Final Report

Effects of Molecular and Environmental Properties on Removal of Pharmaceuticals, Endocrine Disruptors and Disinfection Byproducts by Polyamide RO Membranes

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Executive Summary

Introduction

Membrane treatment technology such as reverse osmosis (RO) has gained widespread acceptance and is used in a variety of industries. While its original application was centered on desalting seawater, RO is being challenged with treating more complex waters such as municipal wastewater. The profiles of municipal wastewater streams (and a host of other water sources) have become more complex, as previously undetected organic compounds are now being detected in trace quantities. These compounds are ubiquitous because of their widespread use in a number of areas such as domestic, industrial and agricultural applications. The ultimate fate of these compounds, however, is municipal wastewater. Organic compounds, including disinfection byproducts, pharmaceuticals and endocrine disrupting chemicals are all classes of compounds now readily detected in municipal wastewater (1-4). Removal of these and other unregulated compounds that pose potential human health risks is critical if RO is to remain a viable treatment technology for municipal wastewater.

Objectives

Four objectives were undertaken in order to gain an understanding of the complex relationship between organic compound physicochemical properties and removal by RO membranes:

- Determination of rejection of trace-organics of interest by Federal and State regulatory agencies using exemplary RO membranes
- Identification of significant compound and membrane physicochemical properties
- Correlation of membrane performance (compound removal) with compound physicochemical properties using multivariate methods to elucidate the mechanisms associated with solute transport of trace-organic compounds

- Investigation of the influence of water quality parameters on the rejection behavior of membranes.

Approach

Cross-flow membrane test cells designed to hydraulically simulate a spiral-wound RO element and manufactured by OCWD were used to conduct the bench-scale experiments. The cells were connected to a common feed source designed to operate in a closed-loop configuration (RO brine and permeate returned to the feed tank during operation). Feedwater exposure to air was minimized to limit test compound volatilization and feedwater temperature was controlled. Each test cell was independently adjusted to operate all membrane swatches at constant water production (flux) and crossflow velocity.

Three commercial standard, high-rejection polyamide RO membranes were evaluated: ESPA-2 (Hydranautics), TFC-HR and TFC-ULP (Koch Membrane Systems). Membranes were provided by the manufacturers in the form of flat-sheets. Organic compounds studied included disinfection byproducts (DBPs), simple aromatics, pesticides and other compounds considered of interest by State and Federal regulatory agencies added to the feedwater at 26.4 – 35.2 ug/L (ppb). In addition, this list also included several unregulated endocrine disruption compounds (EDCs) added at 500 ug/L (ppb). Organic compound physicochemical descriptors were obtained by visual assessment of molecular structures and by searching various readily available resources and databases of molecular properties.

Compound rejection (expressed as log removal) was measured under nominal cross-flow conditions. These data were compiled and a quantitative structure activity relationship (QSAR) approach involving an artificial neural network (ANN)-based empirical multivariate model was utilized to elucidate relationships between compound properties and membrane rejection.

RO removal data for many of these compounds by test membranes were also available from a previous laboratory bench scale study at OCWD supported by a USEPA grant awarded to OCWD through the Desalination Research Innovation Partnership (6), as well as from field observations at the pilot scale (Santa Clara Water Authority, SCWA) and full scale (West Basin Municipal Water District, WBMWD) for comparison to OCWD bench-scale results obtained in this study.

A second objective of this study, representing an extension of previous work at OCWD (6), involved determination of the influence of the feedwater matrix on RO compound rejection. Several compounds identified in that study, along with the same RO membranes, were tested in the cross-flow membrane test unit used in this study under varying salinity and pH conditions. These analyses were used to estimate the degree to which variations in feedwater pH and salinity influence organic compound removal efficiency by RO membranes. Also, conducting these trials under cross-flow conditions helped validate the rejection data obtained from the rapid dead-head radiometric assay method utilized in the former OCWD USEPA study.

Results

RO performance was expressed as log removal as opposed to percent rejection to improve representation of more highly rejected compounds during modeling. Additionally, a categorical analysis was performed in which compound removal was categorized in seven (7) bins: >0 – 0.5 log, 0.5 – 1.0 log, 1.0 – 2.0 log, 2.0 - 3.0 log, 3.0 – 4.0 log, >4.0 log or "membrane accumulation" if log removal was negative (compounds released rather than rejected by the membrane).

The different types of RO membranes exhibited similar compound removal; differences of one log removal or less were observed between the membrane types for the compounds studied.

Compound removal could be described well by an ANN model constructed by incorporating all of the removal data from the three different membranes and including the membrane parameters to the list of potential inputs. Parameters included in the model as predictors of compound removal included: compound log P, compound molecular weight , the number of compound methyl groups and RO membrane roughness. A correlation value of 0.97 was obtained for the resultant model, indicating good agreement between the predicted and the measured log removal values.

Sensitivity analysis and scatter plot analysis revealed a positive relationship between log removal and both log P and molecular weight. The poorest removal of contaminants occurred in where log P <2 and MW <150. DBPs and many endocrine disruptors fall in this category. Higher values for log P and MWs higher than 150 Daltons were correlated with higher compound removal. The log P sensitivity index value suggests that it is the most influential descriptor in the model, and is likely the primary driver when compounds are small and log P is high. In this case, passage of compounds through the membrane may be retarded by membrane adsorption as opposed to steric exclusion, and exhibit high apparent rejection until membrane saturation occurs. Sensitivity analysis indicated a positive relationship between compound removal and both, molecular weight and the number of methyl groups on the compound; likely this is related to increased steric hindrance encountered when larger and more complex structures pass through the RO membrane polymer matrix. The slight negative relationship indicated between membrane roughness and compound removal is more difficult to explain. The effect may be direct (e.g., related to increased membrane surface area which also results in increased probability of membrane/compound interactions), indirect (roughness acts as an indirect indicator of differences in internal membrane matrix structure that affects compound diffusion) or only fortuitous (the ANN used roughness only to identify the membrane).

Membrane rejection behavior for the trace-organic compounds studied was nearly independent of pH and salinity values typically encountered in municipal wastewater treatment applications; predictions of maximum and minimum removal values differed by less than a log in most cases – far less than effects of varying chemical structure.

Variations in pH and salinity did not reduce rejection of highly rejected compounds so that they became poorly rejected, or vice versa.

Conclusions

An empirical QSAR model predicting RO organic rejection using readily obtainable physicochemical properties was developed. Good agreement was observed between empirical data and model predictions for EPA methods 508 and 524 compounds (e.g., DBPs, some EDCs and PCPs), as well as some hormones. However, it is also likely that the model is limited in application to compounds similar to the exemplars used in this study. Further studies are needed if more general predictions of organic compound rejection are desired; however, this study demonstrates that a QSAR approach based on simple physicochemical descriptors may be used to describe and predict rejection of many compounds by thin film composite polyamide RO membranes. The study also indicates that in many cases, variations in feedwater pH and salinity encountered in a typical multi-pass RO installation purifying wastewater do not seriously alter compound rejection, and do not compromise rejection of many highly rejected organic compounds. However, because the scope of study compounds was limited, it may not be possible to generalize this observation. For instance, small, highly charged organic salts were not included in this study; these might be expected to react more strongly with membrane surface and internal charges modulated by both feedwater pH and salinity.

Recommendations

Although this study produced an explanatory and generally predictive model, the finite scope of exemplary compound properties (and possibly test membrane properties) limit general model application; further studies are needed using a wider variety of molecular exemplars with a broader range of physicochemical properties. Also, after examining and comparing organic removal data at the bench, pilot and field scale, it is apparent that current grab-sampling methodologies and use of short term spiking may be adequate for inorganic salts with low membrane affinity, but likely poorly represent membrane

removal of organic compounds with strong membrane affinity. Grab sample measurements may be susceptible to historical biases caused by feed concentration variation and previous membrane accumulation if compounds have large membrane affinities. In this case, a protocol compositing (integrating) feedwater and product water concentration over time may prove superior by allowing membranes time to equilibrate.

Abstract

Removal by thin film composite polyamide reverse osmosis (RO) membranes of a number of trace-organic compounds and hormones considered of interest by State and Federal regulatory agencies was studied using cross-flow membrane test cells. Compounds in RO feed and product water were analyzed using EPA methods 508 and 524 as well as methods developed by OCWD for hormones and endocrine disrupting compounds (EDCs). An empirical artificial neural network (ANN) model relating log compound removal to compound physicochemical properties and membrane properties was successfully constructed. Log removal was used as a transformation function instead of the traditional expression of percent rejection to provide a more even representation of performance value variations across the range of observed compound removal values. Log P most strongly influenced RO removal, followed by molecular weight and the number of methyl groups on the compound. Membrane roughness was weakly related to compound removal.

The rejection behavior of membranes in response to altering feedwater quality parameters (pH and salinity) was also investigated. A surface-response statistical approach in which the range between the minimum and maximum predicted removal of the compound over a range of pH and salinity was used to define influence of these parameters. It was typically observed that variation in compound removal due to these environmental properties was not dramatic; overall, changes in removal over the study range of pH and salinity was less than one log. Highly rejected compounds were not observed to become poorly rejected, and vice versa.

Observations and conclusions were limited by the range of compounds, membranes and environmental variations employed in the study, but nonetheless help expand understanding of principals governing RO rejection of organic substances of public health concern.

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1.0 Introduction

Meeting the demand for potable water is becoming an increasing challenge for water municipalities. Traditionally, this demand has been met using surface water and groundwater supplies, but in arid and semi-arid regions, such as the southwest United States, these supplies are increasingly becoming less reliable and less capable of meeting the demands of the growing regional populations. As a result, municipalities are turning to the use of recycled wastewater as a reliable source to augment traditional drinking water supplies.

Membrane treatment technology such as reverse osmosis (RO) has gained widespread acceptance and is used today in a variety of industries. While its original application was centered on desalting seawater, RO is now being challenged with removing more complex organic chemicals such as those found in municipal wastewater. This is especially true as new, more sensitive analytical detection methodologies are developed, and previously undetected organic compounds are now being detected in trace quantities, making chemical profiles of municipal wastewater streams (and a host of other water sources) more complex. The ultimate fate of many of these compounds that are nearly ubiquitous because of their widespread use in domestic, industrial and agricultural applications is municipal wastewater. Organic compounds, including disinfection byproducts (DBPs), pharmaceuticals and personal care products (PPCPs) and endocrine disrupting chemicals (EDCs) are all readily detected in municipal wastewater (1-4). Removal of these and other unregulated compounds that pose potential human health risks is critical if RO is to remain a viable treatment technology for municipal wastewater.

1.1 Background

The Orange County Water District (OCWD) has been successfully purifying municipal wastewater since the commissioning of Water Factory 21 (WF-21), where secondary municipal wastewater was treated using conventional clarification followed by cellulose acetate RO treatment and disinfection. The 5 million gallon per day (mgd) RO system served as the final filtration step to reclaim municipal wastewater for the maintenance of a seawater intrusion barrier along the coast of Southern California. WF-21 was decommissioned in January 2004, after 27 years in service. It will be replaced by an advanced water treatment facility known as the Groundwater Replenishment System (GWR System), an integrated membrane system (IMS) that will purify close to 100-mgd of municipal wastewater using microfiltration (MF) pretreatment followed by RO and advanced oxidation. The success of the GWR System and other IMS facilities treating similar waters is dependent on maintaining high removal efficiencies for regulated organic contaminants. The removal of unregulated trace organic compounds such as endocrine disruptors and those on state and federal lists such as the U.S. Environmental Protection Agency's (USEPA) candidate-contaminant list are of increasing importance when considering the application of membrane technologies.

Currently it is difficult to know a priori how effective RO (and other treatment technologies) will be in removing compounds which have recently adopted regulatory limits. Given the size and capital cost of municipal water treatment plants, rapid modifications to meet changing regulatory requirements can be difficult and costly. For example, in 1998, N-nitrosodimethylamine (NDMA) was discovered in a northern California drinking water well, and was identified as a byproduct of water treatment. Shortly thereafter, the California Department of Public Health (CDPH) established a notification level (NL; health-based advisory levels established for chemicals that lack maximum contaminant levels (MCL) – an enforceable standard). As a result of reclassifying this compound, OCWD could not successfully remove NDMA to the

specified level and therefore had to abandon the use of its 10-mgd carbon adsorption treatment process. NDMA is only one of many organic compounds of interest by the USEPA and the CDPH. Furthermore, the significance and impact of disinfection byproducts, pharmaceuticals, endocrine disrupting chemicals and other organic compounds is yet to be determined. Given the potential impacts associated with these compounds in the water supply, efforts to better understand their persistence and behavior are needed. In a dynamic regulatory environment, research efforts will benefit water agencies and industries faced with the inevitable issue of removing organic contaminants from their process streams.

1.2 Project Objective

The collective aims of this study were to gain an understanding of the complex relationship between organic compound physicochemical properties and interaction(s) (rejection) by RO polyamide membranes. To achieve this, four objectives were undertaken:

1. Determination of the rejection of trace-organic compounds of interest by Federal and State regulatory agencies using exemplary RO membranes;
2. Identification of significant compound and membrane physicochemical properties;
3. Development of models that correlate membrane performance, i.e. rejection, with compound physicochemical properties to elucidate the mechanisms associated with membrane transport of trace-organic compounds
4. Investigation of the influence water quality parameters have on modulating membrane rejection behavior.

These objectives were met through bench-scale testing at OCWD utilizing membrane swatch test cells designed to simulate the hydrodynamic environment encountered in commercial spiral-wound RO membrane modules. An advanced artificial neural network (ANN) multivariate model and surface-response analysis were then used to describe RO

removal behavior of selected trace-organic compounds. In addition, organic rejection data obtained from Sonoma County Water Agency (SCWA) in northern California (a pilot-scale testing facility) and West Basin Municipal Water District (WBMWD) in southern California (full-scale testing) for comparison to and validation of OCWD results.

2.0 Project Approach

2.1 RO Membranes

Three RO membranes were selected for study (Table 1): ESPA-2 (Hydranautics, Oceanside, CA), TFC-HR and TFC-ULP membranes (Koch Membrane Systems, San Diego, CA). These are standard, high-rejection thin film polyamide RO membranes, and were provided by the manufacturers in the form of flat-sheets from which swatches were obtained. Membranes selected for bench-scale testing were in use at SCWA and WBMWD, so that performance comparison between OCWD bench scale experimental data, and field pilot-scale and full-scale data would be possible. The list of membranes in Table 1 represents a revision of the original list proposed in the project quality assurance project plan (QAPP), which included a cellulose acetate (CA) RO membrane and a nanofiltration (NF) membrane. Issues beyond the control of the investigators, however, required that the scope of the bench-scale project be revised downward, and as a result of this approved revision, the CA and NF membranes were not included in this study.

2.2 Cross-flow Membrane Test Cell

The bench-scale experiments were conducted using cross-flow membrane test cells designed and manufactured by OCWD (Figure 1). Each cell generates accurate performance data rapidly and without significant expense commonly associated with operating larger pilot-scale systems, and the operating conditions within the cell can be varied to simulate a wide range of flow hydraulic conditions (5). The cell is entirely constructed of 316-stainless steel for maximum durability and chemical resistance. A flat

sheet (swatch) of membrane material approximately 97-cm^2 and a shim spacer are placed between the top and bottom plates and secured. The shim is made of Teflon© of varying thicknesses (typically 30-60 mil) and is used to set the flow channel height to match that of a typical spiral RO element feed spacer. A permeate (product water) carrier consisting of uniformly porous sintered 316-stainless steel (100 micron pore size) has been engineered into the top plate of the unit. This serves not only to direct permeate to the product tube (while minimizing the hold-up volume due to the large pore size) but provides structural support critical for maintaining the integrity of the membrane (the membrane is only 150 microns thick and the rejecting layer is even thinner, typically 0.2 microns). Flexible tubing consisting of Viton (Cole-Parmer, Vernon Hills, IL) or material with similar chemical resistance, slips on the end of the product tube for sample collection. A stainless steel rotary vane pump (Fluid-o-Tech, Plantsville, CT) or multistage centrifugal pump (Grundfos Pumps Corporation, Olathe, KS) maintains pulseless cross-flow hydraulic conditions across the membrane surface. A 316-stainless steel concentrate flow control valve (Swagelok Company, Solon, OH) restricts the flow exiting the cell to create the required pressure and flow conditions needed to drive the RO process. The feed pressure into and across the membrane is monitored using stainless steel pressure gauges (NOSHOK, Berea, OH). Validation trials were previously conducted (data not shown) and verified that the performance characteristics of the test cell simulates a spiral RO element (5).

A system consisting of twelve stainless steel cells was constructed by OCWD to test multiple membrane samples and/or operating conditions simultaneously (Figure 2). All cells were connected to a common feed source, with each cell capable of operating independently. This arrangement allowed membrane samples to operate at constant water production (flux) and crossflow velocity throughout the duration of each trial. Feedwater was provided by a 60-gallon stainless steel reservoir tank. Heat generated by the feedwater centrifugal pump was removed using a refrigeration unit coupled to a stainless steel cooling coil that maintained constant feedwater temperature during each test. The system was designed to operate in a batch-mode, or a closed-loop configuration in which both RO permeate and brine was returned to the feedwater reservoir. To avoid

the possibility of contamination and/or loss of test compounds through adsorption, all wettable materials within the system were constructed of 316-stainless steel and the reservoir tank headspace was minimized by a cover plate in contact with the water surface to reduce loss of volatile compounds.

2.3 Experimental Plan

The experimental plan for the first three objectives outlined in Section 1.2 is illustrated in Figure 3. A list of regulated (i.e., those containing MCLs or NLs) organic compounds of interest by State and Federal regulatory agencies and several unregulated endocrine disruption compounds (hormones) was compiled. The OCWD water quality laboratory would conduct analyses for all compounds tested at OCWD, and also assisted WBMWD and SCWA with analysis of hormones.

Organic compound physicochemical properties would be obtained by visual examination of the molecular structure and by searching various readily available resources and databases. Membrane rejection would be measured under cross-flow conditions utilizing the test cell and system described earlier. These data would be compiled and multivariate analyses performed to establish relationships between compound properties and membrane rejection.

The experimental plan to satisfy the final objective is outlined in Figure 4. This objective represents an extension of a previous USEPA grant awarded to OCWD through the Desalination Research Innovation Partnership (6) in which a rapid laboratory assay to measure removal of organic compounds by RO membranes was developed and utilized to provide data for a quantitative structure activity relationship (QSAR) model relating RO removal to fundamental molecular properties (obtained through molecular modeling). Through these analyses, a number of compounds were preliminarily identified containing diverse molecular properties influencing rejection by RO membranes. These compounds, along with the same RO membranes used in the initial study, would be tested in the cross-flow membrane test unit (Figure 1) under varying salinity and pH conditions.

These trials would help elucidate the rejection behavior of RO membranes under varying operational conditions. Conducting these trials under cross-flow conditions would also validate the rejection data obtained from the rapid laboratory assay method developed in the former USEPA study.

2.4 Planned Approach for Evaluating Project Objectives

2.4.1 Task 1 – Compilation of Trace-Organic Compound List and Identification of Compound Properties

2.4.1.1 Organic Compound List

The list of organic compounds used for the study was generated from a search of applicable USEPA and CDPH databases and included constituents with and without established MCLs. It included USEPA Method compounds, including Method 524 volatile organic compounds and Method 508 organo-chlorinated compounds (Table 2). The compounds were provided by Ultra Scientific (N. Kingstown, RI) and Sigma-Aldrich (St. Louis, MO) and consisted of USEPA 500 method standards used to identify and quantify organic compounds in municipal drinking water. All constituents in the standards were pre-analyzed; most were >99% pure. Certificates of analyses were provided with each standard (See Appendix 2 for exemplars). The list of compounds used for the study was limited by analytical ability and sample load constraints of the OCWD water quality laboratory.

Many contaminants of possible public health concern exist which are absent from both Federal and State regulatory guidelines. These classes of compounds include prescription and non-prescription drugs, steroids, hormones, and a host of other chemicals associated with human and industrial usage. A study conducted by the U.S. Geological Survey demonstrated the detection of many synthetic organic compounds in water sources across the United States (7). The criteria used to select compounds for inclusion were (a) the probability of existence in wastewater streams (based on quantities used), (b) possible

human health implications, (c) broad representation of compound classes (thorough the use of surrogates), and (d) the analytical methodologies to measure the compound. Based on these selection criteria, a list of 95 compounds was generated for this study. Even though it was fairly limited in size, it represents one of the few databases of its kind currently in existence.

Analytical methods for these unregulated compounds were developed by OCWD. Nine (9) hormones and potential endocrine-disrupting compounds (Table 3) were utilized for this study. Since standard analytical methods for these unregulated compounds are not widely adopted, the OCWD water quality laboratory conducted analyses for OCWD, SCWA and WBMWD. The laboratory standard operating procedures (SOPs) are included in Appendix 1. Other organic compound analyses reported in this document related to SCWA and WBMWD used as a comparison with OCWD model results were derived by analysis of water samples submitted to contract laboratories utilizing standard EPA methods.

2.4.1.2 Organic Compound Properties

Compounds may be characterized by physical and chemical properties that describe behavior in the environment. Such properties include molecular weight, melting point (MP), water solubility (WS), log P, vapor pressure (VP), Henry's Law constant (HLC), atmosphere OH rate constant (OHA), density (D), etc. A series of readily available references were utilized in an attempt to obtain these data for study compounds. The Syracuse Research Corporation maintains an interactive physical properties database (PHYSPROP) which contains chemical structures, names and physical properties for over 25,000 chemicals (http://www.syrres.com). Other resources included those maintained by CambridgeSoft Corporation (http://chemfinder.cambridgesoft.com) and ChemZoo Corporation (http://www.chemspider.com). In addition, simple visual inspection of molecular structures reveals information that may affect interactions of compounds with membranes, including the number different elements, number and type

of rings, number and type of side chains, etc. Compound properties used in this study are summarized in Appendix 3.

2.4.2 Task 2 – Bench-Scale Membrane Performance Analysis

2.4.2.1 Task 2.1 – Membrane Screening Analysis Using Simple Matrix

A screening analysis was conducted to determine rejection of the test compounds by the test RO membranes using the system illustrated in Figures 1-2. Given the number of compounds that were screened, this represents one of the largest studies of its kind to date.

Membranes selected for this study consist of high solute rejection, high throughput commercial PA membranes in use at OCWD and SCWA and WBMWD. The target operating water flux (i.e., water production) was 12 gfd (20 L/m^2h), which is typical for RO membranes treating filtered municipal wastewater. Prior to conducting the trials, membrane swatches were loaded into each of the 12 test cells and operated under cross-flow conditions at a pressure of 150 psi for a minimum of 15 hours on deionized water. This process was necessary to extract any unreacted monomers (e.g., trimesolyl chloride and *m*-phenylenediamine) and other chemical substances (e.g., sodium bisulfite, methylene blue, etc.) that might remain associated with the membranes following their production. As part of the membrane preparation procedure, initial membrane performance (water flux and solute rejection) of each swatch was measured upon completion of the 15 hour rinse and compared to the specifications provided by the manufacturer. If performance was out of specification, the membrane swatch was rejected. A total of 4 replicate membrane swatches were prepared for each membrane type and experimental condition tested in the study.

After this initial membrane preparation step, the contents of the feed tank were discarded and replaced with a matrix consisting of 1,000 mg/L reagent-grade sodium chloride (ACS reagent, > 99.0%, Sigma-Aldrich, St. Louis, MO) in deionized water. The pH was

adjusted to 6.0 – 6.5 with reagent-grade HCl (ACS reagent, 36.5-38%, Sigma-Aldrich, St. Louis, MO) to reflect that typical of municipal RO feedwater in wastewater reclamation.

Test compounds were added, and the feedwater tank thoroughly mixed to establish uniform concentration. The tank was then secured and the system started. The system was operated for 4-5 hours prior to sample collection (8) to ensure that the membranes had attained a steady-state condition. During this period, both the concentrate (brine) and permeate were returned to the feed tank until sample collection was initiated so that solute feed concentration remained constant. Approximately 5% of the total feed tank volume was produced as RO product water. Based on previous studies conducted at OCWD, was shown that displacing up to 10% of the tank volume over the course of any experiment would negligibly affect results.

Multivariate modeling required determination of numerical values for removal. Since rejection values for many compounds are unknown, all compounds were assumed to potentially be rejected at 99.9% (3-log removal). The concentration of organic compounds added to the feed tank depended on the calibration range of the laboratory analytical instrumentation and the expected range of rejection for each analyte. Compounds were added to the feed so that 99.9% removal represented the mid-point in each analyte's instrument calibration range. Feed concentrations determined by this method for the study were 26.4 ug/L (ppb) for EPA Method 508 compounds, 35.2 ug/L (ppb) for EPA Method 524 compounds, and 500 ug/L (ppb) for the hormones.

Compound removal was calculated based on percent rejection and log removal by the membrane using the following calculations:

(1) % Rejection = ((Feed Concentration - Product Concentration)/Feed Concentration)*100

(2) *n*-fold reduction = initial concentration/final concentration

(3) Log Removal = log (*n*-fold reduction)

It was anticipated that a limited number of USEPA Method 524 compounds would exhibit some degree of volatilization due to elevated vapor pressures, thus resulting in a loss of concentration in the feedwater (personal communication with OCWD laboratory director and staff). A strict sampling protocol was followed to help reduce this problem. Sampling of both the feedwater and RO product water commenced simultaneously. Further, the feedwater sample was collected at the same rate (mL/minute) as the RO product sample in an effort to prevent differential volatilization in each of the two samples. Other measures included reducing the feed tank surface area with a cover resting on the liquid surface, sealing sample bottle openings (with inserted RO product tubing) using Teflon©-faced septa and locating the test system in an area void of direct sunlight.

2.4.2.2 Task 2 – Evaluating Effects of pH and Salinity on Organic Compound Rejection

It is well known that membrane performance may be affected by a host of parameters including feedwater temperature, pH and salinity. As the temperature of the feedwater increases, water flux increases due to increased permeate flow rates. This increase generally results in lower salt rejection (higher salt passage) as the solute diffusion rate increases. PA membranes are considered tolerant over a broad pH range; however the ionic environment of the feedwater has been shown to influence RO membrane rejection (9). Altering the ionic concentration changes the osmotic pressure of the feedwater. An increase in the feedwater ionic concentration increases the osmotic pressure, thus requiring a larger applied pressure to overcome (or reverse) the natural osmotic flow. If the applied pressure gradient remains constant, however, the water flux would begin to decrease, thus resulting in a decrease in salt rejection as well. While these general trends have been observed and are well understood, what has not been examined in greater detail is the influence each of these parameters has on the rejection of trace-organic

compounds. Further, the influence of each parameter on the other and the subsequent impact on solute rejection has also not been extensively investigated.

This task investigated RO membrane rejection behavior as a function of feedwater pH and salinity. A statistical software package (Statgraphics Centurion version XV, Statpoint, Inc., Herndon, VA) was employed to design an experiment to conduct a surface-response analysis (see Section 2.5.2). Experimental trials were conducted in a similar fashion to those outlined in Section 2.4.2.1 Task 2.1 above. Constituents used for the task consisted of the EPA Method 524 compounds (see Table 2). This represents a deviation from what was proposed in the initial QAPP; there, approximately 7-10 compounds were preliminarily selected as well as three water quality parameters - temperature, pH and salinity. Final selection was to be based on the following considerations: (a) interest by both OCWD and regulatory agencies as compounds of public health concern, (b) ability of the OCWD laboratory facilities to analyze the compounds and (c) generated sample workload. Modifications in the workplan were necessary to reflect a reduction in OCWD's water quality laboratory capacity for research samples. However, while the number of parameters was reduced to two (pH and salinity), the number of constituents analyzed was increased from the 7-10 proposed in the QAPP to more than 50 compounds by analyzing multiple compounds simultaneously during experiments. This greatly expanded the scope of the investigation. Feed concentration of these compounds was 44 ug/L (ppb).

2.5 Modeling Approaches

2.5.1 Artificial Neural Network (ANN) Quantitative Structure-Activity Relationship (QSAR) Model

2.5.1.1. Selection of Model Input Parameters

Empirical quantitative structure-activity relationship (QSAR) models that employed a generic algorithm (GA) to select optimal inputs and an artificial neural network (ANN) to

describe interactions of organic compounds with RO membranes have been previously constructed by our laboratory (6). This previous study used fundamental molecular descriptors as inputs to predict the interactions of organic compounds with TFC and CA RO membranes. A similar strategy was employed in the current study to produce an empirical model capable of describing the observed removal of the test compounds by the test membranes; however, in this instance, organic compound physicochemical properties such as molecular weight, log P, water solubility, etc. were employed as model inputs. Although physicochemical properties of compounds may be less precise in defining the molecular properties involved in determining diffusion of organic compounds through RO membranes, they are commonly available to the water professional via the Internet and they may be obtained with no special knowledge of numerical chemistry or use of molecular modeling or molecular dynamics software. Descriptions of the molecular skeleton were also employed in the study (e.g., the number of methyl groups or aromatic rings) and are also simple to determine with only a fundamental knowledge of organic chemistry. Input data used in construction of the model are shown in Table 4.

Membrane properties represented in the model are indicated in Table 5. These were derived previously by OCWD.

2.5.1.2 Model Output Considerations – Timing of Measurements and Choice of Log Removal as a Model Output

Efficiency of organic compound removal was used as the model output; however, some consideration had to be made as to how this was both measured and expressed. Membrane performance needed to be expressed in such a way that a few compounds removed very well or very poorly did not seriously bias the data to be modeled. Also, interactions of the compound with the membrane could significantly affect the apparent membrane performance depending on when product concentration was determined.

When small organic compounds (such as DBPs) strongly associate with the RO membrane, it is possible for the membrane to remove the compound from the RO product

mainly by absorption. In such an instance, initially very little of the compound is observed in the product. Later, however, as the RO membrane loads to saturation, the compound begins to break through and the concentration in the product rises. Thus, initially the membrane appears to perform quite well, but with time as the membrane begins to saturate, RO removal declines severely. In order to avoid this condition, RO membrane performance data used for model construction was obtained after five hours of membrane exposure to organic contaminants. Previous research suggested that this exposure time was sufficient for equilibration of the membrane to occur (1).

Another consequence of strong interactions between compounds and the RO membrane may be a significant time lag between variations in compound concentration in the feed and consequent variation in concentration in the product. If compound affinity is very great and concentration declines in the feed (perhaps due to absorption to the membrane surfaces) to levels below that observed in the product, the RO membrane appears to produce rather than attenuate the compound, though a mass balance of the compound involving integration over an appropriate length of time would reveal that this is not at all actually the case. However, an expression of compound removal would yield a negative value. Although association of compounds with the RO membrane were not directly observed during this study, a negative value for organic contaminant attenuation was attributed to strong association between the compound and the membrane.

Efficiency of compound removal by RO is traditionally expressed as the percent rejection, which is defined as:

$$100-(([Product]/[Feed])*100)$$

This expression assumes a value less than one hundred (100), but can be less than zero (0) if the compound in question is being released from the membrane into the product at a concentration exceeding the feed at the time of measurement. The difficulty with using this expression as a measurement of RO membrane performance for modeling purposes is that the rejection of a majority of organic compounds fall between 90% and 100%, which only represents 10% of the percent rejection range. Moreover, removal of 90%

represents merely a log reduction in compound concentration. Thus, with this expression, 90% of the observed variation available for modeling is provided by compounds removed relatively poorly. Moreover, variations in compounds exceeding an order of magnitude are seriously deemphasized. For example, improving removal of a compound by 10 fold above 90% rejection only increases percent rejection to 99%.

In order to avoid biasing the model with the most poorly rejected compounds, log removal, defined as:

$$\text{Log}_{10}\ ([\text{Feed}]/[\text{Product}])$$

was used to describe compound removal. In this case, a more even representation of performance value variations is obtained across the range of observed compound removal values, and thus there is no tendency for more poorly removed compounds to bias a model constructed using these values. Feed concentrations employed in the study and detection limits of analytical equipment made possible detection of between 3 and 4 logs removal for many organic micropollutants. The overall detection limits for compounds in practice were on the order of 4.3 logs removal; on rare instances where product concentration proved non-detectable, a removal value of 4.3 logs was assigned to the compound for modeling purposes.

Membrane removal of compounds was also expressed on a categorical basis in this study; organic compound removal was categorized as being >0 – 0.5 log, 0.5 – 1.0 log, 1.0 – 2.0 log, 2.0 - 3.0 log, 3.0 – 4.0 log, or >4.0 log. Compounds with removal <0 log (negative values) were categorized as "membrane accumulation" (Table 8).

2.5.1.3 Selection of Compounds for Model Validation

Validation data for an empirical model are often a subset of the information upon which the model is based that is not used in the construction of the model. Subsequently, the model is challenged with these data and its prediction of the dependent variable

compared to the measured values. Close agreement with the validation set indicates a predictive model.

If the experimental data set available for model construction consists of numerous exemplars broadly representative of the full spectrum of variations in the input variables, the validation set may be derived via a simple random sampling. However, with limited experimental data sets, random derivation of the validation set becomes more problematic. The principal difficulty becomes the probable loss of critical information from the remainder of the data set, and subsequent crippling of the model by removal of unique training exemplars.

When small data sets are to be used, it is possible to non-randomly choose the validation exemplars such that the choice does not hamper the knowledge of the model, but still provides a challenge of model predictive ability. In this study, validation exemplars were chosen from the total list of experimental compounds such that as much as possible their structures and properties were flanked by compounds included in model construction. In this fashion, the probability of losing critical input information for model construction was minimized, and the validation compounds tested the ability of the model to derive compound behavior by interpolation, which an ANN should be able to accomplish, as opposed to risk predicting from extrapolation, which is most often beyond the capabilities of a neural network.

2.5.1.4 Use of a Genetic Algorithm (GA) to Select Model Inputs Best Correlated with RO Removal of Organic Compounds

Prior to construction of the ANN, an initial selection process was required to identify the subset of molecular descriptors best correlated with log removal of organic compounds. This operation was carried out using a GA.

2.5.1.4.1. Choice of Exemplars and Randomization of Order

All numerical operations were carried out using Microsoft Excel (Microsoft Corp., Redmond, WA). For all the individual membrane models, data spreadsheets were created containing a line of data for each individual exemplar. Exemplars were constructed for each test compound by combining the molecular descriptors with the measured log removal values. For each RO membrane, the numerical measurements related to specific membrane properties were also included in the input parameter set, the a priori assumption being that one or more of these membrane properties would prove capable of differentiating behavior of the individual test membranes in the resultant model.

The original laboratory replicates were used in this process rather than averages of the data. Each of the test compounds was typically represented by 4 laboratory replicates. This approach increased the number of available exemplars for modeling as well as captured the full range of statistical variation present in the laboratory measurements which otherwise would have been lost in an averaging process. Altogether, a total of 774 exemplars were used for model construction.

The order of the exemplars was randomized prior to any input winnowing or modeling efforts. This was achieved by first creating random numbers using the Excel randomization function and assigning these numbers to each line of exemplar data, then sorting the exemplars using these random numbers. This resulted in a complete randomization of the order of the exemplars in the data spreadsheet. Randomization of the order of the exemplars was performed before each input selection or modeling effort as an additional precaution to insure that the order in which data were presented did not influence the final results.

2.5.1.4.2 Identification of Subsets of Influential Descriptors Using a Genetic Algorithm (GA)

Genetic algorithms (GA) are commonly being used to find a set of parameters that optimize a complex multiparameter function, especially when there is a large number of potential input parameters and a restricted number of exemplars to analyze. Details regarding how GAs operate have been described elsewhere (10). A GA was previously successfully used by our laboratory to identify optimal input parameters for a previous USEPA QSAR study describing RO membrane-organic compound interactions (6).

Selection of input parameters for this study was achieved using a GA provided as part of the NeuralWorks Predict package (NeuralWorks Predict v3.12, Neuralware, Carnegie, PA). This program utilized a logistic multiple linear regression fitness evaluation. In addition to the normal GA selection criteria, an additional "Cascaded Variable Selection" was employed to rapidly eliminate inputs with a low probability of inclusion in the optimum input set (a function especially useful with large input arrays). Inclusion of inputs by the GA was detected by construction of a single ANN and performing a sensitivity analysis to detect influential inputs (methods described below). The GA eliminated descriptors that did not predict compound-membrane interactions, and typically reduced the initial descriptor set down to subsets of less than 6 descriptors.

2.5.1.4.3 Identification of Most Influential Input Parameters

The GA converges on an optimum fit between the input parameters and the output parameter, but it does not necessarily predict a globally optimum input set. The GA uses a random start point, and noise in the data set can result in some inputs being included that are only weakly related to the output variable. However, it was expected that statistically the GA should choose the most highly influential inputs most frequently. We have found that a histogram constructed from multiple, independent GA selections reveals the most influential input parameters for modeling (6). This histogram was

constructed for this study by operating the GA for 10 iterations. For each of these iterations, the order of exemplars in the data spreadsheet was re-randomized, ensuring that the GA started with a completely different and randomized seed population each time.

"Influential" inputs were identified for construction of the ANN model by using a simple filter based on inclusion of the input in ≥ 50% of the input sets (6).

2.5.1.4.4 Construction of an Artificial Neural Network (ANN) Model

Neural network computing is less susceptible to many of the difficulties encountered with other methods of multivariate analysis, including dealing with partially correlated input variables, as may be the case with molecular physicochemical properties. In addition, neural computing methods are capable of describing the behavior of highly complex, nonlinear systems in which the exclusive rules of the interaction are either unknown or difficult to quantify.

As with GAs, the details regarding how ANNs are designed and constructed is outside the scope of this report (11); however for descriptive purposes ANNs may be considered virtual models of biological brains, and are comprised of a network of virtual neurons ("perceptrons"). Information enters each perceptron via "synapses"; each feeding a simple function with a weighting factor that can emphasize or de-emphasize the overall influence of the function. The effects of all the input functions are summed in the perceptron, then fed to an output function (often sigmoidal) by which the perceptron passes information to units further down in the network. The neural net is constructed by interconnecting layers of these perceptrons. Although highly complex multlayered networks are possible, the design adopted for this study was a three-layered network consisting of an input layer, a "hidden" processing layer and an output layer (a single output perceptron in this case). The relationship between inputs and the outputs of a complex system are embossed upon the network by "training" it using concrete exemplars from the real world. During the training process, perceptrons are added and

the values of the weighting factors are adjusted until the behavior of the network converges on the behavior of the real system as determined by one or more correlative comparisons. At this point, the network has "learned" to recognize patterns in the input data that predict the output data. As with any empirical mathematical modeling method, challenging the network with a "test" set of exemplars evaluates the predictive ability of the network. Test data typically consist of 10% to 20% of the exemplars that were not present during training. A well-trained network will predict behavior of the test exemplars as well as it did the training exemplars.

2.5.1.4.5 Randomization of Exemplars Prior to Model Construction

As before, the order of exemplars was randomized prior to GA selection and ANN model construction. This ensured that any ordering of the exemplars would not influence selection of inputs by the GA or training of the ANN.

2.5.1.4.6 Construction of ANN Model

An ANN model was constructed from the surviving input parameters using NeuralWorks Predict v3.12 (Neuralware, Carnegie, PA).

2.5.1.4.6.1 Assigning a Data Noise Level

Although the input data were theoretically "clean", the output data were considered to be "moderately noisy". The software settings were adjusted accordingly to help prevent model over fitting (modeling variations caused by noise).

2.5.1.4.6.2 Assignment of I/O Transformation Functions

Input data entering the network had to be transformed from real world values to the relative input values required by the ANN. This was accomplished by use of one or more transformation functions. Whereas during selection of salient inputs the choice of

transforms was limited to one, in this case up to three transforms could be assigned per input (thus, there could be up to three input perceptrons per input descriptor in the ANN). Transformation functions could either be linear (scaling only), or nonlinear (log, ln, exponential, power, inverse, inverse power or hyperbolic tangent) expressions. The software automatically optimized the choice of functions by regression analysis.

2.5.1.4.6.3 Selection of Model Inputs Using the GA

The method used was more extensive than that for identification of salient input parameters described above in an attempt to further reduce the number of input parameters. Once again a multiple logistic linear regression routine was employed with the cascade variable selection activated.

2.5.1.4.6.4 Selecting Training and Test Exemplar Pools

Input data were divided into two sets using a round robin selection criterion that eliminated every fifth exemplar from the training pool and used these eliminated exemplars to create a testing pool. As the data were previously randomized, this process yielded a random selection of 20% of the exemplars for testing. This process did not specifically remove data for entire compounds from the training pool. The number of experimental compounds included in the study was sufficiently small that complete elimination of any compound from the exemplar database could seriously affected the experience of the ANN. Thus, the model was tested for its ability to predict around noise variations in the exemplar data. Model validation was achieved using the validation set previously described (Section 2.5.1.3).

2.5.1.4.6.5 Training and Selecting the Best ANN Model

Three networks were constructed using the training data. Construction and training the networks proceeded using an adaptive gradient learning rule in which back-propagated gradient information was used to guide an iterative search algorithm. Back-propagation

involves determining the difference between the desired output (the actual laboratory result) and the network prediction, then adjusting the output layer (perceptron) weighting factors in proportion to the difference. The calculations involved in this correction are then used as a basis for making correction to weights in the hidden layer and finally in the input layer (11).

Performance of the networks was evaluated by comparison of the linear correlation (R) between the predicted outputs and the actual laboratory removal data, and the best of the three ANNs chosen.

2.5.1.4.6.6 Testing the Selected Network

The test exemplar set previously described was used to determine the ability of the ANN to predict log removal of the compounds. Comparison of the correlation coefficient to the training set results was used as a measure of overall performance. A close match between training and test data sets was taken as an indication of a good model. In this case, the training and test R values were within 0.02.

2.5.1.4.6.7 Using Sensitivity Analysis to Eliminate Non-Influential ANN Inputs

Due to the more stringent GA settings and the ability to employ more than one transformation function during ANN model construction, the possibility existed that not all of the descriptors provided to the model would be chosen for inclusion in the model. In order to eliminate inputs that had been rejected by the ANN, a sensitivity analysis was performed on the entire data set. This analysis generally indicates the degree and direction of influence that each input in the ANN model has on the model output. If the sensitivity analysis is zero, the input likely has no overall significant effect on the model and may be eliminated without a significant change in model fitness.

In this instance, no inputs were eliminated from the input data set and the ANN model was adopted as-is.

2.5.1.4.6.8 Producing an Excel-Enabled Exportable ANN Model Describing Log Removal of Organic Compounds by RO Membranes

The ANN model was converted to Visual Basic (VB) source code using a Visual Basic compiler provided with NeuralWorks Predict. This source code was imported as a macro function into an Excel spreadsheet designed to include input cells allowing the user to manually enter the relevant input data for any compound of interest, including membrane and compound properties and compound feed concentrations. The embedded ANN VB program then calculates the predicted log removal of the compound and projects membrane performance in terms of percent removal, concentration in the product, and compound mass fluxes.

This exportable ANN model is capable of running under Windows on any PC computer running a macro enabled version of Excel (version for Office 2000 or later).

2.5.1.4.7 Validation of the ANN Model

2.5.1.4.7.1 Validation of the ANN Model Using the Validation Set

The ANN model was validated by challenging it with the exemplars contained in the validation set, and its prediction of the dependent variable compared to the measured values. Close agreement with the validation set indicates a predictive model.

2.5.1.4.7.2 Validation of the ANN Model Using Field Data

Validation of the model was also attempted utilizing field data obtained from RO operations at WBMWD and at SCWA, where RO membranes used at these facilities were also used in this study. In the case of WBMWD, compounds examined included a large number of DBPs naturally present in the feedwater. In the case of SCWA, the compounds consisted mostly of PPCPs, and included both baseline feed concentrations

and spike data. In a number of cases, compounds detected in the field at these facilities were also contained in the ANN model experimental data set from OCWD so that both the predicted values from the ANN model and laboratory values could be compared with the field data.

