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Using Factor Analysis to Assess Bioremediation Performance at a Contaminated Site in South America

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Positive Matrix Factorization (PMF)

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Using positive matrix factorization to investigate microbial dehalogenation of chlorinated benzenes in groundwater at a historically contaminated site

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- Leverage existing investment in data collection!
- Improves understanding and interrogation of the data:
  - Can determine how much of a contaminant is from multiple primary sources vs. degradation; and
  - Can reveal trends in redox conditions.
- Harnesses existing information through meta-analysis.

PMF Workflow Diagram

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Field sampling
-Soil or sediment
-Surface water
-Waste water
-Ground water
-Air
-Biota

Database
-Conc. data
-Analytical method
-Ancillary data
-Spatial Coordinates

Analysis:

Positive Matrix Factorization

PMF2 model

Eqn: X = G F + E

Input Matrices
-Data (Conc.)
-Detection Limit
-Uncertainty

Model Output
- Source profiles or "fingerprints"
- Loading amount of each source

Study Site in South America

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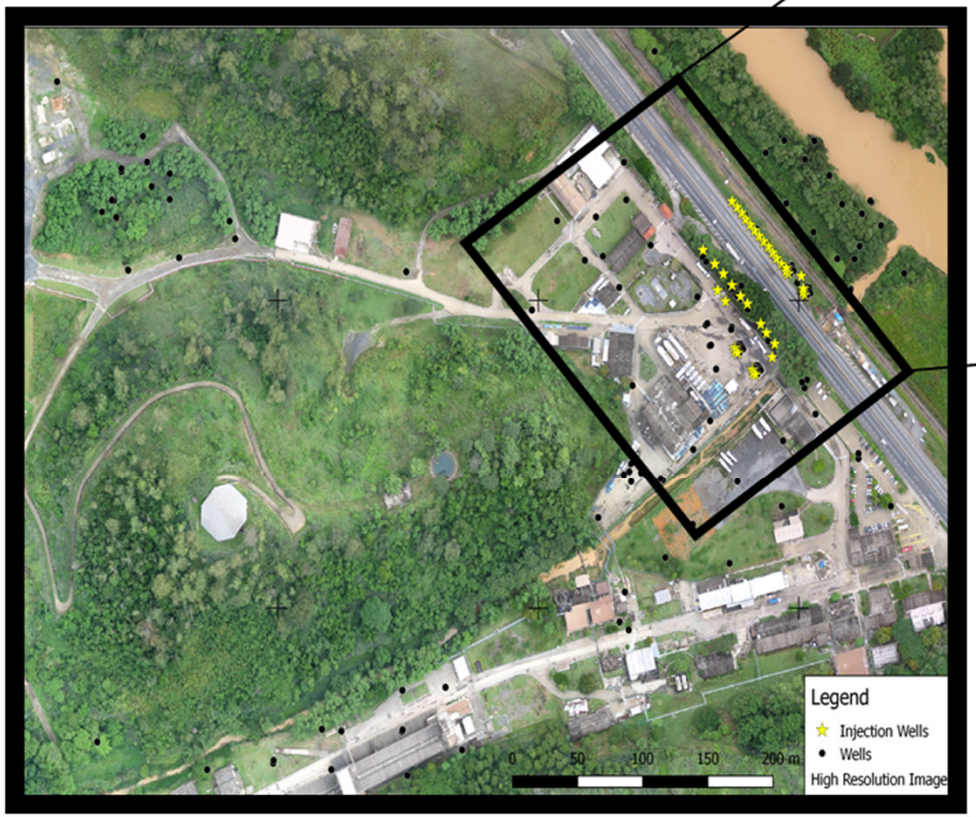

- Specialty chemical manufacturing facility
- Biotreatment system operating since 2011

History of Electron Donor Injections

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Remedy	Time Interval
MNA	Jan. 2004 – Dec. 2010
ERD Donor solution #1	Jan. 2011 – Nov. 2013
MNA	Dec. 2013 - May 2015
ERD Donor solution #2	June 2015 - April 2017
ERD Donor solution #3	May 2017 - Present

- MNA – Monitored Natural Attenuation
- ERD – Enhanced Reductive Dechlorination

Objectives

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- Analyze groundwater database using PMF2;
- Examine fingerprints indicative of dechlorination or other transformations;
- Examine time trends of fingerprints;
- Look at spatial trends;
- Investigate the relationships between contaminant fingerprints and secondary data; and
- Use results from the above tasks and assess bioremediation performance.

