PREDICTING THE PERFORMANCE OF FIXED-BED GRANULAR ACTIVATED CARBON ADSORBERS

D. W. Hand, J. C. Crittenden, D. R. Hokanson, and J. L. Bulloch

Dept. of Civil and Environmental Engineering
Michigan Technological University
Houghton, Michigan 49931
USA

Presented at *First IAWQ Specialized Conference on Adsorption in Water Environment and Treatment Processes*; Shirahama, Wakayama Japan
November 1996

MichiganTech

OUTLINE

Competitive Interactions Between Known Components

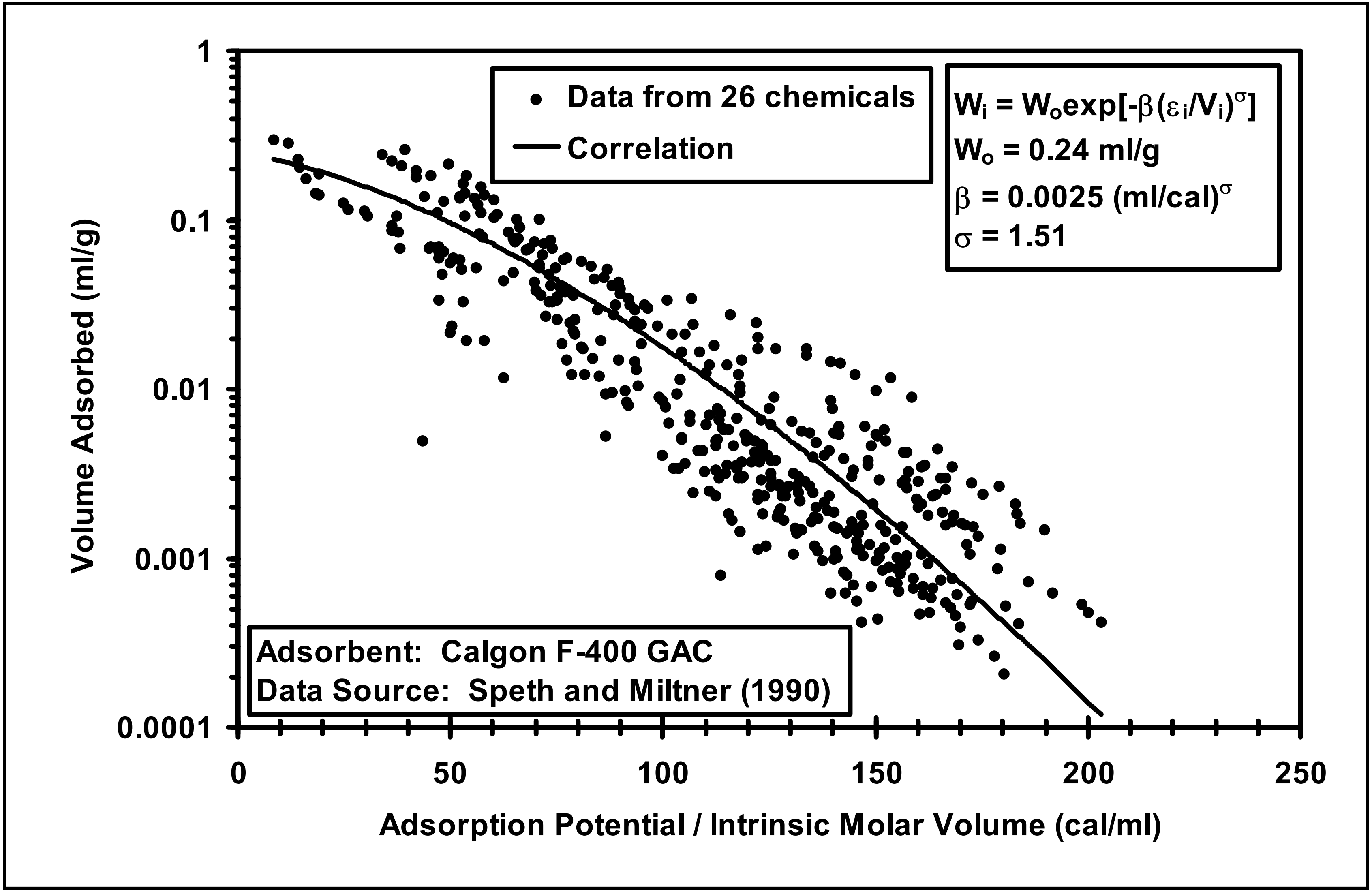
- Correlation of Single Solute Adsorption Equilibria
- Prediction of Multicomponent Equilibria of Known Components
- Model Predictions Using the Equilibrium Column Model
- Model Predictions Using the Pore Surface Diffusion Model

OUTLINE (continued)

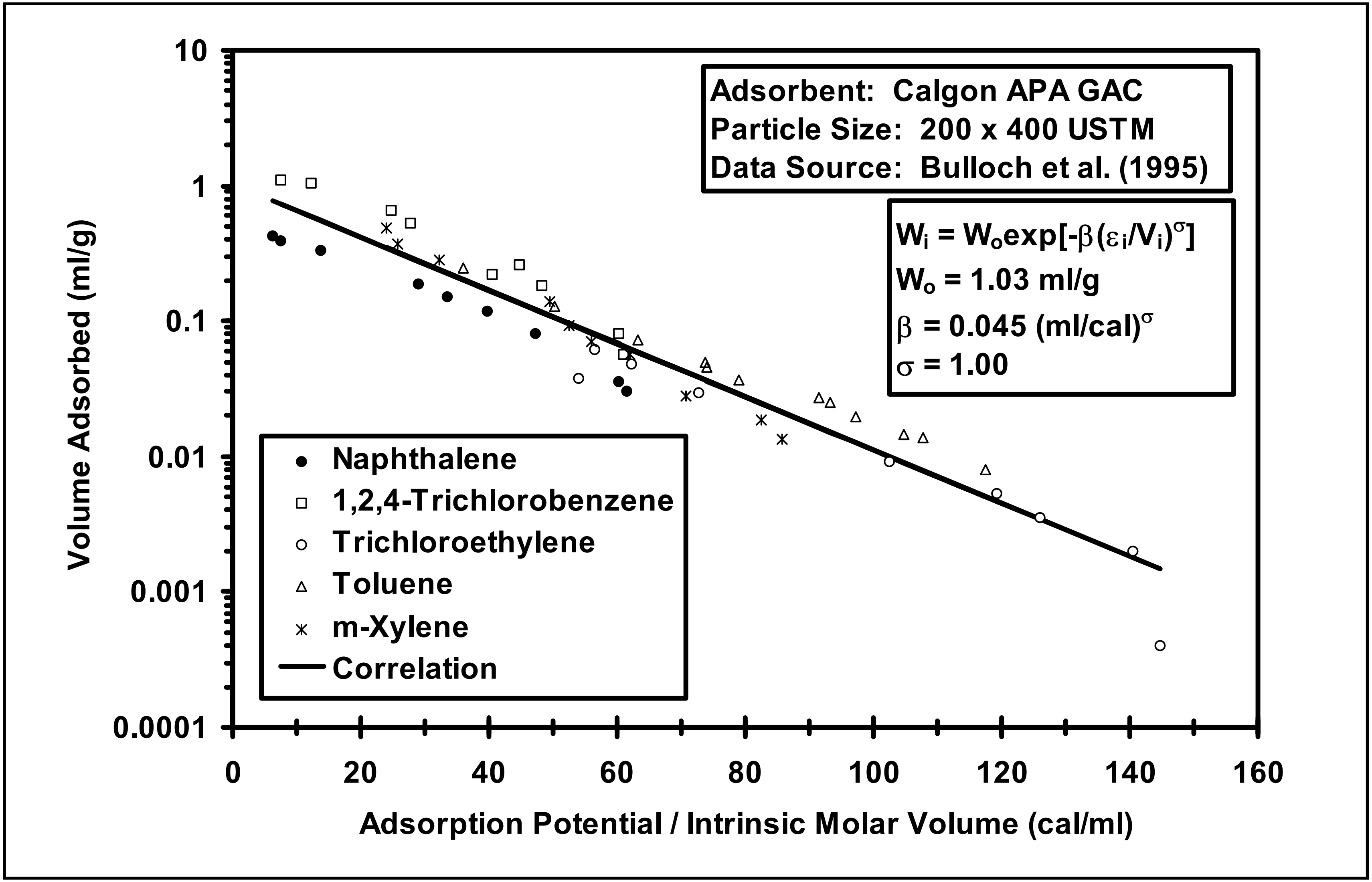
Synthetic Organic Compound (SOC) and Unknown Background Organic Matter (BOM) Interactions

- Impact of BOM on Fixed Bed Adsorption Capacity of SOCs
  - Influence of Exposure Time
  - Influence of Compound Type
  - Influence of Water Type
- Impact of BOM on Adsorption Rate
- Model Simulations for a Variety of Waters

ISOTHERM CORRELATION



MTU DATA FOR SIX COMPONENTS



IDEAL ADSORBED SOLUTION THEORY

$$C_i = \frac{\gamma_i q_i}{\sum_{j=1}^{N} q_j} \left[\frac{\sum_{j=1}^{N} n_j q_j}{n_i K_i} \right]$$