The properties of all the compounds identified at these field sites were obtained and the ANN model was used to predict log removal. A comparison with measured field values of log removal (when obtained) was performed both for WBMWD and for SCWA.

2.5.2 Use of Statistical Experimental Design and Surface-Response Analysis to Study Effects of pH and Salinity

The influence of pH and salinity (over a range typically observed in RO systems engaged in wastewater reclamation) on log removal of selected micropollutants was examined using methods of statistical experimental design and analysis. A statistical package (Statgraphics Centurion XV, Statpoint, Inc., Herndon, VA) was utilized to design a two factor experimental matrix with pH and salinity. After operating the test cells under conditions called out in the matrix, resultant log removal data for each of the study compounds were analyzed using a surface-response approach and the magnitude of influence of pH and salinity on log compound removal by RO determined.

2.5.2.1 Design of the Experimental Matrix

Two experimental factors, pH and salinity, were chosen for water matrix effect evaluations. Salinity of municipal reclaimed wastewater is about 1,000 mg/L, and varies over a factor of over six (6) fold through the feed of an RO plant processing reclaimed wastewater at 85% recovery. Values for pH encountered in RO plants commonly range from 6 to 8. For this reason, the water matrices used in these experiments consisted of pH of 6.0, 7.0 or 8.0 and salinities of 1,000 mg/L, 3,500 mg/L or 6,000 mg/L.

Combinations of pH and salinities chosen for experimentation were established statistically using a 3-level factorial experimental design based on 4 replicate inputs for each condition. This resulted in a randomized experimental design consisting of 36 runs with 27 degrees of freedom. This was a level V design; it could be used to test for all main effect and two-factor interactions. Analysis of a correlation matrix revealed that this design was fully orthogonal.

2.5.2.2 Analysis of Experimental Results Using a Surface-Response Approach

Following execution of the experimental matrix for all test compounds and all test membranes, data were analyzed and a surface-response diagram generated for each compound and each membrane. In performing this analysis, a standardized Pareto chart which displayed a value for each single effect or two-effect combination proportional to its t-statistic was used to ascertain whether or not both single factors and two factor combinations showed a statistically significant influence on log removal of the test compound (statistical significance was defined at the 95% confidence level for this study). Effects that were not statistically significant were removed from the analysis.

2.5.2.2.1 Creating Surface-Response Models for Compound Removal

Compound response was modeled using a best-fit to a polynomial equation incorporating all statistically significant main and two-factor effects. A surface-response plot was generated from this model expressing log removal of the test compound as a function of salinity and pH. In addition, main effects plots were also generated to allow evaluation of the relative influence of both salinity and pH on organic compound removal.

2.5.2.2.2 Determining and Analyzing Overall Influence of pH and Salinity on Compound Removal

In order to facilitate evaluation of the potential for variations of pH and salinity to influence compound removal by the test RO membranes, the surface-response analysis was used to identify the minima and maxima from each surface-response chart. These data were tabulated for each compound on each test membrane. For each case, the values of pH and salinity corresponding to the minimum and maximum removal of each compound were also evaluated. The difference between the minimum and maximum values of compound removal was taken as an indicator of the relative strength of influence that these environmental variables have over compound removal.

3.0 Project Outcomes

3.1 Membrane Solute Rejection Related to Organic Compound Physicochemical Properties

3.1.1 Compound Rejection and Physicochemical Properties

The list of organic compounds and associated physicochemical properties used for this study is shown in Tables 6a-6d. RO performance (expressed as log removal, see Section 2.5.1.2) for each of the three RO membranes is shown in Tables 7a-7b. The different types of RO membranes exhibited similar compound removal; differences of one log removal or less were typically observed between the membrane types for the compounds studied.

3.1.2 ANN Membrane Model Describing Organic Compound Rejection

The ANN best describing variations in log removal of the test compounds by the test membranes had a 5-29-1 structure (5 input nodes, 29 hidden layer nodes and 1 output node). It included as inputs the values of log P, the number of methyl groups, compound molecular weight and membrane roughness. Transformation functions were applied to

these parameters to couple them to the ANN inputs: linear scaling and x^2 functions both were applied to membrane roughness, x^2 to the compound molecular weight and log P, and natural log to the number of methyl groups. The output parameter (log removal) was transformed by a square root function. Although it is not possible to reproduce a mathematic representation of the ANN model in this report as with other types of multivariate models, OCWD will supply upon request an Excel spreadsheet containing the model and a user interface for programming input data and obtaining output data. Contact Don Phipps, Research Director, OCWD, 18700 Ward Street, Fountain Valley, CA 92708 or email dphipps@ocwd.com.

Performance of this ANN model is summarized in Figure 5. The graph provides a visual indication of the fitness of the model by displaying the predicted values of log removal against the actual values (mean plus standard deviation) obtained experimentally for all membranes. Open symbols represent training/test data that were employed by the GA and ANN in input selection and model construction, while closed symbols represent validation compounds which were withheld from all model construction activities and hence indicate predictive abilities of the model (see Section 3.1.4 below). From this visual presentation it may be seen that the model appeared to describe and predict log removal of organic compounds fairly well.

Statistical analysis of model performance is indicated in the table below the graph. Results are presented for the whole data set (all 774 input exemplars), for the training data set (541 exemplars used to construct the ANN) and for the test data set (233 exemplars randomly removed prior to ANN construction used to test ANN predictive ability). Good agreement between training and test set data statistics indicates a predictive model. In all cases with this model, agreement between training and test data is very good.

The R statistic shown here represents the linear correlation between the real world target output and real world model output, where 1.00 indicates a perfect correlation. The high correlation for all data (0.97), for training data (0.98) and for test data (0.96) show that

the ANN model adequately described variations observed in organic compound removal by all the test membranes. The average absolute error between the real world target outputs and the real world model outputs is on the order of 0.2 log removal (average difference between what the model predicted and the real data). The root mean square error between the predicted and actual compound removal was on the order of 0.3 – 0.4 log. The 95% confidence interval is on the order of 0.6 log for the ANN model; this may be interpreted as the overall limit of model prediction or alternatively the "noise band" of the model.

The lower table shows the results of a sensitivity analysis which calculates in general how influential each input is by determining the magnitude of change in model output as a function of changes in the values of each input. This is somewhat similar to a derivative analysis. The sign of the value indicates overall direction of the influence with respect to the model output. Although this type of analysis may be fooled by small, rapid changes, it can be a fair indicator of the importance of a particular input. Results of this analysis will be discussed in Section 3.1.3 below.

Tables 9a - 9c compare the measured and predicted values of log compound removal by the three study membranes. A categorical analysis of the model output compared to measured results is shown in Tables 10a and 10b. In this table, the Percent Exact (% Exact) column indicates how often the measured category matched exactly with the predicted category. Generally, the measured and predicted values were in the same category. In all cases, the difference in log removal was within one category (1 log difference), which is anticipated by the model 95% confidence interval.

3.1.3 Most Influential Model Input Parameters

As indicated earlier, the inputs to the ANN model acting as predictors of compound removal by RO included the compound log P, the number of methyl groups, compound molecular weight and RO membrane roughness. Sensitivity analysis suggests that

differences in log removal by the membranes could be mostly attributed to compound physicochemical properties.

Log P appeared the most positively influential molecular physicochemical property in the model by the results of the sensitivity analysis (value = 1.15). This molecular parameter has been shown in the previous USEPA study at OCWD (6) to be an important predictor of RO removal efficiency. As log P increases, compound hydrophobicity increases. The interaction between hydrophobic compounds and the hydrophobic polyamide polymer likely results in a general tendency for these compounds to strongly associate with the membrane, either by adsorbing on the membrane surface if they are large and complex, or absorbing within the membrane matrix if molecular structure is smaller and simpler.

The number of methyl groups (value = 0.73) was indicated by sensitivity analysis to be the second most positively influential parameter and the molecular weight (value = 0.30) the third most positively influential variable in the model. Molecular mass and complexity are known to affect organic rejection (12-17). Berg et al. (18) determined that molecular structure, such as the number of methyl groups, may be an important parameter for predicting the rejection of non-charged molecules by NF membranes. Non-charged compounds with a higher number of methyl groups were reportedly rejected at higher levels than ones with lower numbers of methyl groups. In the case of this study, the sensitivity analysis also revealed a positive relationship overall between both molecular weight and the number of methyl groups on the molecule, and log compound removal – the larger and more complex the molecule, the greater the tendency for the RO membrane to retard its passage. The primary mechanism in both cases may be attributed to steric hindrance as the molecule diffuses through the membrane matrix.

A direct comparison of compound log removal as a function of log P and molecular weight are illustrated in Figure 6 and 7, respectively. The data shown here represent the average of the replicate analyses performed for all compounds in all experiments. The log P data show a direct and relatively strong relationship to compound removal, which is anticipated by the model sensitivity analysis results (Figure 5). Molecular weight tends

to follow a similar trend - the more massive the compound, the greater the removal. Although the data in these direct comparisons are much noisier, as they contain other factors affecting compound removal, the relationships are visually compelling and tend to support conclusions suggested by modeled results. Looking at the ESPA-2 membrane alone as an example (Figure 8), a categorical analysis of removal which tends to eliminate small perturbations caused by other factors, demonstrates a reasonably positive relationship between log removal and both log P and molecular weight. The poorest removal of contaminants occurs in general with log P <2 and MW <150. DBPs and many endocrine disruptors fall in this category. Higher values for log P and MWs higher than 150 Daltons show higher compound removal. Many pharmaceuticals tend to fall in this category.

The above observations and large value shown in the sensitivity analysis in the model suggests that with the compounds included in this study, log P is likely the primary driving parameter. A small compound that could easily pass through an RO membrane by steric considerations alone would pass slowly if it had a large log P. Rejection values of small molecules with large log P may be at least initially very large as these compounds concentrate in the RO membrane. However, once the membrane is saturated the compounds will break through into the feed, and continue to do so even if the feed concentration is non-detectable, as the membrane and not the feed becomes their source. This is the likely mechanism resulting in the apparent "negative rejection" observed in this study. Small compounds of less than 150 Daltons with higher log P values such as 4-isopropyltoluene, N-butylbenzene, sec-butylbenzene and t-butylbenzene may exemplify this class of compound. Alternatively, small simple compounds with lower log P values such as 1,2-dibromoethane and dibromomethane were not removed well (see Table 11).

Of the membrane parameters considered in the study, only roughness appeared as a predictor of compound removal, and judging by the low sensitivity index value (value = -0.06), it was overall a rather weak predictor. Rejection of most of the test compounds by the test membranes was observed to be very similar, so this result is not altogether surprising. That the sensitivity index is negative indicates that the greater the membrane

roughness, the less the test compounds were rejected. Unlike with the other model input parameters, the reason for this is less clear. The effect could be direct; increased roughness leads to an overall increase in membrane surface area, which increases the probability of molecular interactions of all kinds at the feedwater/membrane interface, including absorption and diffusion into the membrane. The effect could be indirect; increased roughness may reflect variances in the internal membrane chemistry associated with compound diffusion, for example. If, for instance, increased surface roughness was associated with decreased internal cross-linking of the polyamide polymer, steric resistance to compound passage may be reduced in rougher membranes. Or, the association might be fortuitous; differences in roughness values of the three membranes might have acted as a categorical sorting mechanism in the ANN. Since there were only a small number of exemplars of different membrane types, it is possible that the ANN simply identified classes of membrane behavior using roughness. In this case, the numerical value of roughness would have no relationship at all to compound removal, but merely act as a label for the ANN with which to identify membranes of a particular class. The weakness of the response and the fact that visually the data do not appear to vary strongly between the membranes suggests this is not a likely mechanism, but lacking a continuum of roughness exemplars, it is difficult to rule out entirely.

3.1.4 Validation of the ANN Model Using the Validation Set

In this study, validation exemplars were chosen from the total list of experimental compounds such that as much as possible their structures and properties were flanked by compounds included in the model construction. The probability of losing critical input information for model construction was then minimized, and the validation compounds tested the ability of the model to derive compound behavior by interpolation. The model was challenged with these data and its prediction of the dependent variable compared to the measured values. Results of prediction of validation set compounds are indicated by filled symbols in Figure 5. In most instances, predictions of log removal of the validation compounds agreed well with observed compound behavior, indicating that the ANN model was capable of predicting the behavior of compounds closely resembling the

structure and properties of compounds in the experimental data set. So long as new compounds meet this criterion, this sort of empirical multivariate ANN modeling approach utilizing easily obtainable physicochemical compound properties and membrane properties should be able to predict removal of any new organic micropollutants by RO membranes. However, application of this model beyond the experimental data set must be done with reservation. With any empirical model of this type, there are limitations to the universality of its predictions which are a function of its experience. In this instance, the values of inputs for the compound and membrane properties must fall within the range of the model training set or the model will very likely fail.

The model scope is also limited by the RO system properties. In this study, a simple feedwater matrix (de-ionized water and sodium chloride) and new membranes were used. Additionally, although steps were taken to equilibrate the membranes, the possibility remains that compounds with highest membrane affinities were not in equilibrium at the time samples were taken for performance analysis. This can be problematic, especially where results are to be compared with field data; removal may appear high when in reality it could be very low.

Another consideration is the potential presence of model biases as a consequence of the training data set. With a small training set as was utilized in this study, model bias is certainly a concern. In this study, exemplary compounds were limited to those detectable using EPA Methods 524 and 508 and hormones, many of which are neutral or only slightly polar. While it is anticipated that the model should have little difficulty predicting the behavior of compounds detected via these methods (with presumably similar properties), it certainly might fail to predict the behavior of compounds with strong centers of charge, such as strong organic acids or bases, or strongly polar compounds. In this case, the lack of charged moieties in the exemplary compounds may have failed to provide the ANN with the experience needed to predict membrane-compound charge interactions.

Finally, it must be recognized that although model inputs serve as predictors of compound removal, there is no implication of direct mechanism. Clearly inputs such as molecular weight and log P may imply direct steric or affinity types of interactions. However, it is quite possible that rather than a direct relationship with attenuation of organic compound diffusion through the membrane, there is an indirect relationship which may be comlex. This is particularly an issue with membrane roughness, where there are only three variations in the data set. Although able to predict behavior of any of the three exemplary membranes whose performance served in its construction, predictions made for a membrane with intermediate roughness values might not be very accurate. A complete set of validation compounds from a membrane not used in the construction of the model were not available; therefore, this possible limitation of the ANN cannot be ruled out.

3.1.5 Overall Effects of Physicochemical Properties

Physicochemical properties by far best predicted compound removal by RO membranes, and it is encouraging that given the quantity and variety of potential inputs, a fairly robust model could be constructed with only a few simple physicochemical parameters related to hydrophobic and steric interactions. Though the model was likely limited to compounds detectable by EPA methods 524 and 508 (e.g., DBPs), some EDCs and PPCPs, it may prove very useful in dealing with these classes of contaminants, and moreover illustrates the value of this approach to predict RO rejection behavior. One of the appealing characteristics of this model is the ease with which input data may be obtained for its application; parameters such as molecular weight, log P and the number of methyl groups on the molecule may be obtained for a large number of compounds by any water engineer without special software or knowledge of advanced chemical theory or methodologies.

Finally, although it is unwise to apply this particular model to predict RO removal of classes of compounds not included in the study, a broader effort using the same basic approach but encompassing a test compound database with a far wider variety of

physicochemical properties might prove very fruitful, and result in a model with far broader applicability.

3.2 Influence of Water Matrix on Organic Compound Rejection

3.2.1 Compound Rejection as a Function of pH and Salinity

The composition of the different RO feedwater matrices are illustrated in Table 12. The ranges of pH and salinity used in this study were those typically encountered in RO treatment plants engaged in water reuse.

Results of water matrix variations did not seem to have a dramatic effect on organic compound rejection (Tables 13a-13aa). RO rejection of most of the test compounds appeared to be relatively independent of pH and salinity within the range of values employed in the study. Moreover, no cases were observed where shifting pH or salinity altered the performance of the membranes such that a compound initially well rejected became poorly rejected, or vice versa.

3.2.2 Performance of Surface-Response Models

In order to facilitate evaluation of the potential for variations of pH and salinity to influence compound removal by the test RO membranes, surface-response analysis was employed to characterize the overall influence of both parameters on compound removal. Polynomial models were constructed to examine the magnitude of maxima and minima of rejection resulting as pH and salinity were varied over their test ranges. The magnitude of separation between the maxima and minima values were used as an index relating removal of each compound to salinity and pH variations.

Results of this analysis are tabulated for each compound on each test membrane in Tables 14a-14e.

3.2.3 Overall Influence of pH and Salinity on Organic Compound Rejection

Overall, pH and salinity variations did not greatly alter RO compound removal. Insensitivity of RO rejection to changes in water quality parameters is an advantage for treatment plant operations, especially with respect to salinity, which increases significantly along the RO train from the feed end to the brine end of the plant. However, this observation is limited by the range of compounds examined in this study. Most notable, no highly charged organic molecules were examined, and these may well be more sensitive to both pH and salinity shifts, both of which could alter the RO membrane surface charge and influence charge-charge interactions with more highly charged organic contaminants.

The study was limited to the practical values for pH and salinity expected in secondary treated wastewater purification, and it was also limited by a simple feed matrix (sodium chloride and compounds). Actual matrices that define RO feedwater are far more complex, and certainly may be capable of modifying the behavior of organic compounds and RO membranes (18-19). Other limitations are the simple membrane matrix (unexposed clean membrane) and the equilibration of the membrane in the system. Although the compounds used in this study appear relatively insensitive to pH and salinity shifts, complexity of environmental parameters in the field might greatly complicate general prediction of RO removal of many organic contaminants, making experiments involving more complex feedwater matrices and a wider variety of contaminants highly desirable.

3.2.4 Comparison of previous USEPA project results with this Study

The initial USEPA funded work at OCWD examining RO removal of organic compounds (6) focused on developing a rapid radiometric potential assay (RMP assay) to measure interaction of organic compounds with RO membranes and to relate the interactions (removal or association) to fundamental molecular properties of the compounds. QSAR models were developed that enabled prediction of compound rejection. In this study,

compound exposure to the membrane was relatively short (30 minutes), although compound concentration in the feed ranged from 414 ug/L (t-butyl alcohol) to 4,986 ug/L (erythromycin). It was possible that this was not enough time for the membranes to be at equilibrium. In addition, the RMP assay system was not a cross-flow system. The cross-flow component is required for prevention of significant formation of a polarization layer on the membrane, which degrades RO performance. This issue was considered during the initial studies and it was concluded that since the feed matrix was ASTM I de-ionized water with the sole solute the test contaminant, membrane polarization would be minimized. Observed values of rejection by the RMP assay tended to correspond with values observed in a standard RO unit. However, it was desirable to validate results of this initial study by comparing the RMP assay to a more traditional cross-flow RO system.

Seven surrogate compounds from the original study were also included in this study using the cross-flow membrane test cell under varying salinity and pH conditions (Table 15). In general, the compounds that were rejected well in the initial study were also well rejected in this study. The absolute values differ, but categorical analysis (the log removal ranges) show the compound behavior was very similar. The assays were in the same range or differ by one range (or < 0.6 logs) in general. As a result of this comparison, the RMP assay utilized in the initial OCWD study could definitely be considered capable of generally predicting RO rejection, and with the added advantage that the fate of the organic contaminant could be ascertained (whether membrane-bound, capable of penetrating the membrane, or remaining in the feed).

3.3 Comparison of Predicted Organic Compound Rejection with Field Data

Organic compound rejection data obtained from SCWA in Northern California (pilot-scale testing) and WBMWD in Southern California (full-scale testing) were also compared with results from this study to examine the effective ability of both the bench scale assay and the model to describe organic rejection in the field.

Comparisons between the SCWA field data and model predictions (Tables 16a-16b) were often limited by poor resolution of field rejection values. This was the case because with the field data, product contaminant values often fell below instrument detection limits. In such cases, the detection limits were used to define the upper potential limit for compound removal. For instance, if a compound were present in the feed at 10 ng/L and undetected in the product, but the detection limit was 0.1 ng/L, then the removal was said to be ">2.00 logs." In this case, a model prediction of anything >2.00 logs removal would be entirely consistent with the field observation.

Usually, when the ANN model predicted rejection less than the level measured in the field, the model predicted poor compound removal overall. In many cases the model was able to predict the trends observed in the field, which is very good given the fact that only estrone, estriol and progesterone were included in the construction of the ANN model.

Another issue affecting model prediction accuracy is the difference in historical exposure of membranes to compounds with high affinities for the RO membrane. Large temporal shifts in the feed concentrations of these compounds result in the membrane not being in equilibrium with the feed. Grab samples of feed and product taken under these conditions could show artificially good or poor rejection. Differences in membrane equilibrium between the field and bench system would result in serious disagreement between measured laboratory and field values of compound attenuation. The compounds that exhibited "negative rejection" in the laboratory are especially problematic; poor agreement with the field may be anticipated, as the kinetics of RO membrane exposure to these compounds is likely quite different under field conditions and the RO membranes may be nowhere near "equilibrated" with respect to these compounds in either case. If the concentration in the feed is temporally decoupled from that in the product, traditional methods of determining rejection by comparing spot feed and product concentrations are not likely to yield good results. This can particularly become an issue with spiking studies, which were carried out at SCWA. The model predictions indeed failed often where data suggest compounds strongly interacted with the RO membrane.

The WBMWD results for pharmaceuticals represent the actual background of materials present in the RO feedwater (Table 17). No spike study was conducted at this location. There were instances where the observed field measurement agreed with the model predictions (e.g., acetone, carbon disulfide, formaldehyde, and trichloroethene). In many instances the model predicted poorer removal than was observed in the field, but again this was associated with compounds showing evidence of strong affinity for the RO membrane. Most of these compounds fall in the categories of DBPs and carcinogens. As with SCWA data, field measurement resolution was limited by detection sensitivity (e.g., N-nitrosodi-n-butylamine, MTBE, Di-n-butyl phthalate, dalapon, etc.).

In some cases, however, the model failed by overpredicting compound removal from that observed in the field. Examples include bis(2-ethylhexyl)adipate, bis(2-ethylhexyl)phthalate, butyl benzyl phthalate, dimethyl phthalate, and polybrominated diphenyl ether; these compounds were predicted to be more effectively removed than the field measurements indicated. Poor removal in the field may have been due to lack of equilibrium if feed concentrations were not constant, but as these were not spiked compounds, it is also likely that this failure represents deficiencies in the model due to perhaps the test system used to construct the model not being completely at equilibrium.

4.0 Project Conclusions and Recommendations

4.1 Conclusions

4.1.1 Construction of Model for Prediction of Organic Rejection by RO Membranes

This study demonstrated the value of a QSAR approach using an ANN model to describe and ultimately predict the behavior of polyamide RO membranes removing organic compounds. Additionally, unlike the former models constructed at OCWD to describe

RO membrane behavior, the model described in this study utilized as inputs readily obtainable compound physicochemical properties. The model predicted behavior of new compounds (those not used in model construction) fairly well, providing the compounds fell within the scope of experience of the model.

The model was, however, limited by several factors. First, the test compound list was constrained to organics detectable by EPA methods 508 and 524 (e.g., DBPs), some EDCs and PPCPs as well as some hormones. Second, the RO test system feedwater matrix was simple, consisting of only de-ionized water and sodium chloride, and the membrane surfaces were clean. Finally, though steps were taken to the contrary, the system was potentially not at equilibrium with respect to organics exhibiting strong membrane affinity. All of these factors could have introduced potential biases in data, and these biases would have been inherited by the ANN model constructed from them.

It is notable that often when the model failed to predict field observations, it failed in a conservative way by underestimating compound removal. The discrepancies with field observations may be linked to membrane affinity by some compounds biasing results by delaying the observation of organic compound release to the product so that the feed loading of a compound and diffusion into the product become temporally decoupled. This can be especially a problem with spiking studies.

4.1.2 Influence of pH and Salinity on Organic Compound Rejection

Surface-response type statistical analyses demonstrated that in general the compounds examined in this study did not exhibit dramatic variations in removal due over the ranges of pH and salinity investigated; typically, change in removal was less than one log. These observations are likely biased by the overall nature of the study compounds (compounds detectable by EPA method 524) and the biases of the analytical system (the feed is a simple matrix and only clean membranes were used), but for molecules of the variety used in the study, variations in pH and salinity were not nearly as influential on rejection as were physicochemical factors such as log P. In general, highly rejected

compounds remained highly rejected over the variations of pH and salinity examined in this study, and vice versa.

4.2 Recommendations

New micropollutants are continuously being added to the list of compounds of concern that must be addressed by RO membranes during water reuse. A model capable of accurately determining whether or not these new compounds will be effectively removed by RO membranes commonly used in water purification would be of great value to water engineers, especially if it could be easily implemented. This study demonstrated the possibility of constructing such a model using a QSAR approach with an ANN providing the multivariate analysis. The model created in this study describing selected micropollutant removal by TFC polyamide RO membranes is descriptive and predictive, and its implementation requires knowledge of only a few compound physicochemical data readily obtainable by any RO plant engineer.

The use of artificial neural networks offers a particularly attractive solution to empirical multivariate modeling of compound removal. Implementation of ANN models is aided by inclusion of numerous and highly diverse exemplars in the training set used for model construction; if the training set is richly populated with compounds of differing properties, the resultant model will represent the broadest range of compound/membrane interactions available. In addition, inclusion of sufficient compounds to provide "clusters" of compound structures and properties may also greatly improve the model, as the accurate prediction of rejection of molecules whose properties lie between a pair of exemplar molecules is far more likely than if they lie outside the test compounds. Also, expanding the list of exemplary membranes is necessary to thoroughly examine the influence that differing membrane properties have on rejection. Nonetheless, if research reveals that, as this work suggests, variations in commercial polyamide RO membranes have only a weak effect on compound rejection, then it should be possible to construct a general model capable of predicting removal of organic micropollutants by any

polyamide RO membrane by sufficiently expanding the list of exemplary organic compounds.

Results of this study also suggest that a modification of sampling protocols may improve assessment of RO membrane removal of micropollutants. Although grab sampling of RO feedwater and product water may be adequate for determination of rejection of salts that have little or no membrane affinity, in cases where micropollutants exhibit very large membrane affinities, the membrane may buffer variations in contaminant concentration in the product. As a result, concentrations of compounds in the feedwater and in the product water may not co-vary, and calculations of rejection based on the assumption that they do could be considerably in error. A solution to this problem might involve buffering the feedwater and product water data by use of sample compositing methods or mass averaging techniques to remove temporal differences between variations in feedwater concentration of compounds and variations in product concentrations of compounds caused by slower membrane uptake/release. As a result, even in situations where feed concentrations continuously vary, observed rejection should be relatively unaffected by membrane uptake of micropollutants and reflect the actual ability of the membrane to limit diffusion of the compound into the product water.

This work suggests that variations in pH and salinity may not exert a profound influence over organic compound removal, at least by the test membranes and compounds examined in this study. Certainly in cases of neutral or only slightly polar organic contaminants this is not a particularly surprising result, as these compounds would be anticipated to be least affected by membrane surface and internal charge. Choice of test compounds likely biased observations in this study; inclusion of small organic acids (e.g., haloacetic acids) or bases may be of interest in future studies, as membrane interactions of more highly charged molecules of small size and lack of complexity might be expected to be most affected by membrane surface and internal charge which could in turn be influenced by feedwater pH and salinity. In addition, the feedwater matrices examined in the study were simple, and the presence of organic and biological matter present in actual feedwater and/or on the RO membrane could modulate effects of pH and salinity

variations over that observed in the simple matrix employed in this study. Given the potential complexity of RO feedwaters encountered in water reuse, a systematic study of the effects of these elements would require many complex matrices to be examined with a broad variety of compounds, resulting in a very large and costly study. Examination of variance of rejection values for individual contaminants observed in actual RO plants using similar membranes but operated with disparate feedwater matrices might be used to partially elucidate the overreaching effects that feedwater matrix variations have on rejection. Alternatively, laboratory studies using a handful of compounds with structures specifically selected to probe rejection dominated by size, charge or hydrophobic interactions under a variety of differing complex (but defined) feedwater matrices might also prove fruitful.

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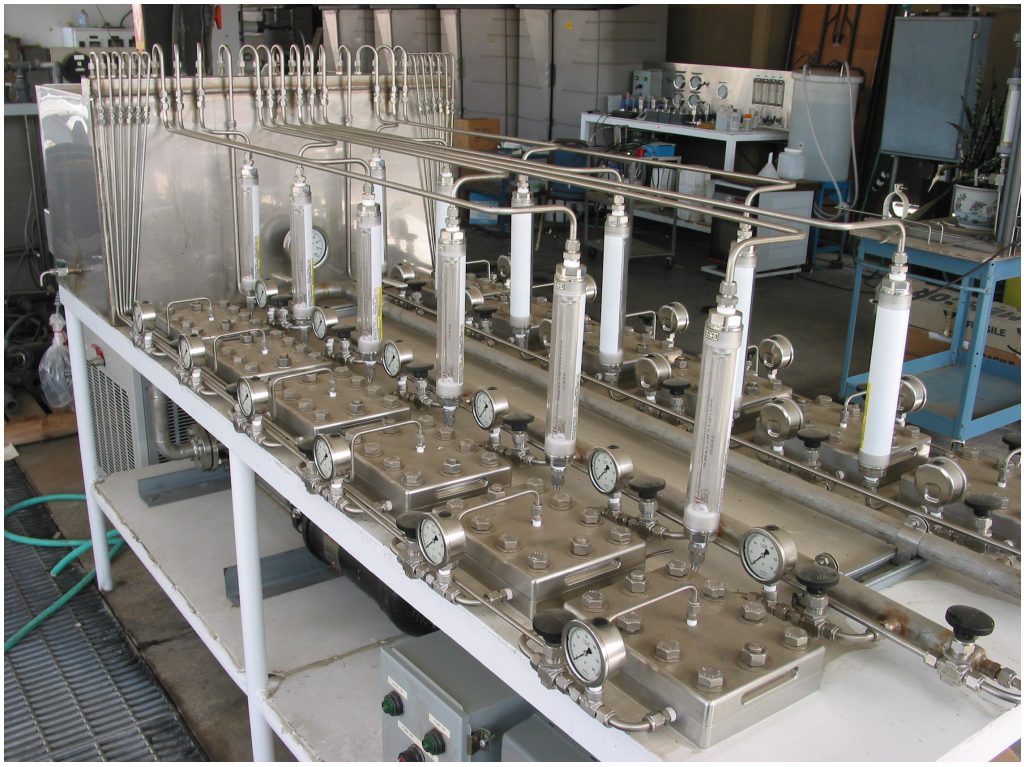
Glossary

ANN	Artificial Neural Network
BP	Boiling point
CA	Cellulose Acetate
CCL	Contaminant Candidate List
CDPH	California Department of Public Health
DBP	Desinfection By-Products
DRIP	Desalination Research and Innovation Partnership

EDC	Endocrine Disrupting Compounds
ESPA	Energy Saving Polyamide
GA	Genetic Algorithm
GWR	Groundwater Replenishment
HLC	Henry's Law Constant
IMS	Integrated Membrane Systems
L/m^2h	Liters per square meter per hour
Log P	Octanol-Water Partition Coefficient value
MCL	Maximum Contaminant Level
MF	Microfiltration
mgd	Million-gallon-per-day
mg/L	Milligrams per liter
MP	Melting point
MW	Molecular Weight
NDMA	N-nitrosodimethylamine
NF	Nanofiltration
NL	Notification Level
OCWD	Orange County Water District
OHA	OH Atmospheric Rate Constant
OWPP	Octanol-Water Partition Coefficient
PPCP	Pharmaceuticals and Personal Care Products
QSAR	Quantitative Structure-Activity Relationship
PA	Polyamide
pKa	Negative Logarithm of the Dissociation Constant
QAPP	Quality Assurance Project Plan
QA/QC	Quality Assurance/Quality Control
R	Linear Correlation
RMP	Radiometric Potential
RMS	Root Mean Squared
RO	Reverse osmosis
SCWA	Sonoma County Water Agency

SOP	Standard Operating Procedure
TDS	Total Dissolved Solids
TFC	Thin Film Composite
TFC-HR	Thin Film Composite-High Rejection
TFC-ULP	Thin Film Composite-Ultra Low Pressure
UCMR	Unregulated Contaminant Monitoring Regulation
USEPA	United States Environmental Protection Agency
USGS	United States Geological Survey
VB	Visual Basic
VP	Vapor Pressure
WBMWD	West Basin Municipal Water District
WF-21	Water Factory-21
WS	Water Solubility



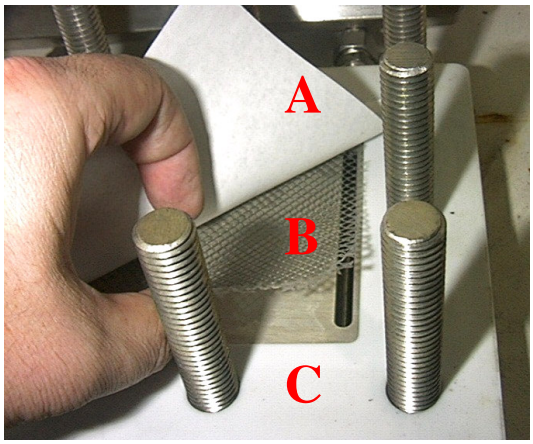


Figure 1. Image of the RO test system equipped with 12 RO test cells (above). Close-up image (below) of the test cell components including the membrane flat sheet (A), feed spacer (B) and the Teflon shim (C).

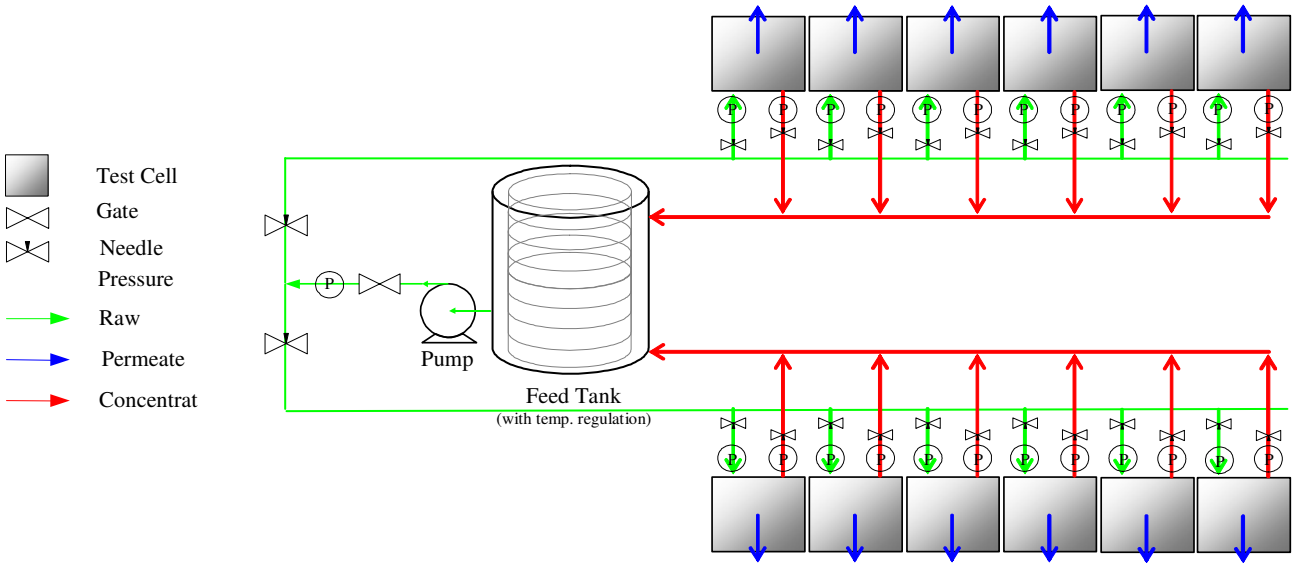


Figure 2. Schematic of the membrane test system designed and constructed by OCWD. The system contains twelve cells that can independently operate under varying conditions of flow and pressure. Brine was continuously returned to the feed tank; permeate was returned to the feed tank when not being sampled.

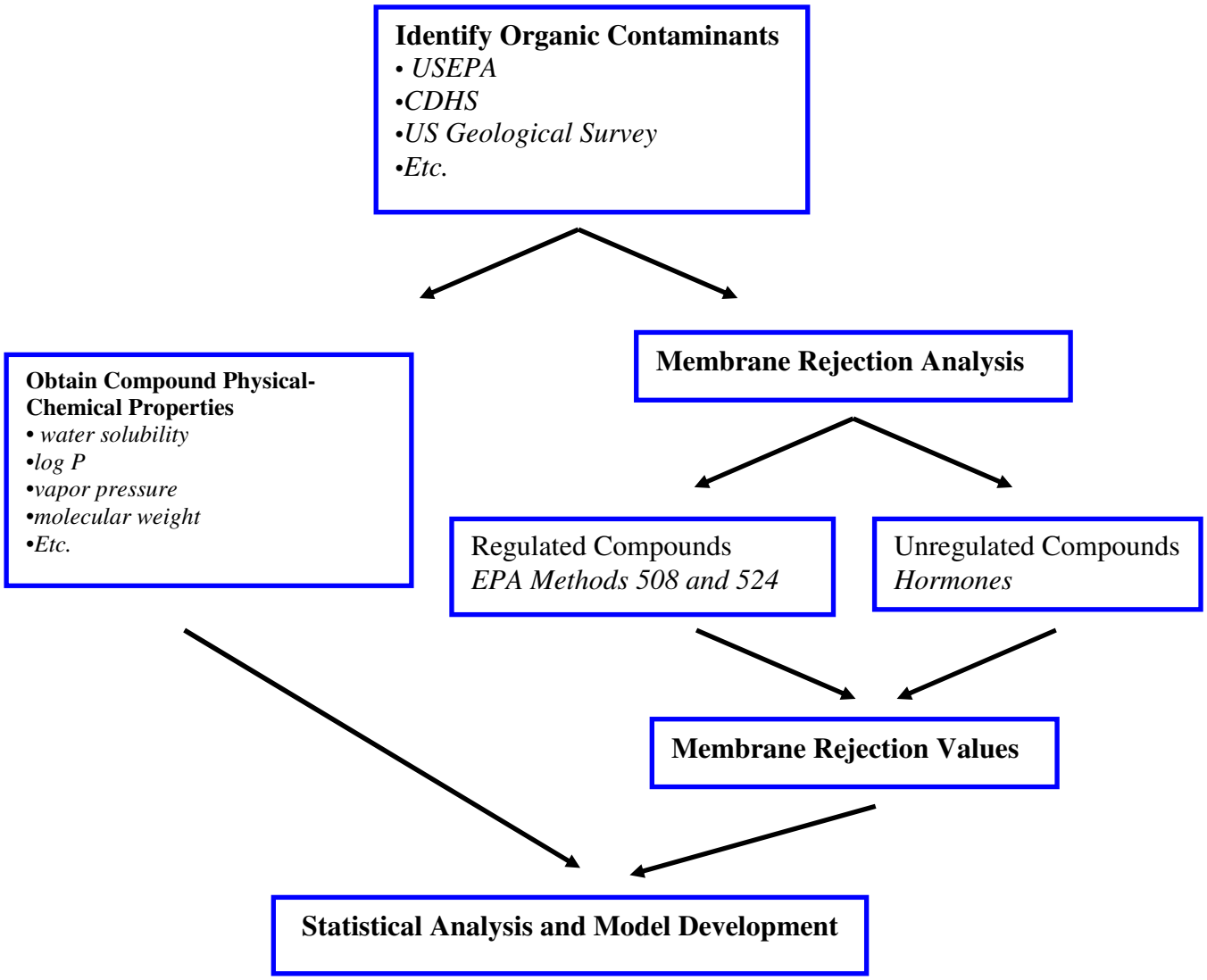


Figure 3. Experimental Plan for objectives 1-3.

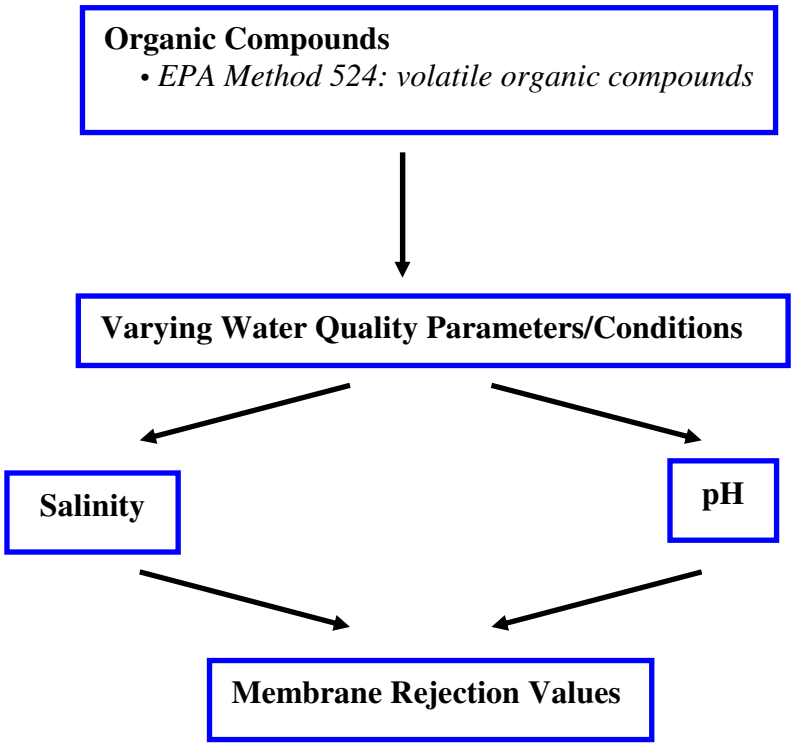
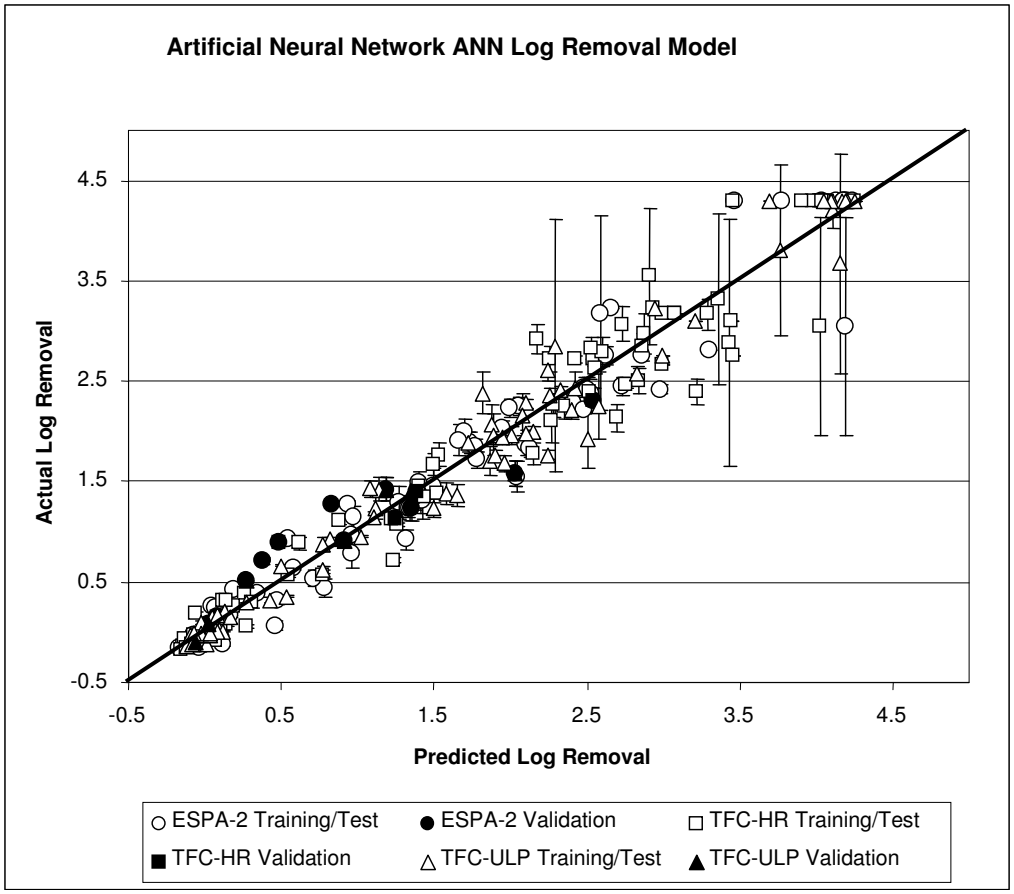


Figure 4. Experimental Plan for objective 4.



