

Source Allocation of PCBs Derived from Quantile Analysis of Cumulative Response Curves Combined with Monte Carlo Analysis

Eric L. Butler, Ph.D.; Gradient

Jeffrey T. Rominger, Ph.D.; Gradient

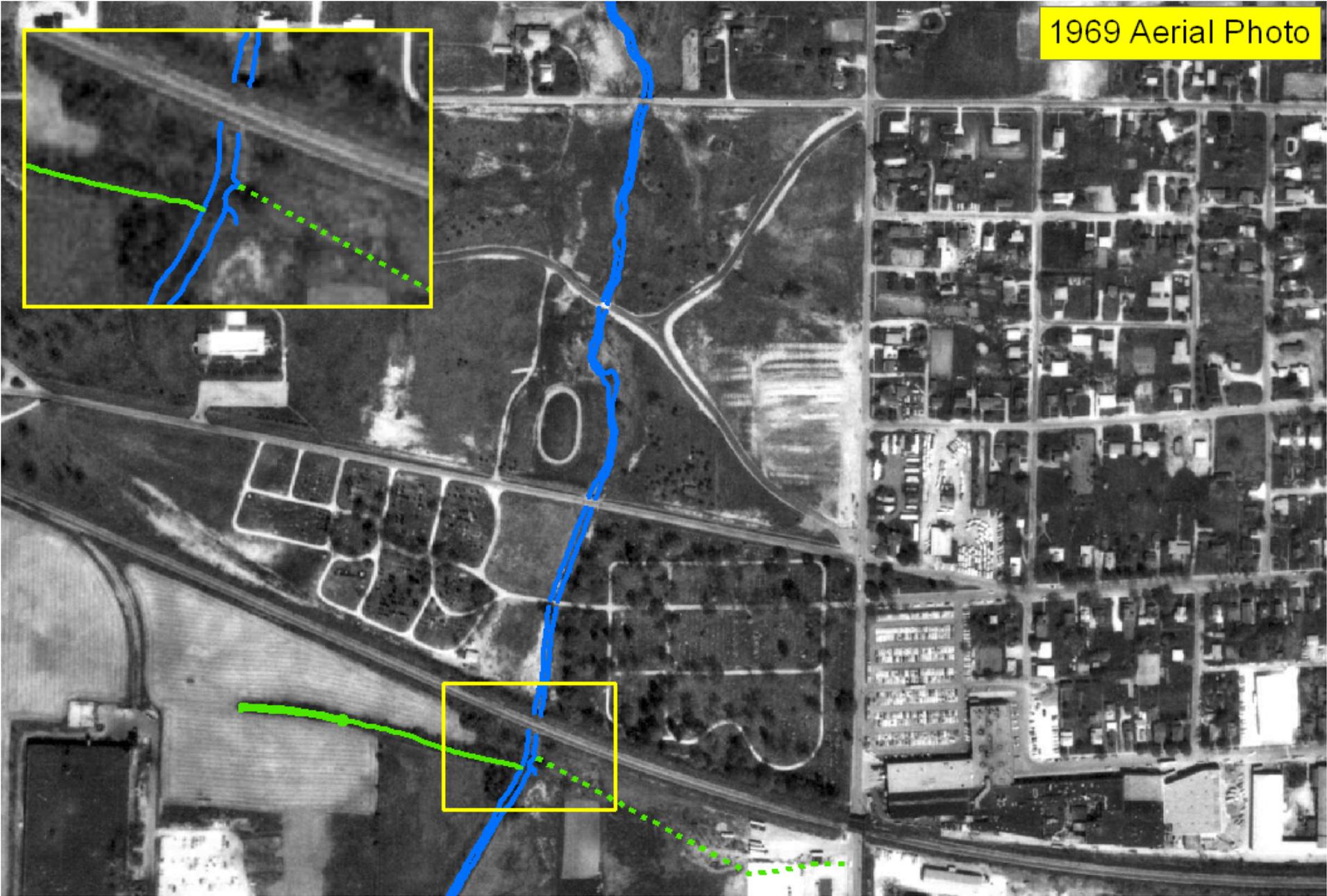
Kim Reynolds Reid; Gradient

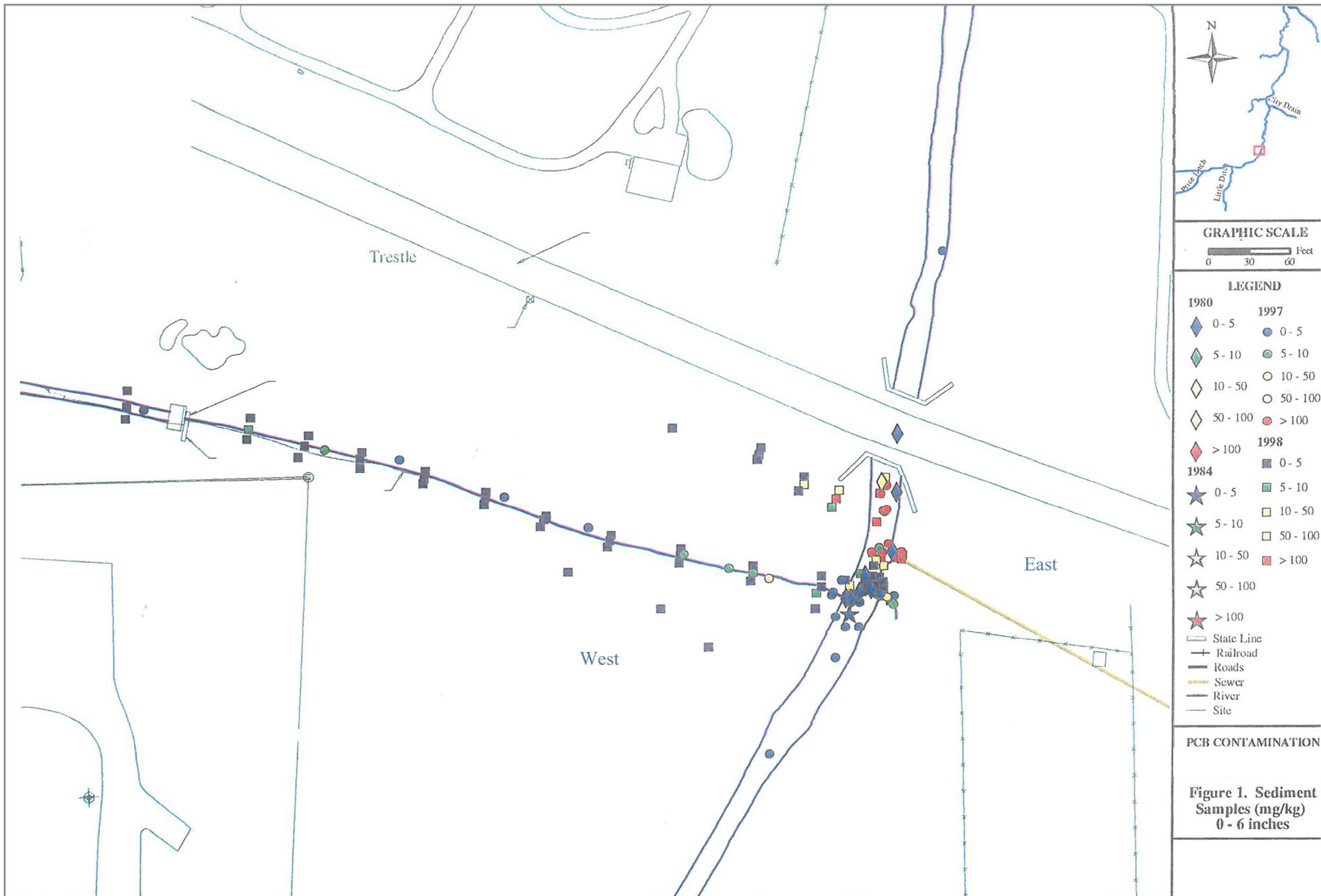
Kathleen A. Radloff, Ph.D.

