.02 | 6.36 | 9.46 |
| 48 | 0.00 | 0.00 | 0.00 | 0.05 | 6.38 | 9.87 |
| 96 | 0.00 | 0.00 | 0.00 | 0.06 | 5.87 | 9.63 |
| 168 | 0.00 | 0.00 | 0.00 | 0.10 | 5.84 | 9.83 |
| 336 | 0.00 | 0.00 | 0.04 | 0.17 | 4.71 | 8.86 |
| 504 | 0.00 | 0.00 | 0.01 | 0.25 | 3.99 | 9.22 |
| 744 | 0.00 | 0.00 | 0.05 | 0.33 | 3.23 | 9.30 |
| 1153 | 0.00 | 0.00 | 0.02 | 0.38 | 2.10 | 8.54 |
| 1344 | 0.00 | 0.00 | 0.03 | 0.37 | 1.51 | 7.68 |
| 1512 | 0.00 | 0.00 | 0.03 | 0.40 | 1.29 | 7.78 |

| NL-P9 | | | | | | |
|---|---|---|---|---|---|---|
| Time | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 0 | 0.00 | 0.00 | 0.00 | 0.00 | 5.28 | 8.16 |
| 24 | 0.00 | 0.00 | 0.00 | 0.03 | 5.33 | 8.07 |
| 48 | 0.00 | 0.00 | 0.00 | 0.05 | 5.60 | 8.90 |
| 96 | 0.00 | 0.00 | 0.00 | 0.00 | 4.89 | 8.12 |
| 168 | 0.00 | 0.00 | 0.02 | 0.09 | 5.28 | 9.05 |
| 336 | 0.00 | 0.00 | 0.00 | 0.18 | 4.33 | 8.68 |
| 504 | 0.00 | 0.00 | 0.01 | 0.21 | 3.68 | 8.43 |
| 744 | 0.00 | 0.00 | 0.00 | 0.23 | 3.00 | 7.99 |
| 1153 | 0.00 | 0.00 | 0.01 | 0.25 | 2.16 | 7.16 |
| 1344 | 0.00 | 0.00 | 0.00 | 0.22 | 1.67 | 6.48 |
| 1512 | 0.00 | 0.00 | 0.00 | 0.24 | 1.54 | 6.42 |

| NC-P1 | | | | | | |
|---|---|---|---|---|---|---|
| Time | CO (μM) | Acet (μM) | CS2 (μM) | CF (μM) | CT (μM) | TCE (μM) |
| 5 | 1.13 | 0.00 | 0.00 | 0.00 | 47.30 | 57.60 |
| 24 | 0.00 | 0.00 | 0.00 | 0.00 | 41.88 | 52.18 |
| 46 | 1.24 | 0.00 | 0.37 | 0.06 | 42.18 | 53.02 |
| 94 | 0.00 | 0.00 | 0.70 | 0.17 | 39.41 | 52.79 |
| 171 | 1.55 | 0.00 | 1.02 | 0.26 | 32.74 | 49.05 |
| 338 | 1.72 | 0.00 | 1.52 | 0.49 | 24.19 | 45.95 |
| 509 | 1.56 | 0.00 | 2.00 | 0.69 | 18.78 | 43.65 |
| 742 | 1.50 | 0.00 | 2.43 | 1.04 | 13.00 | 46.19 |
| 1078 | 0.00 | 0.00 | 2.17 | 1.22 | 7.10 | 40.40 |
| 1270 | 1.14 | 0.00 | 2.14 | 1.28 | 4.85 | 38.44 |
| 1486 | 0.00 | 0.00 | 2.12 | 1.48 | 3.26 | 38.79 |

| NC-P3 | | | | | | |
|---|---|---|---|---|---|---|
| Time | CO (μM) | Acet (μM) | CS2 (μM) | CF (μM) | CT (μM) | TCE (μM) |
| 5 | 1.25 | 0.00 | 0.15 | 0.02 | 42.28 | 54.22 |
| 24 | 1.47 | 0.00 | 0.37 | 0.05 | 43.95 | 55.15 |
| 46 | 0.00 | 0.00 | 0.63 | 0.15 | 40.18 | 52.89 |
| 94 | 0.00 | 0.00 | 0.89 | 0.24 | 39.89 | 52.99 |
| 171 | 1.38 | 0.00 | 1.25 | 0.32 | 35.65 | 52.24 |
| 338 | 1.71 | 0.00 | 1.93 | 0.61 | 28.95 | 51.20 |
| 509 | 1.16 | 0.00 | 2.63 | 0.85 | 26.35 | 54.34 |
| 742 | 1.09 | 0.00 | 2.81 | 1.15 | 15.98 | 48.96 |
| 1078 | 0.00 | 0.00 | 2.55 | 1.35 | 9.58 | 44.18 |
| 1270 | 0.00 | 0.00 | 2.57 | 1.31 | 7.33 | 42.78 |
| 1486 | 0.00 | 0.00 | 2.58 | 1.51 | 4.88 | 43.22 |