Log Removal*	R	Avg. Abs.	RMS	Conf. Interval (95%)	Records
All	0.97	0.21	0.32	0.61	774
Train	0.98	0.20	0.29	0.56	541
Test	0.96	0.23	0.37	0.73	233

	Sensitivity Index		
Roughness (nm)	**Mol Weight**	**Log P**	**# Methyl Groups**
-0.06	0.30	1.15	0.73

Figure 5. Statistics for artificial neural network (ANN) membrane model describing organic compound log removal.

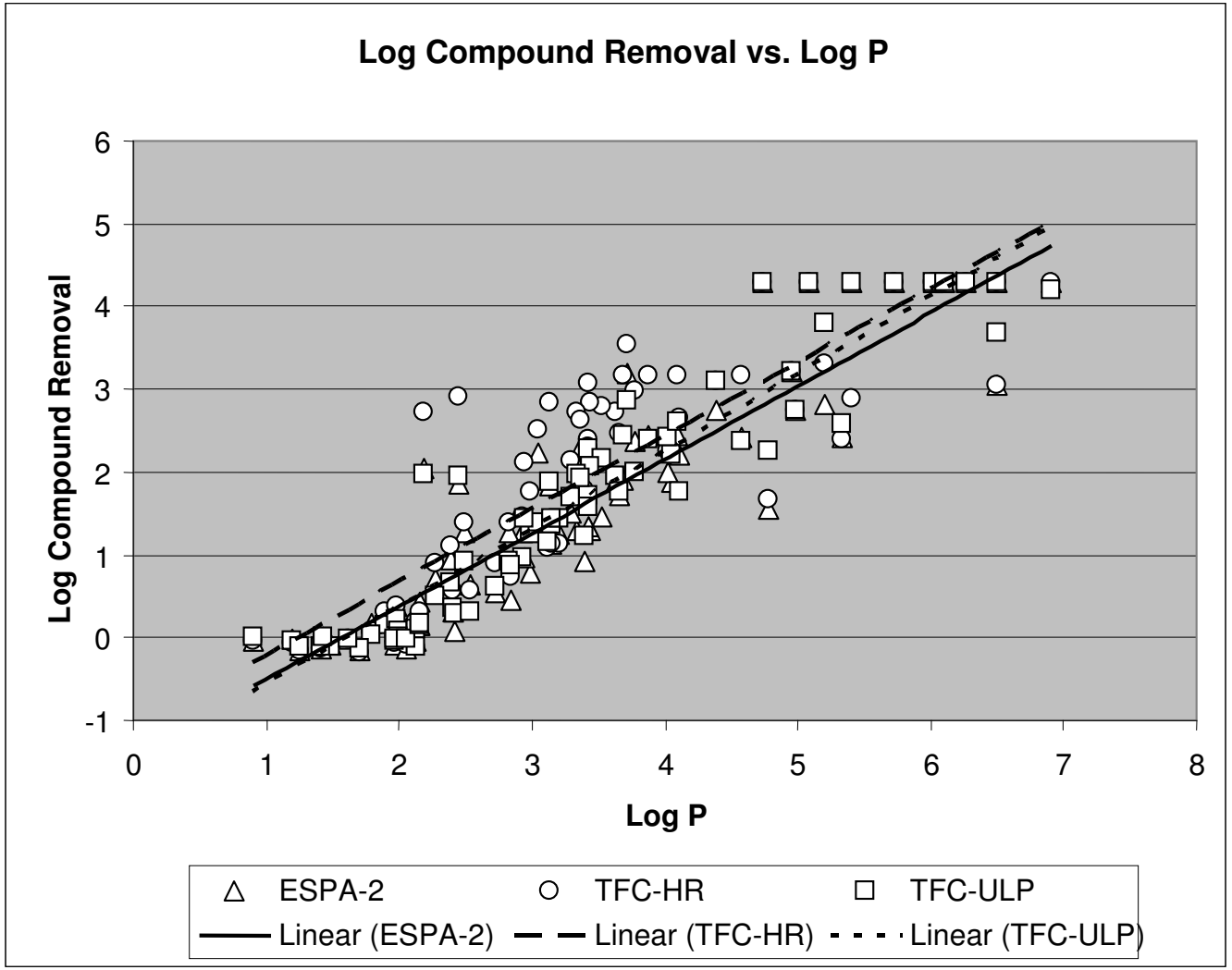


Figure 6. Log removal of test compounds as a function of log P.

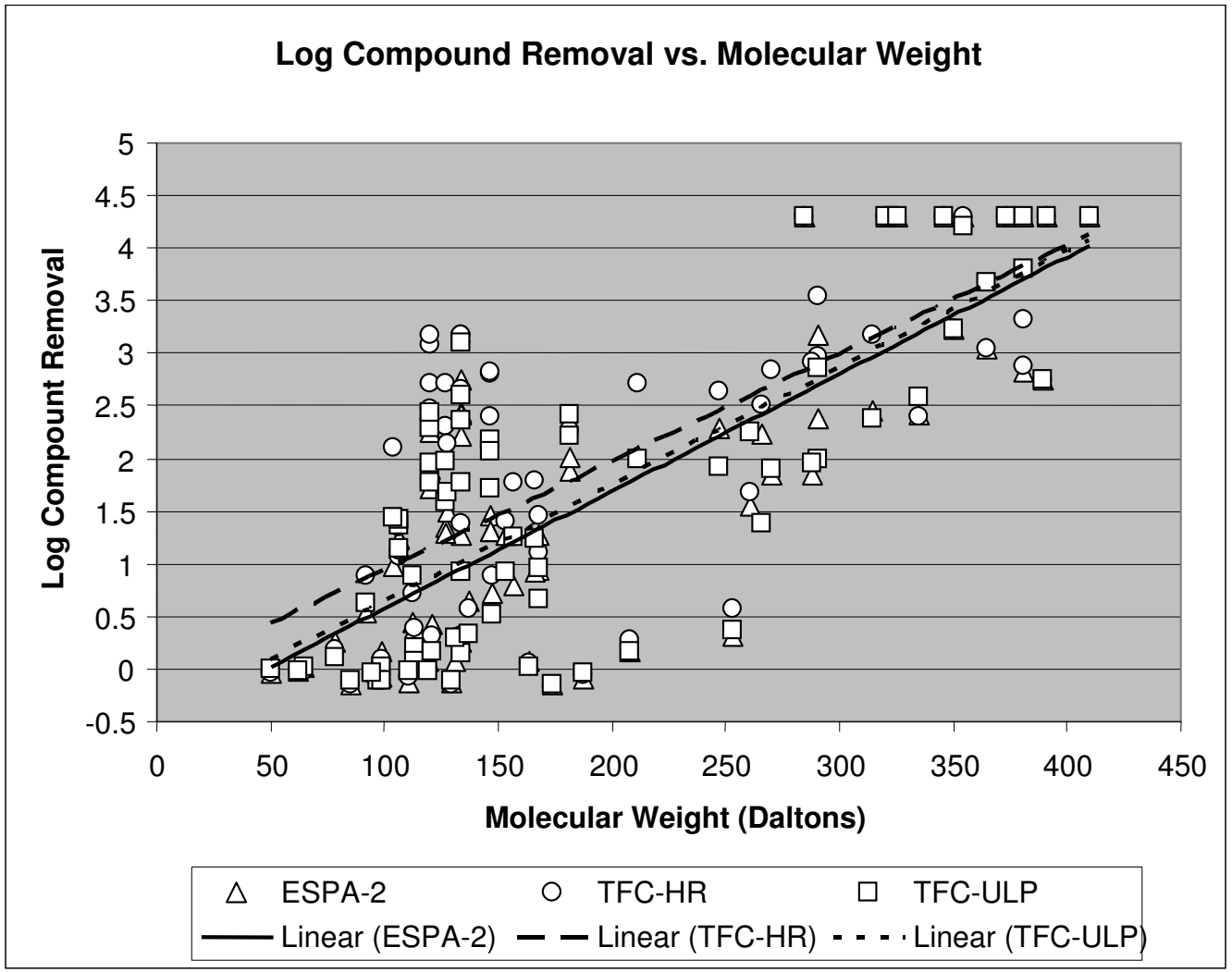


Figure 7. Log removal of test compounds as a function of molecular weight.

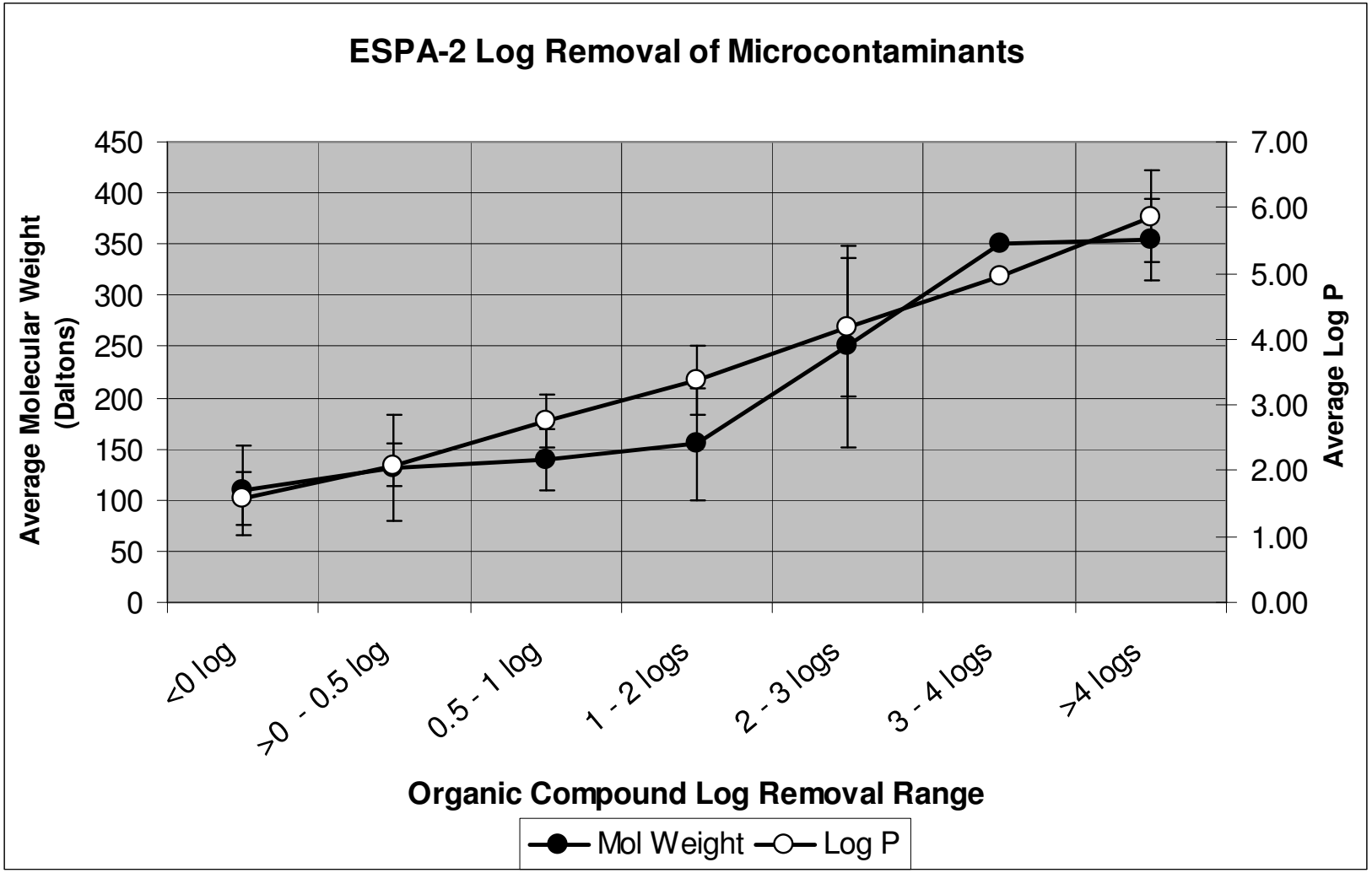


Figure 8. Organic compound log removal on ESPA-2 membrane.

Table 1. Commercial RO membranes used in the study.

Membrane	Manufacturer	Type	Material
ESPA-2	Hydranautics, Oceanside, CA	RO	polyamide
TFC-HR	KMS, San Diego, CA	RO	polyamide
TFC-ULP	KMS, San Diego, CA	RO	polyamide

Table 2. List of trace-organic compounds used in the study: USEPA Method 524 (volatile organic compounds) and USEPA Method 508 (organo-chlorinated compounds).

EPA Method 524	
1,1,1,2-Tetrachloroethane	Carbon tetrachloride
1,1,1-Trichloroethane	Chlorobenzene
1,1,2,2-Tetrachloroethane	Chloroethane
1,1,2-Trichloroethane	Chloroform
1,1-Dichloroethane	Chloromethane
1,1-Dichloroethene	cis-1,3-Dichloropropene
1,2,3-Trichlorobenzene	Dibromochloromethane
1,2,3-Trichloropropane	Dibromomethane
1,2,4-Trichlorobenzene	Dichlorodifluoromethane
1,2,4-Trimethylbenzene	Ethylbenzene
1,2-Dibromoethane	Hexachlorobutadiene
1,2-Dichlorobenzene	isopropylbenzene
1,2-Dichloroethane	m,p-xylene
1,2-Dichloropropane	Methylene chloride
1,3,5-Trimethylbenzene	Naphthalene
1,3-Dichlorobenzene	n-butylbenzene
1,3-Dichloropropane	o-xylene
1,4-Dichlorobenzene	Propylbenzene
2-Chlorotoluene	sec-butylbenzene
4-isopropyltoluene	Styrene
Benzene	tert-butylbenzene
Bromobenzene	Tetrachloroethene
Bromochloromethane	Toluene
Bromodichloromethane	Trichloroethene
Bromoform	Trichlorofluoromethane
Bromomethane	Vinyl chloride

EPA Method 508	
4,4'-DDD	HCH-beta (Beta-BHC)
4,4'-DDT	HCH-gamma (Lindane)
Aldrin	Heptachlor
Chlordane	Heptachlor epoxide
Chlorobenzilate	Hexachlorobenzene
Chlorothalonil	Methoxychlor
Chlorpyrifos	Permethrin-(total of cis/trans)
Dieldrin	Propachlor
Endrin	Trifluralin
Etridiazole	

Table 3. List of trace-organic compounds used in the study: hormones and potential endocrine-disrupting compounds.

Hormones and Potential EDCs
Estriol
Estrone
Progesterone
17b-Estradiol
17a-Estradiol
17a-Ethynylestradiol
Diethylstilbestrol
Epitestosterone
trans-Testosterone

Table 4. Physicochemical properties used as molecular descriptors in the study.

Molecular Structure/Complexity
C=C
C=C
C=N
Molecular Weight
Aromatic Rings
5-Member Aromatic Rings
6-Member Aromatic Rings
Aliphatic Rings
Conjugated Rings
Alkane Groups
Alkene Groups
Nitrile Groups
Methyl Groups

Charge/Polarity
Nitrate Groups
Hydroxyl Groups
Carboxylic Groups

Hydrophobicity
Log P
Water Solubility (mg/L)

Other
Density (g/cc)
Melting Point (^{o}C)
Vapor Pressure (mm Hg)
Henry's Law Constant (atm-m^3/mole)
Atmospheric OH Rate Constant (cm^3/molecule-sec)

Table 5. Physicochemical properties of commercial RO membranes used in the study.

Membrane Properties	ESPA-2	TFC-HR	TFC-ULP
Specific Water Flux (GFD/psi)	0.137	0.138	0.254
Contact Angle (degrees)	60.63	61.15	61.27
Zeta Potential (mV)	-19.03	-13.86	-16.27
Zeta Potential Slope (pH 5-7)	-5.92	-2.14	-2.27
COO/Amide I Ratio	0.274	0.173	0.168
COO/Amide II Ratio	0.254	0.186	0.177
OH/Amide I Ratio	0.487	0.737	0.724
Polyamide Thickness	1.584	0.864	1.059
Roughness (nm)	78.75	38.96	52.57

Table 6a. Physicochemical properties of trace-organic compounds of interest.

COMPOUND	Molecular Weight	Melting Point (°C)	H_2O Solubility (mg/L)	Log P	Vapor Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density	C=C	C=O	C=N
1,1,1,2-Tetrachloroethane	167.85	-70.2	1070.0000	2.93	1.20E+01	0.00245	1.80E-14	1.553	0	0	0
1,1,1-Trichloroethane	133.41	-30.4	1290.0000	2.49	1.24E+02	0.0172	9.43E-15	1.338	0	0	0
1,1,2,2-Tetrachloroethane	167.85	-43.8	2830.0000	2.39	4.62E+00	0.000367	2.50E-13	1.595	0	0	0
1,1,2-Trichloroethane	133.41	-36.6	4590.0000	1.89	2.30E+01	0.000824	1.96E-13	1.441	0	0	0
1,1-Dichloroethane	98.96	-96.9	5040.0000	1.79	2.27E+02	0.00562	2.74E-13	1.176	0	0	0
1,1-Dichloroethene	96.94	-122.5	2420.0000	2.13	6.00E+02	0.0261	1.09E-11	1.213	1	0	0
1,2,3-Trichlorobenzene	181.45	53.5	18.0000	4.05	2.10E-01	0.00125	2.82E-13	1.690	3	0	0
1,2,3-Trichloropropane	147.43	-14.7	1750.0000	2.27	3.69E+00	0.000343	3.51E-13	1.389	0	0	0
1,2,4-Trichlorobenzene	181.45	17.0	49.0000	4.02	4.60E-01	0.00142	5.50E-13	1.463	3	0	0
1,2,4-Trimethylbenzene	120.20	-43.8	57.0000	3.63	2.10E+00	0.00616	3.25E-11	0.876	3	0	0
1,2-Dibromoethane	187.86	9.9	3910.0000	1.96	1.12E+01	0.00065	2.50E-13	2.170	0	0	0
1,2-Dichlorobenzene	147.00	-16.7	156.0000	3.43	1.36E+00	0.00192	4.20E-13	1.306	3	0	0
1,2-Dichloroethane	98.96	-35.5	8600.0000	1.48	7.89E+01	0.00118	2.48E-13	1.253	0	0	0
1,2-Dichloropropane	112.99	-100.0	2800.0000	1.98	5.33E+01	0.00282	4.42E-13	1.156	0	0	0
1,2-Dichlroroethene	96.94	-80.0	6410.0000	1.86	2.00E+02	0.00408	2.62E-12	1.284	1	0	0
1,3,5-Trimethylbenzene	120.20	-44.7	48.2000	3.42	2.48E+00	0.00877	5.75E-11	0.865	3	0	0
1,3-Dichlorobenzene	147.00	-24.8	125.0000	3.53	2.15E+00	0.00263	7.20E-13	1.288	3	0	0
1,3-Dichloropropane	112.99	-99.5	2750.0000	2.00	1.82E+01	0.000976	7.80E-13	1.188	0	0	0
1,4-Dichlorobenzene	147.00	52.7	81.3000	3.44	1.74E+00	0.00241	3.20E-13	1.247	3	0	0
1,2-Dibromo-3-chloropropane	236.33	6.0	1230.0000	2.96	5.80E-01	0.000147	4.35E-13	2.050	0	0	0
2-Chlorotoluene	126.59	-35.6	374.0000	3.42	3.43E+00	3.57E-03	1.82E-12	1.082	3	0	0
4,4-DDD	320.05	109.5	0.0900	6.02	1.35E-06	6.60E-06	4.34E-12	1.385	6	0	0
4,4'-DDT	354.49	108.5	0.0055	6.91	1.60E-07	8.32E-06	3.44E-12	1.560	6	0	0
4-Chlorotoluene	126.59	7.5	106.0000	3.33	2.69E+00	4.38E-03	1.82E-12	1.070	3	0	0
4-Isopropyltoluene	134.22	-68.9	23.4000	4.10	1.46E+00	0.011	1.51E-11	0.860	3	0	0
Aldrin	364.92	104.0	0.0170	6.50	1.20E-04	4.40E-05	6.46E-11	1.600	2	0	0
Benzene	78.12	5.5	1790.0000	2.13	9.48E+01	5.55E-03	1.23E-12	0.879	3	0	0
Beta-BHC	290.83	314.5	0.2400	3.78	3.60E-07	4.40E-07	5.73E-13	1.890	0	0	0
Bromobenzene	157.01	-30.6	446.0000	2.99	4.18E+00	2.47E-03	7.70E-13	1.495	3	0	0
Bromochloromethane	129.38	-87.9	16700.0000	1.41	1.43E+02	1.46E-03	8.80E-14	1.991	0	0	0
Bromodichloromethane	163.83	-57.0	3030.0000	2.00	5.00E+01	2.12E-03	7.84E-14	1.971	0	0	0
Bromoform	252.73	8.0	3100.0000	2.40	5.40E+00	5.35E-04	4.26E-14	2.890	0	0	0
Bromomethane	94.94	-93.7	15200.0000	1.19	1.62E+03	7.34E-03	4.02E-14	1.732	0	0	0
Carbon tetrachloride	153.82	-23.0	793.0000	2.83	1.15E+02	2.76E-02	1.20E-16	1.594	0	0	0
Chlordane	409.78	106.0	0.0130	6.26	9.90E-06	7.03E-05	5.04E-12	1.600	0	0	0
Chlorobenzene	112.56	-45.2	498.0000	2.84	1.20E+01	3.11E-03	7.70E-13	1.107	3	0	0
Chlorobenzilate	325.19	37.0	13.0000	4.74	2.20E-06	7.24E-08	5.09E-12	1.282	6	1	0
Chloroethane	64.52	-138.7	6710.0000	1.43	1.01E+03	1.11E-02	4.11E-13	0.920	0	0	0

6b. Physicochemical properties of trace-organic compounds of interest.

COMPOUND	# Aromatic Rings	# 5-member Arom. Rings	# 6-member Arom. Rings	# Aliphatic Rings	# Conjugated Rings	# Carboxilic Acid Groups	# Hydroxyl Groups	# Alkane Groups	# Alkene Groups	# Nitrate Groups	# Nitrile Groups	# Methyl Groups
1,1,1,2-Tetrachloroethane	0	0	0	0	0	0	0	0	0	0	0	0
1,1,1-Trichloroethane	0	0	0	0	0	0	0	0	0	0	0	1
1,1,2,2-Tetrachloroethane	0	0	0	0	0	0	0	0	0	0	0	0
1,1,2-Trichloroethane	0	0	0	0	0	0	0	0	0	0	0	0
1,1-Dichloroethane	0	0	0	0	0	0	0	0	0	0	0	1
1,1-Dichloroethene	0	0	0	0	0	0	0	0	1	0	0	0
1,2,3-Trichlorobenzene	1	0	1	0	0	0	0	0	0	0	0	0
1,2,3-Trichloropropane	0	0	0	0	0	0	0	0	0	0	0	0
1,2,4-Trichlorobenzene	1	0	1	0	0	0	0	0	0	0	0	0
1,2,4-Trimethylbenzene	1	0	1	0	0	0	0	0	0	0	0	3
1,2-Dibromoethane	0	0	0	0	0	0	0	1	0	0	0	0
1,2-Dichlorobenzene	1	0	1	0	0	0	0	0	0	0	0	0
1,2-Dichloroethane	0	0	0	0	0	0	0	1	0	0	0	0
1,2-Dichloropropane	0	0	0	0	0	0	0	1	0	0	0	1
1,2-Dichlroroethene	0	0	0	0	0	0	0	0	1	0	0	0
1,3,5-Trimethylbenzene	1	0	1	0	0	0	0	0	0	0	0	3
1,3-Dichlorobenzene	1	0	1	0	0	0	0	0	0	0	0	0
1,3-Dichloropropane	0	0	0	0	0	0	0	0	0	0	0	0
1,4-Dichlorobenzene	1	0	1	0	0	0	0	0	0	0	0	0
1.2-Dibromo-3-chloropropane	0	0	0	0	0	0	0	0	0	0	0	0
2-Chlorotoluene	1	0	1	0	0	0	0	0	0	0	0	1
4,4-DDD	2	0	2	0	0	0	0	1	0	0	0	0
4,4'-DDT	2	0	2	0	0	0	0	1	0	0	0	0
4-Chlorotoluene	1	0	1	0	0	0	0	0	0	0	0	1
4-Isopropyltoluene	1	0	1	0	0	0	0	0	0	0	0	3
Aldrin	2	0	2	0	0	0	0	0	0	0	0	0
Benzene	1	0	1	0	0	0	0	0	0	0	0	0
Beta-BHC	0	0	0	1	0	0	0	0	0	0	0	0
Bromobenzene	1	0	1	0	0	0	0	0	0	0	0	0
Bromochloromethane	0	0	0	0	0	0	0	0	0	0	0	0
Bromodichloromethane	0	0	0	0	0	0	0	0	0	0	0	0
Bromoform	0	0	0	0	0	0	0	0	0	0	0	0
Bromomethane	0	0	0	0	0	0	0	0	0	0	0	0
Carbon tetrachloride	0	0	0	0	0	0	0	0	0	0	0	0
Chlordane	0	0	0	0	0	0	0	0	0	0	0	0
Chlorobenzene	1	0	1	0	0	0	0	0	0	0	0	0
Chlorobenzilate	2	0	2	0	0	0	1	0	0	0	0	1
Chloroethane	0	0	0	0	0	0	0	0	0	0	0	1

6c. Physicochemical properties of trace-organic compounds of interest.

COMPOUND	Molecular Weight	Melting Point (°C)	H_2O Solubility (mg/L)	Log P	Vapor Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density	C=C	C=O	C=N
Chloroform	119.38	-63.6	7950.0000	1.97	1.97E+02	3.67E-03	1.03E-13	1.498	0	0	0
Chloromethane	50.49	-97.7	5320.0000	0.91	4.30E+03	8.82E-03	4.36E-14	0.991	0	0	0
Chlorothanonil	265.91	250.0	0.6000	3.05	5.70E-07	2.00E-06	6.18E-15	1.800	3	0	2
Chlorpyrifos	350.59	42.0	1.1200	4.96	2.03E-05	2.93E-06	9.17E-11	1.398	3	0	0
Cis-1,3-Dichloropropene	110.97	-50.0	2180.0000	2.06	2.63E+01	2.71E-03	8.40E-12	1.220	1	0	0
Dibromochloromethane	208.28	-20.0	2700.0000	2.16	5.54E+00	0.000783	5.78E-14	2.451	0	0	0
Dibromomethane	173.84	-52.5	11900.0000	1.70	4.44E+01	0.000822	1.13E-13	2.497	0	0	0
Dichlorodifluoromethane	120.91	-158.0	280.0000	2.16	4.85E+03	0.343	4.00E-16	1.329	0	0	0
Dieldrin	380.91	175.5	0.1950	5.40	5.89E-06	1.00E-05	9.20E-12	1.750	1	0	0
Endrin	380.91	226.0	0.2500	5.20	3.00E-06	6.36E-06	9.20E-12	1.700	1	0	0
Estriol	288.39	282.0	441.0000	2.45	1.97E-10	1.33E-12	1.29E-10	1.270	3	0	0
Estrone	270.37	260.2	30.0000	3.13	1.42E-07	3.80E-10	1.26E-10	1.236	3	1	0
Ethylbenzene	106.17	-94.9	169.0000	3.15	9.60E+00	0.00788	7.10E-12	0.867	3	0	0
Etridazole	247.53	19.9	117.0000	3.37	1.00E-04	2.78E-07	6.87E-12	1.503	0	0	2
Hepatchlor epoxide	389.32	160.0	0.2000	4.98	1.95E-05	2.10E-05	5.17E-12	1.580	1	0	0
Heptachlor	373.32	95.5	0.1800	6.10	4.00E-04	0.000294	6.11E-11	1.580	1	0	0
Hexachlorobenzene	284.78	231.8	0.0062	5.73	1.80E-05	0.0017	2.70E-14	2.044	3	0	0
Hexachlorobutadiene	260.76	-21.0	3.2000	4.78	2.20E-01	0.0103	3.00E-14	1.680	2	0	0
Isopropylbenzene	120.20	-96.0	61.3000	3.66	4.50E+00	0.0115	6.50E-12	0.862	3	0	0
Lindane	290.83	112.5	7.3000	3.72	4.20E-05	5.14E-06	1.90E-13	1.870	0	0	0
Methoxychlor	345.66	87.0	0.1000	5.08	2.58E-06	2.03E-07	5.35E-11	1.410	6	0	0
Methylene chloride	84.93	-95.1	13000.0000	1.25	4.35E+02	0.00325	1.42E-13	1.326	0	0	0
M-Xylene	106.17	-47.8	161.0000	3.20	8.29E+00	0.00718	2.36E-11	0.868	3	0	0
Naphthalene	128.18	80.2	31.0000	3.30	8.50E-02	0.00044	2.16E-11	0.997	5	0	0
N-Butylbenzene	134.22	-87.9	11.8000	4.38	1.06E+00	0.0159	8.72E-12	0.860	3	0	0
N-Propylbenzene	120.20	-99.5	52.2000	3.69	3.42E+00	0.0105	6.00E-12	0.862	3	0	0
O-Xylene	106.17	-25.2	178.0000	3.12	6.61E+00	0.00518	1.37E-11	0.897	3	0	0
Permethrin	391.30	34.0	0.0060	6.50	2.18E-08	1.87E-06	3.90E-11	1.190	6	1	0
Progesterone	314.47	121.0	8.8100	3.87	1.30E-06	6.49E-08	1.04E-10	1.166	1	2	0
Propachlor	211.69	77.0	700.0000	2.18	2.30E-04	9.15E-08	2.10E-11	1.242	3	1	0
P-Xylene	106.17	13.2	162.0000	3.15	8.84E+00	0.0069	1.43E-11	0.861	3	0	0
Sec-Butylbenzene	134.22	-82.7	17.6000	4.57	1.75E+00	0.0176	8.50E-12	0.862	3	0	0
Styrene	104.15	-31.0	310.0000	2.95	6.40E+00	0.00275	5.80E-11	0.905	4	0	0
T-Butylbenzene	134.22	-57.8	29.5000	4.11	2.20E+00	0.0132	4.60E-12	0.867	3	0	0
Tetrachloroethene	165.83	-22.3	206.0000	3.40	1.85E+01	0.0177	1.67E-13	1.623	1	0	0
Toluene	92.14	-94.9	526.0000	2.73	2.84E+01	0.00664	5.96E-12	0.867	3	0	0
Trichloroethene	131.39	-84.7	1280.0000	2.42	6.90E+01	0.00985	2.36E-12	1.462	1	0	0
Trichlorofluoromethane	137.37	-111.1	1100.0000	2.53	8.03E+02	0.097	5.00E-16	1.494	0	0	0
Trifluralin	335.29	49.0	0.1840	5.34	4.58E-05	0.000103	2.40E-11	1.294	3	0	0
Vinylchloride	62.50	-153.7	8800.0000	1.62	2.98E+03	0.0278	6.96E-12	0.911	1	0	0

6d. Physicochemical properties of trace-organic compounds of interest.

COMPOUND	# Aromatic Rings	# 5-member Arom. Rings	# 6-member Arom. Rings	# Aliphatic Rings	# Conjugated Rings	# Carboxilic Acid Groups	# Hydroxyl Groups	# Alkane Groups	# Alkene Groups	# Nitrate Groups	# Nitrile Groups	# Methyl Groups
Chloroform	0	0	0	0	0	0	0	0	0	0	0	0
Chloromethane	0	0	0	0	0	0	0	0	0	0	0	1
Chlorothanonil	0	0	1	0	0	0	0	0	0	0	2	0
Chlorpyrifos	0	0	0	0	0	0	0	0	0	0	0	0
Cis-1,3-Dichloropropene	0	0	0	0	0	0	0	0	1	0	0	0
Dibromochloromethane	0	0	0	0	0	0	0	0	0	0	0	0
Dibromomethane	0	0	0	0	0	0	0	0	0	0	0	0
Dichlorodifluoromethane	0	0	0	0	0	0	0	0	0	0	0	0
Dieldrin	0	0	0	0	0	0	0	0	1	0	0	0
Endrin	0	0	0	2	0	0	0	0	1	0	0	0
Estriol	1	0	1	3	0	0	3	0	0	0	0	0
Estrone	1	0	1	3	0	0	1	0	0	0	0	0
Ethylbenzene	1	0	1	0	0	0	0	0	0	0	0	1
Etridazole	1	1	0	0	0	0	0	0	0	0	0	1
Hepatchlor epoxide	0	0	0	2	0	0	0	0	0	0	0	0
Heptachlor	0	0	0	2	0	0	0	0	0	0	0	0
Hexachlorobenzene	1	0	1	0	0	0	0	0	0	0	0	0
Hexachlorobutadiene	0	0	0	0	0	0	0	0	0	0	0	0
Isopropylbenzene	1	0	1	0	0	0	0	0	0	0	0	2
Lindane	0	0	0	1	0	0	0	0	0	0	0	0
Methoxychlor	2	0	2	0	0	0	0	0	0	0	0	2
Methylene chloride	0	0	0	0	0	0	0	0	0	0	0	0
M-Xylene	1	0	1	0	0	0	0	0	0	0	0	2
Naphthalene	2	0	2	0	2	0	0	0	0	0	0	0
N-Butylbenzene	1	0	1	0	0	0	0	0	0	0	0	1
N-Propylbenzene	1	0	1	0	0	0	0	0	0	0	0	1
O-Xylene	1	0	1	0	0	0	0	0	0	0	0	2
Permethrin	2	0	2	0	0	1	0	0	0	0	0	3
Progesterone	0	0	0	4	0	0	0	0	0	0	0	3
Propachlor	1	0	1	0	0	0	0	0	0	0	0	2
P-Xylene	1	0	1	0	0	0	0	0	0	0	0	2
Sec-Butylbenzene	1	0	1	0	0	0	0	0	0	0	0	2
Styrene	1	0	1	0	0	0	0	0	1	0	0	0
T-Butylbenzene	1	0	1	0	0	0	0	0	0	0	0	3
Tetrachloroethene	0	0	0	0	0	0	0	0	1	0	0	0
Toluene	1	0	1	0	0	0	0	0	0	0	0	1
Trichloroethene	0	0	0	0	0	0	0	0	1	0	0	0
Trichlorofluoromethane	0	0	0	0	0	0	0	0	0	0	0	0
Trifluralin	1	0	1	0	0	0	0	0	0	2	0	2
Vinylchloride	0	0	0	0	0	0	0	0	1	0	0	0

Table 7a. Statistical analysis of organic compound log removal. Bolded compounds were used as validation exemplars.

COMPOUND	ESPA-2			TFC-HR			TFC-ULP		
	Mean	Std Dev	n	Mean	Std Dev	n	Mean	Std Dev	n
1,1,1,2-Tetrachloroethane	1.28	0.03	4	1.46	0.05	4	0.96	0.01	4
1,1,1-Trichloroethane	1.27	0.01	4	1.38	0.04	4	0.92	0.03	4
1,1,2,2-Tetrachloroethane	0.94	0.03	4	1.11	0.04	4	0.66	0.01	4
1,1,2-Trichloroethane	0.26	0.03	4	0.31	0.02	4	0.15	0.01	4
1,1-Dichloroethane	0.17	0.01	4	0.09	0.03	4	0.02	0.01	4
1,1-Dichloroethene	-0.04	0.04	4	-0.10	0.02	4	-0.12	0.02	4
1,2,3-Trichlorobenzene	1.89	0.12	4	2.26	0.13	4	2.21	0.09	4
1,2,3-Trichloropropane	0.71	0.03	4	0.89	0.04	4	0.51	0.01	4
1,2,4-Trichlorobenzene	2.00	0.13	4	2.26	0.12	4	2.41	0.03	4
1,2,4-Trimethylbenzene	1.87	0.11	4	2.71	0.06	4	1.96	0.09	4
1,2-Dibromoethane	-0.09	0.02	4	-0.05	0.02	4	-0.03	0.02	4
1,2-Dichlorobenzene	1.31	0.14	4	2.40	0.13	4	1.72	0.15	4
1,2-Dichloroethane	-0.08	0.01	4	-0.12	0.02	4	-0.11	0.01	4
1,2-Dichloropropane	0.38	0.03	4	0.38	0.02	4	0.21	0.01	4
1,3,5-Trimethylbenzene	2.25	0.09	4	3.07	0.17	4	2.28	0.05	4
1,3-Dichlorobenzene	1.46	0.17	4	2.80	0.15	4	2.17	0.21	4
1,3-Dichloropropane	0.06	0.03	4	0.16	0.02	4	0.07	0.02	4
1,4-Dichlorobenzene	1.30	0.18	4	2.83	0.10	4	2.07	0.20	4
2-Chlorotoluene	1.34	0.12	4	2.31	0.11	4	1.58	0.13	4
4,4-DDD	4.30	0.00	3	4.30	0.00	3	4.30	0.00	3
4,4'-DDT	4.30	0.00	3	4.30	0.00	3	4.20	0.17	3
4-Chlorotoluene	1.29	0.16	4	2.72	0.12	4	1.97	0.21	4
4-Isopropyltoluene	2.44	0.10	4	3.17	0.00	4	2.61	0.11	4
Aldrin	3.04	1.09	3	3.04	1.09	3	3.67	1.09	3
Benzene	0.25	0.03	4	0.18	0.02	4	0.10	0.01	4
Beta-BHC	2.38	0.05	3	2.98	0.20	3	1.99	0.06	3
Bromobenzene	0.79	0.15	4	1.77	0.12	4	1.24	0.12	4
Bromochloromethane	-0.13	0.02	4	-0.15	0.02	4	-0.11	0.01	4
Bromodichloromethane	0.07	0.02	4	0.05	0.02	4	0.01	0.01	4
Bromoform	0.32	0.05	4	0.57	0.05	4	0.36	0.01	4
Bromomethane	-0.02	0.03	4	-0.06	0.02	4	-0.03	0.02	4
Carbon tetrachloride	1.27	0.02	4	1.40	0.04	4	0.92	0.03	4
Chlordane	4.30	0.00	3	4.30	0.00	3	4.30	0.00	3
Chlorobenzene	0.44	0.10	4	0.72	0.02	4	0.88	0.07	4
Chlorobenzilate	4.30	0.00	3	4.30	0.00	3	4.30	0.00	3
Chloroethane	0.01	0.02	4	-0.01	0.03	4	0.01	0.01	4
Chloroform	0.07	0.01	4	0.00	0.02	4	-0.02	0.00	4
Chloromethane	-0.03	0.02	4	-0.05	0.03	4	0.00	0.01	4

7b.Statistical analysis of organic compound log removal. Bolded compounds were used as validation exemplars.

COMPOUND	ESPA-2			TFC-HR			TFC-ULP		
	Mean	Std Dev	n	Mean	Std Dev	n	Mean	Std Dev	n
Chlorothanonil	2.23	0.08	3	2.51	0.12	3	1.38	0.11	3
Chlorpyrifos	3.23	0.00	3	3.23	0.00	3	3.23	0.00	3
Cis-1,3-Dichloropropene	-0.12	0.02	4	-0.08	0.02	4	-0.02	0.02	4
Dibromochloromethane	0.16	0.04	4	0.27	0.03	4	0.16	0.01	4
Dibromomethane	-0.15	0.01	4	-0.17	0.02	4	-0.14	0.01	4
Dichlorodifluoromethane	0.43	0.04	4	0.32	0.04	4	0.17	0.03	4
Dieldrin	4.30	0.00	3	2.88	1.23	3	4.30	0.00	3
Endrin	2.82	0.00	3	3.31	0.85	3	3.81	0.85	3
Estriol	1.85	0.06	3	2.92	0.15	3	1.95	0.09	3
Estrone	1.84	0.09	3	2.84	0.13	3	1.89	0.10	3
Ethylbenzene	1.14	0.12	4	1.34	0.02	4	1.37	0.11	4
Etridazole	2.29	0.05	3	2.63	0.06	3	1.92	0.28	3
Hepatchlor epoxide	2.75	0.00	3	2.75	0.00	3	2.75	0.00	3
Heptachlor	4.30	0.00	3	4.30	0.00	3	4.30	0.00	3
Hexachlorobenzene	4.30	0.00	3	4.30	0.00	3	4.30	0.00	3
Hexachlorobutadiene	1.55	0.15	4	1.68	0.11	4	2.26	0.34	4
Isopropylbenzene	1.72	0.07	4	2.47	0.04	4	1.76	0.06	4
Lindane	3.18	0.97	3	3.55	0.67	3	2.86	1.25	3
Methoxychlor	4.30	0.00	3	4.30	0.00	3	4.30	0.00	3
Methylene chloride	-0.15	0.04	4	-0.16	0.02	4	-0.11	0.01	4
M-Xylene	1.24	0.12	4	1.12	0.03	4	1.43	0.11	4
Naphthalene	1.50	0.11	4	2.14	0.14	4	1.68	0.09	4
N-Butylbenzene	2.76	0.09	4	3.10	0.00	4	3.10	0.00	4
N-Propylbenzene	1.91	0.15	4	3.17	0.00	4	2.43	0.17	4
O-Xylene	1.23	0.08	4	1.07	0.02	4	1.15	0.05	4
Permethrin	4.30	0.00	3	4.30	0.00	3	4.30	0.00	3
Progesterone	2.45	0.08	3	3.17	0.16	3	2.38	0.21	3
Propachlor	2.03	0.07	3	2.72	0.04	3	1.98	0.04	3
P-Xylene	1.24	0.12	4	1.12	0.03	4	1.43	0.11	4
Sec-Butylbenzene	2.41	0.12	4	3.17	0.00	4	2.36	0.06	4
Styrene	0.97	0.15	4	2.11	0.22	4	1.43	0.08	4
T-Butylbenzene	2.21	0.03	4	2.66	0.00	4	1.77	0.04	4
Tetrachloroethene	0.92	0.10	4	1.78	0.10	4	1.23	0.09	4
Toluene	0.54	0.08	4	0.89	0.06	4	0.62	0.04	4
Trichloroethene	0.07	0.04	4	0.29	0.06	4	0.29	0.01	4
Trichlorofluoromethane	0.64	0.02	4	0.57	0.03	4	0.32	0.03	4
Trifluralin	2.41	0.05	3	2.40	0.13	3	2.58	0.07	3
Vinylchloride	-0.02	0.05	4	-0.02	0.02	4	-0.02	0.02	4

Table 8. Log removal ranges selected for categorical analysis.

Percent Rejection	Log Removal Range
< 0% - 0%	Membrane Accumulation
> 0% - 68.3%	> 0 - 0.5 log
> 68.3 - 90%	0.5 - 1 log
> 90% - 99%	1 - 2 logs
> 99% - 99.9%	2 - 3 logs
> 99.9% - 99.99%	3 - 4 logs
> 99.99%	> 4 logs

Table 9a. Comparison of measured and predicted log removal values. Bolded compounds used as validation exemplars.