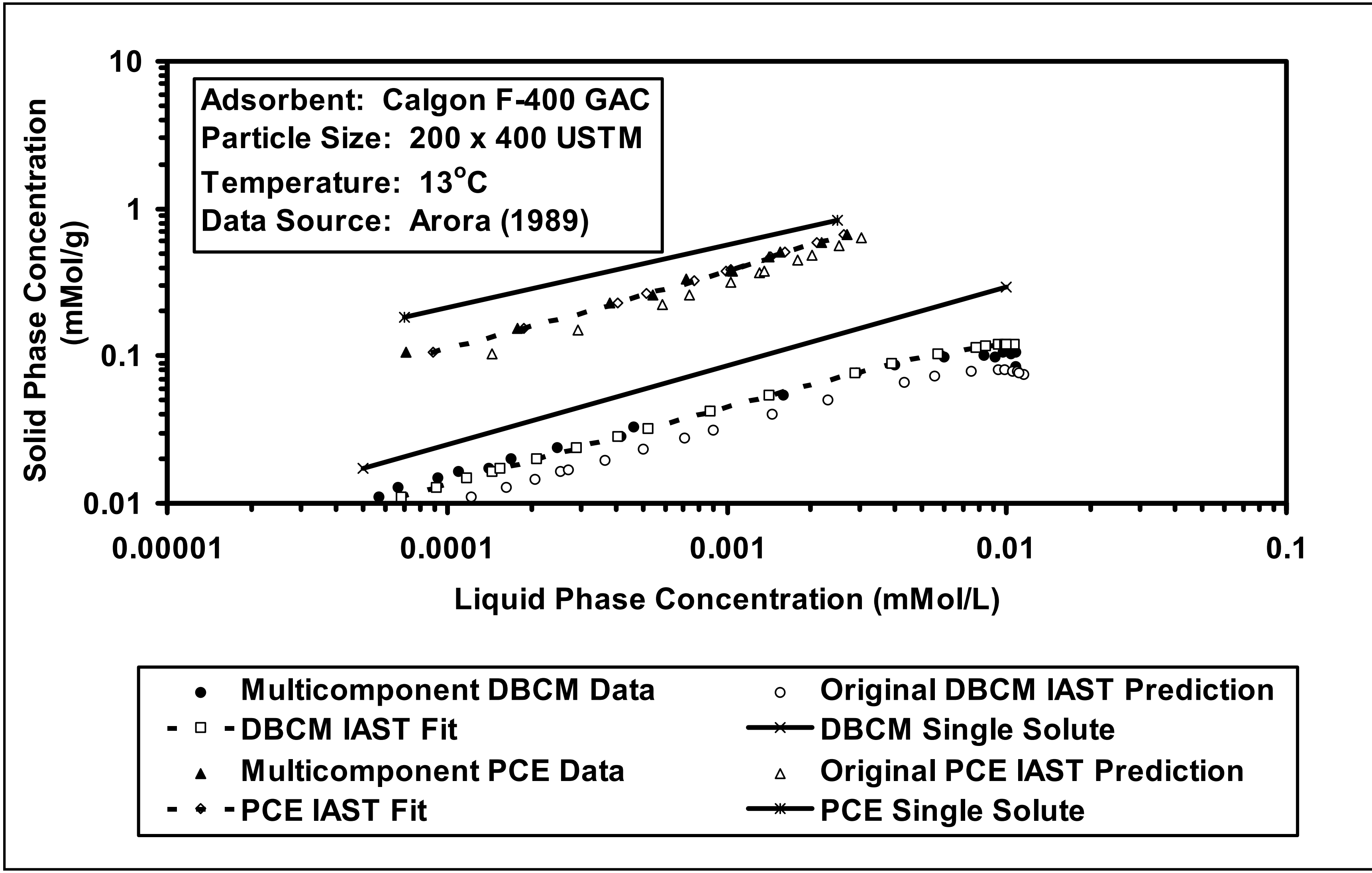
- Wilson Activity Coefficients

$$\ln \gamma_i = 1.0 - \ln \sum_{j=1}^{n} x_j A_{ij} - \sum_{k=1}^{n} \left[\frac{x_k A_{ki}}{\sum_{j=1}^{n} x_j A_{kj}} \right]$$

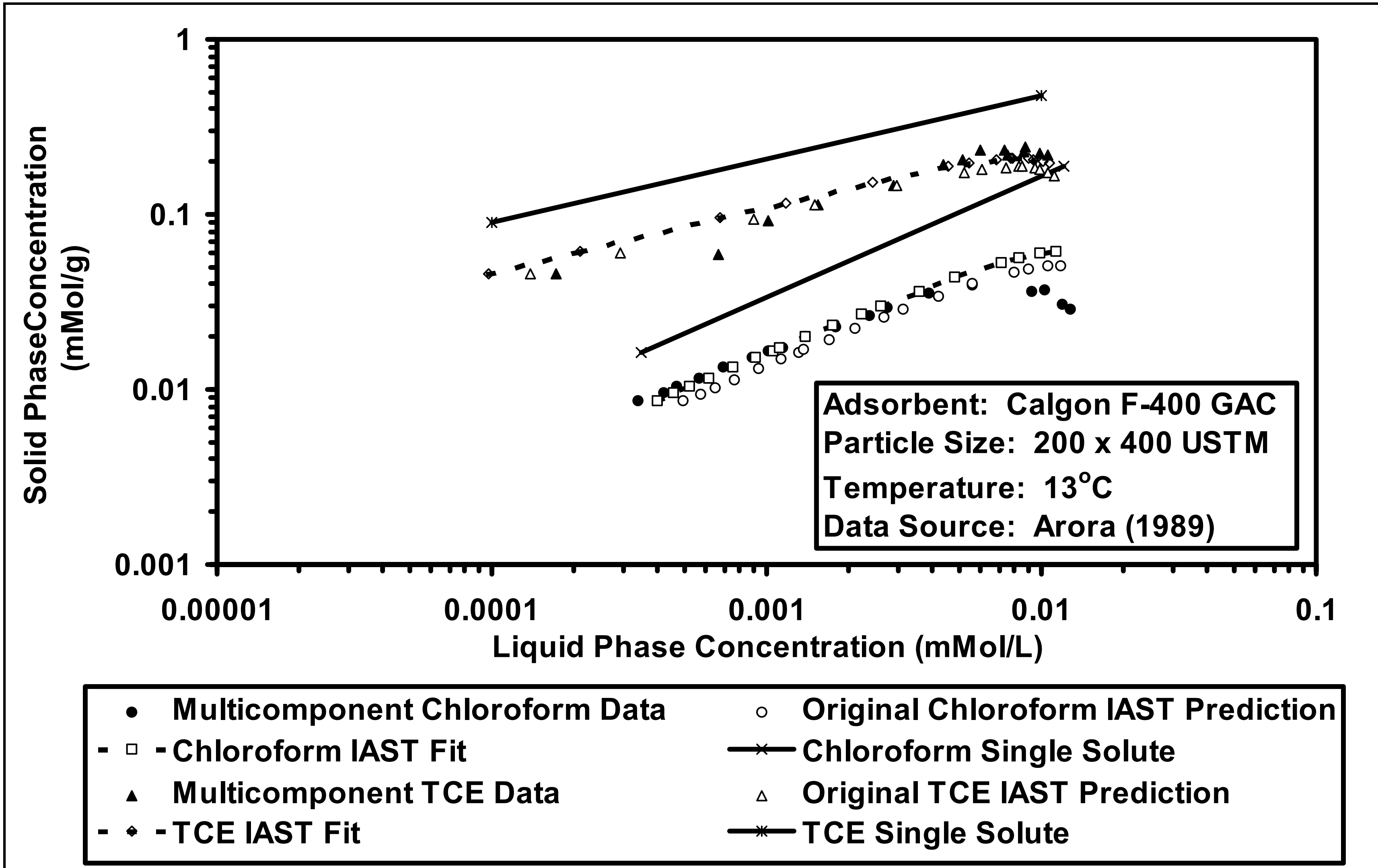
- Empirical Activity Coefficients (less than 1.0)