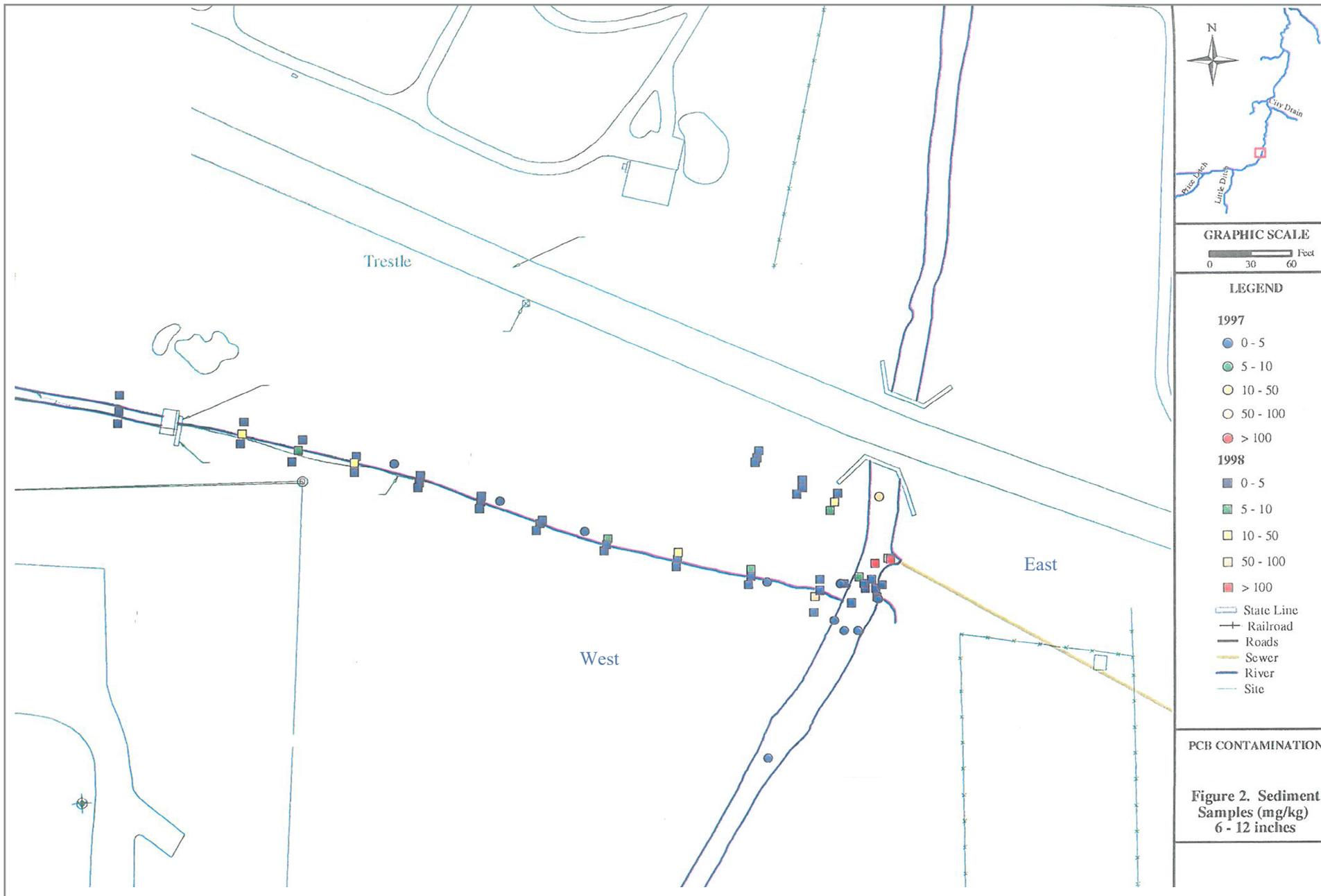
Remy J-C Hennet , Ph.D.; SS Papadopoulos & Associates, Inc.

Battelle International Conference on Remediation and Management of Contaminated Sediments
February 13, 2019

1969 Aerial Photo





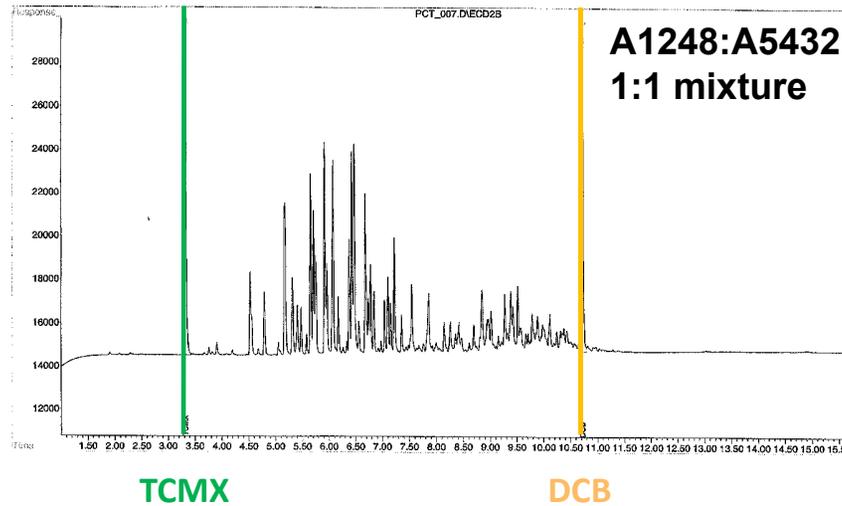
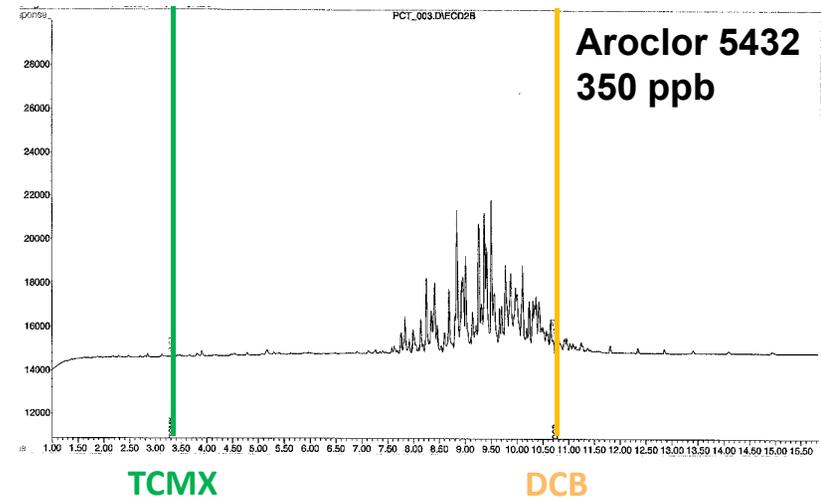
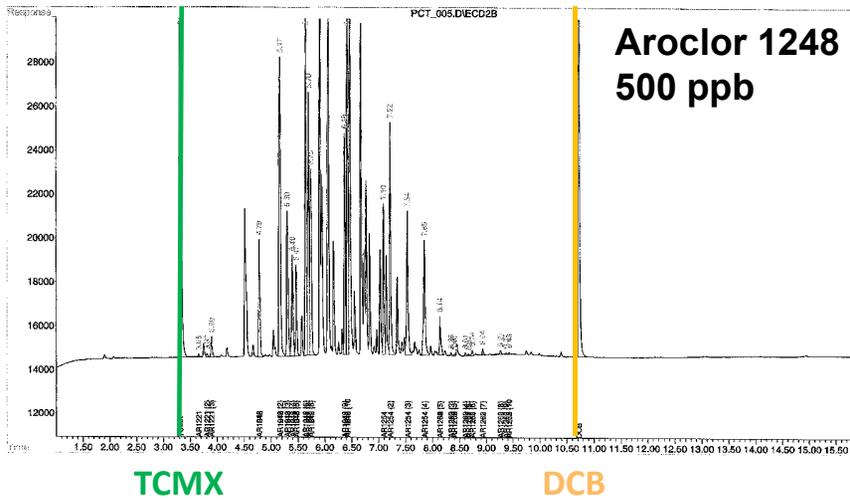


Other Factors in Cost Allocation

- Size of operations: number and type of machines
- Volumes of hydraulic fluids purchased
- Hydraulic fluid storage: drums *vs.* ASTs
- Pathways
- Years of operation