COMPOUND	ESPA-2		TFC-HR		TFC-ULP	
	Measured	Predicted	Measured	Predicted	Measured	Predicted
1,1,1,2-Tetrachloroethane	1.28	0.94	1.46	1.40	0.96	1.02
1,1,1-Trichloroethane	1.27	1.35	1.38	1.52	0.92	0.82
1,1,2,2-Tetrachloroethane	0.94	0.55	1.11	0.88	0.66	0.50
1,1,2-Trichloroethane	0.26	0.05	0.31	0.12	0.15	0.05
1,1-Dichloroethane	0.17	0.16	0.09	0.14	0.02	0.10
1,1-Dichloroethene	-0.04	0.11	-0.10	0.00	-0.12	0.01
1,2,3-Trichlorobenzene	1.89	1.73	2.26	2.35	2.21	2.40
1,2,3-Trichloropropane	0.71	0.38	0.89	0.49	0.51	0.27
1,2,4-Trichlorobenzene	2.00	1.70	2.26	2.28	2.41	2.33
1,2,4-Trimethylbenzene	1.87	2.10	2.71	2.54	1.96	2.00
1,2-Dibromoethane	-0.09	-0.08	-0.05	-0.01	-0.03	-0.01
1,2-Dichlorobenzene	1.31	1.41	2.40	2.51	1.72	1.86
1,2-Dichloroethane	-0.08	-0.02	-0.12	-0.08	-0.11	-0.06
1,2-Dichloropropane	0.38	0.34	0.38	0.26	0.21	0.13
1,3,5-Trimethylbenzene	2.25	2.05	3.07	2.73	2.28	2.10
1,3-Dichlorobenzene	1.46	1.50	2.80	2.60	2.17	2.08
1,3-Dichloropropane	0.06	0.10	0.16	0.08	0.07	0.02
1,4-Dichlorobenzene	1.30	1.42	2.83	2.52	2.07	1.88
2-Chlorotoluene	1.34	1.37	2.31	2.54	1.58	2.03
4,4-DDD	4.30	4.13	4.30	4.03	4.30	4.11
4,4'-DDT	4.30	4.18	4.30	4.03	4.20	4.11
4-Chlorotoluene	1.29	1.27	2.72	2.26	1.97	1.88
4-Isopropyltoluene	2.44	2.48	3.17	2.99	2.61	2.24
Aldrin	3.04	4.19	3.04	4.03	3.67	4.16
Benzene	0.25	0.07	0.18	-0.06	0.10	-0.03
Beta-BHC	2.38	2.53	2.98	2.87	1.99	2.14
Bromobenzene	0.79	0.97	1.77	1.53	1.24	1.12
Bromochloromethane	-0.13	-0.11	-0.15	-0.14	-0.11	-0.07
Bromodichloromethane	0.07	0.05	0.05	0.27	0.01	0.12
Bromoform	0.32	0.47	0.57	0.77	0.36	0.54
Bromomethane	-0.02	-0.05	-0.06	-0.13	-0.03	-0.09
Carbon tetrachloride	1.27	0.83	1.40	1.39	0.92	0.91
Chlordane	4.30	4.20	4.30	3.98	4.30	4.20
Chlorobenzene	0.44	0.79	0.72	1.24	0.88	0.78
Chlorobenzilate	4.30	4.19	4.30	4.05	4.30	4.17
Chloroethane	0.01	0.06	-0.01	0.04	0.01	0.08
Chloroform	0.07	0.09	0.00	0.10	-0.02	0.04
Chloromethane	-0.03	-0.08	-0.05	-0.06	0.00	-0.03

9b. Comparison of measured and predicted log removal values. Bolded compounds used as validation exemplars..

COMPOUND	ESPA-2		TFC-HR		TFC-ULP	
	Measured	Predicted	Measured	Predicted	Measured	Predicted
Chlorothanonil	2.23	2.00	2.51	2.84	1.38	1.57
Chlorpyrifos	3.23	2.66	3.23	2.93	3.23	2.95
Cis-1,3-Dichloropropene	-0.12	0.12	-0.08	0.07	-0.02	0.03
Dibromochloromethane	0.16	0.11	0.27	0.19	0.16	0.16
Dibromomethane	-0.15	-0.17	-0.17	-0.15	-0.14	-0.12
Dichlorodifluoromethane	0.43	0.19	0.32	0.14	0.17	0.08
Dieldrin	4.30	3.78	2.88	3.43	4.30	4.10
Endrin	2.82	3.30	3.31	3.36	3.81	3.76
Estriol	1.85	1.77	2.92	2.17	1.95	1.94
Estrone	1.84	2.12	2.84	2.86	1.89	1.73
Ethylbenzene	1.14	0.97	1.34	1.43	1.37	1.64
Etridazole	2.29	2.41	2.63	2.55	1.92	2.50
Hepatchlor epoxide	2.75	2.86	2.75	3.45	2.75	3.00
Heptachlor	4.30	4.18	4.30	3.91	4.30	4.19
Hexachlorobenzene	4.30	4.03	4.30	4.04	4.30	4.05
Hexachlorobutadiene	1.55	2.04	1.68	1.49	2.26	2.58
Isopropylbenzene	1.72	1.78	2.47	2.75	1.76	1.90
Lindane	3.18	2.59	3.55	2.91	2.86	2.29
Methoxychlor	4.30	3.47	4.30	3.45	4.30	3.70
Methylene chloride	-0.15	-0.04	-0.16	-0.12	-0.11	-0.09
M-Xylene	1.24	1.35	1.12	1.24	1.43	1.19
Naphthalene	1.50	1.40	2.14	2.69	1.68	1.96
N-Butylbenzene	2.76	2.63	3.10	3.45	3.10	3.21
N-Propylbenzene	1.91	1.66	3.17	3.07	2.43	2.42
O-Xylene	1.23	1.32	1.07	1.26	1.15	1.11
Permethrin	4.30	4.23	4.30	4.25	4.30	4.25
Progesterone	2.45	2.73	3.17	3.29	2.38	1.82
Propachlor	2.03	1.95	2.72	2.42	1.98	2.10
P-Xylene	1.24	1.34	1.12	1.22	1.43	1.14
Sec-Butylbenzene	2.41	2.50	3.17	3.07	2.36	2.25
Styrene	0.97	0.96	2.11	2.27	1.43	1.08
T-Butylbenzene	2.21	2.48	2.66	2.99	1.77	2.24
Tetrachloroethene	0.92	1.32	1.78	2.15	1.23	1.49
Toluene	0.54	0.72	0.89	0.61	0.62	0.77
Trichloroethene	0.07	0.46	0.29	0.31	0.29	0.27
Trichlorofluoromethane	0.64	0.58	0.57	0.55	0.32	0.43
Trifluralin	2.41	2.98	2.40	3.22	2.58	2.83
Vinylchloride	-0.02	-0.01	-0.02	-0.07	-0.02	-0.07

Table 10a. Categorical analysis of the model output compared to measured results**.** Bolded compounds used as validation exemplars.

	ESPA-2		TFC-HR		TFC-ULP			% +/-
Compound Name	**Measured**	**Predicted**	**Measured**	**Predicted**	**Measured**	**Predicted**	**% Exact**	**one category**
1,1,1,2-Tetrachloroethane	1 - 2 logs	1 - 2 logs	1 - 2 logs	1 - 2 logs	0.5 - 1 log	1 - 2 logs	67	100
1,1,1-Trichloroethane	1 - 2 logs	0.5 - 1 log	1 - 2 logs	0.5 - 1 log	0.5 - 1 log	0.5 - 1 log	33	100
1,1,2,2-Tetrachloroethane	0.5 - 1 log	>0 - 0.5 log	1 - 2 logs	0.5 - 1 log	0.5 - 1 log	0.5 - 1 log	33	100
1,1,2-Trichloroethane	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	100	100
1,1-Dichloroethane	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	100	100
1,1-Dichloroethene	Memb Accum	Memb Accum	Memb Accum	>0 - 0.5 log	Memb Accum	Memb Accum	33	100
1,2,3-Trichlorobenzene	1 - 2 logs	2 - 3 logs	2 - 3 logs	2 - 3 logs	2 - 3 logs	2 - 3 logs	67	100
1,2,3-Trichloropropane	**0.5 - 1 log**	**>0 - 0.5 log**	**0.5 - 1 log**	**0.5 - 1 log**	**0.5 - 1 log**	**>0 - 0.5 log**	**33**	**100**
1,2,4-Trichlorobenzene	1 - 2 logs	2 - 3 logs	2 - 3 logs	2 - 3 logs	2 - 3 logs	2 - 3 logs	67	100
1,2,4-Trimethylbenzene	1 - 2 logs	1 - 2 logs	2 - 3 logs	2 - 3 logs	1 - 2 logs	2 - 3 logs	67	100
1,2-Dibromoethane	Memb Accum	>0 - 0.5 log	Memb Accum	>0 - 0.5 log	Memb Accum	>0 - 0.5 log	0	100
1,2-Dichlorobenzene	1 - 2 logs	1 - 2 logs	2 - 3 logs	2 - 3 logs	1 - 2 logs	1 - 2 logs	100	100
1,2-Dichloroethane	Memb Accum	**>0 - 0.5 log**	Memb Accum	Memb Accum	Memb Accum	Memb Accum	**67**	**100**
1,2-Dichloropropane	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	100	100
1,3,5-Trimethylbenzene	2 - 3 logs	1 - 2 logs	3 - 4 logs	2 - 3 logs	2 - 3 logs	1 - 2 logs	0	100
1,3-Dichlorobenzene	1 - 2 logs	1 - 2 logs	2 - 3 logs	2 - 3 logs	2 - 3 logs	1 - 2 logs	67	100
1,3-Dichloropropane	**>0 - 0.5 log**	**>0 - 0.5 log**	**>0 - 0.5 log**	**>0 - 0.5 log**	**>0 - 0.5 log**	**>0 - 0.5 log**	**100**	100
1,4-Dichlorobenzene	1 - 2 logs	1 - 2 logs	2 - 3 logs	2 - 3 logs	2 - 3 logs	1 - 2 logs	67	100
2-Chlorotoluene	**1 - 2 logs**	**1 - 2 logs**	**1 - 2 logs**	**2 - 3 logs**	**1 - 2 logs**	**1 - 2 logs**	**67**	**100**
4,4-DDD	>4 logs	3 - 4 logs	>4 logs	3 - 4 logs	>4 logs	3 - 4 logs	0	100
4,4'-DDT	>4 logs	>4 logs	>4 logs	3 - 4 logs	>4 logs	>4 logs	67	100
4-Chlorotoluene	1 - 2 logs	1 - 2 logs	2 - 3 logs	2 - 3 logs	1 - 2 logs	1 - 2 logs	100	100
4-Isopropyltoluene	2 - 3 logs	2 - 3 logs	3 - 4 logs	2 - 3 logs	2 - 3 logs	2 - 3 logs	67	100
Aldrin	2 - 3 logs	3 - 4 logs	2 - 3 logs	3 - 4 logs	2 - 3 logs	3 - 4 logs	0	100
Benzene	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	100	100
Beta-BHC	2 - 3 logs	2 - 3 logs	2 - 3 logs	2 - 3 logs	1 - 2 logs	2 - 3 logs	67	100
Bromobenzene	0.5 - 1 log	0.5 - 1 log	1 - 2 logs	1 - 2 logs	1 - 2 logs	1 - 2 logs	100	100
Bromochloromethane	Memb Accum	Memb Accum	Memb Accum	Memb Accum	Memb Accum	Memb Accum	100	100
Bromodichloromethane	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	100	100
Bromoform	>0 - 0.5 log	>0 - 0.5 log	0.5 - 1 log	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	67	100
Bromomethane	Memb Accum	Memb Accum	Memb Accum	Memb Accum	Memb Accum	Memb Accum	100	100
Carbon tetrachloride	**1 - 2 logs**	**1 - 2 logs**	**1 - 2 logs**	**1 - 2 logs**	**1 - 2 logs**	**1 - 2 logs**	**100**	**100**
Chlordane	>4 logs	3 - 4 logs	>4 logs	3 - 4 logs	>4 logs	3 - 4 logs	0	100
Chlorobenzene	>0 - 0.5 log	0.5 - 1 log	0.5 - 1 log	1 - 2 logs	0.5 - 1 log	1 - 2 logs	0	100
Chlorobenzilate	>4 logs	3 - 4 logs	>4 logs	3 - 4 logs	>4 logs	3 - 4 logs	0	100
Chloroethane	>0 - 0.5 log	>0 - 0.5 log	Memb Accum	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	67	100
Chloroform	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	Memb Accum	>0 - 0.5 log	67	100

10b. Categorical analysis of the model output compared to measured results**.** Bolded compounds used as validation exemplars.

	ESPA-2		TFC-HR		TFC-ULP			% +/-
Compound Name	**Measured**	**Predicted**	**Measured**	**Predicted**	**Measured**	**Predicted**	**% Exact**	**one category**
Chloromethane	Memb Accum	>0 - 0.5 log	Memb Accum	Memb Accum	Memb Accum	Memb Accum	67	100
Chlorothanonil	2 - 3 logs	1 - 2 logs	2 - 3 logs	2 - 3 logs	1 - 2 logs	1 - 2 logs	67	100
Chlorpyrifos	3 - 4 logs	2 - 3 logs	3 - 4 logs	2 - 3 logs	3 - 4 logs	3 - 4 logs	33	100
Cis-1,3-Dichloropropene	Memb Accum	>0 - 0.5 log	Memb Accum	>0 - 0.5 log	Memb Accum	>0 - 0.5 log	0	100
Dibromochloromethane	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	100	100
Dibromomethane	Memb Accum	Memb Accum	Memb Accum	Memb Accum	Memb Accum	Memb Accum	100	100
Dichlorodifluoromethane	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	100	100
Dieldrin	>4 logs	3 - 4 logs	2 - 3 logs	2 - 3 logs	>4 logs	3 - 4 logs	33	100
Endrin	2 - 3 logs	3 - 4 logs	2 - 3 logs	3 - 4 logs	3 - 4 logs	3 - 4 logs	33	100
Estriol	1 - 2 logs	1 - 2 logs	2 - 3 logs	2 - 3 logs	1 - 2 logs	2 - 3 logs	67	100
Estrone	1 - 2 logs	2 - 3 logs	2 - 3 logs	2 - 3 logs	1 - 2 logs	2 - 3 logs	33	100
Ethylbenzene	1 - 2 logs	1 - 2 logs	1 - 2 logs	1 - 2 logs	1 - 2 logs	1 - 2 logs	100	100
Etridazole	2 - 3 logs	2 - 3 logs	2 - 3 logs	2 - 3 logs	1 - 2 logs	2 - 3 logs	67	100
Hepatchlor epoxide	2 - 3 logs	3 - 4 logs	2 - 3 logs	3 - 4 logs	2 - 3 logs	3 - 4 logs	0	100
Heptachlor	>4 logs	3 - 4 logs	>4 logs	2 - 3 logs	>4 logs	3 - 4 logs	0	x
Hexachlorobenzene	>4 logs	3 - 4 logs	>4 logs	2 - 3 logs	>4 logs	2 - 3 logs	0	x
Hexachlorobutadiene	1 - 2 logs	2 - 3 logs	1 - 2 logs	2 - 3 logs	2 - 3 logs	2 - 3 logs	33	100
Isopropylbenzene	1 - 2 logs	1 - 2 logs	2 - 3 logs	2 - 3 logs	1 - 2 logs	2 - 3 logs	67	100
Lindane	2 - 3 logs	2 - 3 logs	3 - 4 logs	2 - 3 logs	2 - 3 logs	2 - 3 logs	67	100
Methoxychlor	>4 logs	3 - 4 logs	>4 logs	3 - 4 logs	>4 logs	3 - 4 logs	0	100
Methylene chloride	Memb Accum	Memb Accum	Memb Accum	Memb Accum	Memb Accum	Memb Accum	100	100
M-Xylene	**1 - 2 logs**	**1 - 2 logs**	**1 - 2 logs**	**1 - 2 logs**	**1 - 2 logs**	**1 - 2 logs**	**100**	**100**
Naphthalene	1 - 2 logs	1 - 2 logs	2 - 3 logs	2 - 3 logs	1 - 2 logs	1 - 2 logs	100	100
N-Butylbenzene	2 - 3 logs	2 - 3 logs	3 - 4 logs	3 - 4 logs	3 - 4 logs	2 - 3 logs	67	100
N-Propylbenzene	1 - 2 logs	2 - 3 logs	3 - 4 logs	2 - 3 logs	2 - 3 logs	2 - 3 logs	33	100
O-Xylene	1 - 2 logs	1 - 2 logs	1 - 2 logs	1 - 2 logs	1 - 2 logs	1 - 2 logs	100	100
Permethrin	>4 logs	3 - 4 logs	>4 logs	3 - 4 logs	>4 logs	3 - 4 logs	0	100
Progesterone	2 - 3 logs	2 - 3 logs	3 - 4 logs	3 - 4 logs	2 - 3 logs	2 - 3 logs	100	100
Propachlor	2 - 3 logs	1 - 2 logs	2 - 3 logs	2 - 3 logs	1 - 2 logs	1 - 2 logs	67	100
P-Xylene	1 - 2 logs	1 - 2 logs	1 - 2 logs	1 - 2 logs	1 - 2 logs	1 - 2 logs	100	100
Sec-Butylbenzene	2 - 3 logs	2 - 3 logs	3 - 4 logs	3 - 4 logs	2 - 3 logs	2 - 3 logs	100	100
Styrene	0.5 - 1 log	0.5 - 1 log	2 - 3 logs	1 - 2 logs	1 - 2 logs	1 - 2 logs	67	100
T-Butylbenzene	2 - 3 logs	2 - 3 logs	2 - 3 logs	2 - 3 logs	1 - 2 logs	2 - 3 logs	67	100
Tetrachloroethene	0.5 - 1 log	0.5 - 1 log	1 - 2 logs	1 - 2 logs	1 - 2 logs	0.5 - 1 log	67	100
Toluene	0.5 - 1 log	0.5 - 1 log	0.5 - 1 log	0.5 - 1 log	0.5 - 1 log	0.5 - 1 log	100	100
Trichloroethene	>0 - 0.5 log	>0 - 0.5 log	>0 - 0.5 log	0.5 - 1 log	>0 - 0.5 log	>0 - 0.5 log	67	100
Trichlorofluoromethane	0.5 - 1 log	0.5 - 1 log	0.5 - 1 log	1 - 2 logs	>0 - 0.5 log	0.5 - 1 log	33	100
Trifluralin	2 - 3 logs	2 - 3 logs	2 - 3 logs	2 - 3 logs	2 - 3 logs	2 - 3 logs	100	100
Vinylchloride	Memb Accum	>0 - 0.5 log	Memb Accum	Memb Accum	Memb Accum	Memb Accum	67	100

Table 11. Comparison of compound removal; high log P vs. low log P.

Log P >4							
				Measured Log Removal			Predicted
Membrane	Compound	Mol Weight	Log_P	Average	Std Dev	n	Log Removal
ESPA-2	4-Isopropyltoluene	134.22	4.10	2.44	0.10	4	2.48
TFC-HR	4-Isopropyltoluene	134.22	4.10	3.17	0.00	4	2.99
TFC-ULP	4-Isopropyltoluene	134.22	4.10	2.61	0.11	4	2.24
ESPA-2	N-Butylbenzene	134.22	4.38	2.76	0.09	4	2.63
TFC-HR	N-Butylbenzene	134.22	4.38	3.10	0.00	4	3.45
TFC-ULP	N-Butylbenzene	134.22	4.38	3.10	0.00	4	3.21
ESPA-2	Sec-Butylbenzene	134.22	4.57	2.41	0.12	4	2.50
TFC-HR	Sec-Butylbenzene	134.22	4.57	3.17	0.00	4	3.07
TFC-ULP	Sec-Butylbenzene	134.22	4.57	2.36	0.06	4	2.25
ESPA-2	T-Butylbenzene	134.22	4.11	2.21	0.03	4	2.48
TFC-HR	T-Butylbenzene	134.22	4.11	2.66	0.00	4	2.99
TFC-ULP	T-Butylbenzene	134.22	4.11	1.77	0.04	4	2.24
Log P <2							
				Measured Log Removal			Predicted
Membrane	Compound	Mol Weight	Log_P	Average	Std Dev	n	Log Removal
ESPA-2	1,2-Dibromoethane	187.86	1.96	-0.09	0.02	4	-0.08
TFC-HR	1,2-Dibromoethane	187.86	1.96	-0.05	0.02	4	-0.01
TFC-ULP	1,2-Dibromoethane	187.86	1.96	-0.03	0.02	4	-0.01
ESPA-2	Dibromomethane	173.84	1.70	-0.15	0.01	4	-0.17
TFC-HR	Dibromomethane	173.84	1.70	-0.17	0.02	4	-0.15
TFC-ULP	Dibromomethane	173.84	1.70	-0.14	0.01	4	-0.12

Table 12. Composition of the different feedwater matrices used in the study.

Feedwater Matrix (Deionized water)	TDS (mg/L)	pH (units)
1	1000	6
2	1000	7
3	1000	8
4	3500	6
5	3500	7
6	3500	8
7	6000	6
8	6000	7
9	6000	8

Table 13a. Effect of feedwater matrix variations on organic compound rejection.

Measured Results for ESPA-2					
		Salinity	Percent Rejection		Log Removal
Compound	pH	(ppm NaCl)	Average	Std Dev	Range
1,1,1,2-Tetrachloroethane	6	1000	95.65	0.40	1 - 2 logs
	6	3500	92.63	0.74	1 - 2 logs
	6	6000	91.68	0.52	1 - 2 logs
	7	1000	93.79	0.46	1 - 2 logs
	7	3500	91.61	0.98	1 - 2 logs
	7	6000	94.67	0.16	1 - 2 logs
	8	1000	93.08	0.30	1 - 2 logs
	8	3500	93.51	0.50	1 - 2 logs
	8	6000	92.75	0.60	1 - 2 logs
1,1,1-Trichloroethane	6	1000	94.94	0.69	1 - 2 logs
	6	3500	92.64	0.62	1 - 2 logs
	6	6000	90.87	0.75	1 - 2 logs
	7	1000	91.84	0.30	1 - 2 logs
	7	3500	92.73	0.85	1 - 2 logs
	7	6000	94.92	0.22	1 - 2 logs
	8	1000	93.04	0.56	1 - 2 logs
	8	3500	91.81	0.46	1 - 2 logs
	8	6000	91.10	0.64	1 - 2 logs
1,1,2,2-Tetrachloroethane	6	1000	89.74	0.58	0.5 - 1 log
	6	3500	87.56	1.62	0.5 - 1 log
	6	6000	80.13	1.41	0.5 - 1 log
	7	1000	87.86	1.48	0.5 - 1 log
	7	3500	85.40	1.51	0.5 - 1 log
	7	6000	87.96	0.34	0.5 - 1 log
	8	1000	86.24	0.71	0.5 - 1 log
	8	3500	84.77	1.24	0.5 - 1 log
	8	6000	85.02	0.55	0.5 - 1 log
1,1,2-Trichloroethane	6	1000	36.37	3.36	>0 - 0.5 log
	6	3500	43.61	1.80	>0 - 0.5 log
	6	6000	29.82	2.62	>0 - 0.5 log
	7	1000	45.57	6.24	>0 - 0.5 log
	7	3500	32.78	4.27	>0 - 0.5 log
	7	6000	49.57	1.79	>0 - 0.5 log
	8	1000	40.12	1.95	>0 - 0.5 log
	8	3500	36.72	3.93	>0 - 0.5 log
	8	6000	36.49	3.39	>0 - 0.5 log
1,1-Dichloroethane	6	1000	36.92	6.76	>0 - 0.5 log
	6	3500	25.44	2.12	>0 - 0.5 log
	6	6000	13.07	6.60	>0 - 0.5 log
	7	1000	14.10	6.57	>0 - 0.5 log
	7	3500	18.25	5.44	>0 - 0.5 log
	7	6000	41.97	4.55	>0 - 0.5 log
	8	1000	19.06	3.83	>0 - 0.5 log
	8	3500	24.57	2.60	>0 - 0.5 log
	8	6000	13.01	4.96	>0 - 0.5 log
1,1-Dichloroethene	6	1000	-7.52	21.57	Membrane Accumulation
	6	3500	-29.03	9.63	Membrane Accumulation
	6	6000	-36.57	7.93	Membrane Accumulation
	7	1000	-26.37	8.93	Membrane Accumulation
	7	3500	-19.25	9.08	Membrane Accumulation
	7	6000	-9.36	3.42	Membrane Accumulation
	8	1000	-11.84	3.01	Membrane Accumulation
	8	3500	-5.12	3.38	Membrane Accumulation
	8	6000	-40.13	8.22	Membrane Accumulation

13b. Effect of feedwater matrix variations on organic compound rejection.

Measured Results for ESPA-2					
		Salinity	Percent Rejection		Log Removal
COMPOUND	pH	(ppm NaCl)	Average	Std Dev	Range
1,2,3-Trichlorobenzene	6	1000	98.95	0.28	1 - 2 logs
	6	3500	99.26	0.36	2 - 3 logs
	6	6000	99.10	0.26	2 - 3 logs
	7	1000	98.31	0.32	1 - 2 logs
	7	3500	97.96	0.28	1 - 2 logs
	7	6000	99.02	0.32	2 - 3 logs
	8	1000	98.76	0.32	1 - 2 logs
	8	3500	99.03	0.33	2 - 3 logs
	8	6000	98.17	0.33	1 - 2 logs
1,2,3-Trichloropropane	6	1000	85.51	0.89	0.5 - 1 log
	6	3500	81.32	2.27	0.5 - 1 log
	6	6000	71.55	1.79	0.5 - 1 log
	7	1000	77.77	2.26	0.5 - 1 log
	7	3500	75.99	1.96	0.5 - 1 log
	7	6000	81.49	0.54	0.5 - 1 log
	8	1000	80.40	1.11	0.5 - 1 log
	8	3500	76.86	1.41	0.5 - 1 log
	8	6000	76.67	0.80	0.5 - 1 log
1,2,4-Trichlorobenzene	6	1000	99.22	0.20	2 - 3 logs
	6	3500	99.61	0.22	2 - 3 logs
	6	6000	99.58	0.16	2 - 3 logs
	7	1000	99.05	0.25	2 - 3 logs
	7	3500	99.13	0.18	2 - 3 logs
	7	6000	99.48	0.21	2 - 3 logs
	8	1000	99.23	0.24	2 - 3 logs
	8	3500	99.38	0.21	2 - 3 logs
	8	6000	98.86	0.24	1 - 2 logs
1,2,4-Trimethylbenzene	6	1000	98.21	0.38	1 - 2 logs
	6	3500	98.63	0.48	1 - 2 logs
	6	6000	98.69	0.38	1 - 2 logs
	7	1000	97.06	0.54	1 - 2 logs
	7	3500	97.77	0.37	1 - 2 logs
	7	6000	98.28	0.44	1 - 2 logs
	8	1000	97.47	0.39	1 - 2 logs
	8	3500	97.42	0.47	1 - 2 logs
	8	6000	98.25	0.49	1 - 2 logs
1,2-Dibromo-3-chloropropane	6	1000	91.79	0.61	1 - 2 logs
	6	3500	90.99	1.41	1 - 2 logs
	6	6000	88.49	1.06	0.5 - 1 log
	7	1000	87.89	1.12	0.5 - 1 log
	7	3500	86.84	1.09	0.5 - 1 log
	7	6000	90.98	0.67	1 - 2 logs
	8	1000	89.68	0.60	0.5 - 1 log
	8	3500	88.17	1.17	0.5 - 1 log
	8	6000	89.66	0.39	0.5 - 1 log
1,2-Dibromoethane	6	1000	-0.77	2.47	Membrane Accumulation
	6	3500	-23.75	6.64	Membrane Accumulation
	6	6000	-41.89	3.02	Membrane Accumulation
	7	1000	-13.77	7.45	Membrane Accumulation
	7	3500	-37.96	6.05	Membrane Accumulation
	7	6000	-5.52	4.68	Membrane Accumulation
	8	1000	-20.93	4.83	Membrane Accumulation
	8	3500	-20.79	3.29	Membrane Accumulation
	8	6000	-28.91	6.63	Membrane Accumulation

13c. Effect of feedwater matrix variations on organic compound rejection.

Measured Results for ESPA-2					
		Salinity	Percent Rejection		Log Removal
COMPOUND	pH	(ppm NaCl)	Average	Std Dev	Range
1,2-Dichlorobenzene	6	1000	95.81	0.94	1 - 2 logs
	6	3500	96.72	1.42	1 - 2 logs
	6	6000	95.53	1.00	1 - 2 logs
	7	1000	95.00	1.42	1 - 2 logs
	7	3500	92.80	1.01	1 - 2 logs
	7	6000	95.08	1.05	1 - 2 logs
	8	1000	95.77	1.14	1 - 2 logs
	8	3500	92.97	1.45	1 - 2 logs
	8	6000	93.69	1.03	1 - 2 logs
1,2-Dichloroethane	6	1000	-19.64	5.28	Membrane Accumulation
	6	3500	-34.39	5.05	Membrane Accumulation
	6	6000	-51.74	8.25	Membrane Accumulation
	7	1000	-25.90	6.20	Membrane Accumulation
	7	3500	-40.99	4.68	Membrane Accumulation
	7	6000	-16.79	7.45	Membrane Accumulation
	8	1000	-17.84	6.57	Membrane Accumulation
	8	3500	-12.82	3.13	Membrane Accumulation
	8	6000	-32.19	6.72	Membrane Accumulation
1,2-Dichloropropane	6	1000	62.40	2.58	>0 - 0.5 log
	6	3500	51.14	1.91	>0 - 0.5 log
	6	6000	40.40	3.90	>0 - 0.5 log
	7	1000	51.99	4.54	>0 - 0.5 log
	7	3500	52.79	4.87	>0 - 0.5 log
	7	6000	60.10	1.66	>0 - 0.5 log
	8	1000	49.23	2.08	>0 - 0.5 log
	8	3500	49.23	2.97	>0 - 0.5 log
	8	6000	50.26	3.39	>0 - 0.5 log
1,3,5-Trimethylbenzene	6	1000	99.62	0.14	2 - 3 logs
	6	3500	99.17	0.15	2 - 3 logs
	6	6000	99.43	0.15	2 - 3 logs
	7	1000	99.08	0.19	2 - 3 logs
	7	3500	99.23	0.20	2 - 3 logs
	7	6000	99.76	0.31	2 - 3 logs
	8	1000	99.26	0.20	2 - 3 logs
	8	3500	99.35	0.22	2 - 3 logs
	8	6000	98.72	0.28	1 - 2 logs
1,3-Dichlorobenzene	6	1000	98.32	0.99	1 - 2 logs
	6	3500	95.47	1.26	1 - 2 logs
	6	6000	96.07	0.87	1 - 2 logs
	7	1000	96.12	1.21	1 - 2 logs
	7	3500	94.74	0.88	1 - 2 logs
	7	6000	96.07	1.08	1 - 2 logs
	8	1000	94.65	1.13	1 - 2 logs
	8	3500	94.38	1.24	1 - 2 logs
	8	6000	93.54	0.98	1 - 2 logs
1,3-Dichloropropane	6	1000	36.73	2.86	>0 - 0.5 log
	6	3500	8.96	3.60	>0 - 0.5 log
	6	6000	1.94	4.24	>0 - 0.5 log
	7	1000	8.82	8.19	>0 - 0.5 log
	7	3500	0.04	6.93	>0 - 0.5 log
	7	6000	20.56	3.78	>0 - 0.5 log
	8	1000	22.84	5.71	>0 - 0.5 log
	8	3500	12.52	3.43	>0 - 0.5 log
	8	6000	4.32	6.97	>0 - 0.5 log

13d. Effect of feedwater matrix variations on organic compound rejection.

Measured Results for ESPA-2					
		Salinity	Percent Rejection		Log Removal
COMPOUND	pH	(ppm NaCl)	Average	Std Dev	Range
1,4-Dichlorobenzene	6	1000	95.23	1.36	1 - 2 logs
	6	3500	100.00	2.88	>4 logs
	6	6000	94.73	1.21	1 - 2 logs
	7	1000	93.70	1.68	1 - 2 logs
	7	3500	92.44	1.27	1 - 2 logs
	7	6000	95.00	1.51	1 - 2 logs
	8	1000	92.91	1.60	1 - 2 logs
	8	3500	93.10	1.58	1 - 2 logs
	8	6000	91.83	1.17	1 - 2 logs
2-Chlorotoluene	6	1000	96.90	0.98	1 - 2 logs
	6	3500	95.40	1.26	1 - 2 logs
	6	6000	95.66	0.82	1 - 2 logs
	7	1000	92.42	1.42	1 - 2 logs
	7	3500	91.80	1.01	1 - 2 logs
	7	6000	95.08	1.09	1 - 2 logs
	8	1000	94.21	1.11	1 - 2 logs
	8	3500	94.83	1.25	1 - 2 logs
	8	6000	92.87	1.06	1 - 2 logs
4-Chlorotoluene	6	1000	93.84	1.46	1 - 2 logs
	6	3500	97.57	1.81	1 - 2 logs
	6	6000	96.59	1.19	1 - 2 logs
	7	1000	92.43	1.77	1 - 2 logs
	7	3500	89.40	1.46	0.5 - 1 log
	7	6000	94.53	1.54	1 - 2 logs
	8	1000	92.35	1.61	1 - 2 logs
	8	3500	94.35	1.66	1 - 2 logs
	8	6000	92.99	1.26	1 - 2 logs
4-Isopropyltoluene	6	1000	99.52	0.12	2 - 3 logs
	6	3500	99.70	0.17	2 - 3 logs
	6	6000	99.72	0.12	2 - 3 logs
	7	1000	99.00	0.20	1 - 2 logs
	7	3500	99.44	0.13	2 - 3 logs
	7	6000	99.68	0.25	2 - 3 logs
	8	1000	99.25	0.18	2 - 3 logs
	8	3500	99.69	0.17	2 - 3 logs
	8	6000	99.58	0.26	2 - 3 logs
Benzene	6	1000	42.41	5.95	>0 - 0.5 log
	6	3500	35.62	3.51	>0 - 0.5 log
	6	6000	49.88	3.16	>0 - 0.5 log
	7	1000	13.51	6.26	>0 - 0.5 log
	7	3500	31.96	5.97	>0 - 0.5 log
	7	6000	41.61	2.48	>0 - 0.5 log
	8	1000	32.68	2.65	>0 - 0.5 log
	8	3500	30.09	3.78	>0 - 0.5 log
	8	6000	30.07	4.85	>0 - 0.5 log
Bromobenzene	6	1000	90.89	2.89	1 - 2 logs
	6	3500	89.85	4.25	0.5 - 1 log
	6	6000	87.88	2.90	0.5 - 1 log
	7	1000	78.70	4.50	0.5 - 1 log
	7	3500	79.28	3.32	0.5 - 1 log
	7	6000	90.85	3.49	1 - 2 logs
	8	1000	78.63	3.75	0.5 - 1 log
	8	3500	79.63	3.50	0.5 - 1 log
	8	6000	78.33	2.89	0.5 - 1 log

13e. Effect of feedwater matrix variations on organic compound rejection.

Measured Results for ESPA-2					
		Salinity	Percent Rejection		Log Removal
COMPOUND	pH	(ppm NaCl)	Average	Std Dev	Range
Bromochloromethane	6	1000	-19.14	6.24	Membrane Accumulation
	6	3500	-40.75	9.18	Membrane Accumulation
	6	6000	-68.11	5.08	Membrane Accumulation
	7	1000	-58.28	9.02	Membrane Accumulation
	7	3500	-62.62	7.75	Membrane Accumulation
	7	6000	-37.77	7.32	Membrane Accumulation
	8	1000	-50.41	10.36	Membrane Accumulation
	8	3500	-37.95	1.77	Membrane Accumulation
	8	6000	-57.12	9.37	Membrane Accumulation
Bromodichloromethane	6	1000	26.27	4.28	>0 - 0.5 log
	6	3500	3.27	3.34	>0 - 0.5 log
	6	6000	-5.99	4.50	Membrane Accumulation
	7	1000	5.88	8.22	>0 - 0.5 log
	7	3500	11.02	7.20	>0 - 0.5 log
	7	6000	29.83	4.37	>0 - 0.5 log
	8	1000	4.85	5.13	>0 - 0.5 log
	8	3500	10.99	3.11	>0 - 0.5 log
	8	6000	3.12	5.68	>0 - 0.5 log
Bromoform	6	1000	67.89	2.72	>0 - 0.5 log
	6	3500	52.63	3.31	>0 - 0.5 log
	6	6000	44.83	1.89	>0 - 0.5 log
	7	1000	61.41	5.73	>0 - 0.5 log
	7	3500	43.63	4.28	>0 - 0.5 log
	7	6000	57.40	2.70	>0 - 0.5 log
	8	1000	53.03	3.24	>0 - 0.5 log
	8	3500	44.88	4.17	>0 - 0.5 log
	8	6000	46.59	3.01	>0 - 0.5 log
Bromomethane	6	1000	-27.33	14.68	Membrane Accumulation
	6	3500	-71.52	15.54	Membrane Accumulation
	6	6000	-73.86	7.80	Membrane Accumulation
	7	1000	-40.39	5.05	Membrane Accumulation
	7	3500	-80.70	11.70	Membrane Accumulation
	7	6000	-43.03	9.13	Membrane Accumulation
	8	1000	-53.01	7.68	Membrane Accumulation
	8	3500	-26.19	4.10	Membrane Accumulation
	8	6000	-68.03	13.72	Membrane Accumulation
Carbon tetrachloride	6	1000	95.04	0.71	1 - 2 logs
	6	3500	92.89	0.66	1 - 2 logs
	6	6000	91.24	0.70	1 - 2 logs
	7	1000	93.55	0.21	1 - 2 logs
	7	3500	91.56	0.63	1 - 2 logs
	7	6000	95.79	0.39	1 - 2 logs
	8	1000	92.43	0.53	1 - 2 logs
	8	3500	92.92	0.70	1 - 2 logs
	8	6000	93.51	0.77	1 - 2 logs
Chlorobenzene	6	1000	65.94	4.05	>0 - 0.5 log
	6	3500	59.95	7.42	>0 - 0.5 log
	6	6000	67.77	3.69	>0 - 0.5 log
	7	1000	55.10	7.76	>0 - 0.5 log
	7	3500	49.15	5.34	>0 - 0.5 log
	7	6000	64.88	4.81	>0 - 0.5 log
	8	1000	63.34	5.60	>0 - 0.5 log
	8	3500	65.29	4.90	>0 - 0.5 log
	8	6000	57.11	4.76	>0 - 0.5 log

13f. Effect of feedwater matrix variations on organic compound rejection.

Measured Results for ESPA-2					
		Salinity	Percent Rejection		Log Removal
COMPOUND	pH	(ppm NaCl)	Average	Std Dev	Range
Chloroethane	6	1000	-2.38	12.37	Membrane Accumulation
	6	3500	-22.36	6.96	Membrane Accumulation
	6	6000	-63.85	7.05	Membrane Accumulation
	7	1000	-16.24	3.70	Membrane Accumulation
	7	3500	-29.60	7.47	Membrane Accumulation
	7	6000	-4.85	4.89	Membrane Accumulation
	8	1000	-13.51	2.68	Membrane Accumulation
	8	3500	-1.48	4.39	Membrane Accumulation
	8	6000	-35.07	7.52	Membrane Accumulation
Chloroform	6	1000	36.54	5.20	>0 - 0.5 log
	6	3500	1.97	2.74	>0 - 0.5 log
	6	6000	2.48	6.95	>0 - 0.5 log
	7	1000	3.22	7.17	>0 - 0.5 log
	7	3500	4.99	4.55	>0 - 0.5 log
	7	6000	21.06	4.91	>0 - 0.5 log
	8	1000	11.38	4.77	>0 - 0.5 log
	8	3500	15.19	2.49	>0 - 0.5 log
	8	6000	-0.79	6.28	Membrane Accumulation
Chloromethane	6	1000	-14.05	14.76	Membrane Accumulation
	6	3500	-42.98	13.14	Membrane Accumulation
	6	6000	-78.48	6.38	Membrane Accumulation
	7	1000	-26.83	6.21	Membrane Accumulation
	7	3500	-53.14	9.19	Membrane Accumulation
	7	6000	-33.23	6.74	Membrane Accumulation
	8	1000	-32.32	5.39	Membrane Accumulation
	8	3500	-15.40	4.82	Membrane Accumulation
	8	6000	-67.99	14.33	Membrane Accumulation
Cis-1,3-Dichloropropene	6	1000	-43.41	5.18	Membrane Accumulation
	6	3500	-38.15	12.32	Membrane Accumulation
	6	6000	-21.11	3.82	Membrane Accumulation
	7	1000	-6.32	8.62	Membrane Accumulation
	7	3500	-33.94	7.38	Membrane Accumulation
	7	6000	-0.90	5.34	Membrane Accumulation
	8	1000	9.62	5.60	>0 - 0.5 log
	8	3500	-9.64	3.13	Membrane Accumulation
	8	6000	-27.15	9.16	Membrane Accumulation
Dibromochloromethane	6	1000	49.68	2.57	>0 - 0.5 log
	6	3500	21.03	3.16	>0 - 0.5 log
	6	6000	21.97	1.64	>0 - 0.5 log
	7	1000	28.72	8.43	>0 - 0.5 log
	7	3500	18.29	6.70	>0 - 0.5 log
	7	6000	37.84	3.20	>0 - 0.5 log
	8	1000	26.23	2.87	>0 - 0.5 log
	8	3500	33.08	4.49	>0 - 0.5 log
	8	6000	22.01	4.29	>0 - 0.5 log
Dibromomethane	6	1000	-21.66	6.78	Membrane Accumulation
	6	3500	-71.16	5.21	Membrane Accumulation
	6	6000	-69.44	6.49	Membrane Accumulation
	7	1000	-36.66	7.17	Membrane Accumulation
	7	3500	-51.24	5.08	Membrane Accumulation
	7	6000	-41.15	7.27	Membrane Accumulation
	8	1000	-57.38	9.26	Membrane Accumulation
	8	3500	-34.72	4.32	Membrane Accumulation
	8	6000	-55.76	8.66	Membrane Accumulation

13g. Effect of feedwater matrix variations on organic compound rejection.