$$\gamma_i = \alpha_i^{(1-z_i)}$$

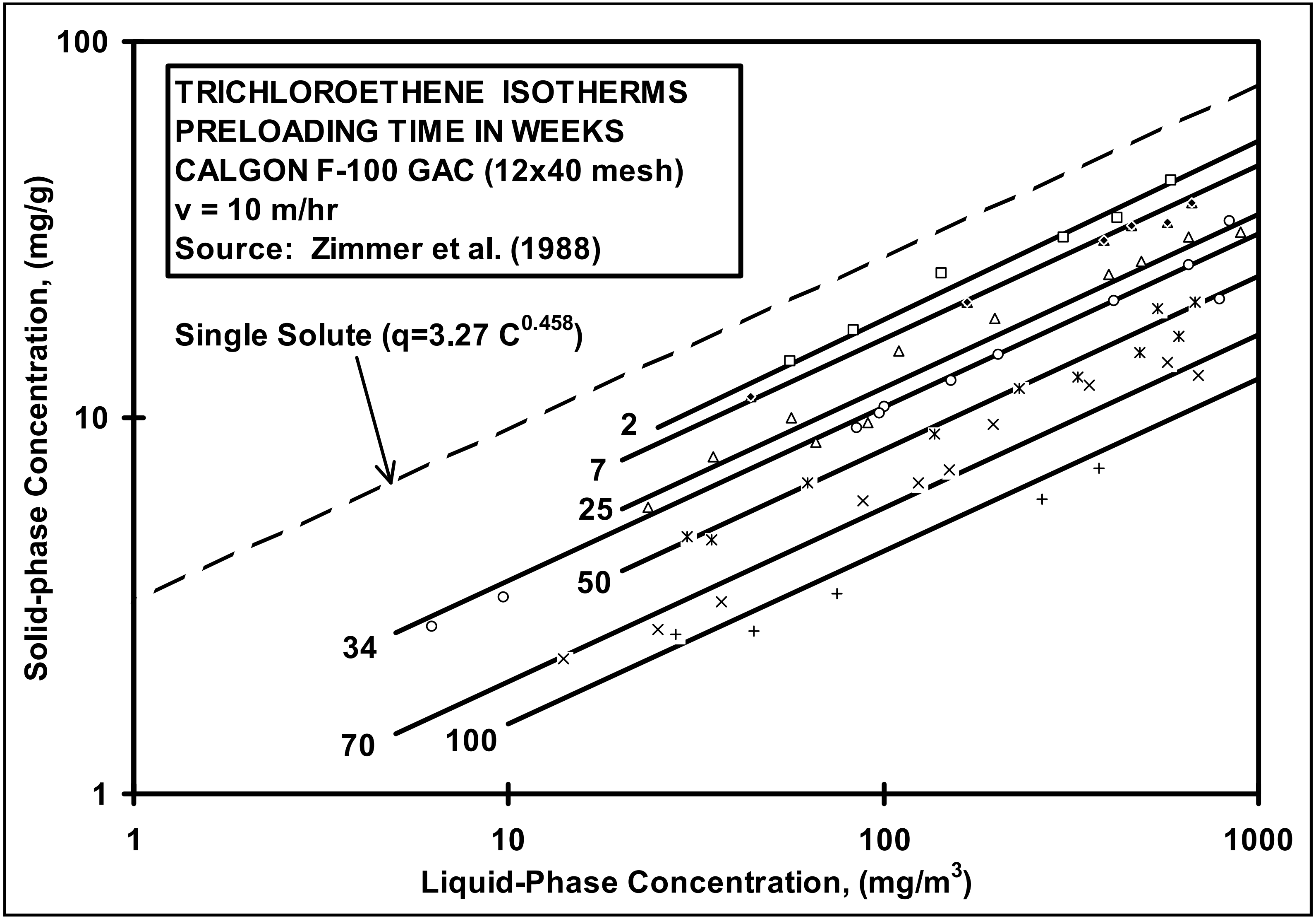
IAST CALCULATIONS SHOWING IMPROVEMENT WITH γ