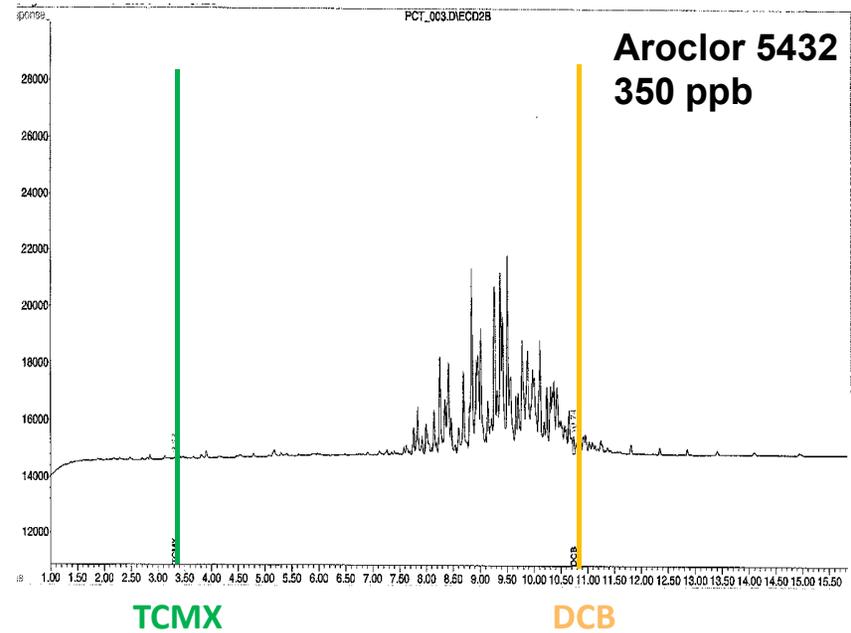
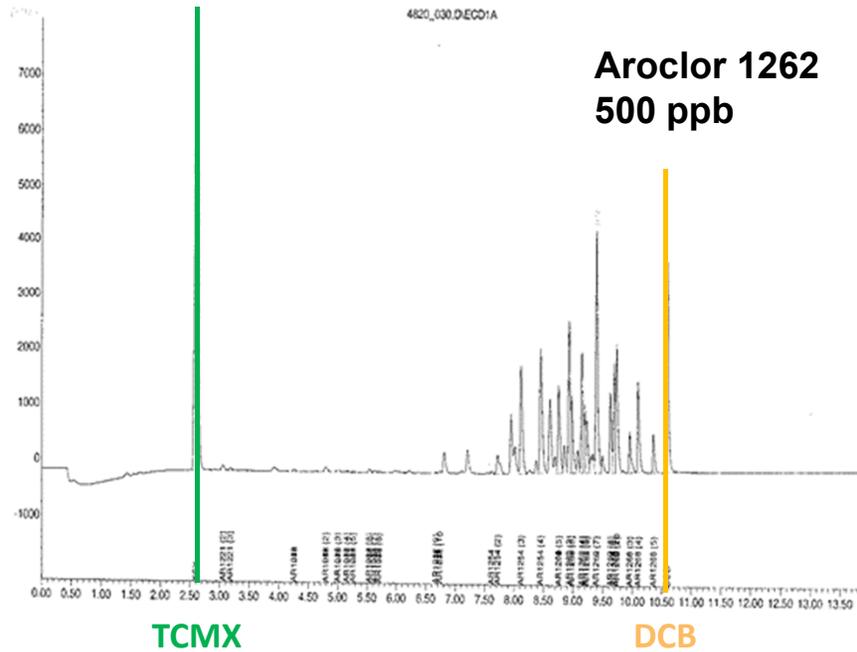
Heritage PCT standards

Heritage Lab Method 8082 DB-5



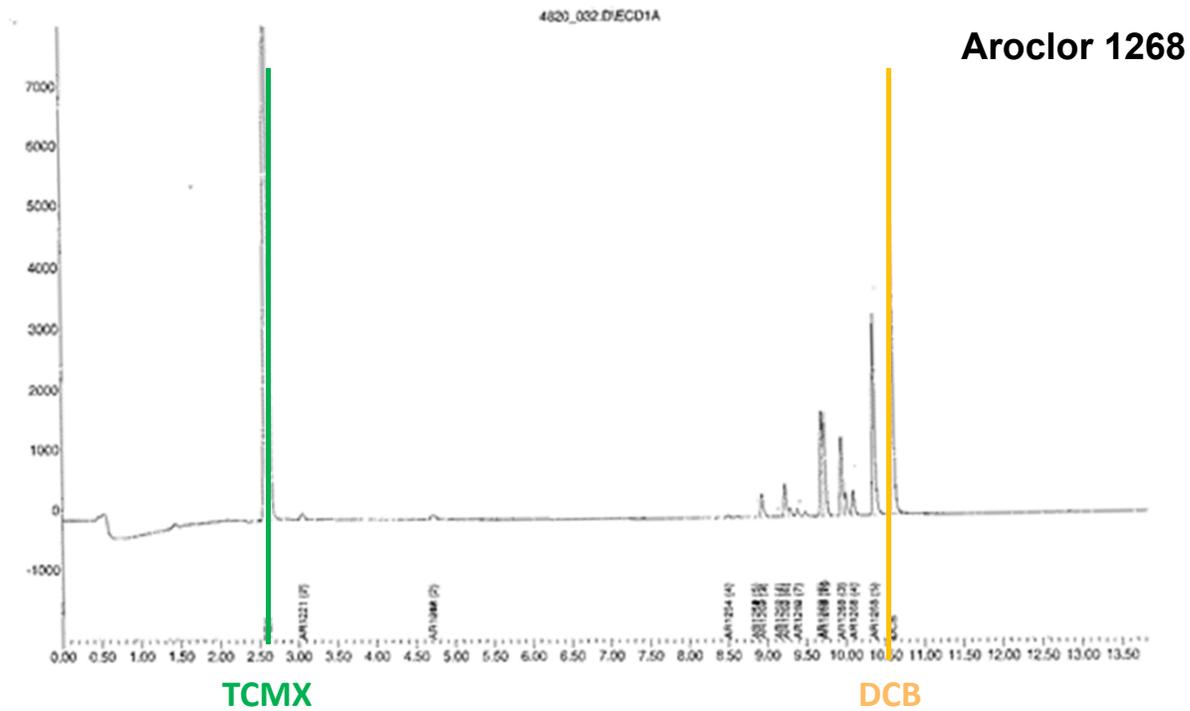
Heritage PCT standards

Heritage Lab Method 8082 DB-5



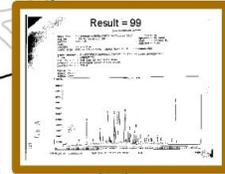
Heritage PCT standards

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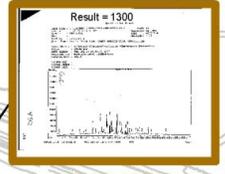
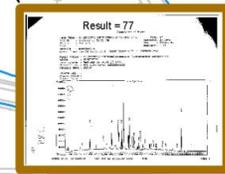


Phase 2 Hardcopy Chromatograms

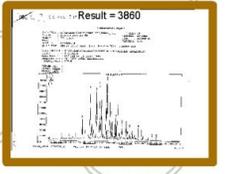
Type B Fingerprint



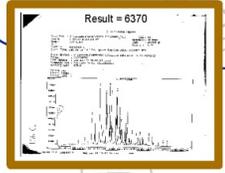
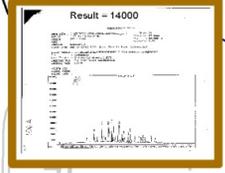
06.48-118A
06.48-118C