Measured Results for ESPA-2					
		Salinity	Percent Rejection		Log Removal
COMPOUND	pH	(ppm NaCl)	Average	Std Dev	Range
Dichlorodifluoromethane	6	1000	55.98	11.10	>0 - 0.5 log
	6	3500	61.80	4.77	>0 - 0.5 log
	6	6000	34.22	10.74	>0 - 0.5 log
	7	1000	60.82	3.15	>0 - 0.5 log
	7	3500	52.99	6.71	>0 - 0.5 log
	7	6000	64.49	1.20	>0 - 0.5 log
	8	1000	66.10	1.50	>0 - 0.5 log
	8	3500	59.26	2.24	>0 - 0.5 log
	8	6000	49.75	1.54	>0 - 0.5 log
Ethylbenzene	6	1000	93.35	1.86	1 - 2 logs
	6	3500	95.10	1.83	1 - 2 logs
	6	6000	92.92	1.23	1 - 2 logs
	7	1000	82.55	3.25	0.5 - 1 log
	7	3500	89.30	1.45	0.5 - 1 log
	7	6000	92.52	1.43	1 - 2 logs
	8	1000	91.72	1.48	1 - 2 logs
	8	3500	92.14	1.70	1 - 2 logs
	8	6000	88.20	1.34	0.5 - 1 log
Hexachlorobutadiene	6	1000	98.47	1.42	1 - 2 logs
	6	3500	99.88	0.32	2 - 3 logs
	6	6000	99.32	0.27	2 - 3 logs
	7	1000	98.98	0.73	3 - 4 logs
	7	3500	99.82	0.17	2 - 3 logs
	7	6000	99.09	0.16	2 - 3 logs
	8	1000	99.82	0.48	2 - 3 logs
	8	3500	99.63	0.08	2 - 3 logs
	8	6000	98.77	0.39	1 - 2 logs
Isopropylbenzene	6	1000	98.62	0.35	1 - 2 logs
	6	3500	98.30	0.46	1 - 2 logs
	6	6000	97.78	0.24	1 - 2 logs
	7	1000	95.76	0.61	1 - 2 logs
	7	3500	96.90	0.41	1 - 2 logs
	7	6000	97.85	0.44	1 - 2 logs
	8	1000	97.69	0.45	1 - 2 logs
	8	3500	97.51	0.49	1 - 2 logs
	8	6000	96.56	0.48	1 - 2 logs
Methylene chloride	6	1000	-220.28	20.34	Membrane Accumulation
	6	3500	-269.39	22.78	Membrane Accumulation
	6	6000	37.91	51.75	>0 - 0.5 log
	7	1000	-42.62	5.37	Membrane Accumulation
	7	3500	-49.60	9.16	Membrane Accumulation
	7	6000	-40.54	8.05	Membrane Accumulation
	8	1000	-253.11	12.58	Membrane Accumulation
	8	3500	-30.76	3.10	Membrane Accumulation
	8	6000	-42.64	10.59	Membrane Accumulation
M-Xylene	6	1000	93.53	2.17	1 - 2 logs
	6	3500	94.76	1.60	1 - 2 logs
	6	6000	94.69	1.06	1 - 2 logs
	7	1000	81.60	3.67	0.5 - 1 log
	7	3500	90.74	1.61	1 - 2 logs
	7	6000	94.08	1.22	1 - 2 logs
	8	1000	93.00	1.37	1 - 2 logs
	8	3500	93.32	1.96	1 - 2 logs
	8	6000	92.74	0.79	1 - 2 logs

13h. Effect of feedwater matrix variations on organic compound rejection.

Measured Results for ESPA-2					
		Salinity	Percent Rejection		Log Removal
COMPOUND	pH	(ppm NaCl)	Average	Std Dev	Range
Naphthalene	6	1000	97.45	0.67	1 - 2 logs
	6	3500	97.95	0.77	1 - 2 logs
	6	6000	97.86	0.61	1 - 2 logs
	7	1000	96.66	0.96	1 - 2 logs
	7	3500	96.11	0.62	1 - 2 logs
	7	6000	98.51	0.60	1 - 2 logs
	8	1000	96.57	0.72	1 - 2 logs
	8	3500	96.94	0.82	1 - 2 logs
	8	6000	97.77	0.58	1 - 2 logs
N-Butylbenzene	6	1000	99.80	0.05	2 - 3 logs
	6	3500	99.95	0.05	3 - 4 logs
	6	6000	99.95	0.04	3 - 4 logs
	7	1000	99.83	0.07	2 - 3 logs
	7	3500	99.75	0.05	2 - 3 logs
	7	6000	99.91	0.12	3 - 4 logs
	8	1000	99.91	0.06	3 - 4 logs
	8	3500	99.88	0.07	2 - 3 logs
	8	6000	99.85	0.11	2 - 3 logs
N-Propylbenzene	6	1000	99.13	0.61	2 - 3 logs
	6	3500	99.28	0.47	2 - 3 logs
	6	6000	98.34	0.38	1 - 2 logs
	7	1000	98.18	0.82	1 - 2 logs
	7	3500	97.41	0.41	1 - 2 logs
	7	6000	98.41	0.48	1 - 2 logs
	8	1000	98.36	0.52	1 - 2 logs
	8	3500	98.84	0.51	1 - 2 logs
	8	6000	98.54	0.46	1 - 2 logs
O-Xylene	6	1000	93.14	0.84	1 - 2 logs
	6	3500	92.76	1.16	1 - 2 logs
	6	6000	93.05	0.61	1 - 2 logs
	7	1000	91.28	1.81	1 - 2 logs
	7	3500	90.27	1.37	1 - 2 logs
	7	6000	93.49	0.75	1 - 2 logs
	8	1000	92.26	0.87	1 - 2 logs
	8	3500	89.68	1.18	0.5 - 1 log
	8	6000	90.00	0.97	0.5 - 1 log
Sec-Butylbenzene	6	1000	99.45	0.15	2 - 3 logs
	6	3500	99.77	0.13	2 - 3 logs
	6	6000	99.68	0.11	2 - 3 logs
	7	1000	99.19	0.19	2 - 3 logs
	7	3500	99.28	0.10	2 - 3 logs
	7	6000	99.71	0.28	2 - 3 logs
	8	1000	99.56	0.15	2 - 3 logs
	8	3500	99.50	0.15	2 - 3 logs
	8	6000	99.57	0.27	2 - 3 logs
Styrene	6	1000	90.77	3.20	2 - 3 logs
	6	3500	86.70	3.38	0.5 - 1 log
	6	6000	93.30	2.65	1 - 2 logs
	7	1000	91.62	3.38	1 - 2 logs
	7	3500	86.19	2.33	0.5 - 1 log
	7	6000	94.44	2.17	1 - 2 logs
	8	1000	90.24	2.93	1 - 2 logs
	8	3500	83.76	2.76	0.5 - 1 log
	8	6000	87.60	2.25	0.5 - 1 log

13i. Effect of feedwater matrix variations on organic compound rejection.

Measured Results for ESPA-2					
		Salinity	Percent Rejection		Log Removal
COMPOUND	pH	(ppm NaCl)	Average	Std Dev	Range
T-Butylbenzene	6	1000	99.38	0.08	2 - 3 logs
	6	3500	99.47	0.19	2 - 3 logs
	6	6000	99.48	0.11	2 - 3 logs
	7	1000	98.93	0.22	1 - 2 logs
	7	3500	99.20	0.18	2 - 3 logs
	7	6000	99.75	0.31	2 - 3 logs
	8	1000	99.39	0.18	2 - 3 logs
	8	3500	99.12	0.16	2 - 3 logs
	8	6000	99.39	0.26	2 - 3 logs
Tetrachloroethene	6	1000	92.73	2.43	1 - 2 logs
	6	3500	93.20	2.37	1 - 2 logs
	6	6000	91.67	1.81	1 - 2 logs
	7	1000	85.31	2.76	0.5 - 1 log
	7	3500	87.58	1.71	0.5 - 1 log
	7	6000	94.21	2.20	1 - 2 logs
	8	1000	88.84	2.65	0.5 - 1 log
	8	3500	86.73	2.32	0.5 - 1 log
	8	6000	85.97	2.08	0.5 - 1 log
Toluene	6	1000	81.76	2.63	0.5 - 1 log
	6	3500	73.41	5.17	0.5 - 1 log
	6	6000	66.40	2.42	>0 - 0.5 log
	7	1000	72.97	4.45	0.5 - 1 log
	7	3500	63.52	4.65	>0 - 0.5 log
	7	6000	74.25	2.99	0.5 - 1 log
	8	1000	70.61	4.14	0.5 - 1 log
	8	3500	66.68	3.59	>0 - 0.5 log
	8	6000	59.44	3.74	>0 - 0.5 log
Trichloroethene	6	1000	23.99	8.01	>0 - 0.5 log
	6	3500	35.24	12.31	>0 - 0.5 log
	6	6000	19.73	4.42	>0 - 0.5 log
	7	1000	4.25	10.13	>0 - 0.5 log
	7	3500	14.99	7.81	>0 - 0.5 log
	7	6000	22.19	7.11	>0 - 0.5 log
	8	1000	19.08	9.65	>0 - 0.5 log
	8	3500	16.57	4.88	>0 - 0.5 log
	8	6000	6.23	10.82	>0 - 0.5 log
Trichlorofluoromethane	6	1000	80.17	4.43	0.5 - 1 log
	6	3500	81.54	2.01	0.5 - 1 log
	6	6000	76.72	2.27	0.5 - 1 log
	7	1000	76.22	1.30	0.5 - 1 log
	7	3500	80.46	2.41	0.5 - 1 log
	7	6000	81.95	0.70	0.5 - 1 log
	8	1000	82.64	1.52	0.5 - 1 log
	8	3500	79.37	1.09	0.5 - 1 log
	8	6000	73.13	1.01	0.5 - 1 log
Vinylchloride	6	1000	23.90	20.63	>0 - 0.5 log
	6	3500	-22.76	11.18	Membrane Accumulation
	6	6000	-68.71	6.14	Membrane Accumulation
	7	1000	-30.09	7.70	Membrane Accumulation
	7	3500	-37.66	7.64	Membrane Accumulation
	7	6000	-14.00	5.89	Membrane Accumulation
	8	1000	-23.14	5.29	Membrane Accumulation
	8	3500	-3.27	4.37	Membrane Accumulation
	8	6000	-37.46	9.02	Membrane Accumulation

13j. Effect of feedwater matrix variations on organic compound rejection.

Measured Results for TFC-HR					
		Salinity	Percent Rejection		Log Removal
Compound	pH	(ppm NaCl)	Average	Std Dev	Range
1,1,1,2-Tetrachloroethane	6	1000	95.00	0.44	1 - 2 logs
	6	3500	95.39	0.23	1 - 2 logs
	6	6000	92.31	0.71	1 - 2 logs
	7	1000	94.59	0.74	1 - 2 logs
	7	3500	95.61	1.11	1 - 2 logs
	7	6000	96.63	0.08	1 - 2 logs
	8	1000	92.73	1.24	1 - 2 logs
	8	3500	95.68	0.27	1 - 2 logs
	8	6000	94.57	0.97	1 - 2 logs
1,1,1-Trichloroethane	6	1000	94.50	0.46	1 - 2 logs
	6	3500	94.64	0.04	1 - 2 logs
	6	6000	91.93	0.61	1 - 2 logs
	7	1000	92.83	0.88	1 - 2 logs
	7	3500	94.53	0.86	1 - 2 logs
	7	6000	96.01	0.09	1 - 2 logs
	8	1000	92.65	1.10	1 - 2 logs
	8	3500	94.80	0.24	1 - 2 logs
	8	6000	92.88	1.09	1 - 2 logs
1,1,2,2-Tetrachloroethane	6	1000	86.76	1.49	0.5 - 1 log
	6	3500	90.64	0.44	1 - 2 logs
	6	6000	78.95	1.93	0.5 - 1 log
	7	1000	86.95	1.72	0.5 - 1 log
	7	3500	90.67	2.95	1 - 2 logs
	7	6000	92.53	0.44	1 - 2 logs
	8	1000	83.31	2.82	0.5 - 1 log
	8	3500	89.46	0.34	0.5 - 1 log
	8	6000	87.62	1.91	0.5 - 1 log
1,1,2-Trichloroethane	6	1000	19.02	8.48	>0 - 0.5 log
	6	3500	52.51	1.75	>0 - 0.5 log
	6	6000	24.12	4.62	>0 - 0.5 log
	7	1000	45.03	6.70	>0 - 0.5 log
	7	3500	54.67	8.57	>0 - 0.5 log
	7	6000	63.27	1.95	>0 - 0.5 log
	8	1000	31.07	6.97	>0 - 0.5 log
	8	3500	53.80	2.55	>0 - 0.5 log
	8	6000	43.12	5.72	>0 - 0.5 log
1,1-Dichloroethane	6	1000	15.95	1.82	>0 - 0.5 log
	6	3500	12.51	4.11	>0 - 0.5 log
	6	6000	-8.95	4.47	Membrane Accumulation
	7	1000	6.80	6.23	>0 - 0.5 log
	7	3500	5.59	2.51	>0 - 0.5 log
	7	6000	21.93	0.63	>0 - 0.5 log
	8	1000	8.86	4.62	>0 - 0.5 log
	8	3500	21.78	4.30	>0 - 0.5 log
	8	6000	0.69	3.06	>0 - 0.5 log
1,1-Dichloroethene	6	1000	-42.99	7.14	Membrane Accumulation
	6	3500	-39.25	13.88	Membrane Accumulation
	6	6000	-65.74	6.31	Membrane Accumulation
	7	1000	-32.06	6.04	Membrane Accumulation
	7	3500	-43.14	3.69	Membrane Accumulation
	7	6000	-22.62	1.34	Membrane Accumulation
	8	1000	-21.90	3.98	Membrane Accumulation
	8	3500	-11.09	6.51	Membrane Accumulation
	8	6000	-62.66	3.40	Membrane Accumulation

13k. Effect of feedwater matrix variations on organic compound rejection.

Measured Results for TFC-HR					
		Salinity	Percent Rejection		Log Removal
Compound	pH	(ppm NaCl)	Average	Std Dev	Range
1,2,3-Trichlorobenzene	6	1000	99.66	0.08	2 - 3 logs
	6	3500	99.58	0.07	2 - 3 logs
	6	6000	99.40	0.19	2 - 3 logs
	7	1000	99.63	0.06	2 - 3 logs
	7	3500	99.84	0.11	2 - 3 logs
	7	6000	99.85	0.05	2 - 3 logs
	8	1000	99.43	0.16	2 - 3 logs
	8	3500	99.87	0.07	2 - 3 logs
	8	6000	99.72	0.27	2 - 3 logs
1,2,3-Trichloropropane	6	1000	79.43	2.67	0.5 - 1 log
	6	3500	86.21	0.72	0.5 - 1 log
	6	6000	70.23	2.47	0.5 - 1 log
	7	1000	80.37	2.45	0.5 - 1 log
	7	3500	86.86	4.39	0.5 - 1 log
	7	6000	89.13	0.54	0.5 - 1 log
	8	1000	75.33	3.93	0.5 - 1 log
	8	3500	84.84	0.41	0.5 - 1 log
	8	6000	81.33	2.70	0.5 - 1 log
1,2,4-Trichlorobenzene	6	1000	99.79	0.08	2 - 3 logs
	6	3500	99.61	0.12	2 - 3 logs
	6	6000	99.71	0.08	2 - 3 logs
	7	1000	99.76	0.03	2 - 3 logs
	7	3500	99.87	0.04	2 - 3 logs
	7	6000	99.88	0.04	2 - 3 logs
	8	1000	99.71	0.09	2 - 3 logs
	8	3500	99.90	0.03	2 - 3 logs
	8	6000	99.82	0.18	2 - 3 logs
1,2,4-Trimethylbenzene	6	1000	99.13	0.14	2 - 3 logs
	6	3500	99.78	0.00	2 - 3 logs
	6	6000	98.97	0.40	1 - 2 logs
	7	1000	99.27	0.27	2 - 3 logs
	7	3500	99.91	0.26	3 - 4 logs
	7	6000	99.96	0.03	3 - 4 logs
	8	1000	98.61	0.52	1 - 2 logs
	8	3500	99.93	0.03	3 - 4 logs
	8	6000	99.73	0.32	2 - 3 logs
1,2-Dibromo-3-chloropropane	6	1000	89.32	1.46	0.5 - 1 log
	6	3500	94.13	0.08	1 - 2 logs
	6	6000	85.99	1.29	0.5 - 1 log
	7	1000	90.37	1.44	1 - 2 logs
	7	3500	95.34	2.43	1 - 2 logs
	7	6000	96.54	0.43	1 - 2 logs
	8	1000	87.59	2.47	0.5 - 1 log
	8	3500	94.79	0.22	1 - 2 logs
	8	6000	93.02	1.33	1 - 2 logs
1,2-Dibromoethane	6	1000	-3.21	10.08	Membrane Accumulation
	6	3500	-6.94	5.06	Membrane Accumulation
	6	6000	-41.80	5.37	Membrane Accumulation
	7	1000	-3.59	10.03	Membrane Accumulation
	7	3500	1.72	12.31	>0 - 0.5 log
	7	6000	19.78	5.21	>0 - 0.5 log
	8	1000	-27.32	8.60	Membrane Accumulation
	8	3500	4.91	7.14	>0 - 0.5 log
	8	6000	-12.61	9.01	Membrane Accumulation

13l. Effect of feedwater matrix variations on organic compound rejection.

Measured Results for TFC-HR					
		Salinity	Percent Rejection		Log Removal
Compound	pH	(ppm NaCl)	Average	Std Dev	Range
1,2-Dichlorobenzene	6	1000	98.68	0.28	1 - 2 logs
	6	3500	99.63	0.27	2 - 3 logs
	6	6000	98.03	0.54	1 - 2 logs
	7	1000	99.01	0.28	2 - 3 logs
	7	3500	99.77	0.48	2 - 3 logs
	7	6000	99.83	0.07	2 - 3 logs
	8	1000	97.63	0.80	1 - 2 logs
	8	3500	99.78	0.08	2 - 3 logs
	8	6000	99.16	0.41	2 - 3 logs
1,2-Dichloroethane	6	1000	-23.94	10.96	Membrane Accumulation
	6	3500	-44.92	6.42	Membrane Accumulation
	6	6000	-62.61	5.34	Membrane Accumulation
	7	1000	-27.71	3.17	Membrane Accumulation
	7	3500	-50.73	4.13	Membrane Accumulation
	7	6000	-34.59	1.41	Membrane Accumulation
	8	1000	-38.83	4.64	Membrane Accumulation
	8	3500	-30.06	4.15	Membrane Accumulation
	8	6000	-40.26	3.22	Membrane Accumulation
1,2-Dichloropropane	6	1000	48.67	4.63	>0 - 0.5 log
	6	3500	54.18	2.23	>0 - 0.5 log
	6	6000	34.79	5.25	>0 - 0.5 log
	7	1000	51.91	5.19	>0 - 0.5 log
	7	3500	59.80	7.63	>0 - 0.5 log
	7	6000	66.31	1.12	>0 - 0.5 log
	8	1000	38.98	7.38	>0 - 0.5 log
	8	3500	59.35	2.29	>0 - 0.5 log
	8	6000	48.28	4.98	>0 - 0.5 log
1,3,5-Trimethylbenzene	6	1000	99.68	0.07	2 - 3 logs
	6	3500	99.91	0.00	3 - 4 logs
	6	6000	99.62	0.15	2 - 3 logs
	7	1000	99.68	0.09	2 - 3 logs
	7	3500	99.95	0.09	3 - 4 logs
	7	6000	99.96	0.00	3 - 4 logs
	8	1000	99.39	0.23	2 - 3 logs
	8	3500	99.96	0.02	3 - 4 logs
	8	6000	99.86	0.28	2 - 3 logs
1,3-Dichlorobenzene	6	1000	99.61	0.07	2 - 3 logs
	6	3500	99.90	0.07	2 - 3 logs
	6	6000	99.35	0.20	2 - 3 logs
	7	1000	99.74	0.11	2 - 3 logs
	7	3500	99.95	0.13	3 - 4 logs
	7	6000	99.95	0.05	3 - 4 logs
	8	1000	99.22	0.28	2 - 3 logs
	8	3500	99.96	0.03	3 - 4 logs
	8	6000	99.78	0.47	2 - 3 logs
1,3-Dichloropropane	6	1000	26.34	6.55	>0 - 0.5 log
	6	3500	33.66	2.07	>0 - 0.5 log
	6	6000	-7.54	7.77	Membrane Accumulation
	7	1000	26.64	8.33	>0 - 0.5 log
	7	3500	37.00	10.70	>0 - 0.5 log
	7	6000	48.80	3.34	>0 - 0.5 log
	8	1000	13.34	7.26	>0 - 0.5 log
	8	3500	36.43	3.94	>0 - 0.5 log
	8	6000	17.88	9.43	>0 - 0.5 log

13m. Effect of feedwater matrix variations on organic compound rejection.

Measured Results for TFC-HR					
		Salinity	Percent Rejection		Log Removal
Compound	pH	(ppm NaCl)	Average	Std Dev	Range
1,4-Dichlorobenzene	6	1000	99.50	0.06	2 - 3 logs
	6	3500	99.86	0.12	2 - 3 logs
	6	6000	99.31	0.25	2 - 3 logs
	7	1000	99.71	0.07	2 - 3 logs
	7	3500	99.90	0.11	2 - 3 logs
	7	6000	99.95	0.05	3 - 4 logs
	8	1000	99.08	0.33	2 - 3 logs
	8	3500	99.92	0.02	3 - 4 logs
	8	6000	99.79	0.37	2 - 3 logs
2-Chlorotoluene	6	1000	97.97	0.51	1 - 2 logs
	6	3500	99.62	0.29	2 - 3 logs
	6	6000	97.03	0.76	1 - 2 logs
	7	1000	98.45	0.46	1 - 2 logs
	7	3500	99.81	0.70	2 - 3 logs
	7	6000	99.87	0.08	2 - 3 logs
	8	1000	96.80	1.11	1 - 2 logs
	8	3500	99.85	0.09	2 - 3 logs
	8	6000	99.08	0.48	2 - 3 logs
4-Chlorotoluene	6	1000	99.28	0.18	2 - 3 logs
	6	3500	100.00	0.18	>4 logs
	6	6000	98.99	0.34	1 - 2 logs
	7	1000	99.53	0.15	2 - 3 logs
	7	3500	99.95	0.18	3 - 4 logs
	7	6000	99.95	0.02	3 - 4 logs
	8	1000	98.66	0.52	1 - 2 logs
	8	3500	99.96	0.02	3 - 4 logs
	8	6000	99.74	0.35	2 - 3 logs
4-Isopropyltoluene	6	1000	99.82	0.00	2 - 3 logs
	6	3500	99.95	0.03	3 - 4 logs
	6	6000	99.81	0.10	2 - 3 logs
	7	1000	99.80	0.08	2 - 3 logs
	7	3500	100.00	0.04	>4 logs
	7	6000	100.00	0.02	>4 logs
	8	1000	99.58	0.19	2 - 3 logs
	8	3500	100.00	0.02	>4 logs
	8	6000	99.95	0.28	3 - 4 logs
Benzene	6	1000	12.82	4.09	>0 - 0.5 log
	6	3500	28.83	3.93	>0 - 0.5 log
	6	6000	36.23	3.12	>0 - 0.5 log
	7	1000	13.27	8.46	>0 - 0.5 log
	7	3500	34.51	9.64	>0 - 0.5 log
	7	6000	48.00	2.71	>0 - 0.5 log
	8	1000	11.58	7.92	>0 - 0.5 log
	8	3500	40.55	4.77	>0 - 0.5 log
	8	6000	12.12	8.94	>0 - 0.5 log
Bromobenzene	6	1000	95.53	1.07	1 - 2 logs
	6	3500	99.05	0.89	2 - 3 logs
	6	6000	93.51	1.38	1 - 2 logs
	7	1000	96.65	0.92	1 - 2 logs
	7	3500	99.31	1.43	2 - 3 logs
	7	6000	99.52	0.23	2 - 3 logs
	8	1000	92.55	2.41	1 - 2 logs
	8	3500	99.42	0.21	2 - 3 logs
	8	6000	97.25	0.92	1 - 2 logs

13n. Effect of feedwater matrix variations on organic compound rejection.

Measured Results for TFC-HR					
		Salinity	Percent Rejection		Log Removal
Compound	pH	(ppm NaCl)	Average	Std Dev	Range
Bromochloromethane	6	1000	-24.96	14.57	Membrane Accumulation
	6	3500	-53.13	8.36	Membrane Accumulation
	6	6000	-66.13	4.96	Membrane Accumulation
	7	1000	-46.91	4.27	Membrane Accumulation
	7	3500	-73.00	6.43	Membrane Accumulation
	7	6000	-43.68	4.80	Membrane Accumulation
	8	1000	-48.82	5.74	Membrane Accumulation
	8	3500	-38.76	1.73	Membrane Accumulation
	8	6000	-58.48	2.16	Membrane Accumulation
Bromodichloromethane	6	1000	11.15	7.33	>0 - 0.5 log
	6	3500	4.90	7.47	>0 - 0.5 log
	6	6000	-11.48	6.32	Membrane Accumulation
	7	1000	13.51	8.80	>0 - 0.5 log
	7	3500	17.07	9.41	>0 - 0.5 log
	7	6000	32.38	2.99	>0 - 0.5 log
	8	1000	-11.20	8.39	Membrane Accumulation
	8	3500	23.54	4.69	>0 - 0.5 log
	8	6000	4.19	6.67	>0 - 0.5 log
Bromoform	6	1000	65.58	4.85	>0 - 0.5 log
	6	3500	71.86	0.95	0.5 - 1 log
	6	6000	52.77	4.31	>0 - 0.5 log
	7	1000	69.96	4.56	0.5 - 1 log
	7	3500	79.05	7.56	0.5 - 1 log
	7	6000	83.11	1.49	0.5 - 1 log
	8	1000	52.62	7.45	>0 - 0.5 log
	8	3500	77.75	1.36	0.5 - 1 log
	8	6000	68.32	5.22	0.5 - 1 log
Bromomethane	6	1000	-24.20	10.10	Membrane Accumulation
	6	3500	-65.38	12.96	Membrane Accumulation
	6	6000	-73.23	3.74	Membrane Accumulation
	7	1000	-26.84	6.88	Membrane Accumulation
	7	3500	-87.94	6.10	Membrane Accumulation
	7	6000	-47.11	3.50	Membrane Accumulation
	8	1000	-41.02	5.66	Membrane Accumulation
	8	3500	-21.08	4.89	Membrane Accumulation
	8	6000	-57.17	3.35	Membrane Accumulation
Carbon tetrachloride	6	1000	93.58	0.71	1 - 2 logs
	6	3500	95.56	0.40	1 - 2 logs
	6	6000	91.74	0.53	1 - 2 logs
	7	1000	93.86	1.06	1 - 2 logs
	7	3500	94.99	0.76	1 - 2 logs
	7	6000	97.29	0.61	1 - 2 logs
	8	1000	91.60	1.72	1 - 2 logs
	8	3500	95.34	0.35	1 - 2 logs
	8	6000	94.68	0.68	1 - 2 logs
Chlorobenzene	6	1000	83.52	4.74	0.5 - 1 log
	6	3500	94.30	1.17	1 - 2 logs
	6	6000	70.63	9.21	0.5 - 1 log
	7	1000	86.41	3.10	0.5 - 1 log
	7	3500	95.46	3.17	1 - 2 logs
	7	6000	93.97	1.52	1 - 2 logs
	8	1000	78.16	6.45	0.5 - 1 log
	8	3500	96.12	0.51	1 - 2 logs
	8	6000	85.63	4.10	0.5 - 1 log

13o. Effect of feedwater matrix variations on organic compound rejection.

Measured Results for TFC-HR					
		Salinity	Percent Rejection		Log Removal
Compound	pH	(ppm NaCl)	Average	Std Dev	Range
Chloroethane	6	1000	-8.34	8.90	Membrane Accumulation
	6	3500	-21.86	7.71	Membrane Accumulation
	6	6000	-61.86	4.15	Membrane Accumulation
	7	1000	-12.33	4.33	Membrane Accumulation
	7	3500	-31.56	1.61	Membrane Accumulation
	7	6000	-20.43	2.27	Membrane Accumulation
	8	1000	-14.57	4.61	Membrane Accumulation
	8	3500	-5.92	2.87	Membrane Accumulation
	8	6000	-35.91	1.25	Membrane Accumulation
Chloroform	6	1000	8.71	4.73	>0 - 0.5 log
	6	3500	-16.27	8.69	Membrane Accumulation
	6	6000	-17.52	3.48	Membrane Accumulation
	7	1000	-3.62	6.46	Membrane Accumulation
	7	3500	-11.07	2.77	Membrane Accumulation
	7	6000	8.80	1.50	>0 - 0.5 log
	8	1000	-15.81	6.13	Membrane Accumulation
	8	3500	3.14	4.96	>0 - 0.5 log
	8	6000	-14.49	3.28	Membrane Accumulation
Chloromethane	6	1000	-12.78	5.57	Membrane Accumulation
	6	3500	-35.73	8.76	Membrane Accumulation
	6	6000	-73.88	4.77	Membrane Accumulation
	7	1000	-22.72	5.54	Membrane Accumulation
	7	3500	-64.60	7.13	Membrane Accumulation
	7	6000	-33.23	1.59	Membrane Accumulation
	8	1000	-29.44	7.16	Membrane Accumulation
	8	3500	-9.63	6.71	Membrane Accumulation
	8	6000	-56.27	2.75	Membrane Accumulation
Cis-1,3-Dichloropropene	6	1000	-45.58	8.29	Membrane Accumulation
	6	3500	-2.33	7.50	Membrane Accumulation
	6	6000	-18.67	6.92	Membrane Accumulation
	7	1000	3.64	10.95	>0 - 0.5 log
	7	3500	15.87	14.15	>0 - 0.5 log
	7	6000	28.92	6.09	>0 - 0.5 log
	8	1000	3.29	7.13	>0 - 0.5 log
	8	3500	19.86	6.44	>0 - 0.5 log
	8	6000	-11.54	9.67	Membrane Accumulation
Dibromochloromethane	6	1000	43.39	6.05	>0 - 0.5 log
	6	3500	43.82	3.42	>0 - 0.5 log
	6	6000	22.33	5.79	>0 - 0.5 log
	7	1000	46.44	7.22	>0 - 0.5 log
	7	3500	55.89	11.26	>0 - 0.5 log
	7	6000	64.17	2.34	>0 - 0.5 log
	8	1000	24.23	8.61	>0 - 0.5 log
	8	3500	57.28	2.64	>0 - 0.5 log
	8	6000	41.16	7.13	>0 - 0.5 log
Dibromomethane	6	1000	-32.49	15.72	Membrane Accumulation
	6	3500	-84.40	16.93	Membrane Accumulation
	6	6000	-78.34	4.40	Membrane Accumulation
	7	1000	-35.85	4.34	Membrane Accumulation
	7	3500	-66.45	4.55	Membrane Accumulation
	7	6000	-51.08	3.46	Membrane Accumulation
	8	1000	-56.31	4.34	Membrane Accumulation
	8	3500	-45.10	2.96	Membrane Accumulation
	8	6000	-54.57	2.39	Membrane Accumulation

13p. Effect of feedwater matrix variations on organic compound rejection.

Measured Results for TFC-HR					
		Salinity	Percent Rejection		Log Removal
Compound	pH	(ppm NaCl)	Average	Std Dev	Range
Dichlorodifluoromethane	6	1000	31.03	4.55	>0 - 0.5 log
	6	3500	51.92	0.60	>0 - 0.5 log
	6	6000	3.47	6.70	>0 - 0.5 log
	7	1000	44.06	2.62	>0 - 0.5 log
	7	3500	42.50	1.72	>0 - 0.5 log
	7	6000	49.87	2.24	>0 - 0.5 log
	8	1000	55.62	2.75	>0 - 0.5 log
	8	3500	52.72	1.38	>0 - 0.5 log
	8	6000	30.61	4.62	>0 - 0.5 log
Ethylbenzene	6	1000	92.59	2.30	1 - 2 logs
	6	3500	98.60	0.31	1 - 2 logs
	6	6000	90.42	2.99	1 - 2 logs
	7	1000	92.76	2.03	1 - 2 logs
	7	3500	99.26	1.27	2 - 3 logs
	7	6000	98.84	0.37	1 - 2 logs
	8	1000	93.26	2.04	1 - 2 logs
	8	3500	99.26	0.12	2 - 3 logs
	8	6000	96.19	1.39	1 - 2 logs
Hexachlorobutadiene	6	1000	97.01	0.42	1 - 2 logs
	6	3500	99.51	0.12	2 - 3 logs
	6	6000	99.21	0.11	2 - 3 logs
	7	1000	98.57	0.31	1 - 2 logs
	7	3500	99.57	0.08	2 - 3 logs
	7	6000	99.32	0.10	2 - 3 logs
	8	1000	99.06	0.31	2 - 3 logs
	8	3500	99.68	0.06	2 - 3 logs
	8	6000	99.22	0.32	2 - 3 logs
Isopropylbenzene	6	1000	98.62	0.25	1 - 2 logs
	6	3500	99.67	0.14	2 - 3 logs
	6	6000	98.07	0.53	1 - 2 logs
	7	1000	98.31	0.42	1 - 2 logs
	7	3500	99.77	0.45	2 - 3 logs
	7	6000	99.87	0.06	2 - 3 logs
	8	1000	97.92	0.70	1 - 2 logs
	8	3500	99.78	0.05	2 - 3 logs
	8	6000	99.26	0.43	2 - 3 logs
Methylene chloride	6	1000	-248.30	29.63	Membrane Accumulation
	6	3500	-53.74	5.43	Membrane Accumulation
	6	6000	38.11	3.00	>0 - 0.5 log
	7	1000	-37.80	11.60	Membrane Accumulation
	7	3500	-50.52	3.64	Membrane Accumulation
	7	6000	-36.55	3.29	Membrane Accumulation
	8	1000	-210.95	19.25	Membrane Accumulation
	8	3500	-31.64	4.87	Membrane Accumulation
	8	6000	-42.44	3.41	Membrane Accumulation
M-Xylene	6	1000	87.87	4.28	0.5 - 1 log
	6	3500	97.81	0.40	1 - 2 logs
	6	6000	87.12	5.21	0.5 - 1 log
	7	1000	87.96	3.75	0.5 - 1 log
	7	3500	98.48	1.26	1 - 2 logs
	7	6000	97.64	0.91	1 - 2 logs
	8	1000	91.75	2.59	1 - 2 logs
	8	3500	98.32	0.25	1 - 2 logs
	8	6000	94.75	1.91	1 - 2 logs

13q. Effect of feedwater matrix variations on organic compound rejection.

Measured Results for TFC-HR					
		Salinity	Percent Rejection		Log Removal
Compound	pH	(ppm NaCl)	Average	Std Dev	Range
Naphthalene	6	1000	98.93	0.14	1 - 2 logs
	6	3500	99.46	0.09	2 - 3 logs
	6	6000	98.38	0.68	1 - 2 logs
	7	1000	99.02	0.20	2 - 3 logs
	7	3500	99.82	0.21	2 - 3 logs
	7	6000	99.89	0.05	2 - 3 logs
	8	1000	98.06	0.65	1 - 2 logs
	8	3500	99.83	0.06	2 - 3 logs
	8	6000	99.70	0.07	2 - 3 logs
N-Butylbenzene	6	1000	100.00	0.06	>4 logs
	6	3500	99.90	0.03	2 - 3 logs
	6	6000	99.95	0.03	3 - 4 logs
	7	1000	99.94	0.00	3 - 4 logs
	7	3500	99.95	0.03	3 - 4 logs
	7	6000	99.95	0.00	3 - 4 logs
	8	1000	99.86	0.05	2 - 3 logs
	8	3500	99.96	0.00	3 - 4 logs
	8	6000	99.95	0.17	3 - 4 logs
N-Propylbenzene	6	1000	99.71	0.07	2 - 3 logs
	6	3500	99.95	0.03	3 - 4 logs
	6	6000	99.67	0.12	2 - 3 logs
	7	1000	99.74	0.08	2 - 3 logs
	7	3500	100.00	0.06	>4 logs
	7	6000	100.00	0.03	>4 logs
	8	1000	99.54	0.18	2 - 3 logs
	8	3500	100.00	0.02	>4 logs
	8	6000	99.90	0.25	2 - 3 logs
O-Xylene	6	1000	88.92	3.05	0.5 - 1 log
	6	3500	94.73	0.69	1 - 2 logs
	6	6000	83.29	5.00	0.5 - 1 log
	7	1000	86.36	3.58	0.5 - 1 log
	7	3500	95.88	3.00	1 - 2 logs
	7	6000	96.33	0.84	1 - 2 logs
	8	1000	85.99	3.26	0.5 - 1 log
	8	3500	95.70	0.34	1 - 2 logs
	8	6000	90.64	2.90	1 - 2 logs
Sec-Butylbenzene	6	1000	99.69	0.00	2 - 3 logs
	6	3500	99.95	0.03	3 - 4 logs
	6	6000	99.68	0.16	2 - 3 logs
	7	1000	99.70	0.09	2 - 3 logs
	7	3500	99.96	0.07	3 - 4 logs
	7	6000	100.00	0.02	>4 logs
	8	1000	99.47	0.21	2 - 3 logs
	8	3500	99.96	0.02	3 - 4 logs
	8	6000	99.90	0.40	2 - 3 logs
Styrene	6	1000	96.25	0.98	1 - 2 logs
	6	3500	99.53	0.35	2 - 3 logs
	6	6000	95.61	1.22	1 - 2 logs
	7	1000	97.84	0.70	1 - 2 logs
	7	3500	99.72	1.20	2 - 3 logs
	7	6000	99.82	0.12	2 - 3 logs
	8	1000	93.91	2.21	1 - 2 logs
	8	3500	99.74	0.11	2 - 3 logs
	8	6000	98.75	0.45	1 - 2 logs

13r. Effect of feedwater matrix variations on organic compound rejection.

Measured Results for TFC-HR					
		Salinity	Percent Rejection		Log Removal
Compound	pH	(ppm NaCl)	Average	Std Dev	Range
T-Butylbenzene	6	1000	99.23	0.20	2 - 3 logs
	6	3500	99.79	0.03	2 - 3 logs
	6	6000	99.31	0.25	2 - 3 logs
	7	1000	99.25	0.13	2 - 3 logs
	7	3500	99.89	0.13	2 - 3 logs
	7	6000	99.95	0.05	3 - 4 logs
	8	1000	99.23	0.27	2 - 3 logs
	8	3500	99.92	0.06	3 - 4 logs
	8	6000	99.78	0.39	2 - 3 logs
Tetrachloroethene	6	1000	95.59	1.10	1 - 2 logs
	6	3500	99.03	0.51	2 - 3 logs
	6	6000	94.93	0.93	1 - 2 logs
	7	1000	97.19	0.75	1 - 2 logs
	7	3500	99.33	1.01	2 - 3 logs
	7	6000	99.49	0.19	2 - 3 logs
	8	1000	94.75	1.64	1 - 2 logs
	8	3500	99.40	0.17	2 - 3 logs
	8	6000	97.35	0.82	1 - 2 logs
Toluene	6	1000	80.54	3.93	0.5 - 1 log
	6	3500	91.01	2.34	1 - 2 logs
	6	6000	71.30	4.05	0.5 - 1 log
	7	1000	86.51	2.93	0.5 - 1 log
	7	3500	92.57	5.79	1 - 2 logs
	7	6000	94.56	1.10	1 - 2 logs
	8	1000	72.41	6.83	0.5 - 1 log
	8	3500	93.26	0.95	1 - 2 logs
	8	6000	81.22	5.08	0.5 - 1 log
Trichloroethene	6	1000	35.64	10.07	>0 - 0.5 log
	6	3500	64.76	2.16	>0 - 0.5 log
	6	6000	37.59	5.52	>0 - 0.5 log
	7	1000	54.30	6.45	>0 - 0.5 log
	7	3500	70.14	8.62	0.5 - 1 log
	7	6000	78.35	3.74	0.5 - 1 log
	8	1000	35.90	9.87	>0 - 0.5 log
	8	3500	74.11	3.66	0.5 - 1 log
	8	6000	46.08	10.16	>0 - 0.5 log
Trichlorofluoromethane	6	1000	68.18	3.68	>0 - 0.5 log
	6	3500	79.47	0.08	0.5 - 1 log
	6	6000	64.74	3.26	>0 - 0.5 log
	7	1000	71.42	3.28	0.5 - 1 log
	7	3500	77.60	2.36	0.5 - 1 log
	7	6000	82.36	0.34	0.5 - 1 log
	8	1000	75.26	3.25	0.5 - 1 log
	8	3500	80.83	0.98	0.5 - 1 log
	8	6000	68.91	3.24	0.5 - 1 log
Vinylchloride	6	1000	-19.94	8.49	Membrane Accumulation
	6	3500	-19.37	7.87	Membrane Accumulation
	6	6000	-68.12	6.92	Membrane Accumulation
	7	1000	-17.23	4.81	Membrane Accumulation
	7	3500	-53.09	8.35	Membrane Accumulation
	7	6000	-24.38	1.86	Membrane Accumulation
	8	1000	-12.64	5.41	Membrane Accumulation
	8	3500	-5.28	7.03	Membrane Accumulation
	8	6000	-57.42	3.58	Membrane Accumulation

13s. Effect of feedwater matrix variations on organic compound rejection.

Measured Results for TFC-ULP					
		Salinity	Percent Rejection		Log Removal
Compound	pH	(ppm NaCl)	Average	Std Dev	Range
1,1,1,2-Tetrachloroethane	6	1000	87.97	1.13	0.5 - 1 log
	6	3500	86.31	4.27	0.5 - 1 log
	6	6000	83.95	0.41	0.5 - 1 log
	7	1000	85.69	0.17	0.5 - 1 log
	7	3500	84.14	1.49	0.5 - 1 log
	7	6000	89.26	1.09	0.5 - 1 log
	8	1000	86.77	0.56	0.5 - 1 log
	8	3500	84.99	1.16	0.5 - 1 log
	8	6000	83.17	2.38	0.5 - 1 log
1,1,1-Trichloroethane	6	1000	86.95	0.23	0.5 - 1 log
	6	3500	84.56	4.26	0.5 - 1 log
	6	6000	81.34	1.25	0.5 - 1 log
	7	1000	84.14	0.19	0.5 - 1 log
	7	3500	82.80	2.27	0.5 - 1 log
	7	6000	88.74	1.16	0.5 - 1 log
	8	1000	85.24	1.08	0.5 - 1 log
	8	3500	82.85	0.86	0.5 - 1 log
	8	6000	80.95	3.21	0.5 - 1 log
1,1,2,2-Tetrachloroethane	6	1000	74.78	2.11	0.5 - 1 log
	6	3500	76.52	6.44	0.5 - 1 log
	6	6000	71.06	1.54	0.5 - 1 log
	7	1000	76.45	0.44	0.5 - 1 log
	7	3500	71.64	1.45	0.5 - 1 log
	7	6000	77.14	1.56	0.5 - 1 log
	8	1000	75.31	0.88	0.5 - 1 log
	8	3500	71.43	1.85	0.5 - 1 log
	8	6000	71.09	2.81	0.5 - 1 log
1,1,2-Trichloroethane	6	1000	-0.09	7.72	Membrane Accumulation
	6	3500	34.29	8.85	>0 - 0.5 log
	6	6000	23.65	4.18	>0 - 0.5 log
	7	1000	32.08	0.86	>0 - 0.5 log
	7	3500	22.32	3.40	>0 - 0.5 log
	7	6000	31.71	4.44	>0 - 0.5 log
	8	1000	31.84	3.08	>0 - 0.5 log
	8	3500	22.86	4.36	>0 - 0.5 log
	8	6000	16.99	7.77	>0 - 0.5 log
1,1-Dichloroethane	6	1000	7.50	4.85	>0 - 0.5 log
	6	3500	2.70	7.11	>0 - 0.5 log
	6	6000	-26.90	1.25	Membrane Accumulation
	7	1000	-14.00	2.71	Membrane Accumulation
	7	3500	-15.70	10.68	Membrane Accumulation
	7	6000	4.33	2.32	>0 - 0.5 log
	8	1000	3.12	1.37	>0 - 0.5 log
	8	3500	-1.65	2.77	Membrane Accumulation
	8	6000	-25.09	17.94	Membrane Accumulation
1,1-Dichloroethene	6	1000	-18.66	9.38	Membrane Accumulation
	6	3500	-15.00	9.71	Membrane Accumulation
	6	6000	-55.16	8.65	Membrane Accumulation
	7	1000	-21.47	2.14	Membrane Accumulation
	7	3500	-34.00	20.16	Membrane Accumulation
	7	6000	-17.82	5.87	Membrane Accumulation
	8	1000	-16.01	3.86	Membrane Accumulation
	8	3500	-22.67	3.96	Membrane Accumulation
	8	6000	-65.74	28.08	Membrane Accumulation

13t. Effect of feedwater matrix variations on organic compound rejection.