| NC-P5 | | | | | | |
|---|---|---|---|---|---|---|
| Time | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 5 | 0.00 | 0.00 | 0.39 | 0.07 | 39.78 | 53.52 |
| 24 | 0.00 | 0.00 | 0.59 | 0.14 | 38.63 | 49.85 |
| 46 | 0.00 | 0.00 | 0.78 | 0.19 | 39.04 | 51.18 |
| 94 | 0.00 | 0.00 | 1.04 | 0.25 | 36.87 | 49.29 |
| 171 | 0.00 | 0.00 | 1.44 | 0.38 | 35.24 | 51.61 |
| 338 | 1.54 | 0.00 | 1.96 | 0.61 | 27.28 | 48.48 |
| 509 | 11.12 | 0.00 | 2.47 | 0.79 | 23.21 | 48.01 |
| 742 | 1.47 | 0.00 | 2.96 | 1.10 | 16.01 | 47.45 |
| 1078 | 0.00 | 0.00 | 2.87 | 1.31 | 9.90 | 43.28 |
| 1270 | 0.00 | 0.00 | 2.73 | 1.33 | 7.04 | 40.15 |
| 1486 | 0.00 | 0.00 | 2.64 | 1.36 | 4.60 | 37.67 |

| NC-P7 | | | | | | |
|---|---|---|---|---|---|---|
| Time | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 5 | 0.00 | 0.00 | 0.57 | 0.10 | 37.20 | 47.46 |
| 24 | 0.00 | 0.00 | 0.82 | 0.13 | 36.03 | 46.51 |
| 46 | 0.00 | 0.00 | 1.01 | 0.23 | 37.08 | 47.57 |
| 94 | 0.00 | 0.00 | 1.35 | 0.35 | 35.48 | 47.23 |
| 171 | 0.88 | 0.00 | 1.63 | 0.45 | 32.80 | 47.79 |
| 338 | 1.42 | 0.00 | 2.24 | 0.72 | 25.90 | 45.37 |
| 509 | 11.31 | 0.00 | 2.80 | 0.93 | 21.18 | 43.57 |
| 742 | 0.84 | 0.00 | 3.02 | 1.32 | 13.86 | 41.78 |
| 1078 | 0.00 | 0.00 | 3.12 | 1.63 | 8.41 | 40.03 |
| 1270 | 0.00 | 0.00 | 2.95 | 1.65 | 5.77 | 37.33 |
| 1486 | 0.00 | 0.00 | 2.86 | 1.86 | 3.69 | 37.18 |

| NC-P9 | | | | | | |
|---|---|---|---|---|---|---|
| Time | CO (µM) | Acet (µM) | CS2 (µM) | CF (µM) | CT (µM) | TCE (µM) |
| 5 | 0.00 | 0.00 | 0.79 | 0.17 | 35.14 | 45.49 |
| 24 | 0.00 | 0.00 | 1.03 | 0.31 | 34.00 | 44.72 |
| 46 | 1.43 | 0.00 | 1.29 | 0.30 | 33.12 | 44.55 |
| 94 | 0.00 | 0.00 | 1.68 | 0.43 | 32.03 | 43.76 |
| 171 | 0.00 | 0.00 | 2.11 | 0.63 | 30.97 | 46.79 |
| 338 | 1.37 | 0.00 | 2.42 | 0.88 | 22.64 | 41.75 |
| 509 | 10.09 | 0.00 | 2.85 | 1.05 | 18.84 | 39.66 |
| 742 | 0.00 | 0.00 | 3.05 | 1.44 | 12.68 | 38.24 |
| 1078 | 0.00 | 0.00 | 2.71 | 1.53 | 7.08 | 32.05 |
| 1270 | 0.00 | 0.00 | 2.39 | 1.34 | 4.54 | 26.85 |
| 1486 | 0.00 | 0.00 | 2.51 | 1.65 | 3.18 | 27.50 |

## Appendix I. DNA Analysis Data

| Sample name | Concentration (ng/uL) |
|---|---|
| NM-P1 | 0.03 |
| NM-P3 | 0.06 |
| NM-P5 | 0 |
| NM-P7 | 0.0672 |
| NM-P9 | 0.225 |
| M2-P1 | 0.11 |
| M2-P3 | 0.141 |
| M2-P5 | 0.352 |
| M2-P7 | 0.234 |
| M2-P9 | 0.088 |
| S2-P1 | 0 |
| S2-P3 | 0.0372 |
| S2-P5 | 0.148 |
| S2-P7 | 0.209 |
| S2-P9 | 0.642 |
| NL-P1 | 0.03 |
| NL-P3 | 0 |
| NL-P5 | 0 |
| NL-P7 | 0 |
| NL-P9 | 0 |
| NC-P1 | 0 |
| NC-P3 | 0 |
| NC-P5 | 0 |
| NC-P7 | 0 |
| NC-P9 | 0 |

# Appendix J. Key Words

Chlorinated solvent

Abiotic degradation

Active to passive transition

Reduction potential

Tricholorethene

Carbon tetrachloride