06.48-105A
06.48-106A

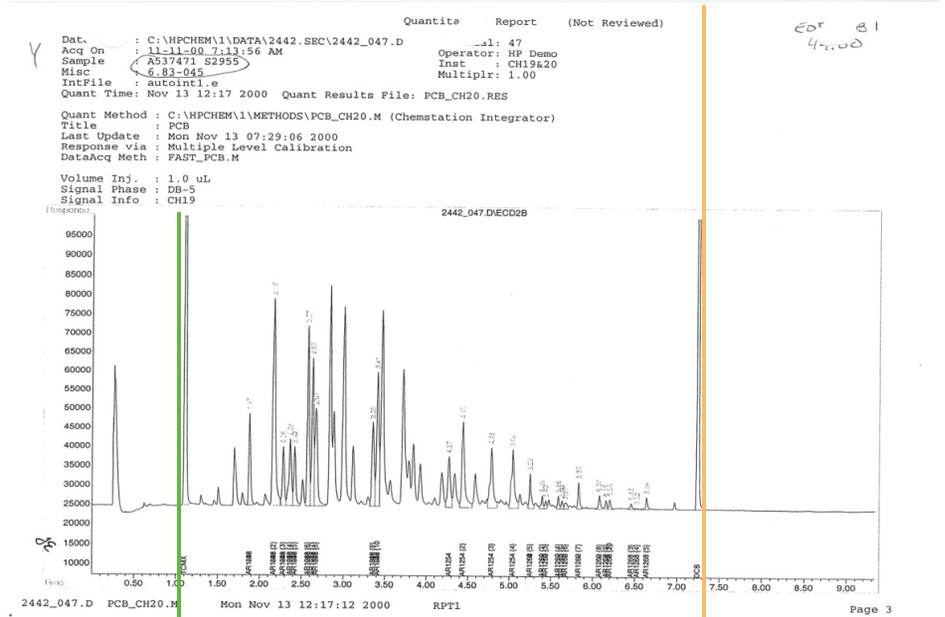


06.48-105C
06.48-106C

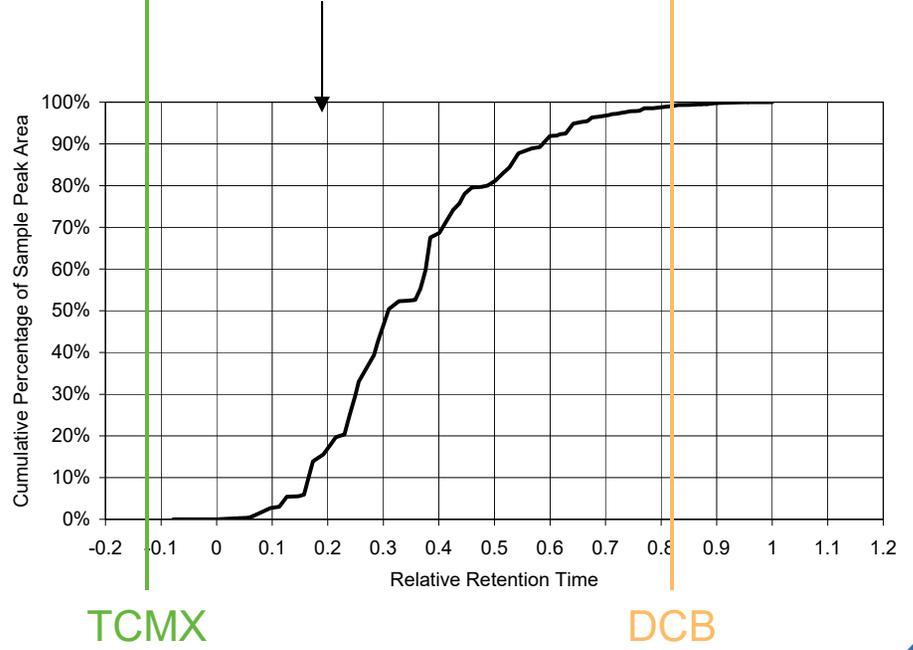


Method 8081 Chromatograms of Sediment Samples

Raw Chromatogram

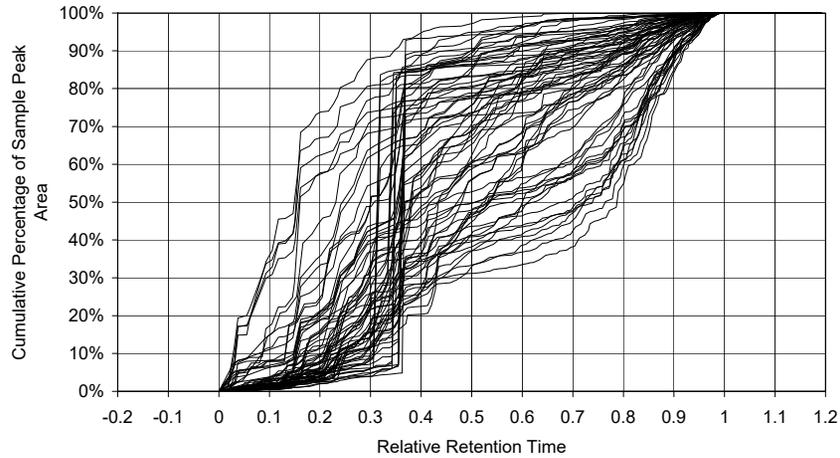


Cumulative Response Curve

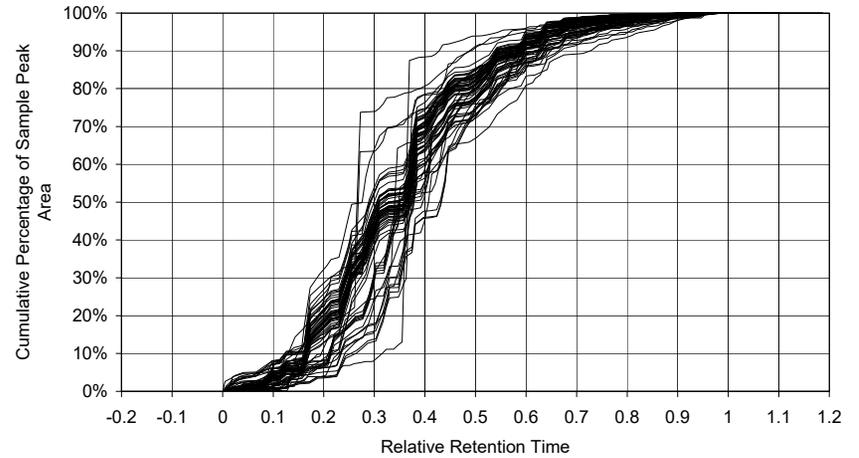


Cumulative Response Curves

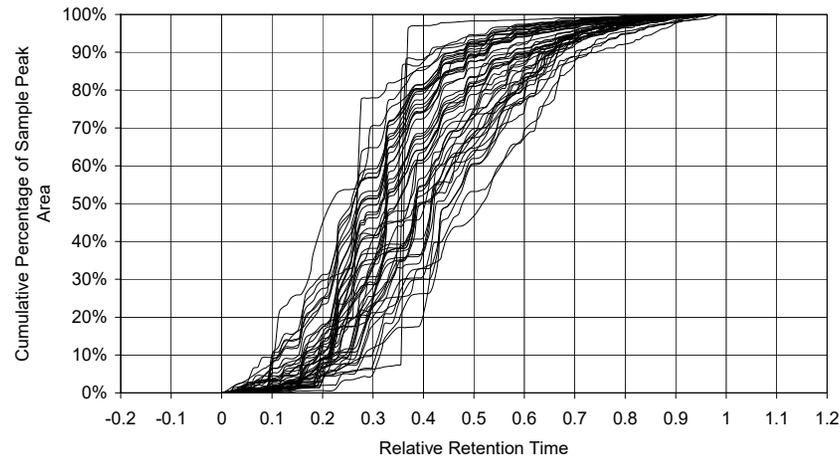
Cumulative Response Curves
West – 71 Samples