Measured Results for TFC-ULP					
		Salinity	Percent Rejection		Log Removal
Compound	pH	(ppm NaCl)	Average	Std Dev	Range
1,2,3-Trichlorobenzene	6	1000	99.32	0.31	2 - 3 logs
	6	3500	99.68	0.04	2 - 3 logs
	6	6000	99.70	0.06	2 - 3 logs
	7	1000	99.45	0.14	2 - 3 logs
	7	3500	99.56	0.04	2 - 3 logs
	7	6000	99.70	0.05	2 - 3 logs
	8	1000	99.60	0.07	2 - 3 logs
	8	3500	99.61	0.24	2 - 3 logs
	8	6000	99.39	0.17	2 - 3 logs
1,2,3-Trichloropropane	6	1000	67.24	2.69	>0 - 0.5 log
	6	3500	71.36	6.97	0.5 - 1 log
	6	6000	64.51	1.89	>0 - 0.5 log
	7	1000	69.44	0.46	0.5 - 1 log
	7	3500	65.71	1.23	>0 - 0.5 log
	7	6000	70.17	1.93	0.5 - 1 log
	8	1000	69.47	1.45	0.5 - 1 log
	8	3500	63.64	3.08	>0 - 0.5 log
	8	6000	61.83	3.97	>0 - 0.5 log
1,2,4-Trichlorobenzene	6	1000	99.75	0.09	2 - 3 logs
	6	3500	99.84	0.03	2 - 3 logs
	6	6000	99.87	0.02	2 - 3 logs
	7	1000	99.72	0.08	2 - 3 logs
	7	3500	99.83	0.00	2 - 3 logs
	7	6000	99.88	0.02	2 - 3 logs
	8	1000	99.82	0.02	2 - 3 logs
	8	3500	99.83	0.06	2 - 3 logs
	8	6000	99.77	0.03	2 - 3 logs
1,2,4-Trimethylbenzene	6	1000	97.72	1.03	1 - 2 logs
	6	3500	99.51	0.20	2 - 3 logs
	6	6000	99.39	0.30	2 - 3 logs
	7	1000	98.42	0.52	2 - 3 logs
	7	3500	98.75	0.28	2 - 3 logs
	7	6000	99.40	0.19	2 - 3 logs
	8	1000	98.95	0.28	1 - 2 logs
	8	3500	98.85	0.74	1 - 2 logs
	8	6000	98.16	0.66	1 - 2 logs
1,2-Dibromo-3-chloropropane	6	1000	80.97	2.26	0.5 - 1 log
	6	3500	85.59	4.01	0.5 - 1 log
	6	6000	84.97	1.47	0.5 - 1 log
	7	1000	83.76	0.51	0.5 - 1 log
	7	3500	83.35	0.80	0.5 - 1 log
	7	6000	85.81	1.14	0.5 - 1 log
	8	1000	84.35	1.10	0.5 - 1 log
	8	3500	83.06	2.26	0.5 - 1 log
	8	6000	81.90	2.44	0.5 - 1 log
1,2-Dibromoethane	6	1000	1.13	7.88	>0 - 0.5 log
	6	3500	10.27	8.22	>0 - 0.5 log
	6	6000	-4.07	7.05	Membrane Accumulation
	7	1000	4.16	2.58	>0 - 0.5 log
	7	3500	-13.42	6.97	Membrane Accumulation
	7	6000	-1.33	6.47	Membrane Accumulation
	8	1000	10.95	5.53	>0 - 0.5 log
	8	3500	-8.23	5.64	Membrane Accumulation
	8	6000	-17.41	11.49	Membrane Accumulation

13u. Effect of feedwater matrix variations on organic compound rejection.

Measured Results for TFC-ULP					
		Salinity	Percent Rejection		Log Removal
Compound	pH	(ppm NaCl)	Average	Std Dev	Range
1,2-Dichlorobenzene	6	1000	96.92	0.98	1 - 2 logs
	6	3500	98.84	0.40	1 - 2 logs
	6	6000	98.73	0.23	1 - 2 logs
	7	1000	98.44	0.47	1 - 2 logs
	7	3500	97.48	0.32	1 - 2 logs
	7	6000	98.46	0.52	1 - 2 logs
	8	1000	98.18	0.66	1 - 2 logs
	8	3500	97.81	1.27	1 - 2 logs
	8	6000	96.45	1.22	1 - 2 logs
1,2-Dichloroethane	6	1000	-31.96	4.54	Membrane Accumulation
	6	3500	-43.66	3.59	Membrane Accumulation
	6	6000	-66.23	3.64	Membrane Accumulation
	7	1000	-42.96	2.23	Membrane Accumulation
	7	3500	-60.08	4.07	Membrane Accumulation
	7	6000	-33.23	4.20	Membrane Accumulation
	8	1000	-35.87	3.63	Membrane Accumulation
	8	3500	-36.65	2.59	Membrane Accumulation
	8	6000	-53.92	10.89	Membrane Accumulation
1,2-Dichloropropane	6	1000	32.42	3.34	>0 - 0.5 log
	6	3500	37.06	8.37	>0 - 0.5 log
	6	6000	26.78	3.00	>0 - 0.5 log
	7	1000	30.40	0.83	>0 - 0.5 log
	7	3500	25.49	5.54	>0 - 0.5 log
	7	6000	40.32	4.15	>0 - 0.5 log
	8	1000	38.30	3.26	>0 - 0.5 log
	8	3500	27.67	4.13	>0 - 0.5 log
	8	6000	20.58	9.79	>0 - 0.5 log
1,3,5-Trimethylbenzene	6	1000	98.97	0.57	1 - 2 logs
	6	3500	99.77	0.10	2 - 3 logs
	6	6000	99.81	0.17	2 - 3 logs
	7	1000	99.19	0.33	2 - 3 logs
	7	3500	99.50	0.12	2 - 3 logs
	7	6000	99.76	0.07	2 - 3 logs
	8	1000	99.56	0.11	2 - 3 logs
	8	3500	99.42	0.36	2 - 3 logs
	8	6000	99.22	0.26	2 - 3 logs
1,3-Dichlorobenzene	6	1000	98.75	0.46	1 - 2 logs
	6	3500	99.61	0.15	2 - 3 logs
	6	6000	99.58	0.09	2 - 3 logs
	7	1000	99.43	0.21	2 - 3 logs
	7	3500	99.13	0.13	2 - 3 logs
	7	6000	99.48	0.24	2 - 3 logs
	8	1000	99.35	0.28	2 - 3 logs
	8	3500	99.22	0.66	2 - 3 logs
	8	6000	98.38	0.64	1 - 2 logs
1,3-Dichloropropane	6	1000	20.41	6.58	>0 - 0.5 log
	6	3500	30.09	4.04	>0 - 0.5 log
	6	6000	19.42	7.56	>0 - 0.5 log
	7	1000	23.05	1.89	>0 - 0.5 log
	7	3500	8.19	5.55	>0 - 0.5 log
	7	6000	21.39	6.77	>0 - 0.5 log
	8	1000	26.14	3.95	>0 - 0.5 log
	8	3500	13.42	7.02	>0 - 0.5 log
	8	6000	5.02	8.41	>0 - 0.5 log

13v. Effect of feedwater matrix variations on organic compound rejection.

Measured Results for TFC-ULP					
		Salinity	Percent Rejection		Log Removal
Compound	pH	(ppm NaCl)	Average	Std Dev	Range
1,4-Dichlorobenzene	6	1000	98.70	0.56	1 - 2 logs
	6	3500	99.63	0.21	2 - 3 logs
	6	6000	99.58	0.09	2 - 3 logs
	7	1000	99.42	0.19	2 - 3 logs
	7	3500	99.14	0.13	2 - 3 logs
	7	6000	99.48	0.24	2 - 3 logs
	8	1000	99.39	0.29	2 - 3 logs
	8	3500	99.27	0.68	2 - 3 logs
	8	6000	98.41	0.63	1 - 2 logs
2-Chlorotoluene	6	1000	95.16	1.65	1 - 2 logs
	6	3500	98.51	0.54	1 - 2 logs
	6	6000	98.11	0.34	1 - 2 logs
	7	1000	97.30	0.74	1 - 2 logs
	7	3500	96.43	0.69	1 - 2 logs
	7	6000	97.91	0.79	1 - 2 logs
	8	1000	97.64	0.88	1 - 2 logs
	8	3500	96.65	1.79	1 - 2 logs
	8	6000	94.57	2.03	1 - 2 logs
4-Chlorotoluene	6	1000	97.95	0.85	1 - 2 logs
	6	3500	99.55	0.20	2 - 3 logs
	6	6000	99.42	0.14	2 - 3 logs
	7	1000	99.15	0.37	2 - 3 logs
	7	3500	98.68	0.26	1 - 2 logs
	7	6000	99.27	0.40	2 - 3 logs
	8	1000	99.08	0.49	2 - 3 logs
	8	3500	98.85	0.97	1 - 2 logs
	8	6000	97.54	1.05	1 - 2 logs
4-Isopropyltoluene	6	1000	99.46	0.52	2 - 3 logs
	6	3500	99.90	0.02	2 - 3 logs
	6	6000	99.91	0.05	3 - 4 logs
	7	1000	99.60	0.24	2 - 3 logs
	7	3500	99.80	0.03	2 - 3 logs
	7	6000	99.91	0.02	3 - 4 logs
	8	1000	99.81	0.02	2 - 3 logs
	8	3500	99.85	0.24	2 - 3 logs
	8	6000	99.69	0.11	2 - 3 logs
Benzene	6	1000	6.44	4.86	>0 - 0.5 log
	6	3500	25.59	3.61	>0 - 0.5 log
	6	6000	29.24	2.48	>0 - 0.5 log
	7	1000	3.59	1.27	>0 - 0.5 log
	7	3500	7.86	9.74	>0 - 0.5 log
	7	6000	23.42	6.91	>0 - 0.5 log
	8	1000	26.64	3.88	>0 - 0.5 log
	8	3500	12.08	3.66	>0 - 0.5 log
	8	6000	-11.34	17.30	Membrane Accumulation
Bromobenzene	6	1000	91.46	2.60	1 - 2 logs
	6	3500	97.16	0.87	1 - 2 logs
	6	6000	96.30	0.73	1 - 2 logs
	7	1000	95.52	0.95	1 - 2 logs
	7	3500	93.08	1.04	1 - 2 logs
	7	6000	95.26	1.81	1 - 2 logs
	8	1000	95.37	1.86	1 - 2 logs
	8	3500	93.99	2.98	1 - 2 logs
	8	6000	89.58	3.73	0.5 - 1 log

13w. Effect of feedwater matrix variations on organic compound rejection.

Measured Results for TFC-ULP					
		Salinity	Percent Rejection		Log Removal
Compound	pH	(ppm NaCl)	Average	Std Dev	Range
Bromochloromethane	6	1000	-20.50	5.98	Membrane Accumulation
	6	3500	-41.72	8.16	Membrane Accumulation
	6	6000	-68.07	1.44	Membrane Accumulation
	7	1000	-52.85	5.34	Membrane Accumulation
	7	3500	-61.13	6.71	Membrane Accumulation
	7	6000	-31.03	4.91	Membrane Accumulation
	8	1000	-30.83	3.45	Membrane Accumulation
	8	3500	-34.80	2.41	Membrane Accumulation
	8	6000	-59.38	15.30	Membrane Accumulation
Bromodichloromethane	6	1000	6.08	7.21	>0 - 0.5 log
	6	3500	3.45	4.66	>0 - 0.5 log
	6	6000	-3.32	4.51	Membrane Accumulation
	7	1000	-0.39	2.47	Membrane Accumulation
	7	3500	-10.28	7.39	Membrane Accumulation
	7	6000	9.50	5.31	>0 - 0.5 log
	8	1000	6.86	4.43	>0 - 0.5 log
	8	3500	-0.72	4.93	Membrane Accumulation
	8	6000	-18.28	13.95	Membrane Accumulation
Bromoform	6	1000	56.22	4.99	>0 - 0.5 log
	6	3500	62.21	5.40	>0 - 0.5 log
	6	6000	62.18	3.61	>0 - 0.5 log
	7	1000	65.08	1.34	>0 - 0.5 log
	7	3500	52.43	3.47	>0 - 0.5 log
	7	6000	59.68	4.46	>0 - 0.5 log
	8	1000	59.70	3.53	>0 - 0.5 log
	8	3500	53.66	5.99	>0 - 0.5 log
	8	6000	47.03	8.43	>0 - 0.5 log
Bromomethane	6	1000	-9.55	13.46	Membrane Accumulation
	6	3500	-38.12	16.82	Membrane Accumulation
	6	6000	-72.68	5.79	Membrane Accumulation
	7	1000	-25.66	3.75	Membrane Accumulation
	7	3500	-69.39	17.51	Membrane Accumulation
	7	6000	-20.31	6.23	Membrane Accumulation
	8	1000	-16.87	4.27	Membrane Accumulation
	8	3500	-25.65	5.10	Membrane Accumulation
	8	6000	-58.75	29.88	Membrane Accumulation
Carbon tetrachloride	6	1000	87.89	1.21	0.5 - 1 log
	6	3500	85.84	4.18	0.5 - 1 log
	6	6000	83.74	1.04	0.5 - 1 log
	7	1000	87.57	0.56	0.5 - 1 log
	7	3500	84.17	2.61	0.5 - 1 log
	7	6000	89.35	3.03	0.5 - 1 log
	8	1000	86.70	1.76	0.5 - 1 log
	8	3500	83.64	0.49	0.5 - 1 log
	8	6000	88.03	2.71	0.5 - 1 log
Chlorobenzene	6	1000	82.01	4.61	0.5 - 1 log
	6	3500	92.06	7.17	1 - 2 logs
	6	6000	87.58	2.09	0.5 - 1 log
	7	1000	88.68	1.61	0.5 - 1 log
	7	3500	84.33	2.21	0.5 - 1 log
	7	6000	88.31	3.75	0.5 - 1 log
	8	1000	89.27	3.22	0.5 - 1 log
	8	3500	85.65	4.61	0.5 - 1 log
	8	6000	76.12	7.59	0.5 - 1 log

13x. Effect of feedwater matrix variations on organic compound rejection.

Measured Results for TFC-ULP					
		Salinity	Percent Rejection		Log Removal
Compound	pH	(ppm NaCl)	Average	Std Dev	Range
Chloroethane	6	1000	0.92	6.57	>0 - 0.5 log
	6	3500	-7.10	8.60	Membrane Accumulation
	6	6000	-56.84	3.82	Membrane Accumulation
	7	1000	-12.87	1.68	Membrane Accumulation
	7	3500	-26.08	11.12	Membrane Accumulation
	7	6000	-9.04	3.60	Membrane Accumulation
	8	1000	-7.21	1.98	Membrane Accumulation
	8	3500	-14.55	3.42	Membrane Accumulation
	8	6000	-37.79	22.09	Membrane Accumulation
Chloroform	6	1000	2.27	5.01	>0 - 0.5 log
	6	3500	-15.49	4.65	Membrane Accumulation
	6	6000	-31.82	1.03	Membrane Accumulation
	7	1000	-22.86	2.74	Membrane Accumulation
	7	3500	-26.64	5.37	Membrane Accumulation
	7	6000	-3.78	5.23	Membrane Accumulation
	8	1000	-10.27	3.47	Membrane Accumulation
	8	3500	-14.51	0.94	Membrane Accumulation
	8	6000	-33.46	12.70	Membrane Accumulation
Chloromethane	6	1000	4.33	10.06	>0 - 0.5 log
	6	3500	-11.34	14.44	Membrane Accumulation
	6	6000	-59.44	4.59	Membrane Accumulation
	7	1000	-17.63	4.41	Membrane Accumulation
	7	3500	-38.08	14.97	Membrane Accumulation
	7	6000	-13.56	6.14	Membrane Accumulation
	8	1000	-8.08	3.07	Membrane Accumulation
	8	3500	-15.34	2.91	Membrane Accumulation
	8	6000	-56.67	31.83	Membrane Accumulation
Cis-1,3-Dichloropropene	6	1000	-31.07	10.94	Membrane Accumulation
	6	3500	23.54	11.77	>0 - 0.5 log
	6	6000	26.51	6.16	>0 - 0.5 log
	7	1000	18.01	2.40	>0 - 0.5 log
	7	3500	3.15	8.10	>0 - 0.5 log
	7	6000	19.93	6.60	>0 - 0.5 log
	8	1000	40.26	3.68	>0 - 0.5 log
	8	3500	9.10	7.48	>0 - 0.5 log
	8	6000	-10.70	14.81	Membrane Accumulation
Dibromochloromethane	6	1000	34.74	6.15	>0 - 0.5 log
	6	3500	36.86	6.12	>0 - 0.5 log
	6	6000	33.52	4.36	>0 - 0.5 log
	7	1000	39.08	0.94	>0 - 0.5 log
	7	3500	23.68	4.82	>0 - 0.5 log
	7	6000	35.24	6.29	>0 - 0.5 log
	8	1000	37.98	4.60	>0 - 0.5 log
	8	3500	27.85	6.64	>0 - 0.5 log
	8	6000	17.80	10.42	>0 - 0.5 log
Dibromomethane	6	1000	-29.27	5.14	Membrane Accumulation
	6	3500	-69.23	11.15	Membrane Accumulation
	6	6000	-78.38	3.22	Membrane Accumulation
	7	1000	-47.18	3.17	Membrane Accumulation
	7	3500	-66.93	4.92	Membrane Accumulation
	7	6000	-47.65	3.51	Membrane Accumulation
	8	1000	-48.75	4.18	Membrane Accumulation
	8	3500	-47.28	2.10	Membrane Accumulation
	8	6000	-61.63	12.31	Membrane Accumulation

13y. Effect of water matrix variations on organic compound rejection

Measured Results for TFC-ULP					
		Salinity	Percent Rejection		Log Removal
Compound	pH	(ppm NaCl)	Average	Std Dev	Range
Dichlorodifluoromethane	6	1000	20.69	3.99	>0 - 0.5 log
	6	3500	32.53	8.37	>0 - 0.5 log
	6	6000	-14.78	7.63	Membrane Accumulation
	7	1000	34.57	4.70	>0 - 0.5 log
	7	3500	25.50	15.40	>0 - 0.5 log
	7	6000	36.65	4.42	>0 - 0.5 log
	8	1000	38.76	2.87	>0 - 0.5 log
	8	3500	27.02	6.16	>0 - 0.5 log
	8	6000	3.79	16.67	>0 - 0.5 log
Ethylbenzene	6	1000	90.51	2.95	1 - 2 logs
	6	3500	97.45	1.35	1 - 2 logs
	6	6000	96.13	0.65	1 - 2 logs
	7	1000	93.83	1.56	1 - 2 logs
	7	3500	94.88	0.93	1 - 2 logs
	7	6000	96.34	1.29	1 - 2 logs
	8	1000	96.12	1.37	1 - 2 logs
	8	3500	95.32	2.09	1 - 2 logs
	8	6000	91.71	2.99	1 - 2 logs
Hexachlorobutadiene	6	1000	98.39	0.53	1 - 2 logs
	6	3500	99.88	0.42	2 - 3 logs
	6	6000	99.77	0.15	2 - 3 logs
	7	1000	99.52	0.10	2 - 3 logs
	7	3500	99.82	0.04	2 - 3 logs
	7	6000	99.77	0.18	2 - 3 logs
	8	1000	99.88	0.03	2 - 3 logs
	8	3500	99.86	0.07	2 - 3 logs
	8	6000	99.61	0.27	2 - 3 logs
Isopropylbenzene	6	1000	97.12	1.34	1 - 2 logs
	6	3500	98.91	0.36	1 - 2 logs
	6	6000	98.84	0.31	1 - 2 logs
	7	1000	97.34	0.65	1 - 2 logs
	7	3500	98.13	0.41	1 - 2 logs
	7	6000	98.93	0.27	1 - 2 logs
	8	1000	98.57	0.32	1 - 2 logs
	8	3500	98.03	0.83	1 - 2 logs
	8	6000	97.15	0.93	1 - 2 logs
Methylene chloride	6	1000	-227.40	14.66	Membrane Accumulation
	6	3500	-254.69	28.51	Membrane Accumulation
	6	6000	-65.84	13.16	Membrane Accumulation
	7	1000	-50.74	1.99	Membrane Accumulation
	7	3500	-49.42	10.20	Membrane Accumulation
	7	6000	-27.94	9.20	Membrane Accumulation
	8	1000	-247.34	23.61	Membrane Accumulation
	8	3500	-31.20	2.19	Membrane Accumulation
	8	6000	-37.94	12.28	Membrane Accumulation
M-Xylene	6	1000	89.17	3.61	0.5 - 1 log
	6	3500	97.48	3.02	1 - 2 logs
	6	6000	95.97	0.68	1 - 2 logs
	7	1000	92.97	1.65	1 - 2 logs
	7	3500	95.09	0.75	1 - 2 logs
	7	6000	96.47	1.23	1 - 2 logs
	8	1000	96.19	1.30	1 - 2 logs
	8	3500	94.77	2.32	1 - 2 logs
	8	6000	94.20	2.24	1 - 2 logs

13z. Effect of water matrix variations on organic compound rejection

Measured Results for TFC-ULP

Compound	pH	Salinity (ppm NaCl)	Average Percent Rejection	Std Dev	Log Removal Range
Naphthalene	6	1000	96.96	0.96	1 - 2 logs
	6	3500	99.35	0.19	2 - 3 logs
	6	6000	99.38	0.28	2 - 3 logs
	7	1000	98.30	0.40	1 - 2 logs
	7	3500	98.79	0.22	1 - 2 logs
	7	6000	99.36	0.13	2 - 3 logs
	8	1000	98.47	0.45	1 - 2 logs
	8	3500	98.65	0.86	1 - 2 logs
	8	6000	98.56	0.49	1 - 2 logs
N-Butylbenzene	6	1000	99.93	0.06	3 - 4 logs
	6	3500	99.95	0.00	3 - 4 logs
	6	6000	99.95	0.00	3 - 4 logs
	7	1000	99.69	0.10	2 - 3 logs
	7	3500			
	7	6000			

13aa. Effect of water matrix variations on organic compound rejection

Measured Results for TFC-ULP					
		Salinity	Percent Rejection		Log Removal
Compound	pH	(ppm NaCl)	Average	Std Dev	Range
T-Butylbenzene	6	1000	97.62	0.91	1 - 2 logs
	6	3500	98.57	0.55	1 - 2 logs
	6	6000	98.67	0.44	1 - 2 logs
	7	1000	96.83	0.62	1 - 2 logs
	7	3500	98.41	0.55	1 - 2 logs
	7	6000	98.98	0.11	1 - 2 logs
	8	1000	98.52	0.14	1 - 2 logs
	8	3500	98.40	0.69	1 - 2 logs
	8	6000	97.57	0.60	1 - 2 logs
Tetrachloroethene	6	1000	91.72	2.25	1 - 2 logs
	6	3500	97.21	0.76	1 - 2 logs
	6	6000	96.32	0.66	1 - 2 logs
	7	1000	96.02	0.86	1 - 2 logs
	7	3500	94.31	1.14	1 - 2 logs
	7	6000	95.95	1.30	1 - 2 logs
	8	1000	95.87	1.43	1 - 2 logs
	8	3500	94.78	2.24	1 - 2 logs
	8	6000	90.47	3.15	1 - 2 logs
Toluene	6	1000	73.99	5.56	0.5 - 1 log
	6	3500	86.57	2.11	0.5 - 1 log
	6	6000	80.70	2.10	0.5 - 1 log
	7	1000	85.17	1.23	0.5 - 1 log
	7	3500	73.89	4.16	0.5 - 1 log
	7	6000	79.93	4.60	0.5 - 1 log
	8	1000	82.19	3.96	0.5 - 1 log
	8	3500	76.36	5.74	0.5 - 1 log
	8	6000	64.22	9.61	>0 - 0.5 log
Trichloroethene	6	1000	41.40	10.23	>0 - 0.5 log
	6	3500	71.01	4.98	0.5 - 1 log
	6	6000	66.19	4.07	>0 - 0.5 log
	7	1000	62.86	1.29	>0 - 0.5 log
	7	3500	56.34	6.94	>0 - 0.5 log
	7	6000	62.54	7.51	>0 - 0.5 log
	8	1000	67.23	5.73	>0 - 0.5 log
	8	3500	56.15	6.91	>0 - 0.5 log
	8	6000	35.18	14.46	>0 - 0.5 log
Trichlorofluoromethane	6	1000	56.06	3.12	>0 - 0.5 log
	6	3500	63.74	7.18	>0 - 0.5 log
	6	6000	51.26	3.34	>0 - 0.5 log
	7	1000	60.85	0.56	>0 - 0.5 log
	7	3500	56.83	7.95	>0 - 0.5 log
	7	6000	65.47	3.29	>0 - 0.5 log
	8	1000	66.10	2.40	>0 - 0.5 log
	8	3500	58.80	2.31	>0 - 0.5 log
	8	6000	42.37	10.66	>0 - 0.5 log
Vinylchloride	6	1000	-0.86	7.84	Membrane Accumulation
	6	3500	-4.75	10.74	Membrane Accumulation
	6	6000	-53.57	6.58	Membrane Accumulation
	7	1000	-15.54	3.45	Membrane Accumulation
	7	3500	-27.68	19.26	Membrane Accumulation
	7	6000	-7.08	5.91	Membrane Accumulation
	8	1000	-2.96	1.95	Membrane Accumulation
	8	3500	-6.63	2.80	Membrane Accumulation
	8	6000	-56.95	31.31	Membrane Accumulation

Table 14a. Data derived from surface-response analysis showing magnitude of influence of pH and salinity on RO removal of compounds. Magnitude of the difference between minimum and maximum predicted compound removal indicates degree of influence.

Compound	Projected Minimum				Projected Maximum			Log Removal Range	
	Membrane	Log Removal	pH	TDS	Log Removal	pH	TDS	Minimum	Maximum
1,1,1,2-Tetrachloroethane	ESPA-2	1.09	8.00	3234	1.35	6.00	1000.00	1 - 2 logs	1 - 2 logs
	TFC-HR	1.22	6.00	6000	1.40	7.71	6000	1 - 2 logs	1 - 2 logs
	TFC-ULP	NA	NA	NA	NA	NA	NA	NA	NA
1,1,1-Trichloroethane	ESPA-2	1.06	8.00	3054	1.29	6.00	1000.00	1 - 2 logs	1 - 2 logs
	TFC-HR	1.20	6.00	6000	1.29	7.41	6000	1 - 2 logs	1 - 2 logs
	TFC-ULP	0.80	8.00	1000	0.86	6.00	1000	0.5 - 1 log	0.5 - 1 log
1,1,2,2-Tetrachloroethane	ESPA-2	0.78	8.00	3232	1.01	6.00	1000.00	0.5 - 1 log	1 - 2 logs
	TFC-HR	0.81	6.00	6000	1.05	7.91	6000	0.5 - 1 log	1 - 2 logs
	TFC-ULP	NA	NA	NA	NA	NA	NA	NA	NA
1,1,2-Trichloroethane	ESPA-2	0.20	6.00	NA	0.25	7.14	NA	>0 - 0.5 log	>0 - 0.5 log
	TFC-HR	0.19	6.00	6000	0.38	7.48	4872	>0 - 0.5 log	>0 - 0.5 log
	TFC-ULP	0.01	6.00	1000	0.17	7.11	3719	>0 - 0.5 log	>0 - 0.5 log
1,1-Dichloroethane	ESPA-2	0.08	6.00	6000	0.17	6.00	1000.00	>0 - 0.5 log	>0 - 0.5 log
	TFC-HR	0.03	6.00	6000	0.08	8.00	1000	>0 - 0.5 log	>0 - 0.5 log
	TFC-ULP	-0.05	6.00	6000	-0.01	6.00	1000	Memb Accumulation	Memb Accumulation
1,1-Dichloroethene	ESPA-2	-0.10	NA	6000	-0.03	NA	1000.00	Memb Accumulation	Memb Accumulation
	TFC-HR	-0.17	6.00	6000	-0.06	7.92	1793	Memb Accumulation	Memb Accumulation
	TFC-ULP	-0.15	8.00	6000	-0.04	7.17	2717	Memb Accumulation	Memb Accumulation
1,2,3-Trichlorobenzene	ESPA-2	1.87	8.00	NA	2.01	6.00	NA	1 - 2 logs	2 - 3 logs
	TFC-HR	2.31	6.00	6000	2.69	7.29	3728	2 - 3 logs	2 - 3 logs
	TFC-ULP	2.08	6.00	1000	2.55	6.00	6000	2 - 3 logs	2 - 3 logs
1,2,3-Trichloropropane	ESPA-2	0.62	8.00	3185	0.81	6.00	1000.00	0.5 - 1 log	0.5 - 1 log
	TFC-HR	0.64	6.00	6000	0.89	7.83	6000	0.5 - 1 log	0.5 - 1 log
	TFC-ULP	NA	NA	NA	NA	NA	NA	NA	NA
1,2,4-Trichlorobenzene	ESPA-2	2.12	8.00	NA	2.26	6.00	NA	2 - 3 logs	2 - 3 logs
	TFC-HR	NA	NA	NA	NA	NA	NA	NA	NA
	TFC-ULP	2.47	6.00	1000	2.88	6.00	6000	2 - 3 logs	2 - 3 logs
1,2,4-Trimethylbenzene	ESPA-2	1.63	8.00	1000	1.89	6.00	6000.00	1 - 2 logs	1 - 2 logs
	TFC-HR	2.01	6.00	1000	3.02	7.57	4516	2 - 3 logs	3 - 4 logs
	TFC-ULP	1.64	6.00	1000	2.40	6.00	6000	1 - 2 logs	2 - 3 logs
1,2-Dibromo-3-chloropropane	ESPA-2	0.91	8.00	2677	1.10	6.00	1000.00	0.5 - 1 log	1 - 2 logs
	TFC-HR	0.99	6.00	6000	1.35	7.99	6000	0.5 - 1 log	1 - 2 logs
	TFC-ULP	0.76	6.00	1000	0.82	6.00	6000	0.5 - 1 log	0.5 - 1 log

14b. Data derived from surface-response analysis showing magnitude of influence of pH and salinity on RO removal of compounds. Magnitude of the difference between minimum and maximum predicted compound removal indicates degree of influence.

Compound	Projected Minimum				Projected Maximum			Log Removal Range	
	Membrane	Log Removal	pH	TDS	Log Removal	pH	TDS	Minimum	Maximum
1,2-Dibromoethane	ESPA-2	-0.14	6.00	6000	-0.01	6.00	1000.00	Memb Accumulation	Memb Accumulation
	TFC-HR	-0.11	6.00	6000	0.04	6.47	1000	Memb Accumulation	>0 - 0.5 log
	TFC-ULP	-0.04	6.00	6000	0.00	6.00	1000	Memb Accumulation	Memb Accumulation
1,2-Dichlorobenzene	ESPA-2	1.16	8.00	3487	1.39	6.00	6000.00	1 - 2 logs	1 - 2 logs
	TFC-HR	1.88	6.00	6000	2.49	7.37	4318	1 - 2 logs	2 - 3 logs
	TFC-ULP	1.54	6.00	1000	1.96	6.00	6000	1 - 2 logs	1 - 2 logs
1,2-Dichloroethane	ESPA-2	-0.17	6.00	6000	-0.07	6.00	1000.00	Memb Accumulation	Memb Accumulation
	TFC-HR	-0.19	6.00	6000	-0.10	6.00	1000	Memb Accumulation	Memb Accumulation
	TFC-ULP	-0.21	6.00	6000	-0.14	8.00	1000	Memb Accumulation	Memb Accumulation
1,2-Dichloropropane	ESPA-2	0.27	8.00	2726	0.41	6.00	1000.00	>0 - 0.5 log	>0 - 0.5 log
	TFC-HR	0.27	6.00	6000	0.41	7.58	6000	>0 - 0.5 log	>0 - 0.5 log
	TFC-ULP	NA	NA	NA	NA	NA	NA	NA	NA
1,3,5-Trimethylbenzene	ESPA-2	2.06	8.00	1000	2.22	6.00	1000.00	2 - 3 logs	2 - 3 logs
	TFC-HR	2.40	6.00	1000	3.32	7.37	4086	2 - 3 logs	3 - 4 logs
	TFC-ULP	1.89	6.00	1000	2.70	6.00	6000	1 - 2 logs	2 - 3 logs
1,3-Dichlorobenzene	ESPA-2	1.34	8.00	NA	1.54	6.00	NA	1 - 2 logs	1 - 2 logs
	TFC-HR	2.52	NA	1000	2.94	NA	3878	2 - 3 logs	2 - 3 logs
	TFC-ULP	1.96	6.00	1000	2.48	6.00	6000	1 - 2 logs	2 - 3 logs
1,3-Dichloropropane	ESPA-2	0.02	8.00	3158	0.16	6.00	1000.00	>0 - 0.5 log	>0 - 0.5 log
	TFC-HR	0.05	6.00	6000	0.22	7.86	6000	>0 - 0.5 log	>0 - 0.5 log
	TFC-ULP	0.03	8.00	6000	0.10	7.03	1000	>0 - 0.5 log	>0 - 0.5 log
1,4-Dichlorobenzene	ESPA-2	1.19	8.00	NA	1.52	6.00	NA	1 - 2 logs	1 - 2 logs
	TFC-HR	2.32	6.00	NA	2.86	7.35	NA	2 - 3 logs	2 - 3 logs
	TFC-ULP	2.00	6.00	1000	2.58	6.00	6000	1 - 2 logs	2 - 3 logs
2-Chlorotoluene	ESPA-2	1.18	8.00	NA	1.32	6.00	NA	1 - 2 logs	1 - 2 logs
	TFC-HR	1.75	6.00	6000	2.59	7.52	4548	1 - 2 logs	2 - 3 logs
	TFC-ULP	1.34	6.00	1000	1.83	6.00	6000	1 - 2 logs	1 - 2 logs
4-Chlorotoluene	ESPA-2	1.17	8.00	NA	1.36	6.00	NA	1 - 2 logs	1 - 2 logs
	TFC-HR	2.20	6.00	6000	3.13	7.56	6000	2 - 3 logs	3 - 4 logs
	TFC-ULP	1.75	6.00	1000	2.37	6.00	6000	1 - 2 logs	2 - 3 logs
4-Isopropyltoluene	ESPA-2	2.19	7.37	1000	2.59	6.00	6000.00	2 - 3 logs	2 - 3 logs
	TFC-HR	NA	NA	NA	NA	NA	NA	NA	NA
	TFC-ULP	2.18	6.00	1000	3.17	6.00	6000	2 - 3 logs	3 - 4 logs

14c. Data derived from surface-response analysis showing magnitude of influence of pH and salinity on RO removal of compounds. Magnitude of the difference between minimum and maximum predicted compound removal indicates degree of influence.

Compound	Projected Minimum				Projected Maximum			Log Removal Range	
	Membrane	Log Removal	pH	TDS	Log Removal	pH	TDS	Minimum	Maximum
Benzene	ESPA-2	0.12	7.14	2265	0.29	6.00	6000.00	>0 - 0.5 log	>0 - 0.5 log
	TFC-HR	0.08	6.00	1000	0.24	6.00	6000	>0 - 0.5 log	>0 - 0.5 log
	TFC-ULP	0.00	6.00	1000	0.17	6.00	6000	Memb Accumulation	>0 - 0.5 log
Bromobenzene	ESPA-2	0.72	8.00	NA	0.87	6.00	NA	0.5 - 1 log	0.5 - 1 log
	TFC-HR	1.36	6.00	6000	2.07	7.56	4674	1 - 2 logs	2 - 3 logs
	TFC-ULP	1.11	6.00	1000	1.50	6.00	6000	1 - 2 logs	1 - 2 logs
Bromochloromethane	ESPA-2	-0.21	6.00	6000	-0.12	6.00	1000.00	Memb Accumulation	Memb Accumulation
	TFC-HR	-0.21	6.71	5441	-0.12	6.00	1000	Memb Accumulation	Memb Accumulation
	TFC-ULP	-0.21	6.24	6000	-0.14	6.00	1000	Memb Accumulation	Memb Accumulation
Bromodichloromethane	ESPA-2	0.01	6.00	5210	0.12	6.00	1000.00	>0 - 0.5 log	>0 - 0.5 log
	TFC-HR	0.00	6.00	6000	0.11	7.65	6000	Memb Accumulation	>0 - 0.5 log
	TFC-ULP	NA	NA	NA	NA	NA	NA	NA	NA
Bromoform	ESPA-2	0.26	8.00	3245	0.44	6.00	1000.00	>0 - 0.5 log	>0 - 0.5 log
	TFC-HR	0.41	6.00	6000	0.69	7.70	6000	>0 - 0.5 log	0.5 - 1 log
	TFC-ULP	0.30	8.00	6000	0.41	6.61	6000	>0 - 0.5 log	>0 - 0.5 log
Bromomethane	ESPA-2	-0.23	6.00	6000	-0.12	6.00	1000.00	Memb Accumulation	Memb Accumulation
	TFC-HR	-0.23	6.00	6000	-0.11	8.00	1000	Memb Accumulation	Memb Accumulation
	TFC-ULP	-0.22	6.00	6000	-0.10	8.00	1000	Memb Accumulation	Memb Accumulation
Carbon tetrachloride	ESPA-2	1.07	8.00	2588	1.33	6.00	1000.00	1 - 2 logs	1 - 2 logs
	TFC-HR	1.17	6.00	6000	1.39	7.52	6000	1 - 2 logs	1 - 2 logs
	TFC-ULP	NA	NA	NA	NA	NA	NA	NA	NA
Chlorobenzene	ESPA-2	0.39	8.00	NA	0.49	6.00	NA	>0 - 0.5 log	>0 - 0.5 log
	TFC-HR	0.76	6.00	6000	1.36	7.34	3953	0.5 - 1 log	1 - 2 logs
	TFC-ULP	0.69	6.00	1000	0.97	6.61	6000	0.5 - 1 log	0.5 - 1 log
Chloroethane	ESPA-2	-0.16	6.00	6000	0.00	6.00	1000.00	Memb Accumulation	Memb Accumulation
	TFC-HR	-0.17	6.00	6000	-0.03	6.00	1000	Memb Accumulation	Memb Accumulation
	TFC-ULP	-0.14	6.00	6000	-0.03	6.00	1000	Memb Accumulation	Memb Accumulation
Chloroform	ESPA-2	0.00	6.00	5557	0.12	6.00	1000.00	Memb Accumulation	>0 - 0.5 log
	TFC-HR	-0.04	6.00	6000	0.02	6.00	1000	Memb Accumulation	>0 - 0.5 log
	TFC-ULP	-0.10	6.00	6000	-0.04	6.00	1000	Memb Accumulation	Memb Accumulation
Chloromethane	ESPA-2	-0.21	6.00	6000	-0.05	6.00	1000.00	Memb Accumulation	Memb Accumulation
	TFC-HR	-0.20	6.00	6000	-0.07	8.00	1000	Memb Accumulation	Memb Accumulation
	TFC-ULP	-0.13	6.00	6000	-0.05	6.00	1000	Memb Accumulation	Memb Accumulation

14d. Data derived from surface-response analysis showing magnitude of influence of pH and salinity on RO removal of compounds. Magnitude of the difference between minimum and maximum predicted compound removal indicates degree of influence.

Compound	Projected Minimum				Projected Maximum			Log Removal Range	
	Membrane	Log Removal	pH	TDS	Log Removal	pH	TDS	Minimum	Maximum
Cis-1,3-Dichloropropene	ESPA-2	-0.15	6.00	1000	0.04	8.00	1000.00	Memb Accumulation	>0 - 0.5 log
	TFC-HR	-0.10	6.00	1000	0.09	7.76	1000	Memb Accumulation	>0 - 0.5 log
	TFC-ULP	-0.12	6.00	1000	0.17	8.00	1000	Memb Accumulation	>0 - 0.5 log
Dibromochloromethane	ESPA-2	0.10	8.00	3185	0.26	6.00	1000.00	>0 - 0.5 log	>0 - 0.5 log
	TFC-HR	0.17	6.00	1000	0.38	7.72	6000	>0 - 0.5 log	>0 - 0.5 log
	TFC-ULP	0.13	8.00	1000	0.18	6.82	3929	>0 - 0.5 log	>0 - 0.5 log
Dibromomethane	ESPA-2	-0.25	6.00	6000	-0.11	6.00	1000.00	Memb Accumulation	Memb Accumulation
	TFC-HR	-0.24	6.00	6000	-0.11	6.00	1000	Memb Accumulation	Memb Accumulation
	TFC-ULP	-0.26	6.00	6000	-0.16	6.00	1000	Memb Accumulation	Memb Accumulation
Dichlorodifluoromethane	ESPA-2	0.29	NA	6000	0.47	NA	1000.00	>0 - 0.5 log	>0 - 0.5 log
	TFC-HR	0.13	6.00	6000	0.36	7.85	2347	>0 - 0.5 log	>0 - 0.5 log
	TFC-ULP	0.00	6.00	6000	0.28	7.26	2894	Memb Accumulation	>0 - 0.5 log
Ethylbenzene	ESPA-2	0.95	7.25	1000	1.18	6.00	6000.00	0.5 - 1 log	1 - 2 logs
	TFC-HR	1.33	6.00	6000	2.08	7.69	4480	1 - 2 logs	2 - 3 logs
	TFC-ULP	1.01	6.00	1000	1.54	6.00	6000	1 - 2 logs	1 - 2 logs
Hexachlorobutadiene	ESPA-2	1.68	6.00	1000	2.71	8.00	2899.14	1 - 2 logs	2 - 3 logs
	TFC-HR	1.64	6.00	1000	2.65	8.00	3119	1 - 2 logs	2 - 3 logs
	TFC-ULP	2.09	6.00	1000	2.91	8.00	2582	2 - 3 logs	2 - 3 logs
Isopropylbenzene	ESPA-2	1.56	8.00	NA	1.68	6.00	NA	1 - 2 logs	1 - 2 logs
	TFC-HR	1.85	6.00	1000	2.58	7.60	4557	1 - 2 logs	2 - 3 logs
	TFC-ULP	1.45	6.00	1000	2.01	6.00	6000	1 - 2 logs	2 - 3 logs
Methylene chloride	ESPA-2	-0.59	6.00	1000	0.04	6.93	6000.00	Memb Accumulation	>0 - 0.5 log
	TFC-HR	-0.46	6.00	1000	0.12	6.00	6000	Memb Accumulation	>0 - 0.5 log
	TFC-ULP	-0.57	6.00	1000	0.00	7.26	6000	Memb Accumulation	Memb Accumulation
M-Xylene	ESPA-2	0.96	6.89	1000	1.34	6.00	6000.00	0.5 - 1 log	1 - 2 logs
	TFC-HR	1.26	8.00	1000	1.91	8.00	4914	1 - 2 logs	1 - 2 logs
	TFC-ULP	0.93	6.00	1000	1.54	6.00	6000	0.5 - 1 log	1 - 2 logs
Naphthalene	ESPA-2	1.40	8.00	2442	1.76	6.00	6000.00	1 - 2 logs	1 - 2 logs
	TFC-HR	2.00	8.00	1000	2.73	7.74	5119	1 - 2 logs	2 - 3 logs
	TFC-ULP	1.51	6.00	1000	2.29	6.52	6000	1 - 2 logs	2 - 3 logs
N-Butylbenzene	ESPA-2	2.77	8.00	NA	2.97	6.00	NA	2 - 3 logs	2 - 3 logs
	TFC-HR	2.40	6.00	1000	3.43	6.81	6000	2 - 3 logs	3 - 4 logs
	TFC-ULP	2.95	6.00	1000	3.38	8.00	3796	2 - 3 logs	3 - 4 logs

14e. Data derived from surface-response analysis showing magnitude of influence of pH and salinity on RO removal of compounds. Magnitude of the difference between minimum and maximum predicted compound removal indicates degree of influence.