IAST CALCULATIONS SHOWING NO IMPROVEMENT WITH γ

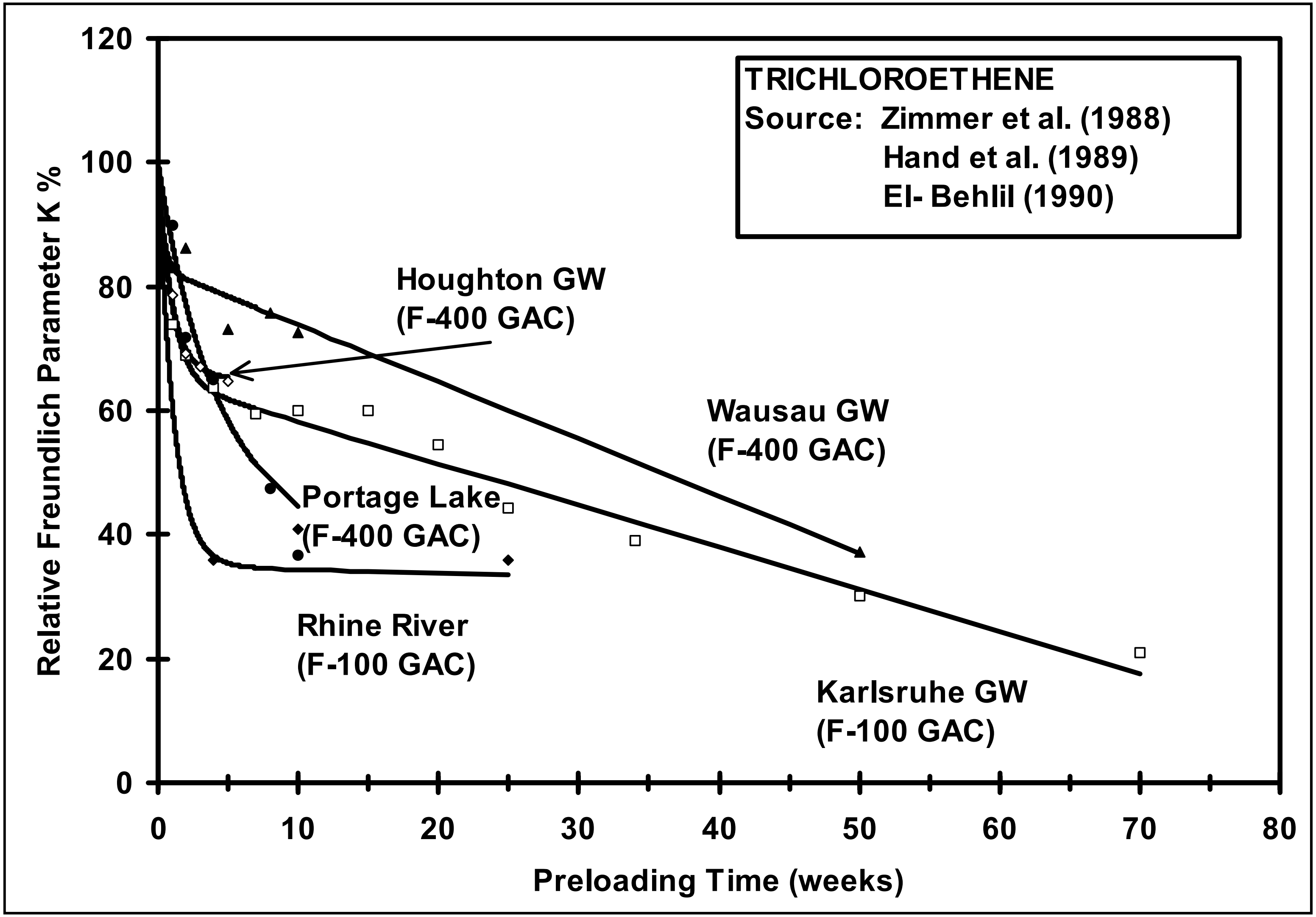


ADSORPTION EQUILIBRIUM ISOTHERM FOR TRICHLOROETHENE

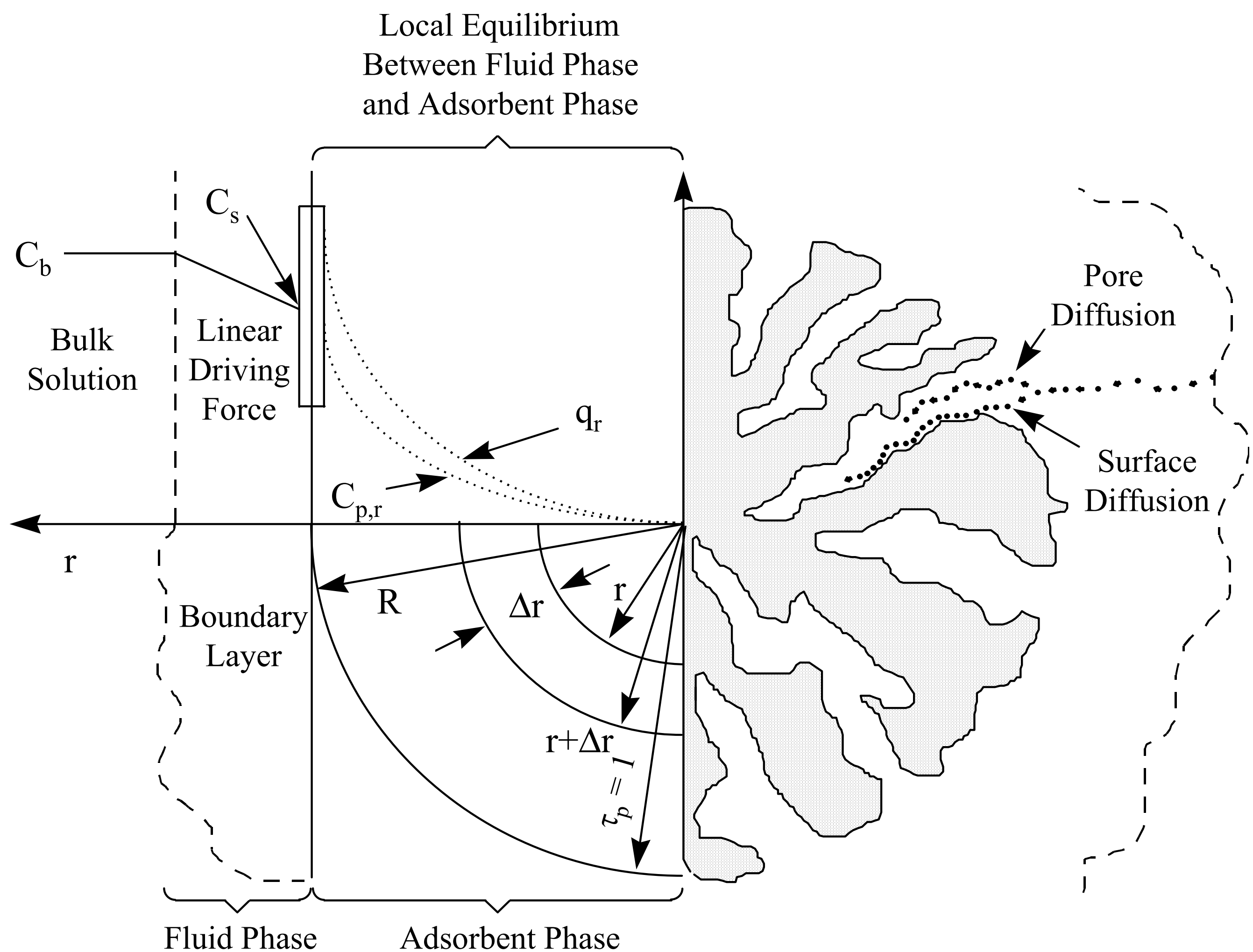


MichiganTech

FREUNDLICH K REDUCTION FOR VARIOUS WATERS



PSDM MECHANISMS



Mass Flux $= k_f(C_b - C_s)$

Mass Flux $= -D_s \rho_a \frac{\partial q_r}{\partial r} - \frac{D_l \varepsilon_p}{\tau_p} \frac{\partial C_{p,r}}{\partial r}$

MASS TRANSFER COEFFICIENTS

- External Mass Transfer Coefficient (Gnielinski, 1978)

$$k_f = \frac{\left[1 + 1.5\left(1 - \varepsilon\right)\right] \phi D_\ell}{2R} \left[2 + 0.644 \, Re^{1/2} \, Sc^{1/3} \right]$$

MASS TRANSFER COEFFICIENTS (continued)

- Intraparticle Surface Diffusion Coefficient

$$D_s = SPDFR * \left[\frac{D_\ell \, \varepsilon_p \, C_0}{\tau_p \, K \, C_0^{1/n} \, \rho_a} \right]$$

  - Single Components:
    - SPDFR between 4 and 8 (mean = 6.58)