Cumulative Response Curves
East – 66 Samples



Cumulative Response Curves
STREAM - 48 Samples

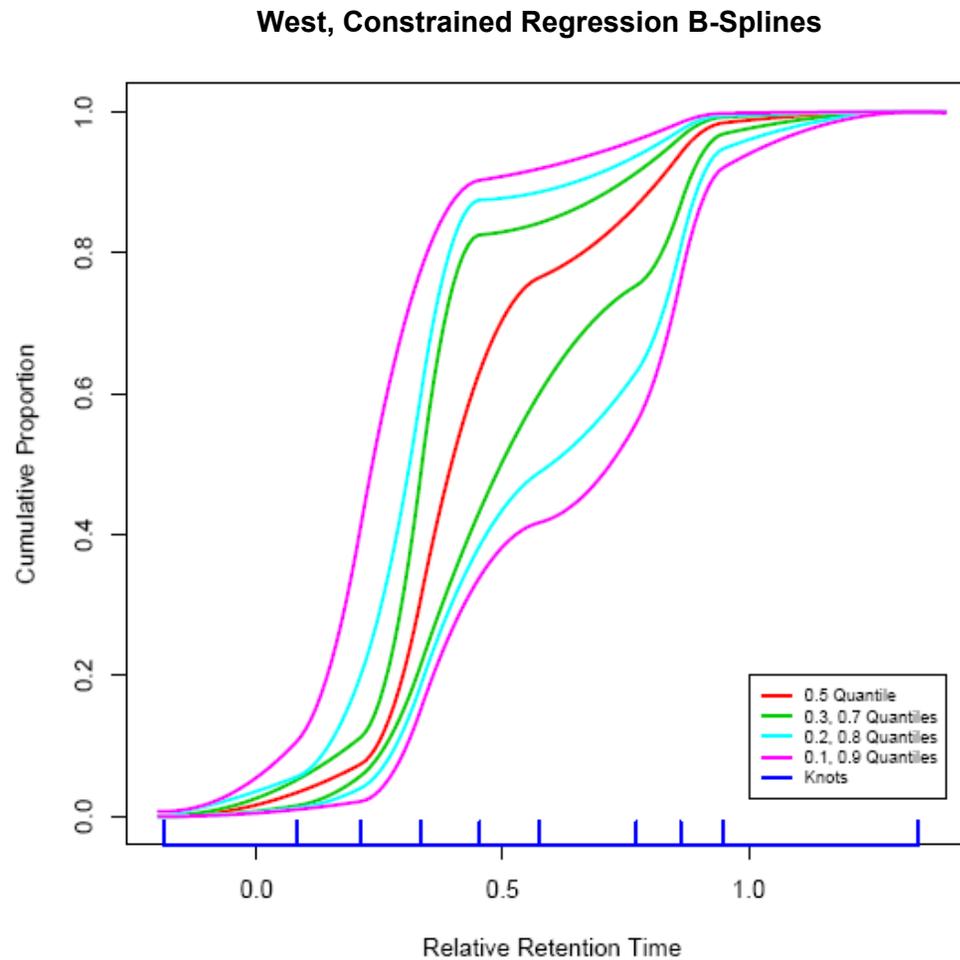


71: West
66: East
48: STREAM

Quantile Regression

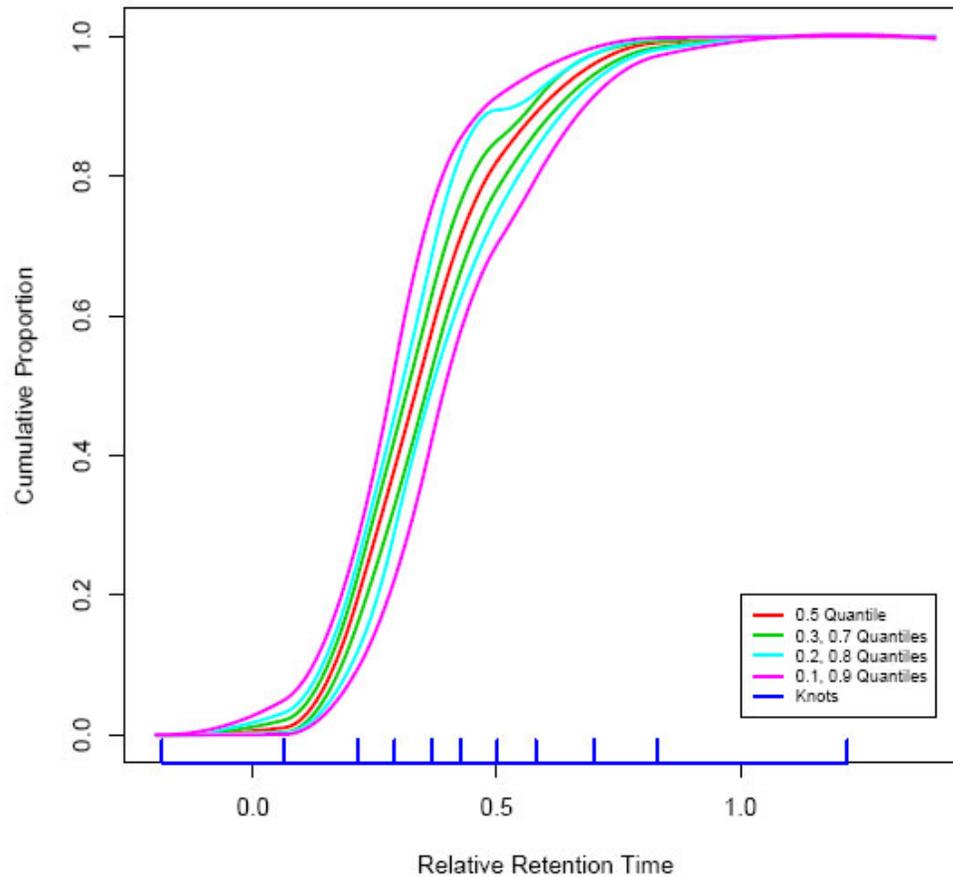
- Fitting a function through the original data so that a certain *proportion* of the data is above or below that line
- For example, for curve of Quantile 0.4, 60% of original data is above the curve, 40% below
- Ng and He (1999)
- Constrained B-splines, using *cobs* (a package of functions)
- All calculations using “R”
- Fitted functions must be increasing
- Equal to zero at relative retention time zero and equal to one at relative retention time one

Constrained Quantile Regression B-splines for West at Various τ (Quantiles)



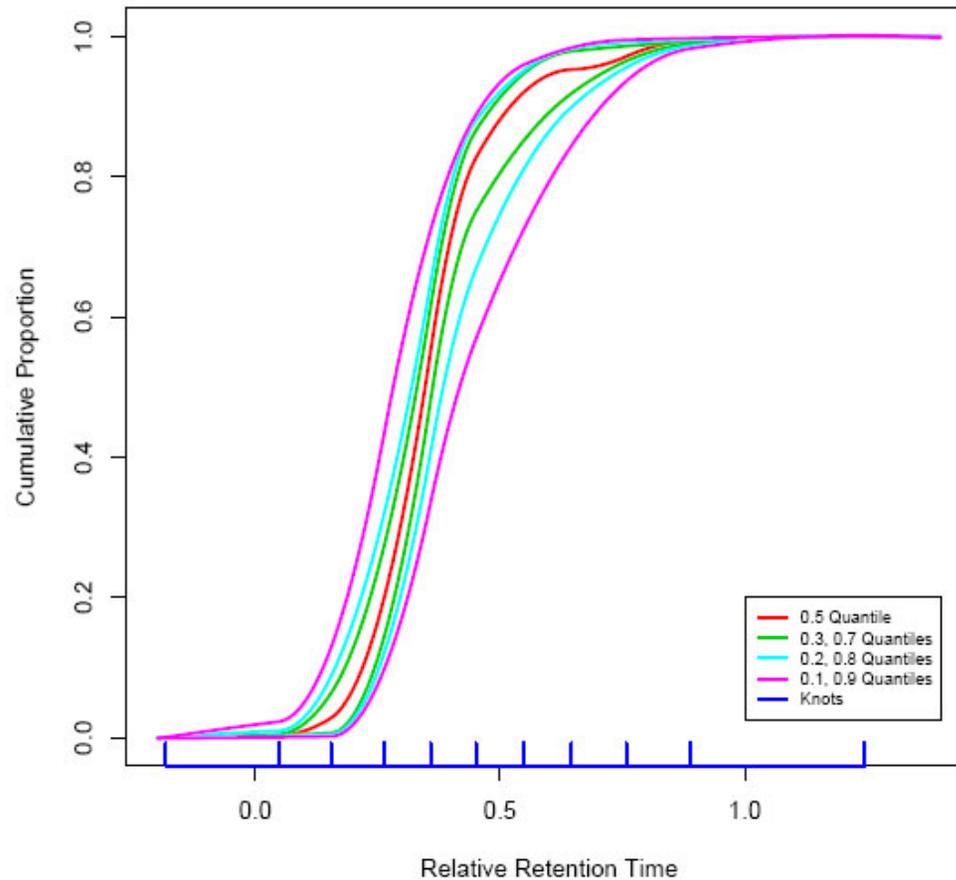
Constrained Quantile Regression B-splines for East at Various τ (Quantiles)

East, Constrained Regression B-Splines



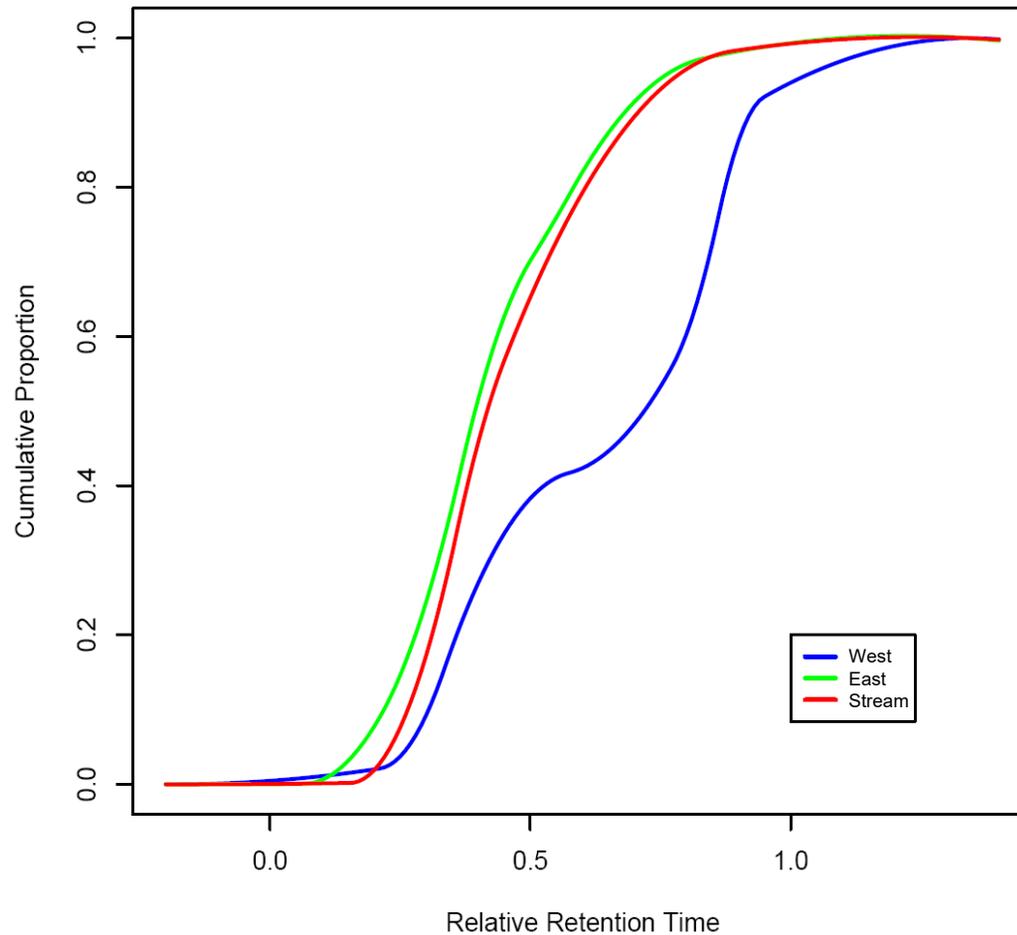
Constrained Quantile Regression B-splines for the Stream at Various τ (Quantiles)