Compound	Projected Minimum				Projected Maximum			Log Removal Range	
	Membrane	Log Removal	pH	TDS	Log Removal	pH	TDS	Minimum	Maximum
N-Propylbenzene	ESPA-2	1.65	8.00	1000	1.99	6.00	6000.00	1 - 2 logs	1 - 2 logs
	TFC-HR	NA	NA	NA	NA	NA	NA	NA	NA
	TFC-ULP	2.02	6.00	1000	3.01	6.00	5314	2 - 3 logs	3 - 4 logs
O-Xylene	ESPA-2	1.05	8.00	NA	1.15	6.00	NA	1 - 2 logs	1 - 2 logs
	TFC-HR	1.06	8.00	1000	1.50	8.00	6000	1 - 2 logs	1 - 2 logs
	TFC-ULP	0.86	6.00	1000	1.14	6.00	6000	0.5 - 1 log	1 - 2 logs
Sec-Butylbenzene	ESPA-2	2.30	8.00	NA	2.46	6.00	NA	2 - 3 logs	2 - 3 logs
	TFC-HR	2.62	NA	1000	3.27	NA	3652	2 - 3 logs	3 - 4 logs
	TFC-ULP	1.93	6.00	1000	2.78	6.00	6000	1 - 2 logs	2 - 3 logs
Styrene	ESPA-2	0.85	8.00	NA	1.05	6.00	NA	0.5 - 1 log	1 - 2 logs
	TFC-HR	1.62	8.00	1000	2.46	7.58	4833	1 - 2 logs	2 - 3 logs
	TFC-ULP	1.19	6.00	1000	1.89	6.00	6000	1 - 2 logs	1 - 2 logs
T-Butylbenzene	ESPA-2	2.12	7.14	NA	2.25	6.00	NA	2 - 3 logs	2 - 3 logs
	TFC-HR	2.10	6.00	1000	3.00	8.00	4060	2 - 3 logs	2 - 3 logs
	TFC-ULP	1.50	6.00	1000	1.98	6.00	4883	1 - 2 logs	1 - 2 logs
Tetrachloroethene	ESPA-2	0.90	8.00	NA	1.02	6.00	NA	0.5 - 1 log	1 - 2 logs
	TFC-HR	1.46	6.00	6000	2.10	7.40	4161	1 - 2 logs	2 - 3 logs
	TFC-ULP	1.11	6.00	1000	1.51	6.33	6000	1 - 2 logs	1 - 2 logs
Toluene	ESPA-2	0.46	8.00	4555	0.67	6.00	1000.00	>0 - 0.5 log	0.5 - 1 log
	TFC-HR	0.67	6.00	6000	1.12	7.34	4177	0.5 - 1 log	1 - 2 logs
	TFC-ULP	0.51	8.00	6000	0.76	6.46	6000	0.5 - 1 log	0.5 - 1 log
Trichloroethene	ESPA-2	0.07	8.00	NA	0.12	6.00	NA	>0 - 0.5 log	>0 - 0.5 log
	TFC-HR	0.29	6.00	6000	0.56	7.31	4129	>0 - 0.5 log	0.5 - 1 log
	TFC-ULP	0.22	6.00	1000	0.49	6.38	6000	>0 - 0.5 log	>0 - 0.5 log
Trichlorofluoromethane	ESPA-2	0.64	NA	6000	0.71	NA	1000.00	0.5 - 1 log	0.5 - 1 log
	TFC-HR	0.53	6.00	1000	0.71	7.59	3183	0.5 - 1 log	0.5 - 1 log
	TFC-ULP	0.32	8.00	6000	0.49	7.07	3191	>0 - 0.5 log	>0 - 0.5 log
Vinylchloride	ESPA-2	-0.18	6.00	6000	-0.05	6.00	1000.00	Memb Accumulation	Memb Accumulation
	TFC-HR	-0.17	6.00	6000	-0.04	8.00	1251	Memb Accumulation	Memb Accumulation
	TFC-ULP	-0.10	6.00	6000	-0.03	6.00	1000	Memb Accumulation	Memb Accumulation

Table 15. Comparison of compound removal determined using the radiometric potential (RMP) assay developed at OCWD during the EPA-1 study (6) and removal results obtained using the cross-flow membrane cell in the current (EPA-2) study.

Compound	Membrane	EPA-2 (RO Cell)			EPA-1 (RMP Assay)			Comparison	Notes
		Avg.% Rej.	Log Rem.	Range	Est. % Rej.	Log Rem.	Range	EPA2 to EPA 1	
Benzene	ESPA-2	43.45	0.25	>0 - 0.5 log	76.68	0.63	0.5 - 1 log	Less	Assays differ by < 0.4 log
	TFC-HR	34.39	0.18	>0 - 0.5 log	78.59	0.67	0.5 - 1 log	Less	Assays differ by <0.5 log
Toluene	ESPA-2	70.53	0.53	0.5 - 1 log	91.63	1.08	1 - 2 logs	Less	Assays differ by < 0.6 log
	TFC-HR	86.93	0.88	0.5 - 1 log	88.09	0.92	0.5 - 1 log	Similar	Both assays in same range
Ethylbenzene	ESPA-2	92.59	1.13	1 - 2 logs	96.81	1.50	1 - 2 logs	Similar	Both assays in same range
	TFC-HR	95.45	1.34	1 - 2 logs	98.39	1.79	1 - 2 logs	Similar	Both assays in same range
Estrone	ESPA-2	98.54	1.84	1 - 2 logs	99.78	2.66	2 - 3 logs	Less	Assays differ by one range
	TFC-HR	99.85	2.83	2 - 3 logs	99.84	2.80	2 - 3 logs	Similar	Both assays in same range
Lindane	ESPA-2	99.84	2.80	2 - 3 logs	97.87	1.67	1 - 2 logs	Greater	Assays differ by one range
	TFC-HR	99.95	3.32	3 - 4 logs	99.06	2.03	2 - 3 logs	Greater	Assays differ by one range
Progesterone	ESPA-2	99.64	2.44	2 - 3 logs	99.75	2.60	2 - 3 logs	Similar	Both assays in same range
	TFC-HR	99.93	3.15	3 - 4 logs	99.96	3.43	3 - 4 logs	Similar	Both assays in same range
Chlorpyrifos	ESPA-2	99.94	3.23	3 - 4 logs	99.34	2.18	2 - 3 logs	Greater	Assays differ by one range
	TFC-HR	99.94	3.23	3 - 4 logs	99.27	2.14	2 - 3 logs	Greater	Assays differ by one range

Table 16a. Comparison of organic compound removal observed at Sonoma County Water Agency with OCWD model predictions.

Compound	Log Removal		Predicted Range	Comparison of	Notes
PPCPs	**Measured**	**Predicted**		**Measured to Predicted**	
Acetaminophen - MSRC	>1.00	-0.04	Membrane Accumulation	Greater	Model predicts poorer removal. Sonoma membrane not at equilibrium?
Acetaminophen - MWH	>1.43	-0.04	Membrane Accumulation	Greater	Model predicts poorer removal. Sonoma membrane not at equilibrium?
Antipyrine -MSRC	>1.22	1.74	1 - 2 logs	Similar?	Observed field range agrees with predicted value
Caffeine - MSRC	>2.29	2.21	2 - 3 logs	Similar?	Observed field range agrees with predicted value
Caffeine - MWH	>1.94	2.21	2 - 3 logs	Similar?	Observed field range agrees with predicted value
Caffeine - OCWD	>1.04	2.21	2 - 3 logs	Similar?	Observed field range agrees with predicted value
Carbamezipine -MSRC	>1.94	0.84	0.5 - 1 logs	Greater	Model predicts poorer removal. Sonoma membrane not at equilibrium?
Cimetidine - MSRC	>2.56	1.30	1 - 2 logs	Greater	Model predicts poorer removal. Sonoma membrane not at equilibrium?
Codeine - MSRC	>2.22	0.65	0.5 - 1 logs	Greater	Model predicts poorer removal. Sonoma membrane not at equilibrium?
Cotinine - MSRC	>1.87	0.01	>0 - 0.5 logs	Greater	Model predicts poorer removal. Sonoma membrane not at equilibrium?
Cotinine - MWH	>1.76	0.01	>0 - 0.5 logs	Greater	Model predicts poorer removal. Sonoma membrane not at equilibrium?
DEET - MWH	>1.62	3.07	3 - 4 logs	Similar?	Observed field range agrees with predicted value
Diazinon - MWH	>0.95	2.66	2 - 3 logs	Similar?	Observed field range agrees with predicted value
Diltiazem - MSRC	>1.88	1.24	1 - 2 logs	Greater	Model predicts poorer removal. Sonoma membrane not at equilibrium?
Erythromycin-18 - MSRC	>1.82	0.92	0.5 - 1 logs	Greater	Model predicts poorer removal. Sonoma membrane not at equilibrium?
Fluoxetine - MSRC	>0.55	3.67	3 - 4 logs	Similar?	Poor field resolution, but observed range could agree with predicted value
Hydrocodone - MSRC	>1.81	1.26	1 - 2 logs	Greater	Model predicts poorer removal. Sonoma membrane not at equilibrium?
Ketoprofen - MSRC	>1.39	2.23	2 - 3 logs	Similar?	Poor field resolution, but observed range could agree with predicted value
Metformin - MSRC	>2.68	0.23	>0 - 0.5 logs	Greater	Model predicts poorer removal. Sonoma membrane not at equilibrium?
Methyl parathion - MWH	>1.30	1.40	1 - 2 logs	Similar?	Observed field range agrees with predicted value
Nicotine - MSRC	>1.49	0.04	>0 - 0.5 logs	Greater	Model predicts poorer removal. Sonoma membrane not at equilibrium?
Paraxanthine - MSRC	>1.85	1.53	1 - 2 logs	Greater	Model predicts within 0.5 logs
Ranitidine - MSRC	>1.62	0.45	>0 - 0.5 logs	Greater	Model predicts poorer removal. Sonoma membrane not at equilibrium?
Sulfamethoxazole - MSRC	>1.33	0.48	>0 - 0.5 logs	Greater	Model predicts poorer removal. Sonoma membrane not at equilibrium?
TBEP - MWH	>0.86	2.13	2 - 3 logs	Similar?	Observed field range agrees with predicted value
TDCPP - MWH	>1.62	3.56	3 - 4 logs	Similar?	Observed field range agrees with predicted value
Triclosan - MWH	>0.96	1.59	1 - 2 logs	Similar?	Observed field range agrees with predicted value
Trimethoprim - MSRC	>2.30	1.04	1 - 2 logs	Greater	Model predicts poorer removal. Sonoma membrane not at equilibrium?
Warfarin - MSRC	>1.19	-0.07	Membrane Accumulation	Greater	Model predicts poorer removal. Sonoma membrane not at equilibrium?
EDCs					
Estrone - MSRC	*>2.41*	*2.86*	*2 - 3 logs*	*Similar*	*Lab Results = 2.84 +/- 0.13 log removal for TFC-HR*
Estrone - OCWD	*>0.64*	*2.86*	*2 - 3 logs*	*Similar?*	*Lab Results = 2.84 +/- 0.13 log removal for TFC-HR*
Beta-estradiol - MSRC	>1.07	3.52	3 - 4 logs	Similar?	Observed field range agrees with predicted value

Italics = Included in OCWD Swatch Studies
Nominal RO Performance

16b. Comparison of organic compound removal observed at Sonoma County Water Agency with OCWD model predictions.

Compound	Log Removal		Range	Comparison of	Notes
	Observed	Predicted		Measured to Predicted	
Diethylstilbestrol	>0.84 - >1.98	3.77	3 - 4 logs	Similar?	Poor field resolution, but observed range could agree with predicted value
Epitestosterone	>2.7	2.89	2 - 3 logs	Similar?	Observed field range agrees with predicted value
Estriol	*>2.00 - >2.30*	*2.16*	*2 - 3 logs*	*Similar?*	*Lab Results = 2.92 +/- 0.15 log removal for TFC-HR*
Estrone	*>2.10 - >2.40*	*2.86*	*2 - 3 logs*	*Similar?*	*Lab Results = 2.84 +/- 0.13 log removal for TFC-HR*
Progesterone	*>2.70 - >3.00*	*3.29*	*3 - 4 logs*	*Similar?*	*Lab Results = 3.17 +/- 0.16 log removal for TFC-HR*
trans-testosterone	>0.78 - >0.89	2.71	2 - 3 logs	Similar?	Poor field resolution, but observed range could agree with predicted value
17a-Estradiol	>2	3.28	3 - 4 logs	Similar?	Observed field range agrees with predicted value
17a-Ethynylestradiol	>2.10 - >2.30	3.00	2 - 3 logs	Similar?	Observed field range agrees with predicted value
17b-Estradiol	>2.05 - >2.40	3.28	3 - 4 logs	Similar?	Observed field range agrees with predicted value
NDMA	>0.52 - >0.71	0.08	>0 - 0.5 logs	Greater	Model predicts poorer removal. Sonoma membrane not at equilibrium?
1,4-Dioxane	>1.85 - >1.89	-0.16	Membrane Accumulation	Greater	Model predicts poorer removal. Sonoma membrane not at equilibrium?

Italics = Included in OCWD Swatch Studies

RO Performance During 35 Minute Spiking Study

Table 17. Comparison of organic compound removal observed at West Basin Municipal Water District with OCWD model predictions.

Compound	Log Removal		Range	Comparison of	Notes
	Measured	Predicted		Measured to Predicted	
1,4-Dichlorobenzene	**0.17**	**1.42**	**1 - 2 log**	**Less**	**Lab Results = 1.3 +/- 0.18 log removal for ESPA-2**
1,4-Dioxane	>0.97	-0.09	Membrane Accumulation	Greater	Model predicts poorer removal. WBMWD membrane not at equilibrium?
4-methyl-2-pentanone	>0.13	0.24	>0 - 0.5 log	Similar?	Poor field resolution, but observed range could agree with predicted value
Acetone	-0.07	-0.02	Membrane Accumulation	Similar	Observed field range agrees with predicted value
Bis(2-ethylhexyl)adipate	0.03	4.22	>4 log	Less	Probable model failure
Bis(2-ethylhexyl)phthalate	>0.015	4.24	>4 log	Less?	Poor field measurement resolution, possible model failure
Bromochloroacetic acid (BCAA)	>0.91	-0.20	Membrane Accumulation	Greater	Model predicts poorer removal. WBMWD membrane not at equilibrium?
Bromochloromethane	**0.02**	**-0.11**	**Membrane Accumulation**	**Similar**	**Lab Results = -0.13 +/- 0.02 log removal for ESPA-2**
Bromodichloromethane	**0.37**	**0.05**	**>0 - 0.5 log**	**Similar**	**Lab Results = 0.07 +/- 0.02 log removal for ESPA-2**
Bromoform	**>0.75**	**0.47**	**>0 - 0.5 log**	**Greater**	**Lab Results = 0.32 +/- 0.05 log removal for ESPA-2; within 0.5 log?**
Butyl benzyl phthalate	>0.19	4.18	> 4 log	Less?	Poor field measurement resolution, possible model failure
Carbon Disulfide	0.09	0.03	>0 to 0.5 log	Similar	Observed field range agrees with predicted value
Chloroform	**0.32**	**0.09**	**>0 to 0.5 log**	**Similar**	**Lab Results = 0.07 +/- 0.01 log removal for ESPA-2**
Chloromethane	**-0.23**	**-0.08**	**Membrane Accumulation**	**Similar**	**Lab Results = -0.03 +/- 0.02 log removal for ESPA-2**
Dalapon	>0.84	0.40	>0 - 0.5 log	Greater	Model predicts poorer removal. WBMWD membrane not at equilibrium?
Dibromoacetic acid (DBAA)	>0.38	-0.20	Membrane Accumulation	Greater	Model predicts poorer removal. WBMWD membrane not at equilibrium?
Dibromochloromethane	**0.44**	**0.11**	**>0 to 0.5 log**	**Similar**	**Lab Results = 0.16 +/- 0.04 log removal for ESPA-2**
Dibromomethane	**0.02**	**-0.17**	**Membrane Accumulation**	**Similar**	**Lab Results = -0.15 +/- 0.01 log removal for ESPA-2**
Dichloroacetic acid (DCAA)	>1.32	-0.17	Membrane Accumulation	Greater	Model predicts poorer removal. WBMWD membrane not at equilibrium?
Diethyl phthalate	0.62	1.80	1 - 2 log	Less	Probable model failure
Dimethyl phthalate	>0*	3.57	3 - 4 log	Less?	Poor field measurement resolution or model failure
Di-n-butyl phthalate	>0.01	2.76	2 - 3 log	Less?	Poor field measurement resolution or model failure
Formaldehyde	-0.12	-0.09	Membrane Accumulation	Similar	Observed field range agrees with predicted value
Methyl tert-butyl ether (MTBE)	>0.69	0.03	>0 to 0.5 log	Greater	Model predicts poorer removal. WBMWD membrane not at equilibrium?
Methylene Chloride	**0.02**	**-0.04**	**Membrane Accumulation**	**Similar**	**Lab Results = -0.15 +/- 0.04 log removal for ESPA-2**
N-Nitrosodiethylamine	>1.84	-0.06	Membrane Accumulation	Greater	Model predicts poorer removal. WBMWD membrane not at equilibrium?
N-Nitrosodimethylamine	0.14	-0.05	Membrane Accumulation	Similar	Observed field range agrees with predicted value
N-Nitrosodi-n-butylamine	>0.47	2.18	2 - 3 log	Similar	Poor field resolution
N-Nitrosomorpholine	>1.31	-0.14	Membrane Accumulation	Greater	Model predicts poorer removal. WBMWD membrane not at equilibrium?
N-Nitrosopiperidine	>1.02	-0.14	Membrane Accumulation	Greater	Model predicts poorer removal. WBMWD membrane not at equilibrium?
N-Nitrosopyrrolidine	>0.55	-0.10	Membrane Accumulation	Greater	Model predicts poorer removal. WBMWD membrane not at equilibrium?
PBDE-154 (Polybrominated diphenyl ether)	0.18	4.21	>4 log	Less	Probable model failure
p-Dichlorobenzene	0.22	1.33	1 - 2 log	Less	Probable model failure
Tert-butyl alcohol	>0.39	0.02	>0 to 0.5 log	Greater	Model predicts within 0.5 log
Tetrachloroethene	**0.74**	**1.32**	**1 to 2 log**	**Less**	**Lab Results = 0.92 +/- 0.10 log removal for ESPA-2; Lab membrane not at equilibrium?**
Toluene	**>0.68**	**0.72**	**0.5 to 1 log**	**Similar**	**Lab Results = 0.54 +/- 0.08 log removal for ESPA-2**
Trichloroacetic acid (TCAA)	>1.55	-0.19	Membrane Accumulation	Less	Model predicts poorer removal. WBMWD membrane not at equilibrium?
Trichloroethene	0.30	0.46	>0 to 0.5 log	Similar	Observed field range agrees with predicted value

Bold = compound included in model construction

Appendix 1

Orange County Water District

Water Quality Laboratory Standard Operating Procedures

ORANGE COUNTY WATER DISTRICT
STANDARD OPERATING PROCEDURE

EPA Method 508

DETERMINATION OF CHLORINATED PESTICIDES IN WATER BY GAS CHROMATOGRAPHY WITH AN ELECTRON CAPTURE DETECTOR

File Name:	M:\Sop\Organic\epa method sop\508_1101.doc	Effective Date:	11/01/2001
Revision:	5	Supersedes:	4 (01/01/1995)

1. SUMMARY OF METHOD

A measured volume of sample of approximately 1 liter is solvent extracted with methylene chloride by shaking in a separatory funnel. The Methylene chloride extract is isolated, dried, and concentrated to a volume of 5 ml after exchanging into methyl tert-butyl ether (MTBE). Chromatographic conditions are described which permit the separation and measurement of the analytes in the extract by GC with an electron capture detector (ECD). 2.0 ul of concentrated sample is injected to the ECD for analysis. EPA method 508 is used for the determination of chlorinated pesticides in groundwater and finished drinking water.

2. ANALYTES

This is a gas chromatographic (GC) method applicable to the determination of certain chlorinated pesticides in groundwater and finished drinking water. The following compounds can be determined using this method:

LIMS code	Analyte

ALACHL	Alachlor
ALDRIN	Aldrin
ClPYRI	Chlorpyrifos
CLTNIL	Chlorothalonil
DDD	4,4'-DDD
DDE	4,4'-DDE
DDT	4,4'DDT
DIELDR	Dieldrin
ENDOI	Endosulfan I
ENDOSL	Endosulfan sulfate
ENDRIN	Endrin
ENDR-A	Endrin Aldehyde
ENDR-K	Endrin Ketone
LINDNE	HCH-gamma (Lindane)
HEPT	Heptachlor
HEPEPX	Heptachlor epoxide
METHOX	Methoxychlor
TOXA	Toxaphene
ClDANE	Chlordane
BHCa	HCH-alpha(Alpha-BHC)
BHCb	HCH-beta(Beta-BHC)
BHCd	HCH-delta(Delta-BHC)
ENDOII	Endosulfan II
CLDA	Chlordane - alpha
CLDG	Chlordane - gamma
CLBZLA	Chlorobenzilate
CLNEB	Chloroneb
DCPA	DCPA - Dacthal
ETRDZL	Etridiazole
PROPCL	Propachlor
TRFLRN	Trifluralin
PMTHRN	Permethrin - (total of cis/trans)
HEXCLB	Hexachlorobenzene
HCLCPD	Hexachlorocyclopentadiene
PCB16	PCB-1016
PCB21	PCB-1221
PCB32	PCB-1232
PCB42	PCB-1242
PCB48	PCB-1248
PCB54	PCB-1254
PCB60	PCB-1260

3. APPARATUS AND EQUIPMENT

3.1 Sample Bottles – 2.5 liter amber glass bottles fitted with a screw cap lined with teflon.

3.2 Autosampler vials - equipped with Teflon-lined septum.

3.3 Concentrator Tube - Zymark 200 mL tubes used with the Zymark Turbo-Vap.

3.4 Analytical Balance: Capable of weighing accurately to nearest 0.0001 g.

3.5 Zymark Turbo-Vap - used to concentrate extracts.

3.6 CP 3800 Varian gas chromatograph with dual columns - electron capture detectors (ECD). Equipped with an CR 8400 autosampler for injecting samples into the GC.

3.7 Column: Fused Silica Capillary column, DB-5 30 meters long x 0.32 mm I.D. with a 0.25 micron film thickness. Alternate column - DB-1701 30 meters long x 0.32 mm I.D. with a 0.25 micron film thickness.

3.8 Disposable Pasteur Pipets and graduated cylinders (1000ml, 100ml, and 10ml).

4. REAGENTS AND CONSUMABLE MATERIALS

4.1 Reagent Water - Millipore Milli-Q System or equivalent.

4.2 Methylene Chloride: Burdick & Jackson - capillary GC^2 solvent.

4.3 Methyl tert-Butyl ether (MTBE): Burdick & Jackson - capillary GC^2 solvent.

4.4 Methanol: Burdick & Jackson - capillary GC^2 solvent.

4.5 Sodium Sulfate: (ACS) Granular, anhydrous. Heat sodium sulfate at 400ºC four hours, and store sodium sulfate at 130^{oo}C.

4.6 Sodium Thiosulfate ($Na_2S_2O_3$) : ACS grade.

4.7 Acetone: Burdick & Jackson - capillary GC solvent.

4.8 Phosphate buffer, pH 7 - Prepare by mixing 29.6 ml of 0.1 N HCl and 50 ml of 0.1 M dipotassium phosphate.

4.9 Sodium chloride, crystal, ACS grade - Heat treat in a shallow tray at 400ºC for a minimum of 4 hours to remove interfering organic substances.

4.10 Sodium thiosulfate, granular, anhydrous, ACS grade.

4.11 Pentachloronitrobenzene (PCNB) -100µg/ml from Ultra Scientific (Cat # PPS-130), for use as internal standard.

4.12 4,4'-Dichlorobiphenyl (DCB) - 500µg/ml from Ultra Scientific (Cat #PPS-120), for use as surrogate standard.

5. SAMPLE COLLECTION, PRESERVATION AND HANDLING

Samples are collected in amber 2.5 liter bottles, fitted with a screw cap lined with teflon. If the samples contain residual chlorine add 80 mg/L of sodium thiosulfate. After addition to the sample, seal the bottle and shake for one minute. Store samples at 4^{o}C. All samples must be extracted within 7 days after collection. The extract should be analyzed within 14 days after extraction.

6. EXTRACTION

6.1 Transfer 1 liter of sample to a 2-L separatory funnel and spike the sample with 2 ul of the surrogate standard spiking solution. Add spiking solution at this time. Adjust the sample to pH7 by addin 25 ml of the phosphate buffer. Check pH. Add 100 g of NaCl. Seal, and shake the separatory to dissolve the salt. Add 60 ml of methylene chloride to the separatory funnel contained the sample. Extract the sample by vigorously shaking the funnel for 2 minutes with periodic venting to release excess pressure. Allow the organic layer to separate from the water phase for a minimum of 10 minutes. If the emulsion interface between layers is more than one third the volume of the solvent layer, the analyst must employ mechanical techniques to complete the phase separation. The optimum technique depends upon the sample, but may include stirring, filtration through glass wool, centrifugation, or other physical methods. Collect the methylene chloride extract in a 250 ml Erlenmeyer flask containing approximately 7 grams of anhydrous sodium sulfate.

6.2 Add a second 60 ml volume of methylene chloride to the separtory funnel and repeat the extraction procedure a second time, combing the extracts in the Erlenmeyer flask. Perform a third extraction in the same manner. Swirl flask to dry extract; allow flask to sit for 15 minutes. Transfer the extract to the 200 ml concentrator tube. Rinse the remaining sodium sulfate with two 25 ml portions of methylene chloride and decant rinses into the concentrator tube.

6.3 Concentrate the extract using Turbo-Vap to 1 ml. Add 10 ml of MTBE and reduce down to 1 ml. Repeat with two more 10 ml of MTBE to completely exchange the solvents. Transfer the solvent extract to the 10 ml graduated tube and add 1 ul of internal standard spiking solution to the sample extract, seal, and shake to distribute the internal standard. Adjust the final volume to 5 ml with MTBE. Transfer the extract to 2 auto sampler vials and store. Refrigerate at 4^{o}C until analysis by GC-ECD.

7. ANALYSIS

7.1 EPA method 508 is used to monitor for low level of chlorinated pesticides in ground water. Because of these low levels, any type of contamination or interferences can cause analytical problems. Thus, reagent blanks must be monitored for every extraction run - monitoring of reagent blanks is essential to the success of this method. If results for reagent blanks rise above this level corrective actions must be performed. Analyze a 5-point calibration at the beginning of each analytical run. Verify the calibration by measurement of two calibration check standards, one at the beginning and one at the end of the run. These check standards should be at two different concentration levels to verify the calibration curve. LFBs (laboratory fortified blanks) should also be analyzed

with each extraction run. Standards used for these QA/QC samples must be ordered from a second source whenever possible. For extended runs, check standards should be interspersed with samples at regular intervals. If the response of any analyte varies from the predicted response by more than +/- 20%, test must be repeated using fresh calibration standards. The five point calibration should be 0.01, 0.05, 0.10, 0.15 and 0.20 ppb. Any results above 0.20 ppb must be confirmed with a standard that is within +/- 20% of the actual result. 2 ul of sample is injected for analysis.

Instrument Conditions:

1.	Initial column temperature:	60°C			
2.	Hold time:	0 min			
3.	Final temperatures:	140ºC	200ºC	220ºC	300ºC
4.	Temperature rates:	25ºC/min	2ºC/min	3ºC/min	15ºC/min
5.	Hold times:	1 min	1 min	8 min	4.81min
6.	Helium linear velocity:	30 cm/sec			
7.	Splitless injection with	45 second delay			
8.	Injector temperature:	250°C			
9.	Detector temperature:	310°C			

8. QA/QC REQUIREMENTS

8.1 Laboratory Reagent Blank - Run before samples. Use to demonstrate that all glassware and reagent interferences are under control. If any contamination peaks are produced, determine source of contamination and eliminate interference.

8.2 Laboratory Fortified Blank - Must analyze at least two laboratory fortified blank (LFB) one after every calibration and one at the end of the analysis. The fortification concentration of each analyte should confirm the ability to detect at the reportable level. If the recovery of any analyte falls outside the control limits, the source of the problem must be identified and corrected.

8.3 Standards –After calibrate the system with 5 point calibration standards, verify calibration standards by analyzing a standard prepared from reference material obtained from an independent or second source for daily analysis, one from the beginning and one at the end. EPA performance evaluations are an excellent process to determine the validity of the method. Results must be within +/- 30% of those used to routinely check calibration. Daily, run a low level standard to check the reportable detection level, RDL.

8.4 Samples - Samples must be extracted within 7 days after collection. Samples must be stored at 4ºC until ready for extraction. Duplicates are run on 10% of samples, or once during run, whichever is greater. Results should be within +/- 20%. Extracts should be analyzed within 14 days after extraction. All positive identifications must be confirmed using the confirmation column or GC/MS method 525.

8.5 Spike Recoveries - The laboratory must add a known concentration of spike solution, the same as used for LFB, to at least 10% of samples or once per analytical run, whichever is greater. Recoveries should be within the acceptable range. Wherever possible, run a second source standard for spikes.

8.6 QC Requirements – The system must pass the Sensitivity, chromatographic, and column performance criteria. Before the sample analysis, inject 1 µl of Laboratory performance check solution from Ultra Scientific Cat # PPM-508 to verify the system suitability ; EPA Method 508, Revision 3.1. Analyze EPA QC check sample with known values if available. The results for each analyte must be within the EPA acceptance criteria. Semi-annually, analyze EPA Performance Evaluation samples. Analyze these check samples whenever major maintenance to the system occurs to ensure the validity of the method.

8.7 Endrin and DDT degradation - Monitor the degradation of both Endrin and DDT by filling out the correct form for each instrument. Breakdown must be adequately consistent during the analysis run. Monitor all spikes and standards for degradation. When consistency is lost - service the injection port of the instrument - (greater than 20% on either target).

9. PREVENTIVE MAINTENANCE AND CORRECTIVE ACTIONS

9.1 Glassware - Glassware must be carefully cleaned. Clean all glassware as soon as practical after use by thoroughly rinsing with last solvent used in it. Follow by washing with hot water and detergent and thoroughly rinsing with tap water followed by reagent water. After drying, heat in oven. Do not heat volumetric glassware above 220^{o}C. Thorough rinsing with acetone may be substituted for heating.

9.2 Reagents - The use of high purity solvents and reagents will help to minimize contamination problems.

9.3 Carryover - Contamination carryover may occur when a sample containing a low concentration of analytes is analyzed immediately following a sample containing a high concentration. Use solvent rinses between samples to minimize carryover.

9.4 All reagents and apparatus must be routinely demonstrated to be free from interferences under the conditions of the analysis by running laboratory method blanks. Minimize contact of the samples, reagents, or solvents with any plastics. This well help reduce contamination. Interferences by phthalate esters can pose a major problem in pesticide analysis when using the electron capture detector.

Record all corrective actions in the maintenance log book. Include a complete description of the problem and what action were taken to correct it.

9.6 No or Poor Chromatography-

Check all the standards. If calibration, LPC, Degradation check and/or QC lie outside the acceptable limits we must first re-run the standards to assure that the injection procedure is working properly. After the re-run if standards still lie

outside the acceptable limits we must make a new standard or conduct instrument maintenance to assure that calibration and QC lie with acceptable parameters. For elevated spike recoveries make sure that the sample matrix is clean. If sample matrix is altering recoveries then a new matrix must be selected. If instrument performance is acceptable the samples must be re-extracted. If the sample lie outside allowable holding time they must be re-sampled.

9.6.2 Request re-sample if it's necessary.

9.6.3 If there's hits, confirm with GC/MS using second Column.

SOP PROCEDURE CHANGE

CHANGE	DATE	INITIALS
Laboratory performance check Verify system suitability	01/02/01	LY
Solution (Ultra Scientific Cat # PPM-508)		
Calibration Check Standard Checking the calibration Curve	01/02/01	

ORANGE COUNTY WATER DISTRICT
STANDARD OPERATING PROCEDURE

EPA Method 524.2
Rev. 4.1

DETERMINATION OF VOLATILE ORGANIC COMPOUNDS IN WATER BY PURGE AND TRAP AND CAPILLARY COLUMN GAS CHROMATOGRAPHY/ MASS SPECTROMETRY

File Name:	M:\SOP\Organic\epa method sop\524_2_1100.doc	Effective Date:	02/19/2003
Revision:	5	Supersedes:	5 (10/28/2002)

1. SUMMARY OF METHOD

EPA method 524.2 is used in the District's monitoring of volatile organic compounds (VOCs) throughout the basin. The method is used as the primary source of data in the analysis of VOCs for the District's main laboratory. Measurement of low levels of VOCs in finished drinking water requires an extensive QA/QC procedure. VOCs are purged from a 25ml sample and trapped onto an absorbent material. This material is then rapidly heated to desorb the VOCs into the system. The column is temperature programmed to separate the target analytes required of the method. Analytes are detected using a mass spectrometer. A data system is used to convert responses into actual concentrations of all analytes. Identification is based on the comparison of the mass spectra and retention time of an unknown to a library of reference mass spectral data of the target analytes. Quantification is based on internal standard. The District's laboratory uses spike samples for additional QA/QC documentation for this method.

2. ANALYTES

This is a gas chromatographic mass spectrometry (GC/MS) method, applicable to the determination of a wide range of volatile organic compounds. The following compounds can be determined using this method:

Lims code	Analyte
BENZ	Benzene

BRBENZ	Bromobenzene
CH2BrC	Bromochloromethane
CHBrCl	Bromodichloromethane
CHBr3	Bromoform
CH3Br	Bromomethane
nBBENZ	n-Butylbenzene
sBBENZ	sec-Butylbenzene
tBBENZ	tert-Butylbenzene
CCl4	Carbon tetrachloride
CLBENZ	Chlorobenzene
ClETHA	Chloroethane
CHCl3	Chloroform
CH3Cl	Chloromethane
2ClTOL	2-Chlorotoluene
4ClTOL	4-Chlorotoluene
CHBr2C	Dibromochloromethane
DBCP	1,2-Dibromo-3-chloropropane
EDB	1,2-Dibromoethane
CH2Br2	Dibromomethane
12DCB	1,2-Dichlorobenzene
13DCB	1,3-Dichlorobenzene
14DCB	1,4-Dichlorobenzene
CCl2F2	Dichlorodifluoromethane
11DCA	1,1-Dichloroethane
12DCA	1,2-Dichloroethane
11DCE	1,1-Dichloroethene
c-12DCE	cis-1,2-Dichloroethene
t-12DCE	trans-1,2-Dichloroethene
12DCP	1,2-Dichloropropane
13DCP	1,3-Dichloropropane
22DCP	2,2-Dichloropropane
11DCP	1,1-Dichloropropene
c13DCP	cis-1,3-Dichloropropene
t13DCP	trans-1,3-Dichloropropene
EtBENZ	Ethylbenzene
HClBut	Hexachlorobutadiene
ISPBNZ	Isopropylbenzene
4IPTOL	4-Isopropyltoluene
CH2Cl2	Methylene chloride
NAP	Naphthalene
NBENZ	Nitrobenzene
PRBNZ	Propylbenzene
STYR	Styrene
1112PC	1,1,1,2-Tetrachloroethane
1122PC	1,1,2,2-Tetrachloroethane
PCE	Tetrachloroethene

TOLU	Toluene
123TCB	1,2,3-Trichlorobenzene
124TCB	1,2,4-Trichlorobenzene
111TCA	1,1,1-Trichloroethane
112TCA	1,1,2-Trichloroethane
TCE	Trichloroethene
CCl3F	Trichlorofluoromethane
123TCP	1,2,3-Trichloropropane
124TMB	1,2,4-Trimethylbenzene
135TMB	1,3,5-Trimethylbenzene
VNYLCL	Vinyl chloride
o-XYL	o-Xylene
mp-XYL	m,p-Xylene
Cl3F3E	Trichlorotrifluoroethane
TOTALX	Total Xylenes
THMS	Total THMs
MEK	MEK (2-Butanone)
MIBK	MIBK (4-Methyl 2-pentanone)
2ClEVE	2-chloroethyl vinyl ether
B2CLEE	bis(2-Chloroethyl)ether
MTBE	Methyl-t-butyl ether
DIPE	Diisopropyl Ether
TAME	Tert Amyl Methyl Ether
ETBE	Ethyl tert Butyl Ether
TBA	Tert-butyl alcohol

(targets in bold represent the custom “EPA-100” mix)
The following analytes do not have a lims code but can be analyzed by 524.2.

Acetone
Acrylonitrile
Allyl chloride
Carbon disulfide
Chloroacetonitrile
trans-1,4-Dichloro-2-butene
1,1-Dichloropropanone
Diethyl ether
Ethyl methacrylate
2-Hexanone
Methacrylonitrile
Methyl acrylate
Methyl iodide
Methylmethacrylate
2-Nitropropane
Pentachloroethane
Propionitrile

Tetrahydrofuran

3. APPARATUS AND EQUIPMENT

3.1 Sample Bottles - 250 ml amber glass bottles & 40 ml amber vials - fitted with an open top screw cap lined with Teflon.

3.2 Purge and Trap unit – Varian Archon Autosampler and Tekmar 3000/3100 Purge and Trap. Use a Vocarb 4000 trap – "I" trap from Supelco.

3.3 Varian Model 3400/ 3800 gas chromatograph with a (Varian) Saturn-3/ Saturn 2000 GC/MS system.

3.4 Column: Fused Silica Capillary column, 60 meter x 0.32 mm ID DB-VRX with 1.8 micron film thickness.

3.5 Volumetric flasks (200ml, 100ml, and 50ml), and Hamilton micro syringes - 10ul to 250ul.

4. REAGENTS AND CONSUMABLE MATERIALS

4.1 Reagent Water - Millipore Milli-Q System or equivalent.

4.2 Standard stock VOCs - 200 ug/ml volatile Aromatics and Haloalkanes mix (Ultra Scientific, Accustandard) and a Custom EPA-100 Mix (Accu-std), TBA Custom std mix, Custom – MEK mix MEK, MIBK, B2ClEE, Custom-Oxy std mix – (Ultra Scientific).

4.3 Internal standard - Fluorobenzene (internal) (Ultra Scientific) 2000 ug/ml. Tune standard – 4-Bromofluorobenzene –diluted to give a 25ng/ul solution. Used to pass EPA tune specifications.

4.4 GC^2 Methanol - Burdick and Jackson.

4.5 Ascorbic acid - ACS grade – if source water is chlorinated.

4.6 UHP grade Helium carrier gas.

4.7 Hydrochloric acid (1+1) - carefully add a measured volume of concentrated HCl to an equal volume of reagent water.

5. SAMPLE COLLECTION, PRESERVATION AND HANDLING

5.1 All samples must be collected in four amber 40ml vials while spikes are collected in 250 mL amber bottles. The 40ml vials and the 250ml amber glass bottles should be filled just to overflowing. If the concentration of the Trihalomethanes is important and the sample is known to be from a chlorinated source, ascorbic acid (25mg/40ml vial) must be added to the sample prior to collection. Do not flush out the rapidly dissolving ascorbic acid. Adjust the pH of all samples to <2 by carefully adding two drops of 1:1 HCl to each 40 ml vial of sample. Mix the sample for 1 min. All samples must be chilled to 4^{o}C at the time of collection, and they must be maintained at that temperature until ready for analysis. Samples must be stored away from all contaminating organic solvent vapors. Total hold time from sample collection to analysis is 14 days. If the samples are not analyzed by this period, they must be discarded. The Water Quality Department must be informed in order to resample the site. A travel blank of the volatile free reagent water must accompany each set of samples brought into the laboratory.

6. ANALYSIS

6.1 Tuning with BFB:

The Saturn-3/ Sauturn 2000 must meet the BFB criteria before analyses are performed. Inject 1.0 ul of a 25ng/ul Bromofluorobenzene (BFB) standard directly into the column. Obtain a background corrected mass spectrum of BFB peak and confirm that all the key M/Z criteria in Table A are achieved. If the tune does not pass, adjust the tune parameters and rerun BFB. Hardcopy the BFB report.

6.2 Calibration Curve:

A three to five point standard calibration curve must be run containing all method analytes, depending upon the concentration range desired. Examples of concentrations used in the curve are: 0.5, 2.0, 5.0, 10.0, 20.0, and 30.0 ppb. You may increase the range of the calibration curve, however a 0.5 ppb standard must be run to confirm the RDL of all analytes. A concentration of 2.0 ppb of the internal is injected into every sample and standard via the Tekmar purge/trap unit. The recoveries and area counts are tracked to insure a properly running instrument. The standard calibration curve for each analyte must be within a +/- 20% relative standard deviation. If not, the analytes which failed (or the entire calibration curve) should be re-analyzed. Once the calibration curve has been established, it must be verified on each working day by analyzing the continuous calibration check standard. Typically, a standard calibration curve can last approximately 2 months.

Standard Preparation:

Calibration standards are prepared from separate stock solutions. The Aromatic stock solution, the Haloalkane stock solution, and the custom MEK mix are combined into one solution for both calibration and for the second source standard. The “Oxy” standard and the TBA standard are both generated separately, based on co-elution problems with other targets. The calibration check solution is analyzed at 2.0ppb – it is the second source standard from Supelco. The custom EPA-100 mix is used for both spikes

and the high LFB check solution – contains 20 targets which are both regulated by the state and have been detected within the District's basin. Working standards shall be made up in batches and verified against the working calibration. Working standards are valid for 14 days from the day they are made. Stock standards are good for one month or when QA/QC data shows they need to be replaced.

Preparing internal and surrogate standards for the AquaTek 50:

The internal standard mix from Ultra Scientific – Fluorobenzene - is at 2000 ug/mL. Add 250uL of this to a 10 ml volumetric flask containing GC grade methanol. Bring to a final volume of 10mls of GC^2 methanol. We have found that this internal is stable and does not interfere with any of the other targets.

Baking the column:

Bake the column whenever any changes are made to the system that introduces air into the system such as cutting the ends of the column or installing a new column, or any work done on the Tekmar autosampler or purge and trap. The system – both purge & trap and the GC/MS, should be periodically baked to remove water vapor and organic interferences.

Notes:

1. Scan numbers of the key targets and the internal standard should be documented so as to monitor the life of the column. The column should be replaced when resolution has dropped below an acceptable level. The early gases are good indicators of the column's age and performance.

2. Data is collected for each run under specific file names within the software system. Mass spectral data are obtained with electron impact (EI) ionization at 70 eV electron energy. For samples that have ion abundance over the system's working range, a dilution with reagent water is necessary. Tentatively identified samples by comparison of mass spectrum (after background subtraction) to a reference spectrum in a user library. Ions above 10% relative abundance in the mass spectrum of the standard must be present in the spectrum of the component and should agree within absolute 10%. The GC retention time of the sample component must be within 10 scans of the time observed for that same compound when a calibration solution was analyzed.

3. Samples should be analyzed as soon as possible after collection –but have a 14 day holding time. Communication between the lab and the water quality department is important to understand each sample. There may be specific conditions or problems associated with each sample – an example would be frothing or very high levels. The more a chemists knows about the sample, the better he or she can provide quality assurance and processes, which can produce reliable results. If data shows that the value of the result is outside the calibration range – the sample must be diluted or additional standards analyzed to bracket the value within +/-20% of the value.