  - Multiple Components:
    - SPDFR = 16.27 EBCT(min)$^{-0.843}$

MASS TRANSFER COEFFICIENTS (continued)

- Intraparticle Pore Diffusion Coefficient

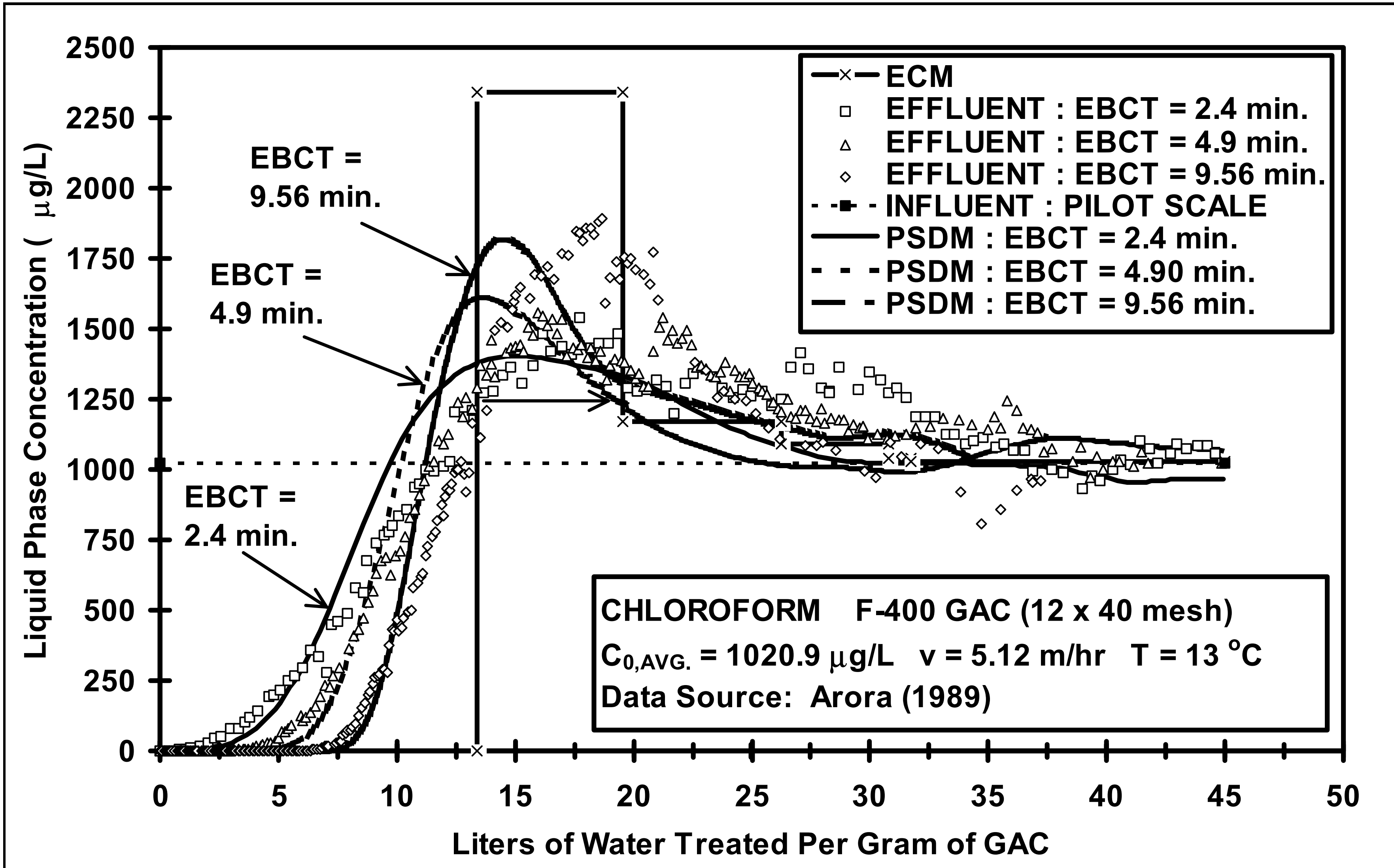
$$D_p = \frac{\varepsilon_p D_\ell}{\tau_p}$$

  - SOCs Alone (maximum pore diffusion flux):
    - $\tau_p = 1.0$
  - SOCs in the Presence of BOM:
    - $\tau_p = 1.0$ when Time < 70 days
    - $\tau_p = 0.334 + 6.61(10^{-6}) * t$ when Time > 70 days

ADSORPTION DESIGN SOFTWARE (AdDesignS™)

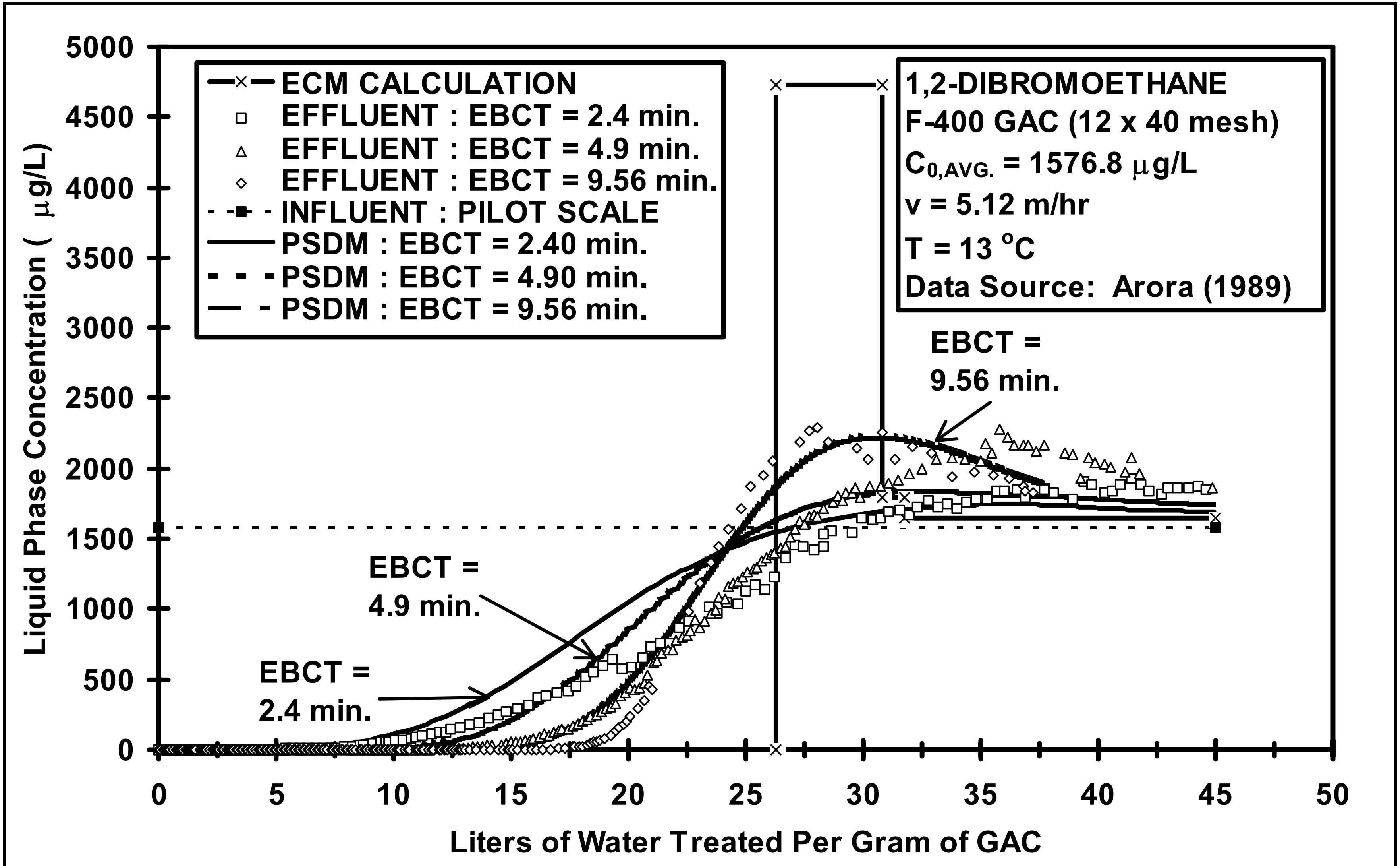
- Gas and Liquid phase
- Visual Basic Front-End with FORTRAN DLLs
- Up To 6 Components (12 PDEs), Solved by Orthogonal Collocation (Up To 18 Axial and 6 Radial Points, Up To 126 ODEs for Each Component, 756 ODEs total)
- Structured Heuristics Based on Experience for Model Parameter Estimation
- Data Base for Isotherms and Adsorbents
- SI and English Units
- 15,000 lines of code