Halomethanes

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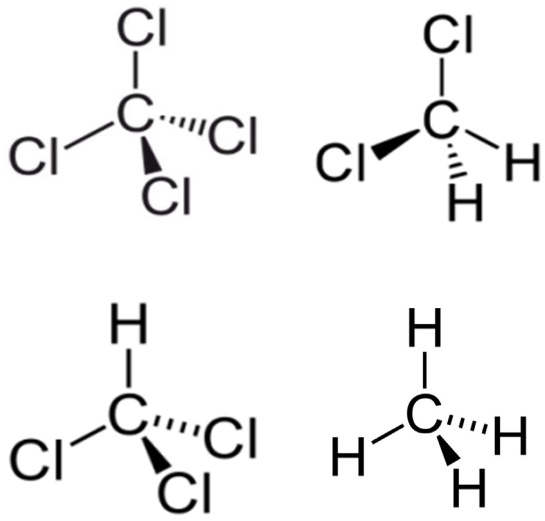
- **Input Data Summary**
  - 177 samples
  - 33% BDL
  - January 29, 2004 - March 24, 2017
  - 65 wells



- **Analytes**:
  - Carbon tetrachloride (CTC)
  - Chloroform, trichloromethane (TCM)
  - Methylene chloride, dichloromethane (DCM)
  - Methane
  - Not included: Chloromethane (n = 7)

4-Factor Halomethane Solution

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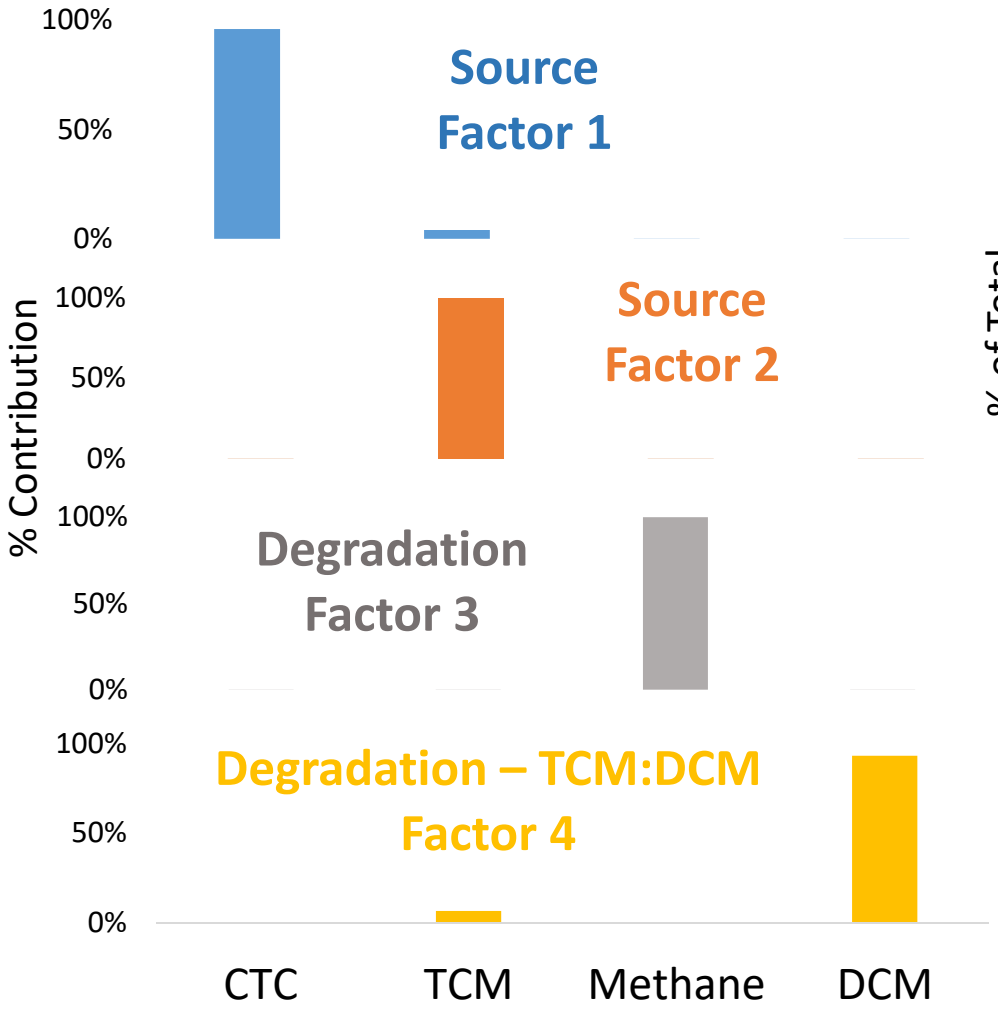
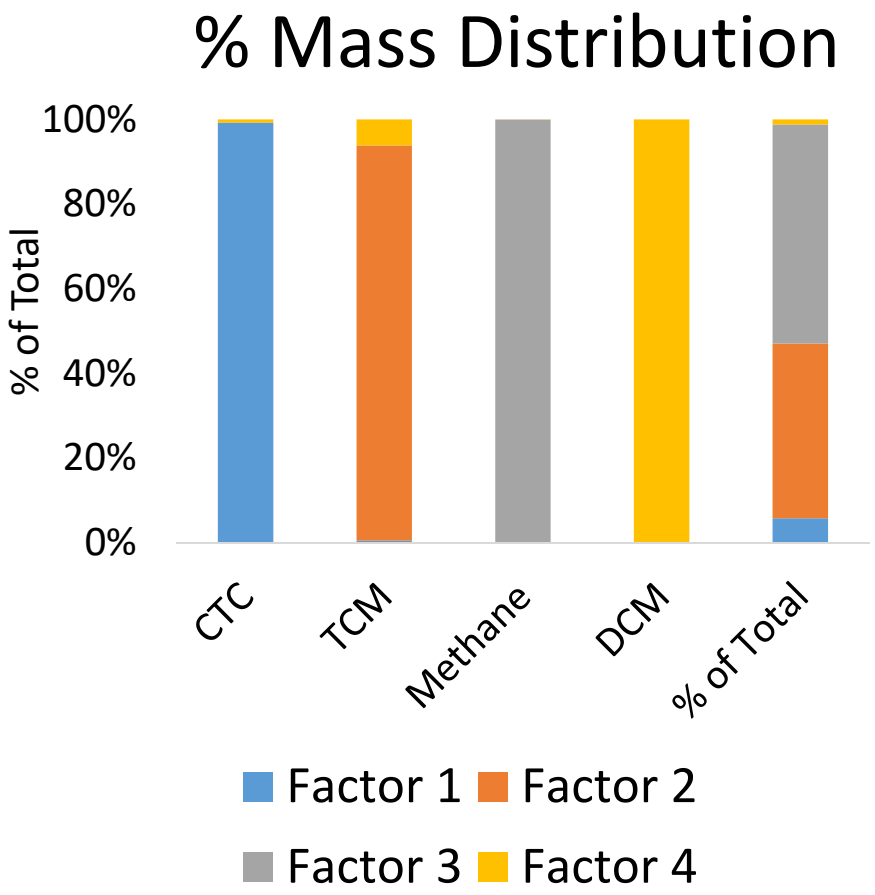
"Fingerprints"