Stream, Constrained Regression B-Splines



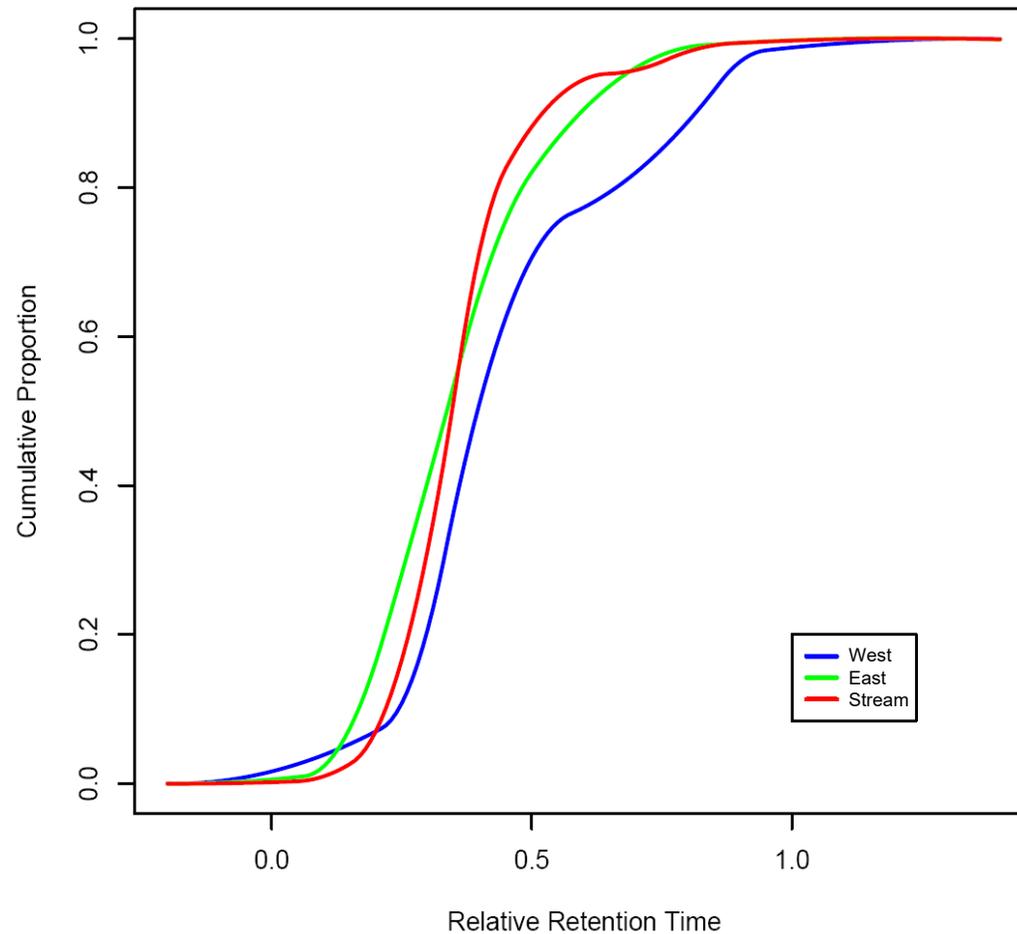
$\tau = 0.1$ Constrained Quantile Regression B-splines, at Three Sites