CHLOROFORM: 6 Component ECM and PSDM Simulations for Organic Free Water

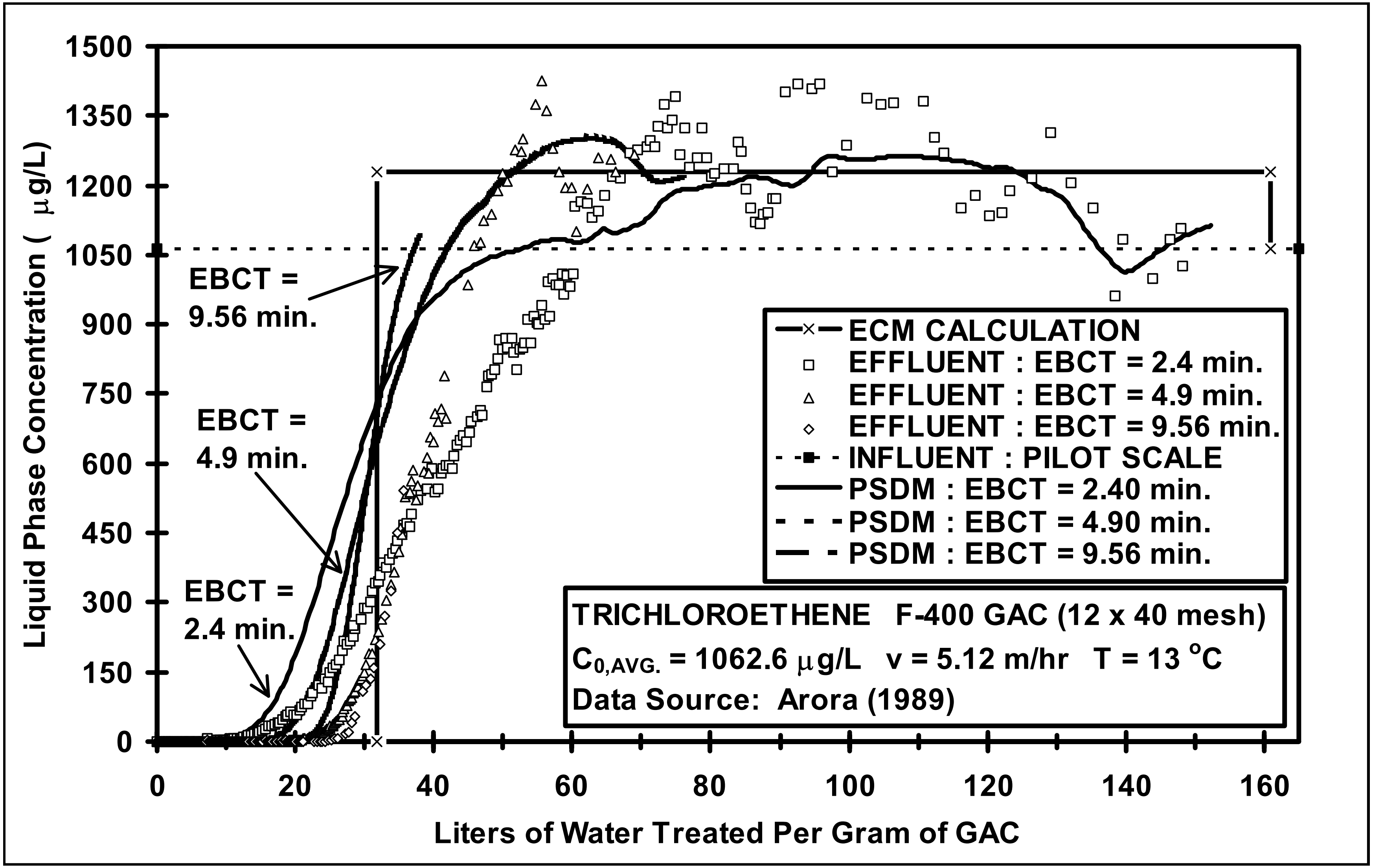


MichiganTech

1,2-DBE RESULT: 6 Component ECM and PSDM Simulations for Organic Free Water



TCE RESULT: 6 Component ECM and PSDM Simulations for Organic Free Water

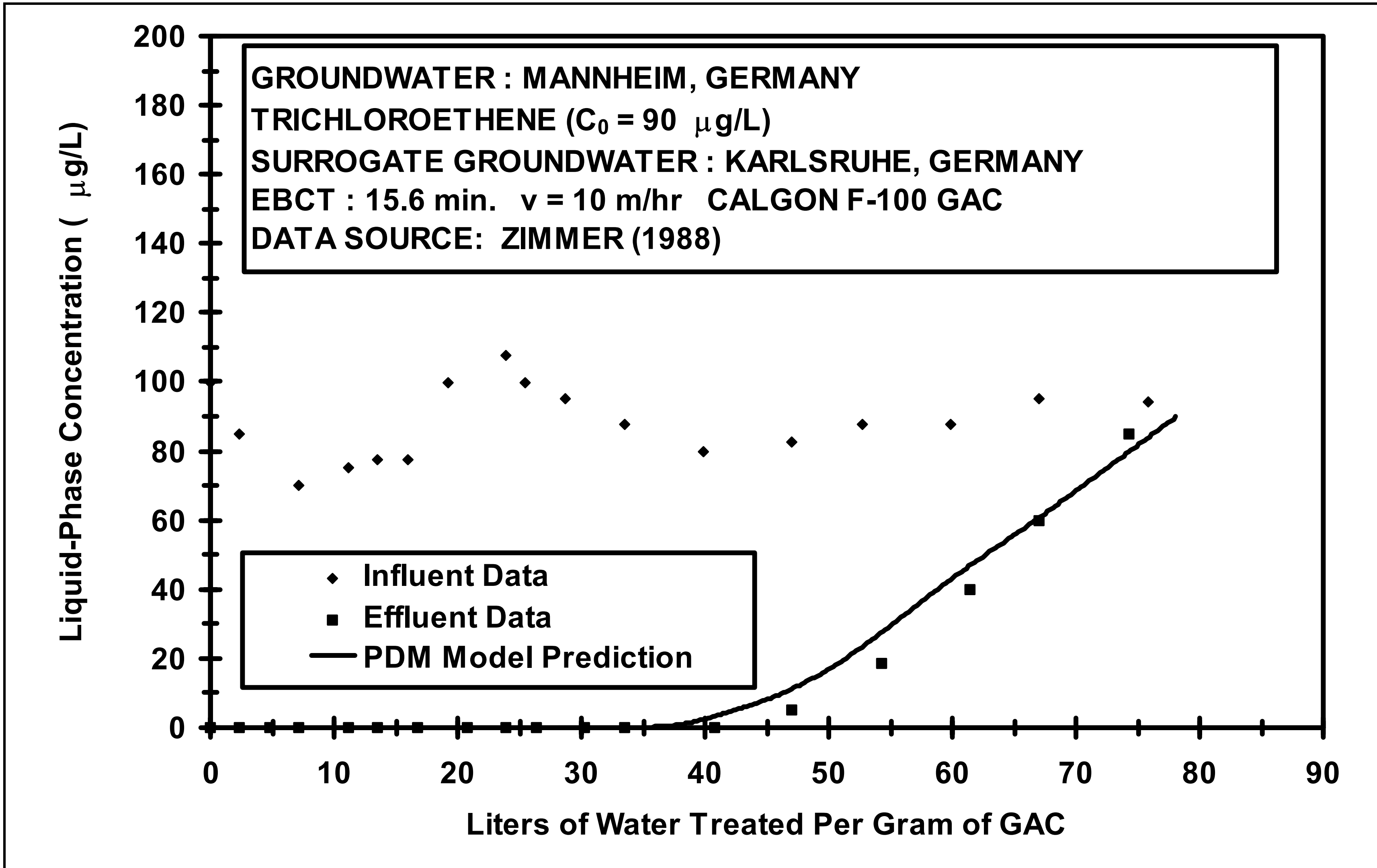


MichiganTech

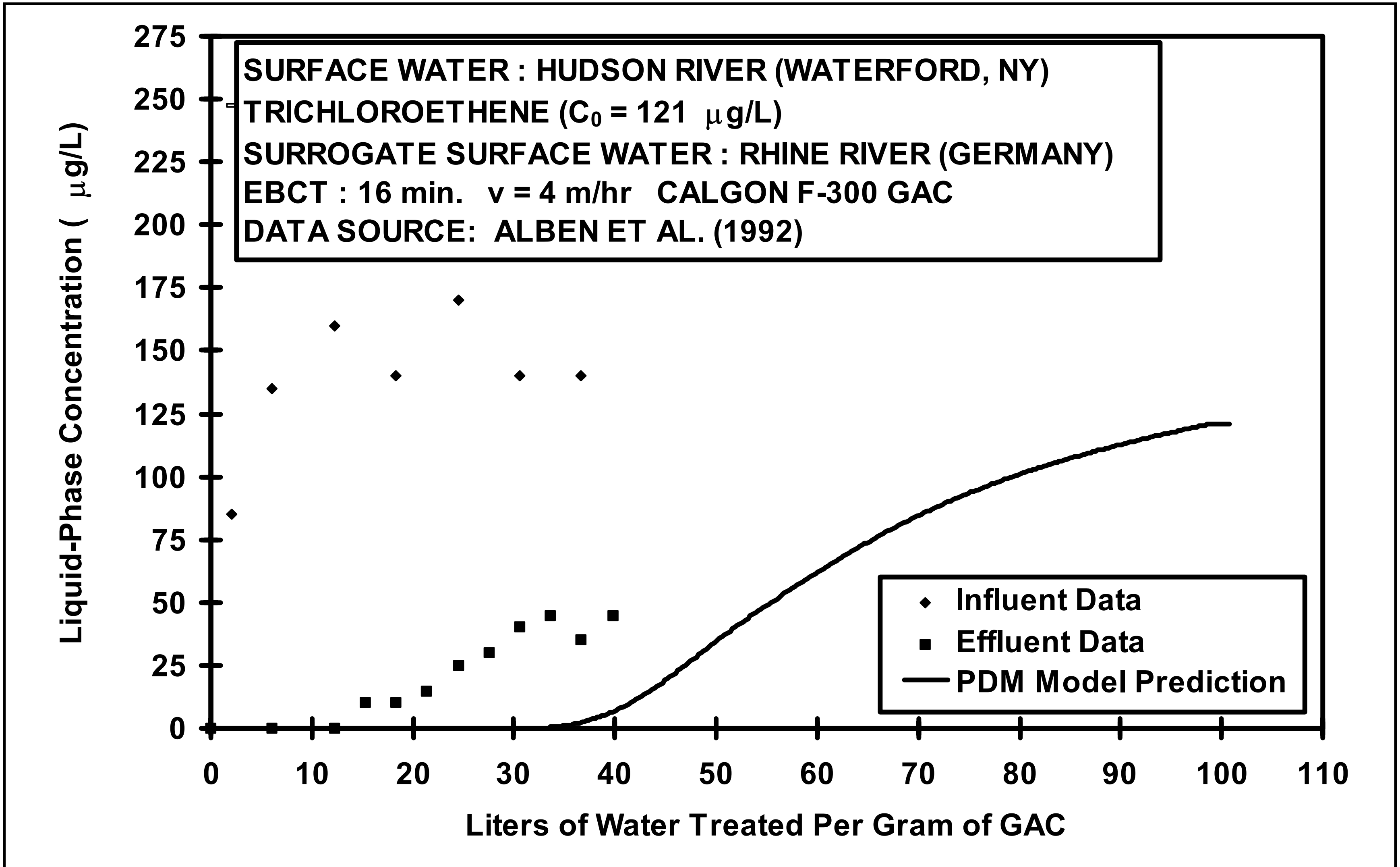
MODEL VERIFICATION EFFORT

- 11 Case Studies
  - 9 Pilot Plant Experiments
  - 2 Full-Scale Plants
- 11 Water Sources (USA, Germany, Netherlands)
  - 8 Groundwaters
  - 3 Surface Waters
- 4 Adsorbents
- 50 Empty Bed Contact Times
- 15 Synthetic Organic Chemicals