Comparison to Another Site

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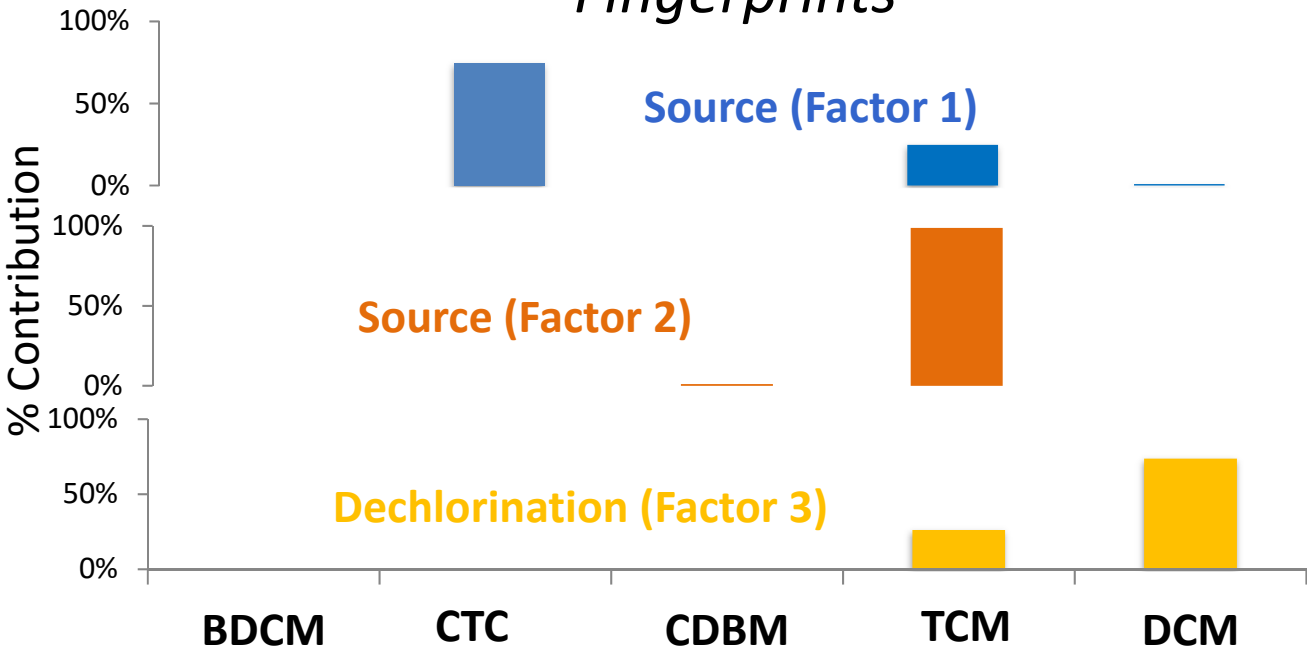
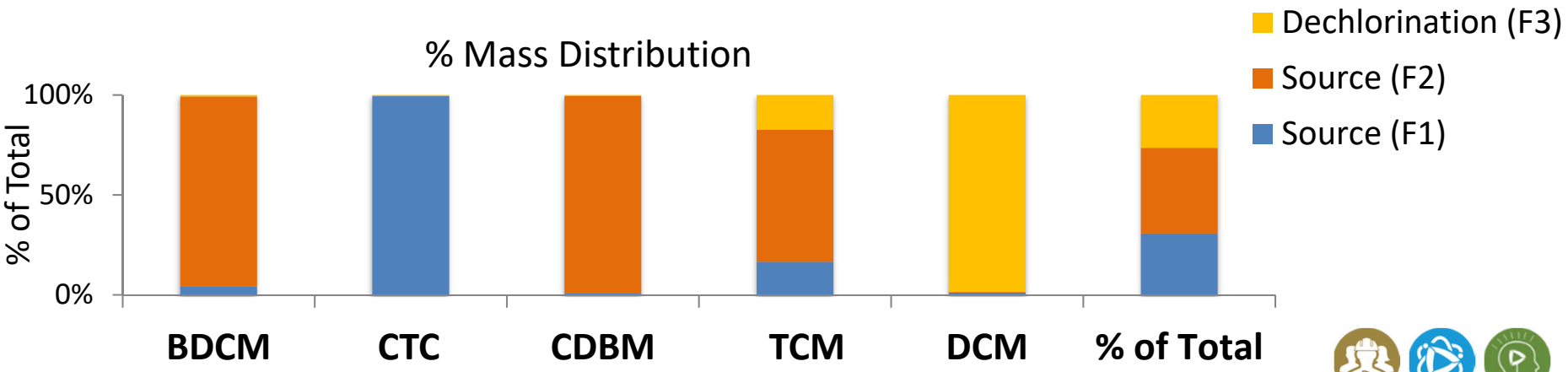
"Fingerprints"