0.1 Quantile Constrained Regression B-Splines, by Site

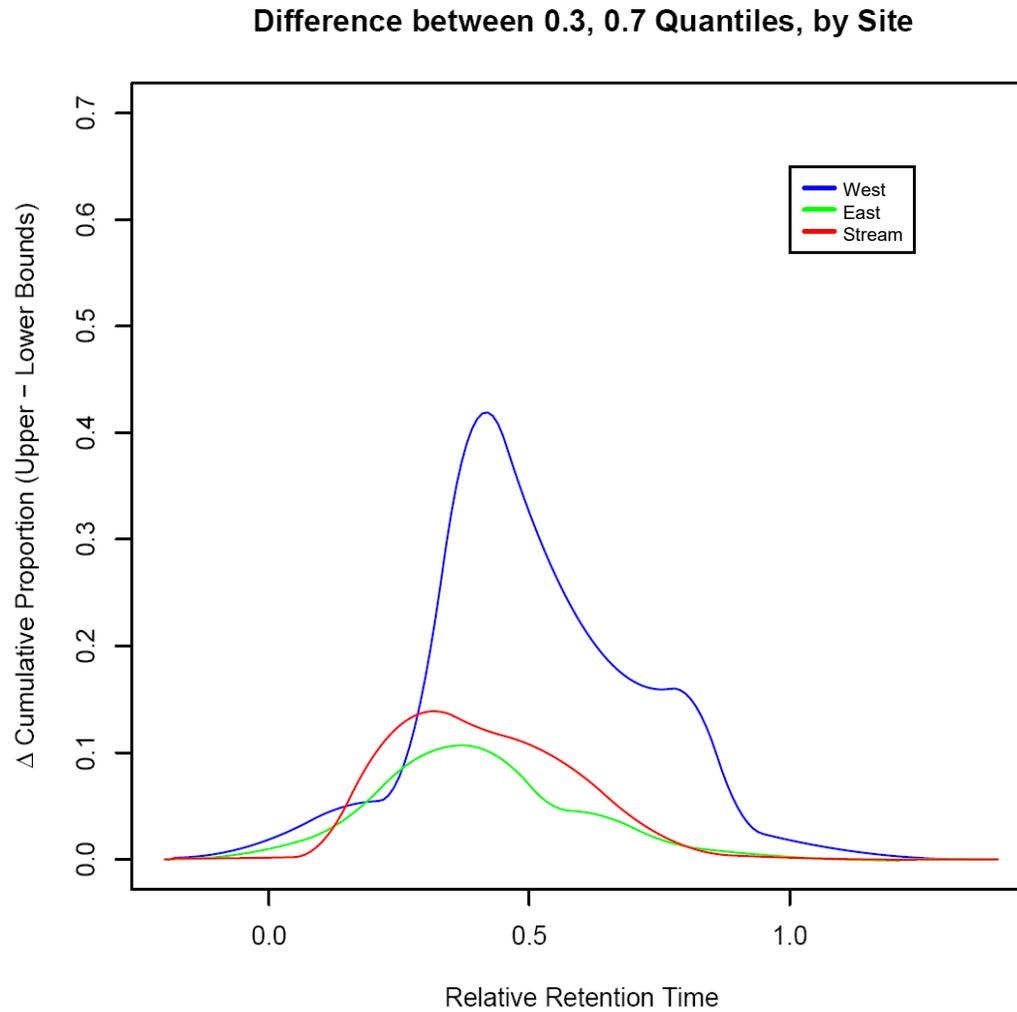


Median ($\tau = 0.5$) Constrained Quantile Regression B-splines, at Three Sites

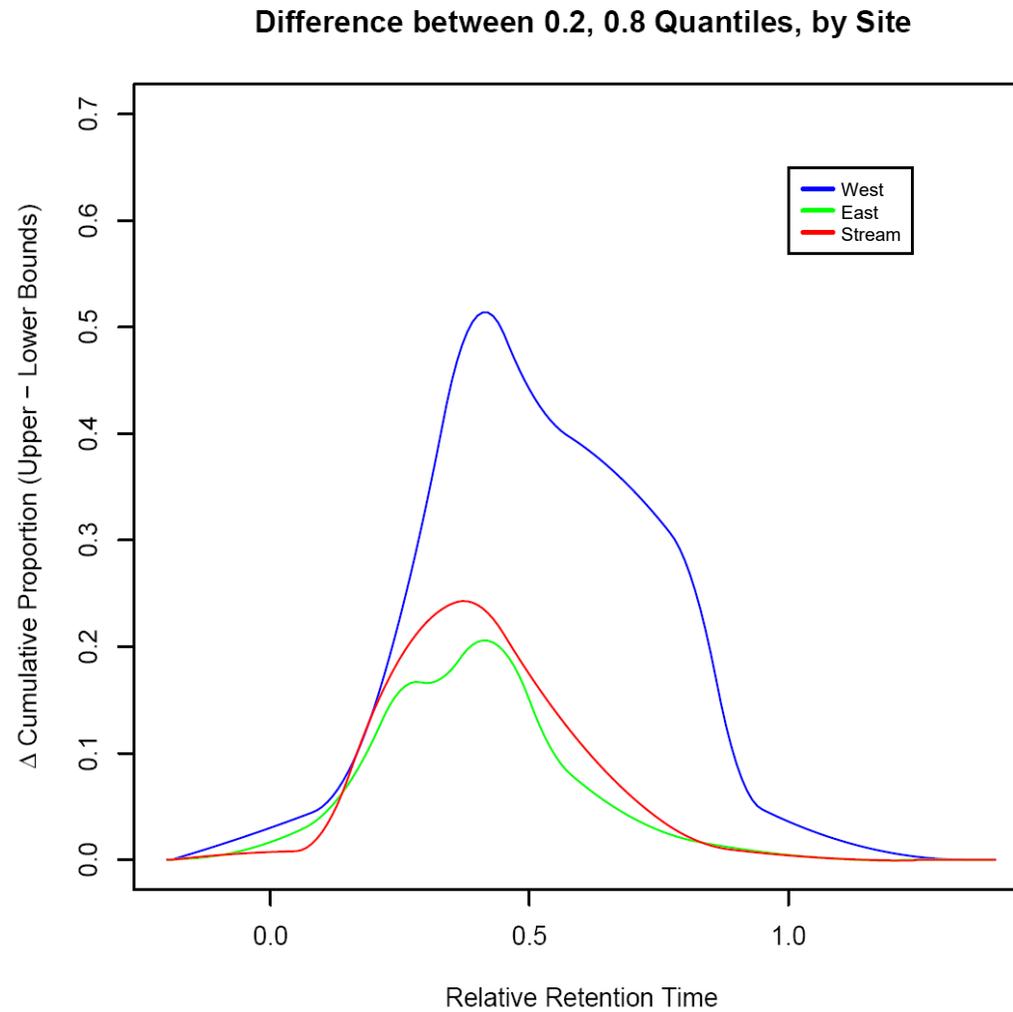
Median Constrained Regression B-Splines, by Site



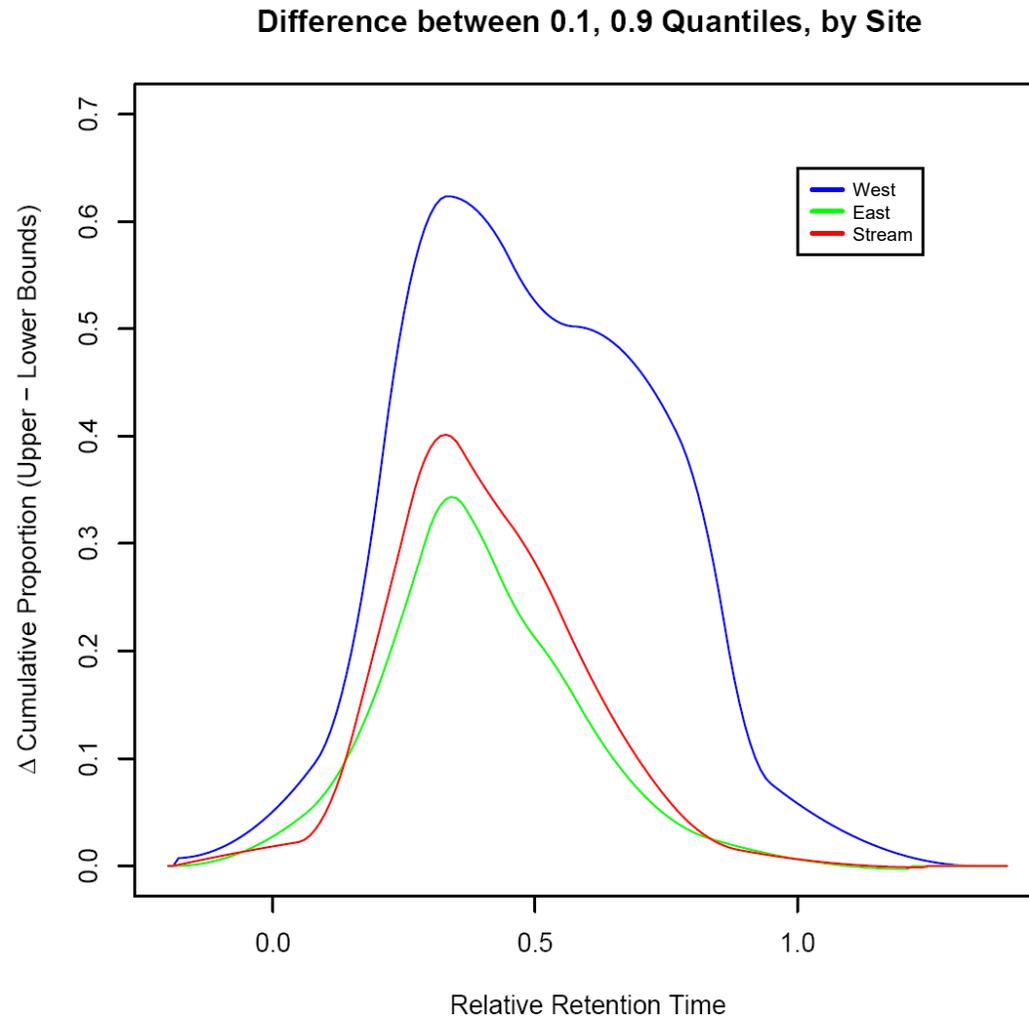
Difference Between 0.3, 0.7 Quantiles, by Site



Difference Between 0.2, 0.8 Quantiles, by Site



Difference Between 0.1, 0.9 Quantiles, by Site

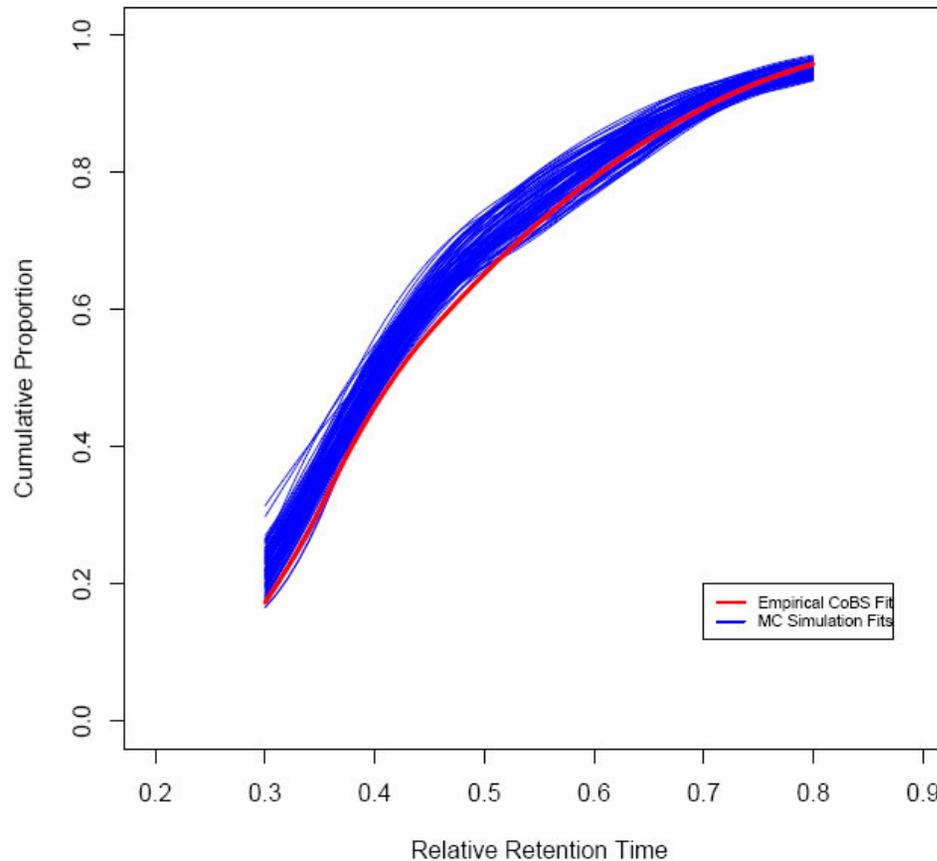


Monte Carlo Simulation

- Randomly selected from West samples and East samples for a total number of samples to match the number of Stream samples
- Varied proportion of West; 2%, 5%, 10%, 15%, 25%, 50%
- 100 iterations
- Compared Simulation to actual