TCE: PSDM PREDICTION - KARLSRUHE TAP WATER CORRELATIONS

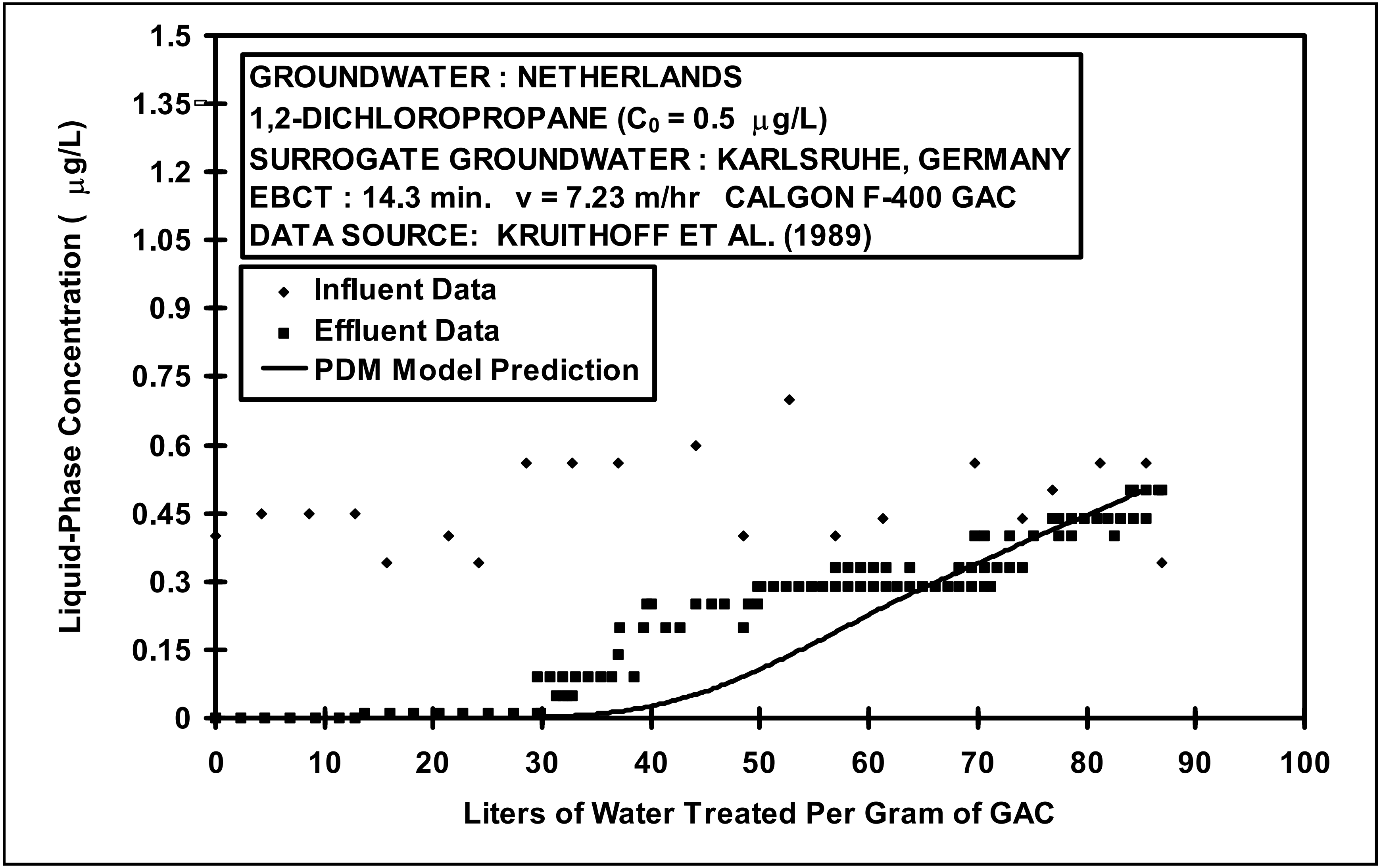


TCE: PSDM PREDICTION - RHINE RIVER WATER CORRELATIONS



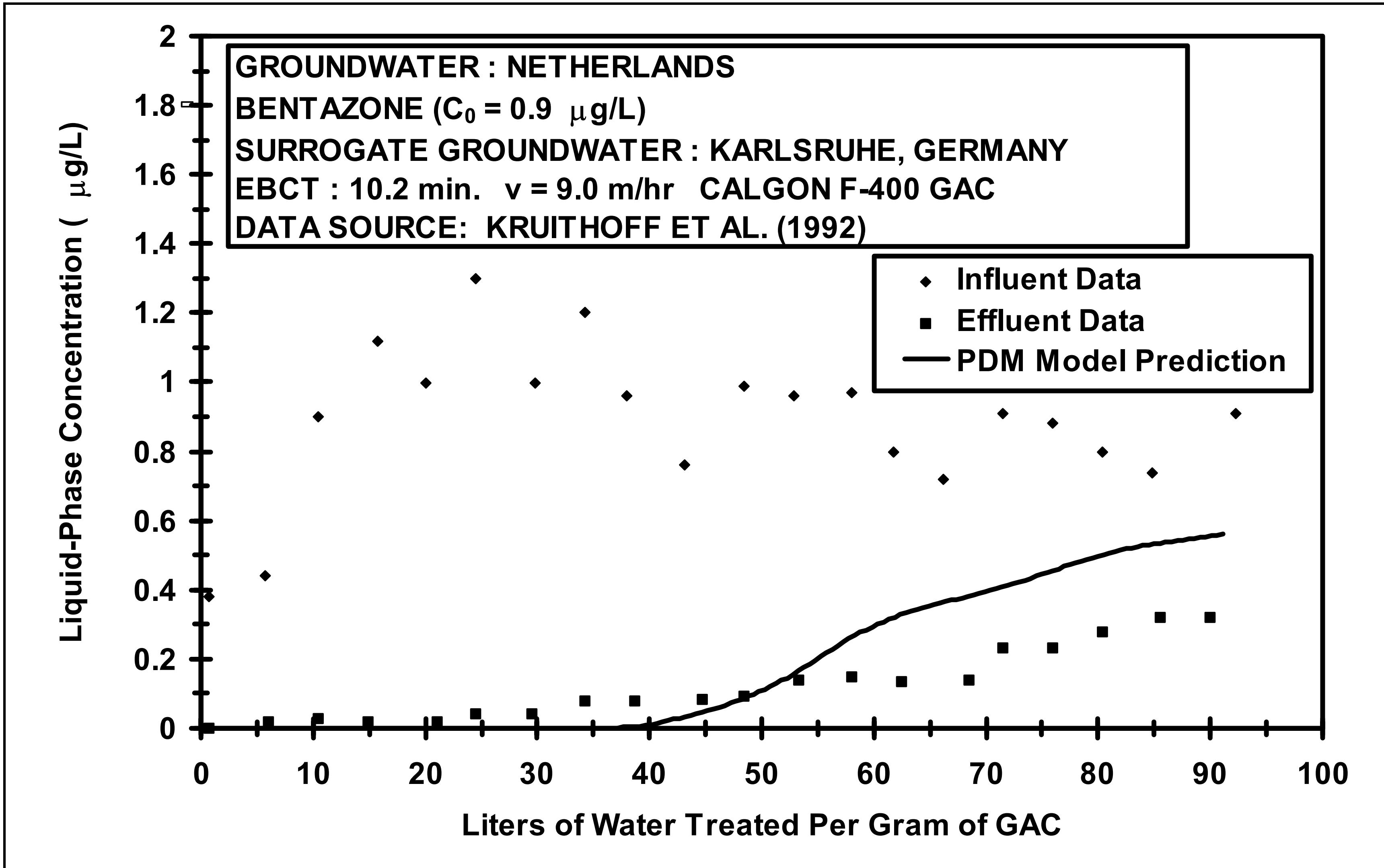
MichiganTech

1,2-DCP: PSDM PREDICTION - KARLSRUHE TAP WATER CORRELATIONS



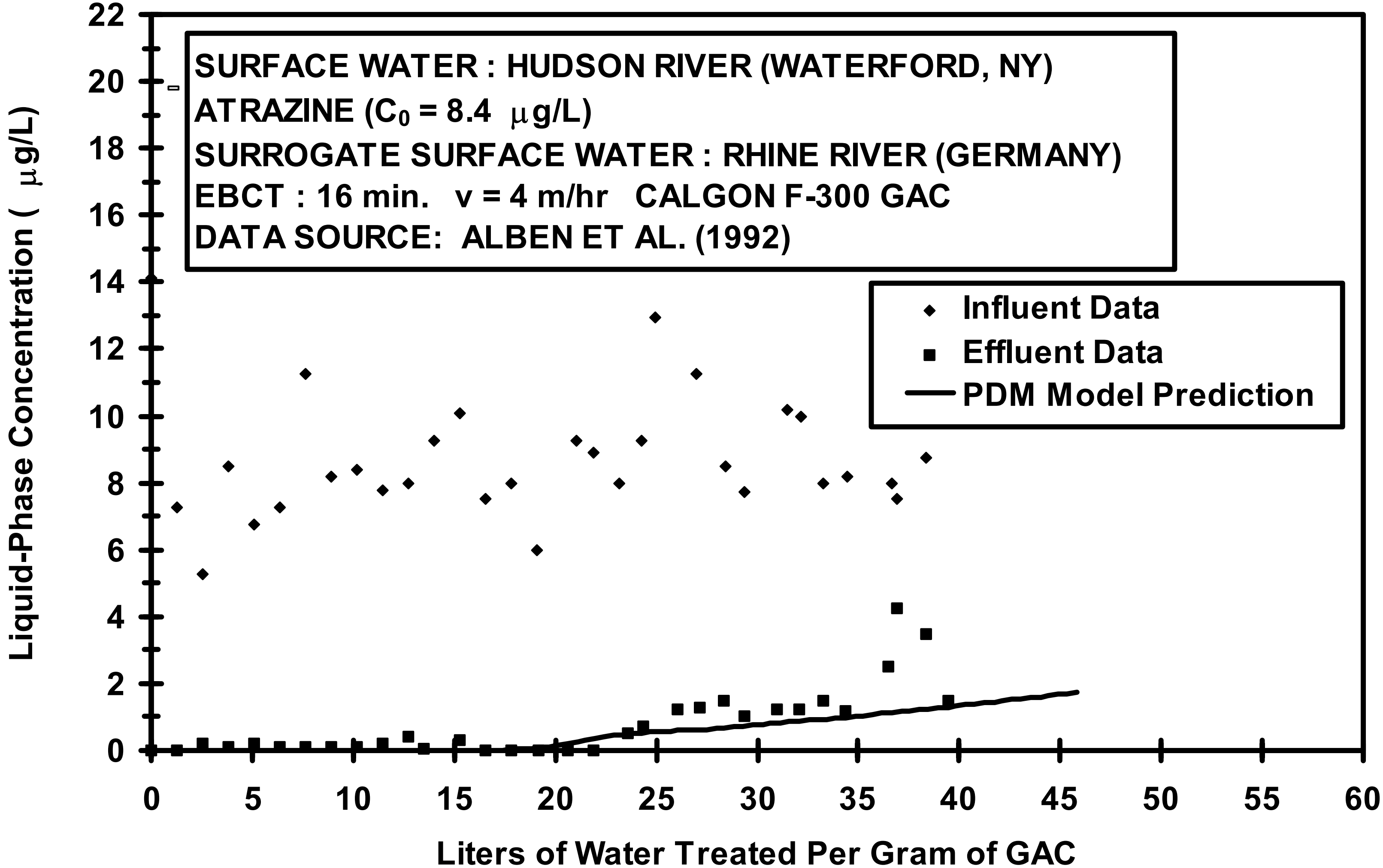
MichiganTech

BENTAZONE: PSDM PREDICTION - KARLSRUHE TAP WATER CORRELATIONS

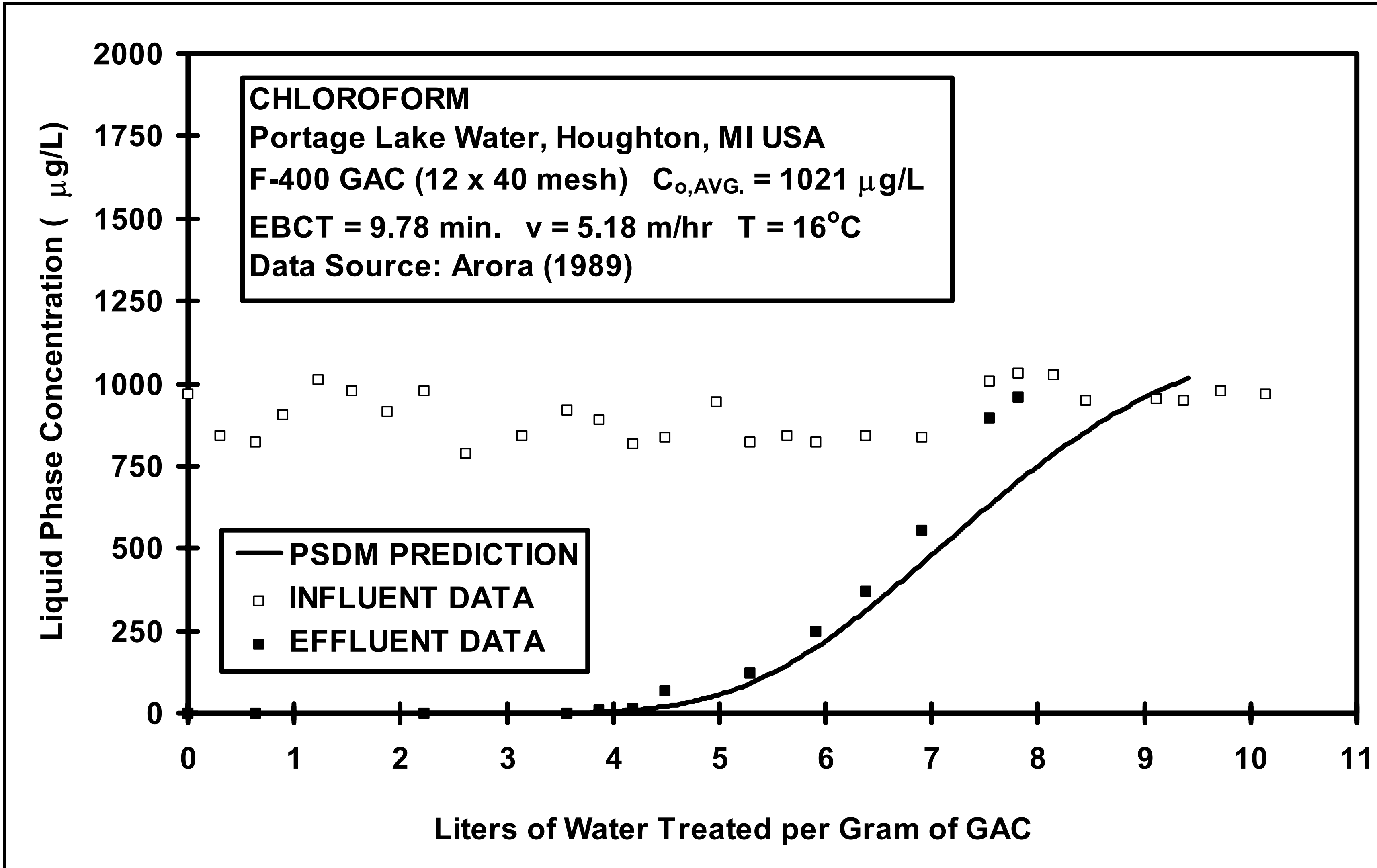


MichiganTech

ATRAZINE: PSDM PREDICTION - KARLSRUHE TAP WATER CORRELATIONS

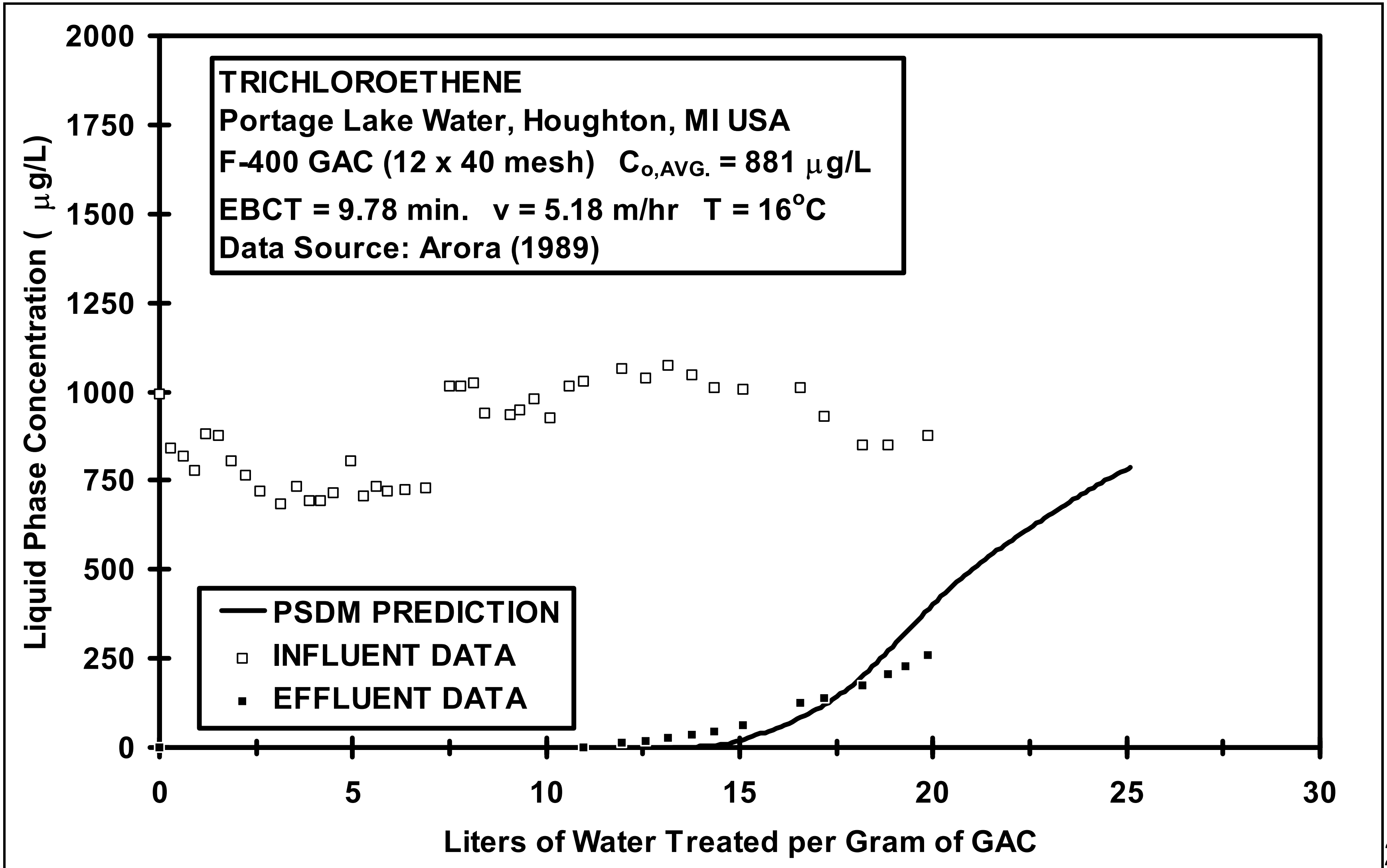


CHLOROFORM: PSDM PREDICTION USING THE RHINE RIVER WATER FOULING CORRELATION



MichiganTech

TCE: PSDM PREDICTION USING THE RHINE RIVER WATER FOULING CORRELATION



CONCLUSIONS

- AdDesignS™ interfaces several fixed bed adsorption models, model parameter estimation methods, and isotherm and adsorbent data bases.
- AdDesignS™ allows the user to make adsorber performance predictions with greater ease and archive the results.
- The heuristics for determining the most appropriate models and parameters should be considered work in progress and the Adsorption Design Software can be greatly improved as more information is gathered on the practical application of the models.

CONCLUSIONS (continued)

- Single component isotherm data can be correlated using the intrinsic molar volume and the Polanyi Potential Theory
- Multicomponent equilibria can be predicted from single solute isotherms using IAST for similar sized molecules
- The Equilibrium Column Model can predict the longest bed life and the highest overshoot concentrations for multicomponent mixtures of known components.

CONCLUSIONS (continued)

- The PSDM can predict the effluent concentration history profiles for multicomponent mixtures of known components.
- The PSDM can simulate the effluent concentration history profiles for SOCs in the presence of BOM.
  - Reductions in capacity and diffusivities which were estimated from a ground water and surface water span the range of fixed bed data from 11 different studies.