Input Data:

- Industrial Site in USA
- 1990-2011
- 87 samples
- 42% BDL
- 52 wells
- 3 Factors Resolved



Take away notes -

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- PMF offer unique ability to resolve the kind of intractable combination of processes that occur in groundwater systems
  - Individual degradation processes can serve as separate ‘sources’
  - The PMF model is a source apportionment tool

Temporal Trends: Monitoring Well

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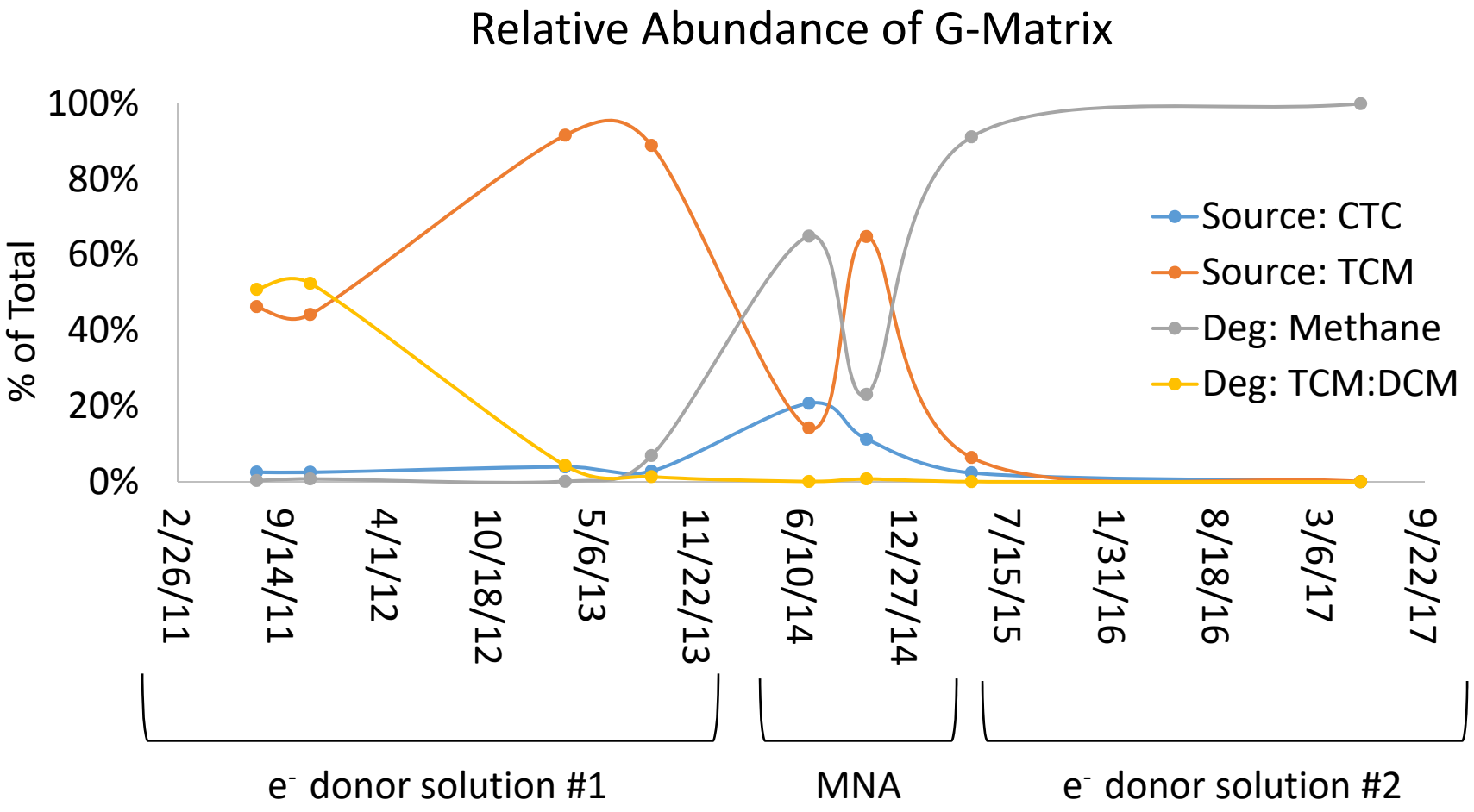