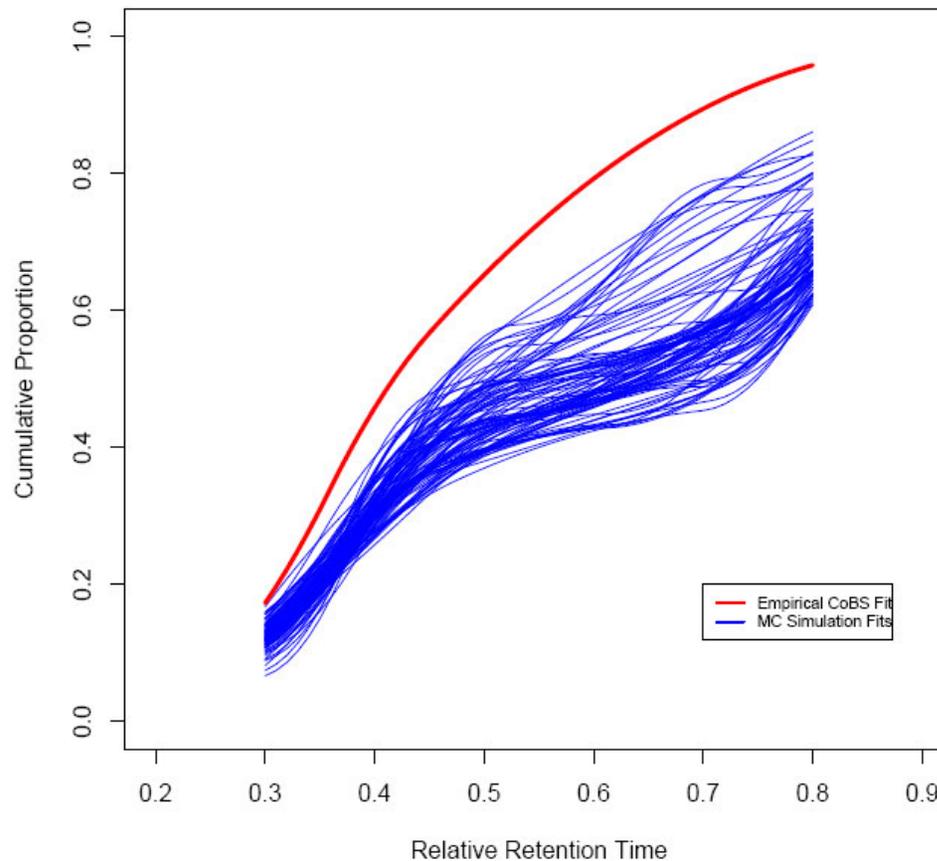
Various Constrained B-spline Quantile Regressions for the Original and Simulated Stream Samples (100 Iterations) for Particular West Shares and τ

Empirical and Simulated Stream Samples (West = 5%, tau = 0.1)



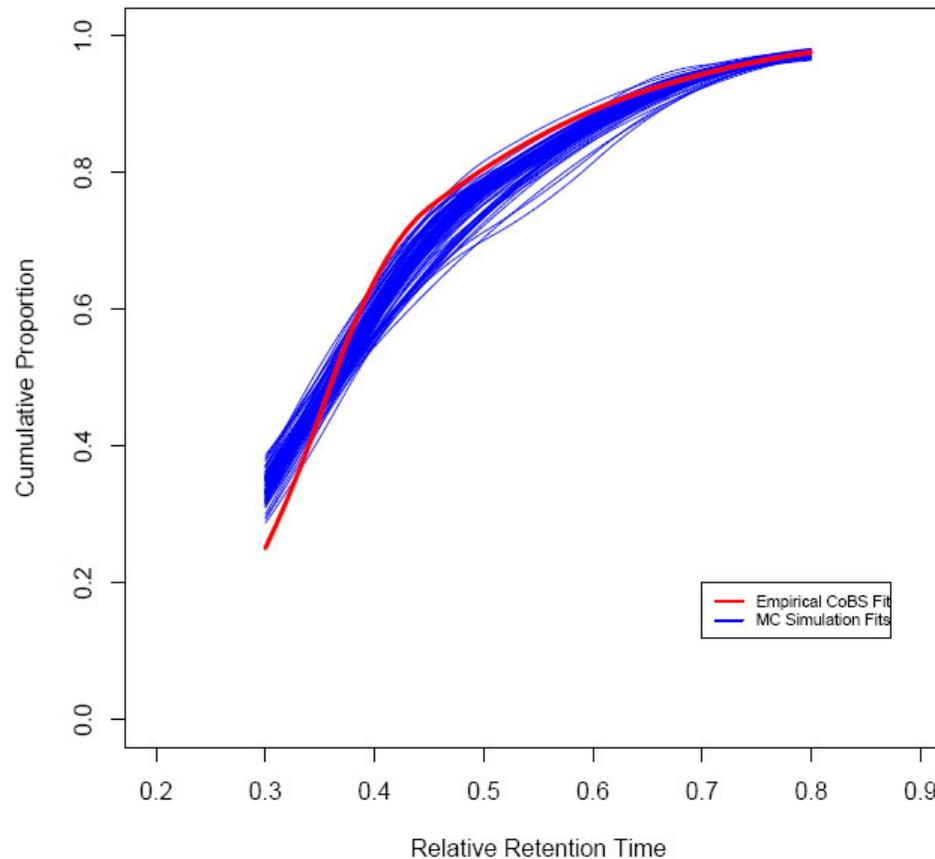
Various Constrained B-spline Quantile Regressions for the Original and Simulated Stream Samples (100 Iterations) for Particular West Shares and τ

Empirical and Simulated Stream Samples (West = 50%, tau = 0.1)



Various Constrained B-spline Quantile Regressions for the Original and Simulated Stream Samples (100 Iterations) for Particular West Shares and τ

Empirical and Simulated Stream Samples (West = 10%, tau = 0.3)



Proportion of Iterations that Fit the Original Data (100 Comparisons)

| Data Type | West Share | Quantile (τ) | | | | | | |
|-----------|------------|---------------------|-------|-------|-------|-------|-------|-------|
| | | 0.1 | 0.2 | 0.3 | 0.5 | 0.7 | 0.8 | 0.9 |
| Empirical | 0% | > 95% | > 95% | > 95% | < 95% | < 95% | < 95% | > 95% |
| Simulated | 2% | 96% | 80% | 47% | 0% | 0% | 20% | 79% |
| Simulated | 5% | 87% | 69% | 38% | 0% | 2% | 16% | 81% |
| Simulated | 10% | 71% | 47% | 17% | 0% | 3% | 24% | 83% |
| Simulated | 15% | 27% | 25% | 9% | 0% | 0% | 18% | 85% |
| Simulated | 25% | 7% | 3% | 0% | 0% | 0% | 19% | 85% |
| Simulated | 50% | 0% | 0% | 0% | 0% | 0% | 13% | 85% |
| Empirical | 100% | < 95% | < 95% | < 95% | < 95% | < 95% | < 95% | > 95% |

Proportion of Iterations that Fit the Original Data (1 Billion Comparisons)

| Data Type | West Share | Quantile (τ) | | | | | | |
|-----------|------------|---------------------|-------|-------|-------|-------|-------|-------|
| | | 0.1 | 0.2 | 0.3 | 0.5 | 0.7 | 0.8 | 0.9 |
| Empirical | 0% | > 95% | > 95% | > 95% | < 95% | < 95% | > 95% | > 95% |
| Simulated | 2% | 100% | 99% | 98% | 45% | 27% | 73% | 99% |
| Simulated | 5% | 100% | 99% | 98% | 33% | 15% | 65% | 99% |
| Simulated | 10% | 94% | 81% | 84% | 30% | 18% | 63% | 98% |
| Simulated | 15% | 53% | 67% | 77% | 29% | 23% | 68% | 99% |
| Simulated | 25% | 23% | 31% | 43% | 8% | 19% | 72% | 99% |
| Simulated | 50% | 0% | 0% | 0% | 0% | 8% | 62% | 100% |
| Empirical | 100% | < 95% | < 95% | < 95% | < 95% | < 95% | < 95% | > 95% |

Conclusions

- West share of 2-5% fit the data best
- Lower bound contribution of 0%
- Upper bound contribution of 10%

Questions?

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Principal

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