  - Additional comparisons are needed to develop more general guidelines.

FURTHER READING

Crittenden, J.C., N.J. Hutzler, D.G. Geyer, J.L. Oravitz, and G. Friedman, "Transport of Organic Compounds with Saturated Groundwater Flow: Model Development and Parameter Sensitivity," *Water Resources Research*, 22 (3), 271-284 (1986).

Crittenden, J.C., T.F. Speth, D.W. Hand, P.J. Luft, and B. Lykins, "Evaluating Multi-component Competition in Fixed Beds," *Journal of Environmental Engineering*, 113 (6), 1363-1375 (1987a).

Crittenden, J.C., D.W. Hand, H. Arora, and B.W. Lykins Jr., "Design Considerations for GAC Treatment of Organic Chemicals," *Jour. of AWWA*, 79 (1), 74-82 (1987b).

Crittenden, J.C., R.D. Cortright, B. Rick, S.R. Tang, and D. Perram, "Using Granular Activated Carbon to Remove Volatile Organic Chemicals from Air Stripping Off-Gas," *Jour. of AWWA*, 80 (5), 73-84 (1988).

Hand, D. W., J. C. Crittenden, and W. E. Thacker, "Simplified Models for Design of Fixed-Bed Adsorbers," *Jour. of Env. Eng. Div., Proceedings of ASCE*, 110 (EE2), 1984.

Hand, D. W., J. C. Crittenden, H. Arora, J. Miller, and B.W.Lykins Jr., "Design of Fixed-Beds to Remove Multi-component Mixtures of Volatile and Synthetic Organic Chemicals," *Jour. of AWWA*, 81(1) 1989.

Hand, D. W., J.C. Crittenden, D.R. Hokanson, and J.L. Bulloch, "Predicting the performance of fixed-bed granular activated carbon adsorbers," *Water Science and Technology*, 35(7), 235-241 (1997).

Sontheimer, H., J.C. Crittenden, and R.S. Summers, "Activated Carbon for Water Treatment," DVGW-Forschungsstelle, Engler-Bunte-Institut, Univ. Karlsruhe, Fed. Rep. of Germany (1988).

ACKNOWLEDGMENTS

- National Center for Clean Industrial and Treatment Technologies (CenCITT)
- U.S. Environmental Protection Agency
- National Science Foundation (No. ECE 8603615)
- Environmental Engineering Center (MTU)
- Some laboratory and field data were analyzed and provided by G. Baldauf, Gerhard Zimmer, and the late Professor Heinrich Sontheimer at Engler-Bunte-Institut, University of Karlsruhe