Located ~1.4m away from an injection well

Annual Trends: Factor Loading Amount

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The average percent of the total concentration of each factor in each year

	Year	Source: CTC	Source: TCM	Degradation: DCM:TCM	Degradation: Methane
MNA	2004	9%	46%	10%	35%
	2009	30%	67%	3%	0%
ERD	2011	5%	67%	27%	0%
	2012	11%	82%	6%	1%
MNA	2013	14%	50%	0%	36%
	2014	12%	29%	0%	59%
	2015	9%	31%	0%	60%
ERD	2016	52%	47%	0%	0%
	2017	9%	37%	0%	54%

Amendments did not promote CTC and TCM dechlorination to DCM

Correlations with Secondary Data

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- Dissolved Oxygen (DO)
- Oxidation Reduction Potential (ORP)
- pH
- Temperature (Temp.)
- Turbidity
- Total Organic Carbon (TOC)
- Total Iron
- Sulfate

Spearman's Rank Order Correlations

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Correlations to the 4-Factor Halomethane PMF Solution
Rank of % of total vs rank of secondary data

% Factor	DO (mg/L)	ORP (mV)	Sulfate (mg/L)	Total Iron (µg/L)	TOC (mg/L)	pH (UPH)	Temp. (℃)	Turbidity (NTU)	Specific Conductance (µS/cm)	Vinyl Chloride (ug/L)
Source: CTC	0	+	0	--	--	0	0	--	--	--
Source: TCM	0	+	0	--	0	--	--	--	--	--
Degradation TCM:DCM	0	0	0	0	0	--	+	+	+	--
Degradation: Methane	0	--	0	+	+	+	0	0	0	+
n	96	71	102	103	95	113	96	101	96	52

+	Positive Correlation
--	Negative Correlation
0	No Correlation

Chlorinated ethenes

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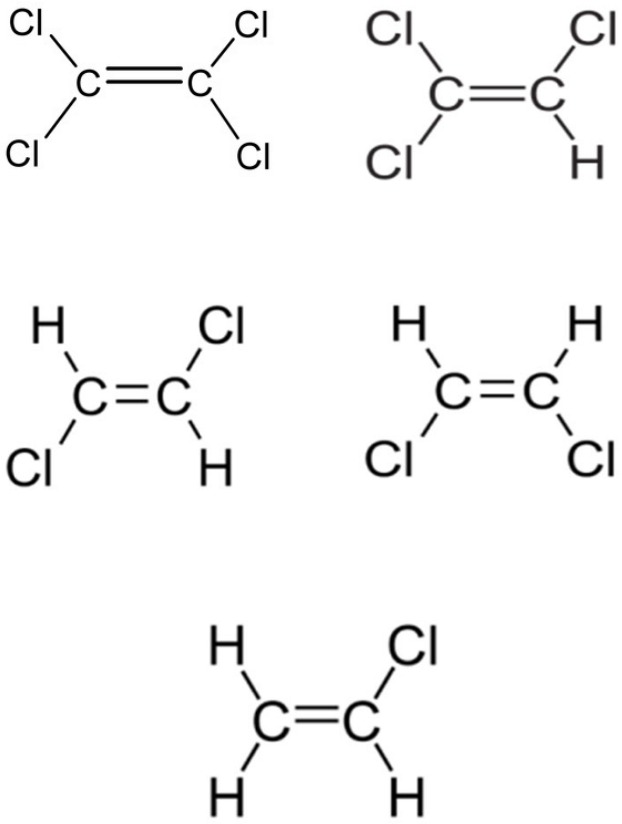
- 81 samples
- Dataset 17% BDL
- January 29, 2004 - March 24, 2017
- 61 wells

- Tetrachloroethene (PCE)
- Trichloroethene (TCE)
- *cis*-1,2-Dichloroethene (cDCE)
- *trans*-1,2-Dichloroethene (tDCE)
- Vinyl Chloride (VC)



<u>Not included</u>

Ethene (n = 20)

Ethane (n = 6)

4-Factor Chlorinated Ethene Solution

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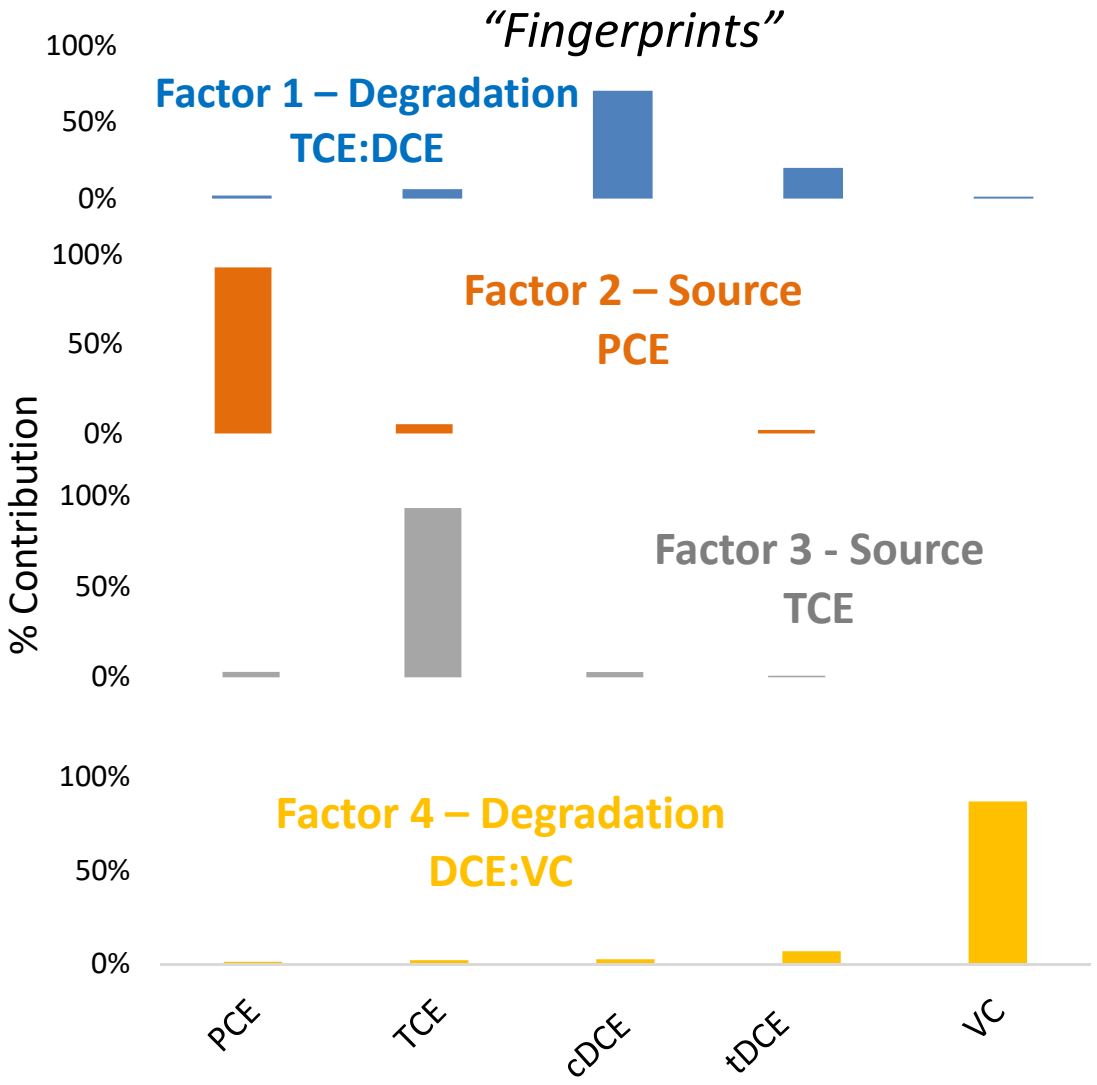

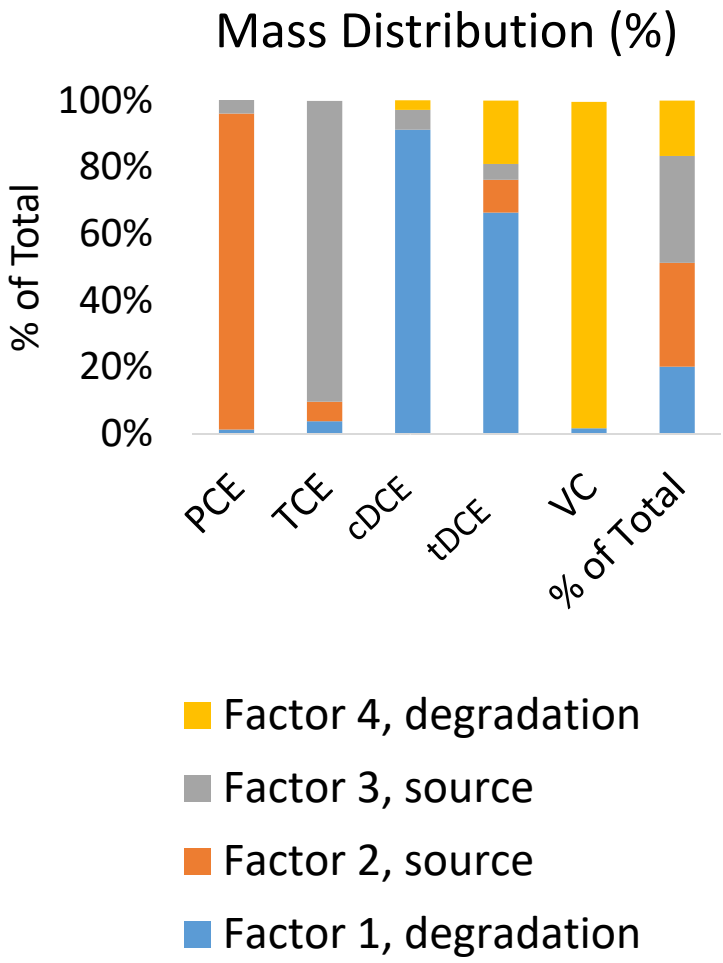

Comparison to Another Site

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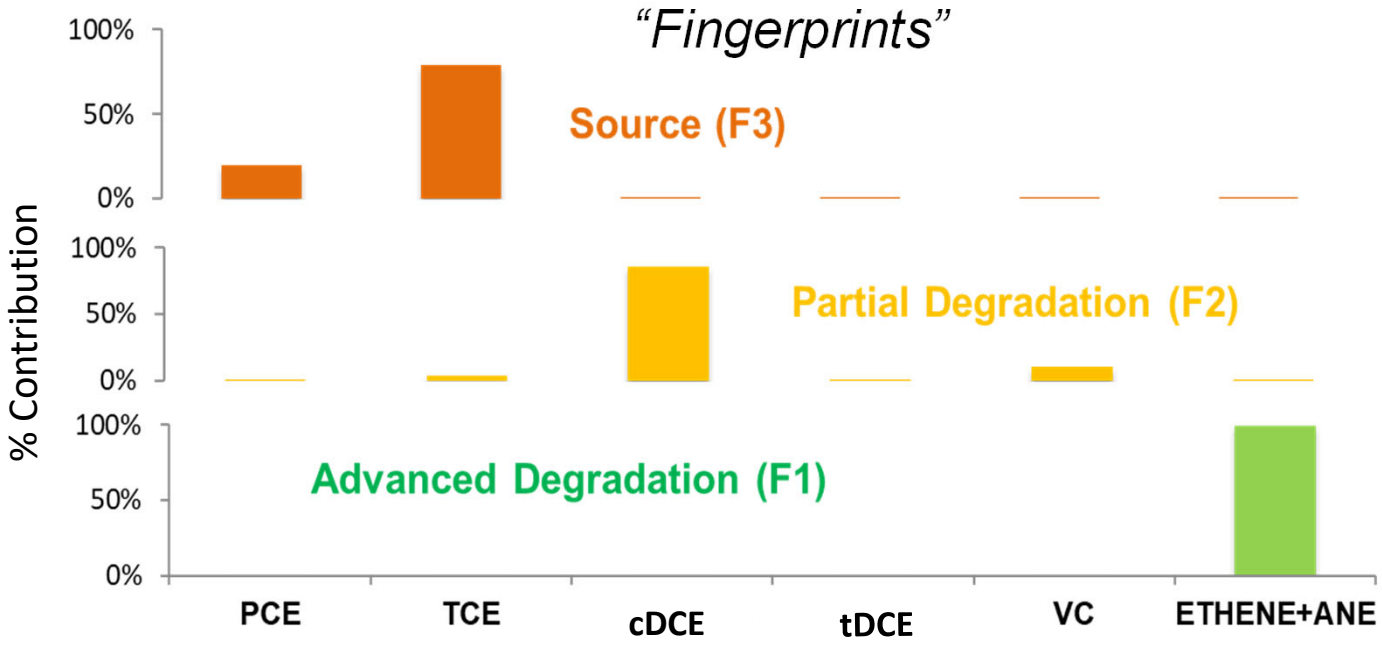
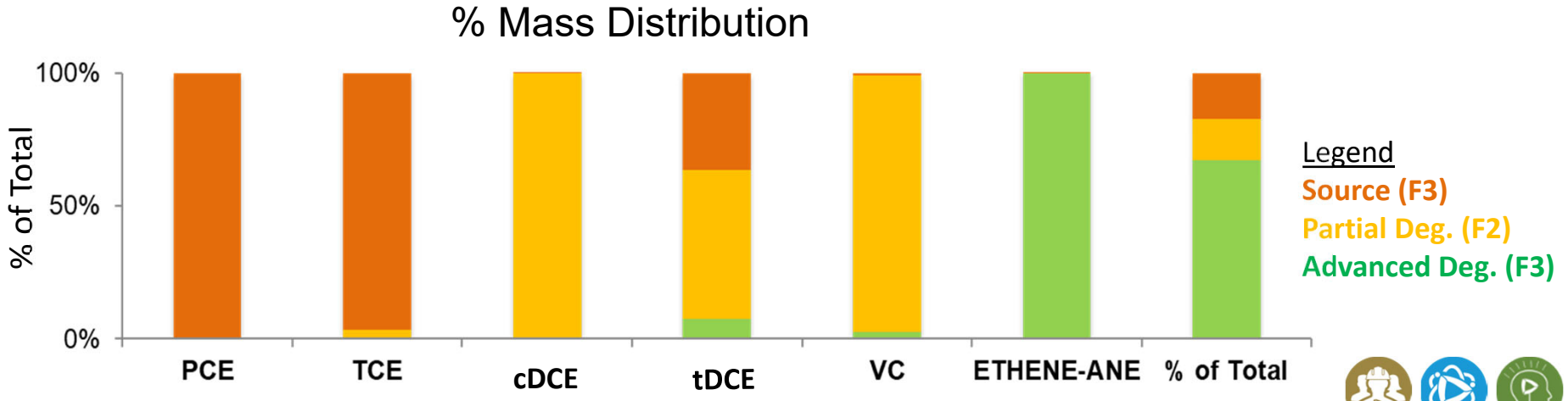


Input Data

- Industrial Site in USA
- Pump and Treat
- 2005-2011
- 76 samples
- 35% BDL
- 41 wells
- 3 Factors Resolved



Annual Trends: Factor Loading Amount

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The average percent of the total concentration of each factor in each year

	Year	Source: PCE	Source: TCE	Degradation: TCE:DCE	Degradation: DCE:VC
MNA	2004	38%	21%	16%	25%
MNA	2009	17%	30%	29%	24%
ERD	2011	31%	60%	6%	3%
ERD	2012	60%	12%	17%	12%
MNA	2013	21%	27%	38%	13%
MNA	2014	29%	14%	36%	21%
ERD	2015	30%	23%	15%	32%
ERD	2016	17%	41%	10%	32%
ERD	2017	34%	41%	15%	11%

Compare Redox Conditions

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Interpretation of Factor	Chlorinated Ethenes		Halomethanes	
South America: Source(s)	**Positive Correlations** **pH, Total Fe, Spec. Cond.**	**Negative Correlations** None	**Positive Correlations** ORP	**Negative Correlations** pH, Total Fe, TOC, Temp., Turbidity, Spec. Cond.
South America: Degradation pathways	**pH, Total Fe,** Methane, Temperature, Spec. Cond.	ORP, Sulfate	**pH, Total Fe,** TOC, Turbidity, Temp., Turbidity, **Spec. Cond.**	ORP
USA: Source(s)	**Positive Correlations** None	**Negative Correlations** ORP, ALK	**Positive Correlations** DO, **Ferric Fe**	**Negative Correlations** TOC, Temp.
USA: Degradation pathways	**Ferric Iron,** Methane, ALK	Sulfate	**pH,** TOC, ORP	None

Benefits & Future Directions

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Benefits

- Leverage existing investment in data collection;
- Improves understanding and interrogation of the data; and
- Motivation of the industry to moving into using meta-analysis in order to harness existing information.

Future Directions

- Closer evaluation the performance of the biotreatment system;
- Explore the spatial analysis;
- Integrate other COCs & evaluate sediment data; and
- Test approach on a unique data set (e.g., $\delta^{13}C$ data) collected from a CSIA study at the Site.

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Questions?

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