TABLE A

BFB KEY M/Z ABUNDANCE CRITERIA

MASS	CRITERIA
50	15 to 40% of mass 95
75	30 to 60% of mass 95
95	base peak, 100% relative abundance
96	5 to 9% of mass 95
173	<2% of mass 174
174	>50% of mass 95
175	5 to 9% of mass 174
176	>95% but <101% of mass 174
177	5 to 9% of mass 176

In order to achieve proper results, a system must be within target analyte contamination or interferences. To this goal, it is mandatory that both a travel blank and a reagent water blank be run with each set of samples. Conditions for the GC/MS system are as follows:

MS and GC Conditions:

1.	Initial column temperature:	35°C
2.	Hold time:	2 minutes
3.	Final temperature:	220°C
4.	Temperature rate:	4°C/minute
5.	Hold time:	1.75 minutes
6.	Helium flow rate:	1.0 ml/minute
7.	Total run time:	50 minutes
8.	Head pressure:	5 PSI
9.	Injector temperature:	125°C
10.	Transfer line GC/MS:	220°C
11.	Total scan time	0.7 seconds
12.	Mass range:	46 to 260 AMU and 35 to 260 AMU
13.	Fil/Mult delay	2.00 minute

Tekmar ALS/3000/3100 Purge and Trap Conditions:

1.	Purge Time:	11.00 minutes
2.	Bake Time:	10.00 minutes
3.	Pre-Heat:	245°C
4.	Desorb:	250°C
5.	Bake:	260°C

Tekmar AquaTek 50 Conditions:

1.	Settle:	0.3 minutes
2.	Prepurge:	30 seconds
3.	Sample Pressurize:	40-60 seconds
4.	Sample Transfer:	75 seconds
5.	Internal Standard Fill:	5 seconds
6.	Internal Standard Trans:	50 seconds
7.	Backflush:	Off
8.	Desorb Time:	4 minutes
9.	Transfer Line Rinse:	Off

7. QA/QC REQUIREMENTS

7.1 Laboratory Reagent Blank - Run before samples. Use to demonstrate that all glassware and reagent interference are under control. If any contamination peaks are produced, determine source of contamination and eliminate interference.

7.2 Laboratory Fortified Blank - The fortification concentration of each analyte should confirm the ability to detect at the reportable level. If the recovery of any analyte falls outside the control limits, +/-30%, the source of the problem must be identified and corrected.

7.3 Standards - Verify calibration standards quarterly by analyzing a standard prepared from reference material obtained from an independent or second source. EPA performance evaluations are an excellent process to determine the validity of the method. Results must be within +/- 30% of those used to routinely check calibration. Daily, run a low level standard to check the reportable detection level, RDL. **% RSD of each calibration curve should be less than 20%. If one or more calibration curve has more than 20% RSD, re-integrate the peak and verify peak integration. If the problems are not solved by reprocess, rerun new calibration curve using freshly made standards to meet the 20% requirement.**

7.4 Samples - Samples must be analyzed within 14 days after collection. Samples must be stored at 4°C or below until ready for analysis. Duplicates are run on 5% of samples, or once during run, whichever is greater. Results should be within +/- 20%.

7.5 Spike Recoveries - The laboratory must add a known concentration of spike solution, the same as used for LFB, to at least 5% of samples or once per analytical run, whichever is greater. Recoveries should be within the acceptable range, +/- 30%. Wherever possible, run a second source standard for spikes.

7.6 QC Requirements - Analyze EPA QC check sample with known values if available. The results for each analyte must be within the EPA acceptance criteria. Semi-annually, analyze EPA Performance Evaluation samples. Analyze additional check samples whenever major maintenance to the system occurs to ensure the validity of the method.

7.7 Continuous Calibration Check Standard: Daily analyze a 2 ppb continuous calibration check standard. Also, confirm the RDL. The concentration measured using the calibration curve must be within +/-30% of the true value of the concentration in the calibration solution. If this condition is not met, recalibration may be required.

7.8 If samples fail any of the above QC requirements, resample request will be followed to re-analyze the sample. Also verify tuning compound, BFB and proceed the system diagnostics to investigate any malfunction of the system.

8. PREVENTIVE MAINTENANCE AND CORRECTIVE ACTIONS

8.1 Glassware - Glassware must be carefully cleaned. Do not heat volumetric glassware above 220^{o}C.

8.2 Reagents - The use of high purity solvents and reagents will help to minimize contamination problems.

8.3 Carryover - Contamination carryover may occur when a sample containing a low concentration of analytes is analyzed immediately following a sample containing a high concentration. Use volatile free reagent water rinses between samples to minimize carryover.

8.4 All reagents and apparatus must be routinely demonstrated to be free from interference under the conditions of the analysis by running laboratory method blanks. Minimize contact of the samples and reagents with solvent vapors (methylene chloride). This well help reduce contamination.

8.5 A refrigerator blank should be run at least once a month. This blank, volatile free reagent water, is sealed in a 40 ml vial and placed in the VOC storage refrigerator for one month. Analyzed each month, it should be free of any organic contamination. Freons are the most likely interference to be picked up by this blank.

8.6 Record all corrective actions in the maintenance log book. Include a complete description of the problem and what action were taken to correct it.

SOP PROCEDURE CHANGE

CHANGE DATE
INITIALS

Appendix 2

Compound Certificate of Analyses

ULTRA SCIENTIFIC
Analytical Solutions

Certificate of Analysis

VOC Mixture

Product DWM-588 **Expiration Date:** Feb-2009
Lot Number: CC-0210 **Page:** 1 of 3

This Certified Reference Material (CRM) was manufactured and verified in accordance with ULTRA's ISO 9001:2000 registered quality system, and the analyte concentrations were verified by our ISO 17025 accredited laboratory. The true value and uncertainty value at the 95% confidence level for each analyte, determined gravimetrically, is listed below.

Analyte	CAS#	Analyte Lot	True Value
bromochloromethane	000074-97-5	JS-16015HS	2006 ± 10 µg/mL
bromodichloromethane	000075-27-4	DU-14522LS	2006 ± 10 µg/mL
bromoform	000075-25-2	DU-06126KS	2006 ± 10 µg/mL
carbon tetrachloride	000056-23-5	01704MF	2006 ± 10 µg/mL
chloroform	000067-66-3	BS-03041BS	2006 ± 10 µg/mL
dibromochloromethane	000124-48-1	DO-12622CI	2006 ± 10 µg/mL
dibromomethane	000074-95-3	EM-01514TJ	2006 ± 10 µg/mL
methylene chloride	000075-09-2	45139	2006 ± 10 µg/mL
trichlorofluoromethane	000075-69-4	DR-16417BR	2006 ± 10 µg/mL
1,2-dibromoethane	000106-93-4	TB-101777	2006 ± 10 µg/mL
1,1-dichloroethane	000075-34-3	64552/1	2006 ± 10 µg/mL
1,2-dichloroethane	000107-06-2	KN-09446KN	2006 ± 10 µg/mL
1,1-dichloroethene	000075-35-4	01218EC	2007 ± 10 µg/mL
cis-1,2-dichloroethene	000156-59-2	13707BO	2006 ± 10 µg/mL
trans-1,2-dichloroethene	000156-60-5	DO-07817JR	2006 ± 10 µg/mL
1,1,1,2-tetrachloroethane	000630-20-6	CO-12312LI	2006 ± 10 µg/mL
1,1,2,2-tetrachloroethane	000079-34-5	10917TB	2006 ± 10 µg/mL
tetrachloroethene	000127-18-4	PS-00344BR	2006 ± 10 µg/mL
1,1,1-trichloroethane	000071-55-6	LU-13149TR	2006 ± 10 µg/mL
1,1,2-trichloroethane	000079-00-5	JB-0701HH	2006 ± 10 µg/mL
trichloroethene	000079-01-6	KN-08846KN	2006 ± 10 µg/mL

Balances used in the manufacture of this standard are calibrated with weights traceable to NIST in compliance with ANSI/NCSL Z-540-1 and ISO 9001.

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ISO 17025
Cert. No. 0851- 01

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Dr. Edward Fitzgerald,
Senior Scientist

ULTRA SCIENTIFIC
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Certificate of Analysis

VOC Mixture

Product DWM-588 **Expiration Date:** Feb-2009
Lot Number: CC-0210 **Page:** 2 of 3

Analyte	CAS#	Analyte Lot	True Value
1,2-dibromo-3-chloropropane	000096-12-8	FBL-01	2005 ± 10 µg/mL
1,2-dichloropropane	000078-87-5	DC-120777	2006 ± 10 µg/mL
1,3-dichloropropane	000142-28-9	PR-17916MR	2005 ± 10 µg/mL
2,2-dichloropropane	000594-20-7	CI-05304BI	2006 ± 10 µg/mL
1,1-dichloropropene	000563-58-6	34768-21	2005 ± 10 µg/mL
cis-1,3-dichloropropene	010061-01-5	EB-1890	2006 ± 10 µg/mL
trans-1,3-dichloropropene	010061-02-6	34257-41	2005 ± 10 µg/mL
hexachlorobutadiene	000087-68-3	339923/1	2006 ± 10 µg/mL
1,2,3-trichloropropane	000096-18-4	12020TF	2005 ± 10 µg/mL
naphthalene	000091-20-3	14205KB	2007 ± 10 µg/mL
benzene	000071-43-2	31072	2006 ± 10 µg/mL
n-butylbenzene	000104-51-8	AA-28519CO	2006 ± 10 µg/mL
sec-butylbenzene	000135-98-8	MR-11305DN	2006 ± 10 µg/mL
tert-butylbenzene	000098-06-6	MQ-04010MQ	2007 ± 10 µg/mL
ethylbenzene	000100-41-4	033067	2006 ± 10 µg/mL
isopropylbenzene	000098-82-8	EN-00621TG	2006 ± 10 µg/mL
4-isopropyltoluene	000099-87-6	PP-05104CP	2006 ± 10 µg/mL
n-propylbenzene	000103-65-1	LO-14513MR	2006 ± 10 µg/mL
styrene	000100-42-5	MQ-11228MQ	2006 ± 10 µg/mL
toluene	000108-88-3	43045	2006 ± 10 µg/mL
1,2,4-trimethylbenzene	000095-63-6	BO-13528BI	2007 ± 10 µg/mL
1,3,5-trimethylbenzene	000108-67-8	KM-02011KM	2006 ± 10 µg/mL
o-xylene	000095-47-6	DI-00459CJ	2006 ± 10 µg/mL
m-xylene	000108-38-3	DO-06834CO	2006 ± 10 µg/mL

Balances used in the manufacture of this standard are calibrated with weights traceable to NIST in compliance with ANSI/NCSL Z-540-1 and ISO 9001.

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Certificate of Analysis

VOC Mixture

Product DWM-588 **Expiration Date:** Feb-2009
Lot Number: CC-0210 **Page:** 3 of 3

Analyte	CAS#	Analyte Lot	True Value
p-xylene	000106-42-3	03747LN	2007 ± 10 µg/mL
1,4-dichlorobenzene	000106-46-7	05205KA	2006 ± 10 µg/mL
bromobenzene	000108-86-1	CG-02513MF	2006 ± 10 µg/mL
chlorobenzene	000108-90-7	03148HZ	2006 ± 10 µg/mL
2-chlorotoluene	000095-49-8	10018BC	2006 ± 10 µg/mL
4-chlorotoluene	000106-43-4	CR-14512LQ	2006 ± 10 µg/mL
1,2-dichlorobenzene	000095-50-1	089469KY	2006 ± 10 µg/mL
1,3-dichlorobenzene	000541-73-1	JN-05902LZ	2006 ± 10 µg/mL
1,2,3-trichlorobenzene	000087-61-6	LI-12912PF	2006 ± 10 µg/mL
1,2,4-trichlorobenzene	000120-82-1	00334TQ	2006 ± 10 µg/mL
bromomethane	000074-83-9	06623AQ	2008 ± 10 µg/mL
chloroethane	000075-00-3	00223KG	2009 ± 10 µg/mL
chloromethane	000074-87-3	3-2296	2009 ± 10 µg/mL
dichlorodifluoromethane	000075-71-8	N960053	2009 ± 10 µg/mL
vinyl chloride	000075-01-4	RM00068	2009 ± 10 µg/mL

Matrix: methanol (methyl alcohol)

Balances used in the manufacture of this standard are calibrated with weights traceable to NIST in compliance with ANSI/NCSL Z-540-1 and ISO 9001.

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Analytical Solutions

Certificate of Analysis

Organochlorine Pesticides Mixture

Product PPM-508B **Expiration Date:** Sep-2007
Lot Number: CA-1509A **Page:** 1 of 1

This Certified Reference Material (CRM) was manufactured and verified in accordance with ULTRA's ISO 9001:2000 registered quality system, and the analyte concentrations were verified by our ISO 17025 accredited laboratory. The true value and uncertainty value at the 95% confidence level for each analyte, determined gravimetrically, is listed below.

Analyte	CAS#	Analyte Lot	True Value
aldrin	000309-00-2	ER082003-01	1004 ± 5 µg/mL
alpha-BHC	000319-84-6	CAP-27275-15	1004 ± 5 µg/mL
beta-BHC	000319-85-7	35072-32	1002 ± 5 µg/mL
delta-BHC	000319-86-8	35097-03	1004 ± 5 µg/mL
gamma-BHC	000058-89-9	NT01899	1003 ± 5 µg/mL
4,4'-DDD	000072-54-8	22599-62	1002 ± 5 µg/mL
4,4'-DDE	000072-55-9	13125HR	1004 ± 5 µg/mL
4,4'-DDT	000050-29-3	MD-101797	1003 ± 5 µg/mL
dieldrin	000060-57-1	35006-40	1002 ± 5 µg/mL
endosulfan I	000959-98-8	BCD-29550-56	1003 ± 5 µg/mL
endosulfan II	033213-65-9	29494-55	1002 ± 5 µg/mL
endosulfan sulfate	001031-07-8	3245501	1004 ± 5 µg/mL
endrin	000072-20-8	34701-41	1003 ± 5 µg/mL
endrin aldehyde	007421-93-4	33381-04	1003 ± 5 µg/mL
heptachlor	000076-44-8	333379-48	1003 ± 5 µg/mL
heptachlor epoxide - isomer B	001024-57-3	31337-33	1003 ± 5 µg/mL
methoxychlor	000072-43-5	29550-70	1004 ± 5 µg/mL

Matrix: methyl tert-butyl ether (MTBE)

Balances used in the manufacture of this standard are calibrated with weights traceable to NIST in compliance with ANSI/NCSL Z-540-1 and ISO 9001.

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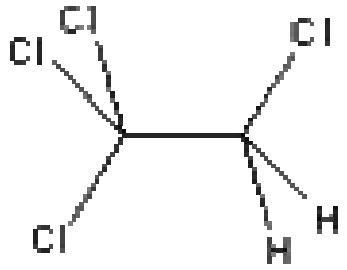
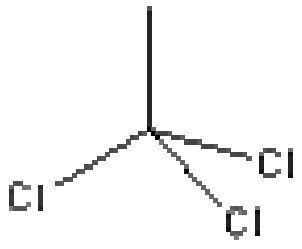
Appendix 3

Structures and Molecular Descriptors of the Compounds Used for Modeling



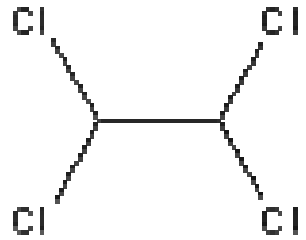
1,1,1,2 Tetrachloroethane

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
167.85	-70.2	1070.0000	2.93	1.20E+01	0.00245	1.80E-14	1.553
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
0	0	0	0	0	0	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	0	



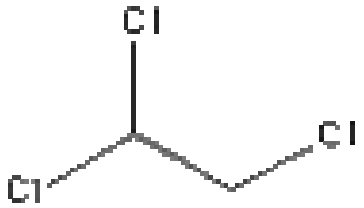
1,1,1-Trichloroethane

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
133.41	-30.4	1290.0000	2.49	1.24E+02	0.0172	9.43E-15	1.338
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
0	0	0	0	0	0	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	0	



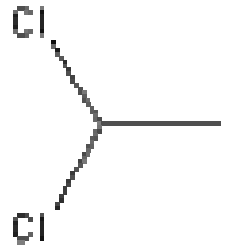
1,1,2,2-Tetrachloroethane

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
167.85	-43.8	2830.0000	2.39	4.62E+00	0.000367	2.50E-13	1.595
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
0	0	0	0	0	0	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	0	



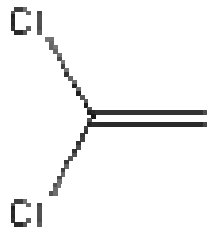
1,1,2-Trichloroethane

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
133.41	-36.6	4590.0000	1.89	2.30E+01	0.000824	1.96E-13	1.441
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
0	0	0	0	0	0	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	0	



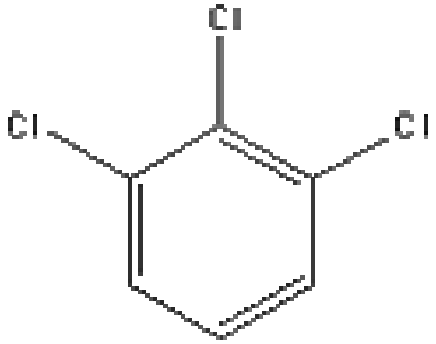
1,1-Dichloroethane

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
98.96	-96.9	5040.0000	1.79	2.27E+02	0.00562	2.74E-13	1.176
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
0	0	0	0	0	0	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	1	



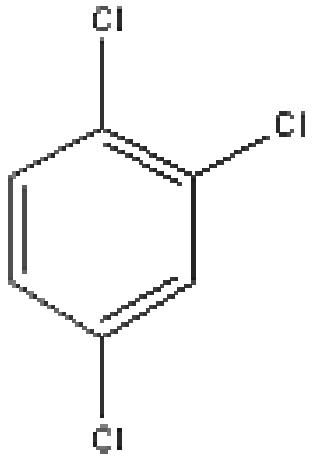
1,1-Dichloroethene

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
96.94	-122.5	2420.0000	2.13	6.00E+02	0.0261	1.09E-11	1.213
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
1	0	0	0	0	0	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	1	0	0	0	



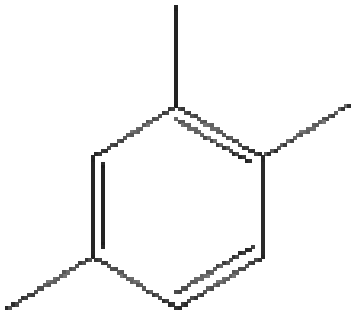
1,2,3-Trichlorobenzene

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
181.45	53.5	18.0000	4.05	2.10E-01	0.00125	2.82E-13	1.690
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
3	0	0	1	0	1	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	1	0	0	0	



1,2,4-Trichlorobenzene

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
181.45	17.0	49.0000	4.02	4.60E-01	0.00142	5.50E-13	1.463
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
3	0	0	1	0	1	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	0	

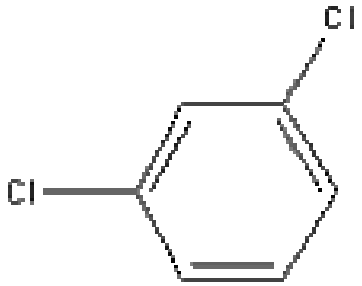


1,2,4-Trimethylbenzene

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
120.20	-43.8	57.0000	3.63	2.10E+00	0.00616	3.25E-11	0.876
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
3	0	0	1	0	1	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	3	

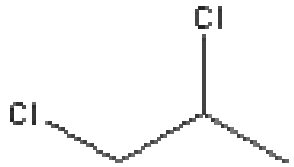
1,2-Dibromoethane

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
187.86	9.9	3910.0000	1.96	1.12E+01	0.00065	2.50E-13	2.170
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
0	0	0	0	0	0	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	1	0	0	0	0	



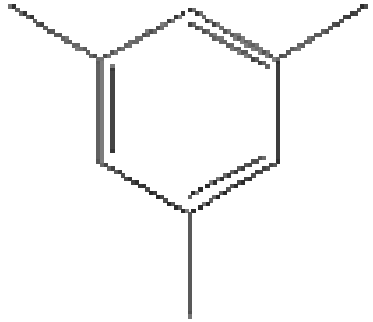
1,2-Dichlorobenzene

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
147.00	-24.8	125.0000	3.53	2.15E+00	0.00263	7.20E-13	1.288
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
3	0	0	1	0	1	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	0	



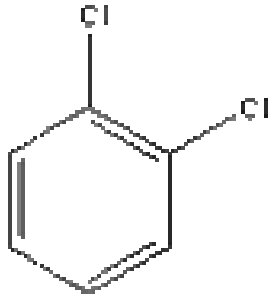
1,2-Dichloropropane

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
112.99	-100.0	2800.0000	1.98	5.33E+01	0.00282	4.42E-13	1.156
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
0	0	0	0	0	0	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	1	0	0	0	1	



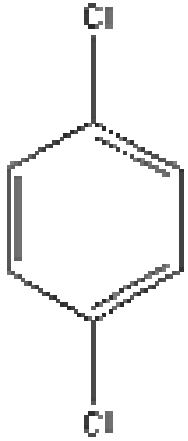
1,3,5-Trimethylbenzene

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
120.20	-44.7	48.2000	3.42	2.48E+00	0.00877	5.75E-11	0.865
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
3	0	0	1	0	1	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	3	



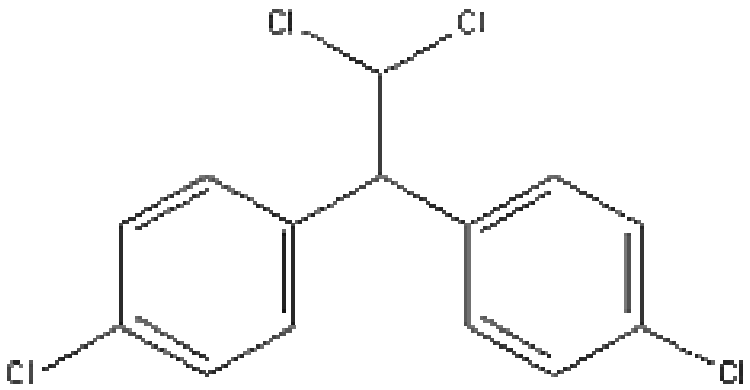
1,3-Dichlorobenzene

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
147.00	-16.7	156.0000	3.43	1.36E+00	0.00192	4.20E-13	1.306
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
3	0	0	1	0	1	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	0	



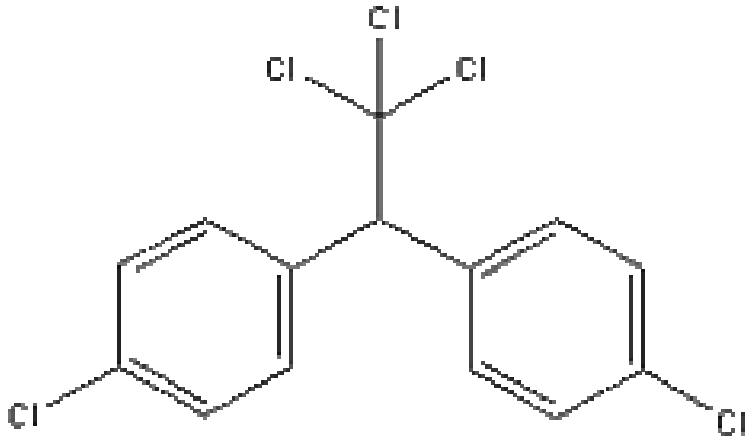
1,4-Dichlorobenzene

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
147.00	52.7	81.3000	3.44	1.74E+00	0.00241	3.20E-13	1.247
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
3	0	0	1	0	1	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	0	



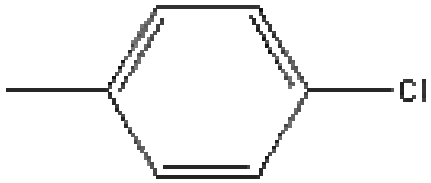
4,4-DDD

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
320.05	109.5	0.0900	6.02	1.35E-06	6.60E-06	4.34E-12	1.385
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
6	0	0	2	0	2	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	1	0	0	0	0	



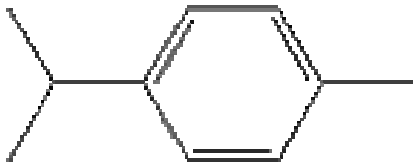
4,4'-DDT

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
354.49	108.5	0.0055	6.91	1.60E-07	8.32E-06	3.44E-12	1.560
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
6	0	0	2	0	2	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	1	0	0	0	0	



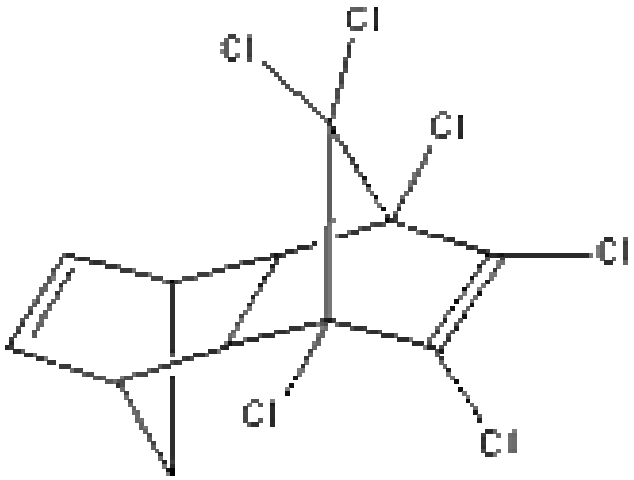
4-Chlorotoluene

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
126.59	7.5	106.0000	3.33	2.69E+00	4.38E-03	1.82E-12	1.070
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
3	0	0	1	0	1	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	1	



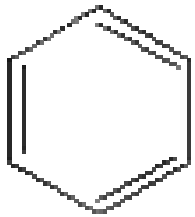
4-Isopropyltoluene

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
134.22	-68.9	23.4000	4.10	1.46E+00	0.011	1.51E-11	0.860
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
3	0	0	1	0	1	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	3	



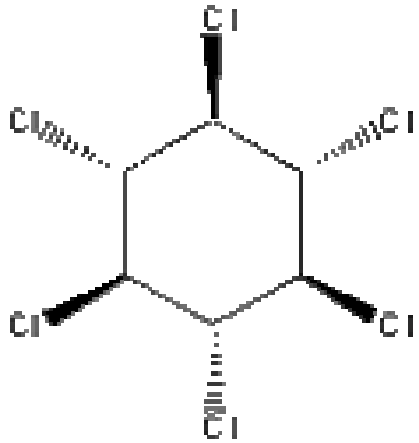
Aldrin

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
364.92	104.0	0.0170	6.50	1.20E-04	4.40E-05	6.46E-11	1.600
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
2	0	0	2	0	2	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	0	



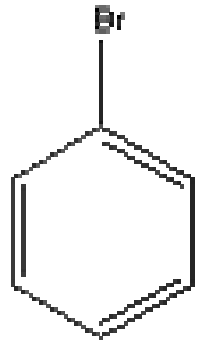
Benzene

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
78.12	5.5	1790.0000	2.13	9.48E+01	5.55E-03	1.23E-12	0.879
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
3	0	0	1	0	1	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	0	



Beta-BHC

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
290.83	314.5	0.2400	3.78	3.60E-07	4.40E-07	5.73E-13	1.890
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
0	0	0	0	0	0	1	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	0	

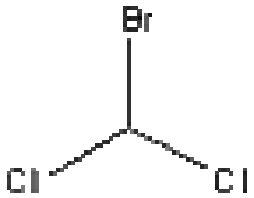


Bromobenzene

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
157.01	-30.6	446.0000	2.99	4.18E+00	2.47E-03	7.70E-13	1.495
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
3	0	0	1	0	1	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	0	

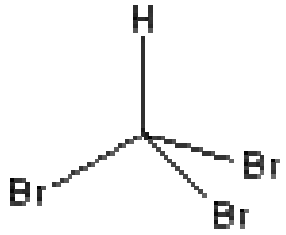
Bromochloromethane

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
129.38	-87.9	16700.0000	1.41	1.43E+02	1.46E-03	8.80E-14	1.991
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
0	0	0	0	0	0	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	0	



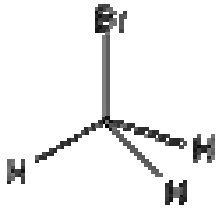
Bromodichloromethane

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
163.83	-57.0	3030.0000	2.00	5.00E+01	2.12E-03	7.84E-14	1.971
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
0	0	0	0	0	0	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	0	



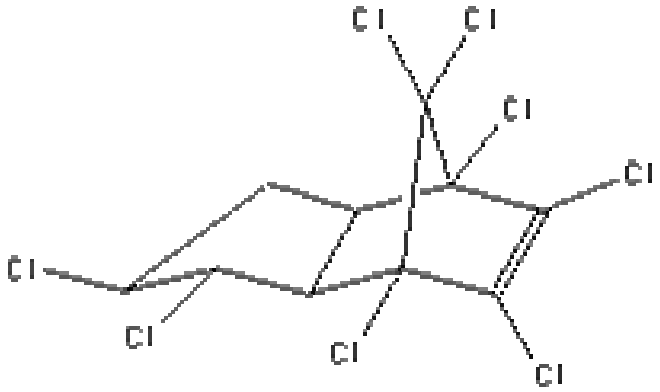
Bromoform

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
252.73	8.0	3100.0000	2.40	5.40E+00	5.35E-04	4.26E-14	2.890
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
0	0	0	0	0	0	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	0	



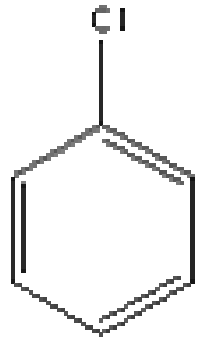
Bromomethane

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
94.94	-93.7	15200.0000	1.19	1.62E+03	7.34E-03	4.02E-14	1.732
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
0	0	0	0	0	0	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	0	



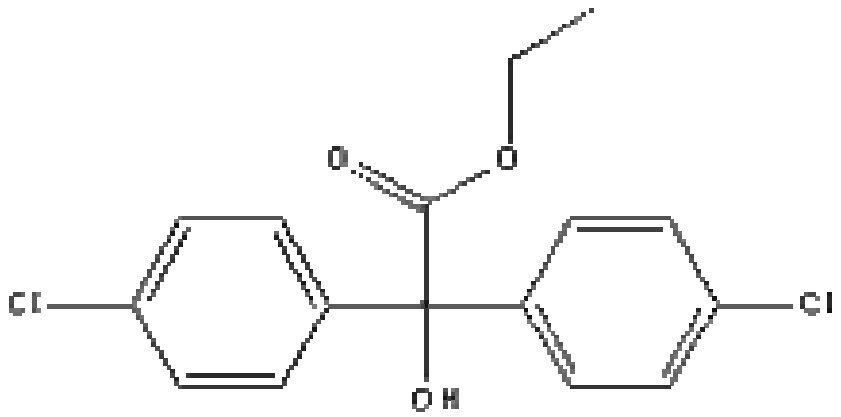
Chlordane

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
409.78	106.0	0.0130	6.26	9.90E-06	7.03E-05	5.04E-12	1.600
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
0	0	0	0	0	0	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	0	



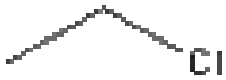
Chlorobenzene

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
112.56	-45.2	498.0000	2.84	1.20E+01	3.11E-03	7.70E-13	1.107
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
3	0	0	1	0	1	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	0	



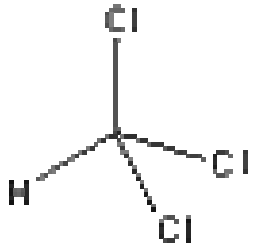
Chlorobenzilate

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
325.19	37.0	13.0000	4.74	2.20E-06	7.24E-08	5.09E-12	1.282
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
6	1	0	2	0	2	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	1	0	0	0	0	1	



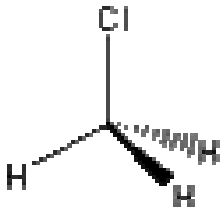
Chloroethane

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
64.52	-138.7	6710.0000	1.43	1.01E+03	1.11E-02	4.11E-13	0.920
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
0	0	0	0	0	0	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	1	



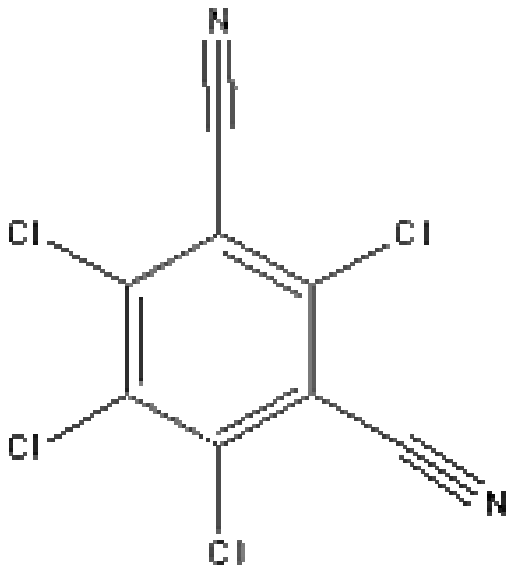
Chloroform

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
119.38	-63.6	7950.0000	1.97	1.97E+02	3.67E-03	1.03E-13	1.498
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
0	0	0	0	0	0	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	0	



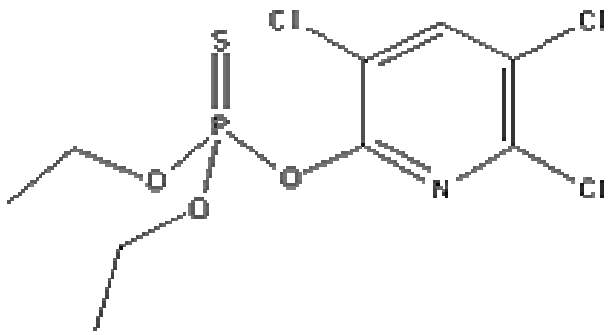
Chloromethane

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
50.49	-97.7	5320.0000	0.91	4.30E+03	8.82E-03	4.36E-14	0.991
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
0	0	0	0	0	0	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	1	



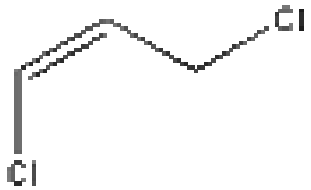
Chlorothanonil

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
265.91	250.0	0.6000	3.05	5.70E-07	2.00E-06	6.18E-15	1.800
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
3	0	2	0	0	1	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	2	0	



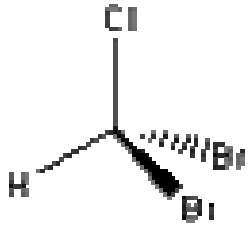
Chlorpyrifos

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
350.59	42.0	1.1200	4.96	2.03E-05	2.93E-06	9.17E-11	1.398
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
3	0	0	0	0	0	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	0	



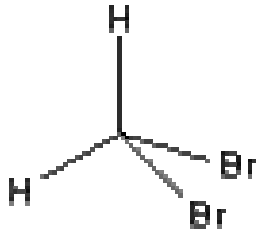
Cis-1,3-Dichloropropene

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
110.97	-50.0	2180.0000	2.06	2.63E+01	2.71E-03	8.40E-12	1.220
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
1	0	0	0	0	0	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	1	0	0	0	



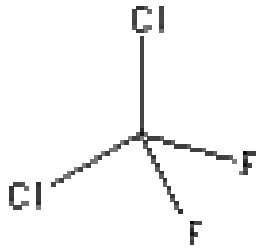
Dibromochloromethane

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
208.28	-20.0	2700.0000	2.16	5.54E+00	0.000783	5.78E-14	2.451
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
0	0	0	0	0	0	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	0	



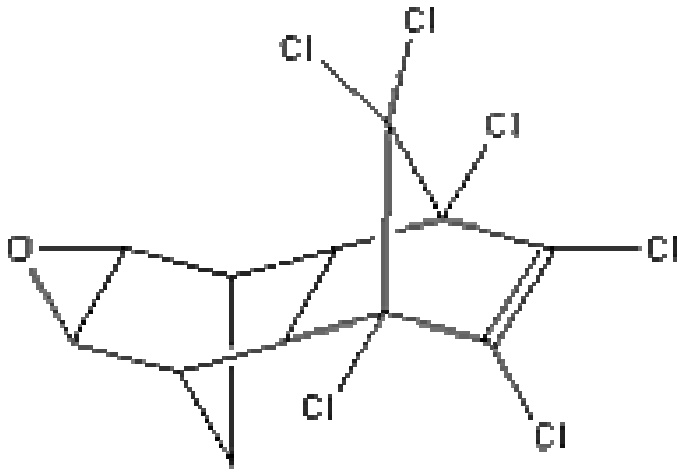
Dibromomethane

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
173.84	-52.5	11900.0000	1.70	4.44E+01	0.000822	1.13E-13	2.497
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
0	0	0	0	0	0	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	0	



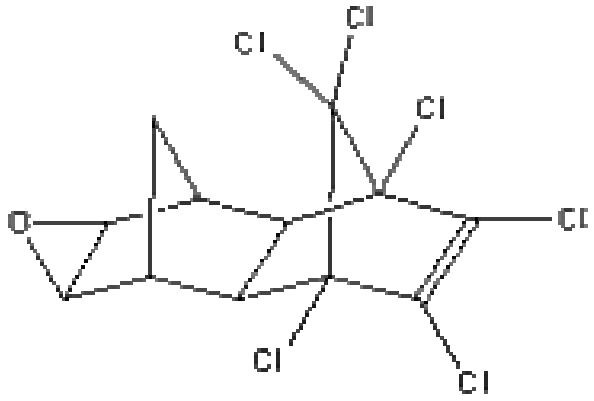
Dichlorodifluoromethane

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
120.91	-158.0	280.0000	2.16	4.85E+03	0.343	4.00E-16	1.329
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
0	0	0	0	0	0	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	0	



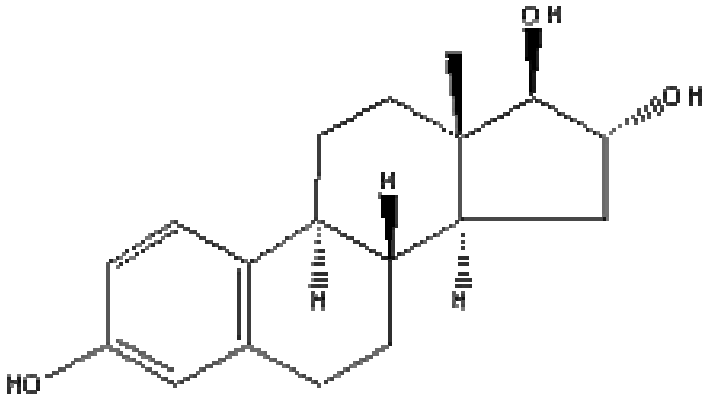
Dieldrin

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
380.91	175.5	0.1950	5.40	5.89E-06	1.00E-05	9.20E-12	1.750
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
1	0	0	0	0	0	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	1	0	0	0	



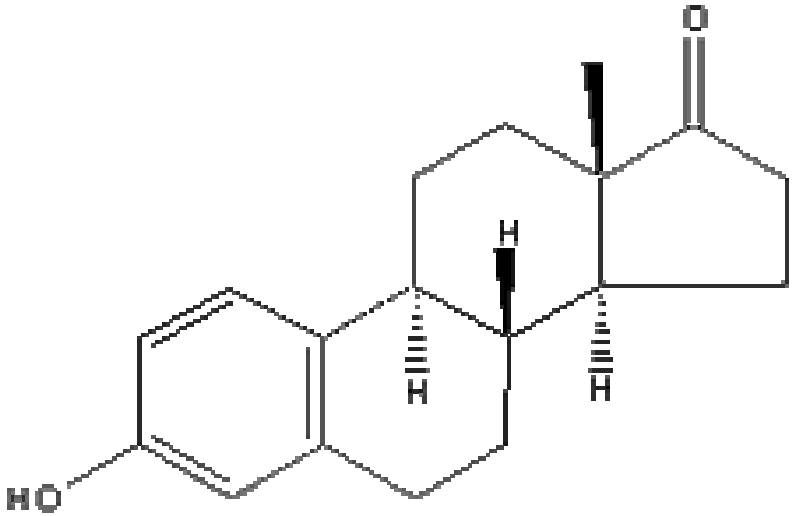
Endrin

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
380.91	226.0	0.2500	5.20	3.00E-06	6.36E-06	9.20E-12	1.700
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
1	0	0	0	0	0	2	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	1	0	0	0	



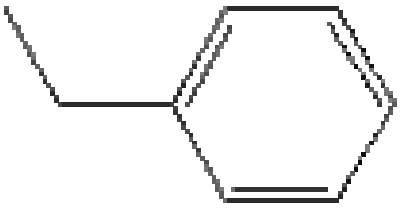
Estriol

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
288.39	282.0	441.0000	2.45	1.97E-10	1.33E-12	1.29E-10	1.270
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
3	0	0	1	0	1	3	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	3	0	0	0	0	0	



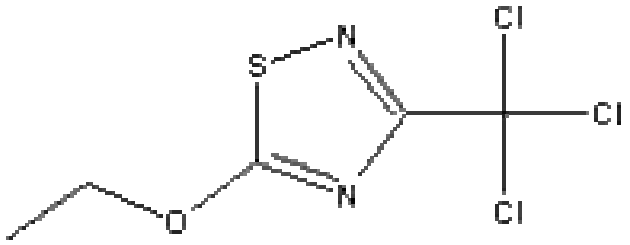
Estrone

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
270.37	260.2	30.0000	3.13	1.42E-07	3.80E-10	1.26E-10	1.236
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
3	1	0	1	0	1	3	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	1	0	0	0	0	0	



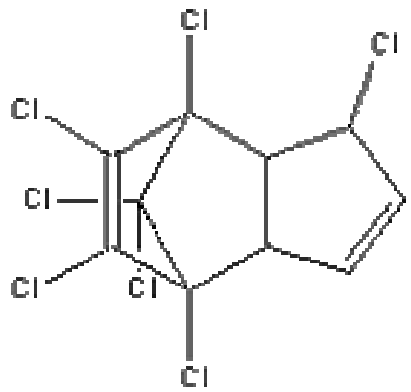
Ethylbenzene

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
106.17	-94.9	169.0000	3.15	9.60E+00	0.00788	7.10E-12	0.867
C=C	C=O	C=N	# Aromatic Rings	# 5-member Arom. Rings	# 6-member Arom. Rings	# Aliphatic Rings	# Conjugated Rings
3	0	0	1	0	1	0	0
# Carboxilic Acid Groups	# Hydroxyl Groups	# Alkane Groups	# Alkene Groups	# Nitrate Groups	# Nitrile Groups	# Methyl Groups	
0	0	0	0	0	0	1	



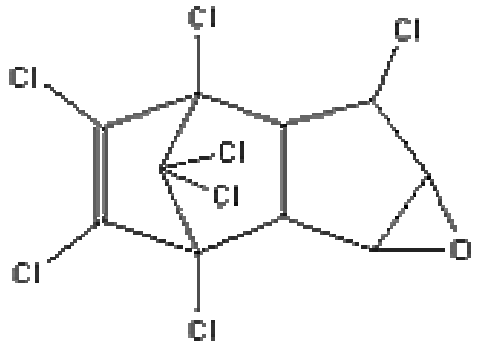
Etridiazole

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
247.53	19.9	117.0000	3.37	1.00E-04	2.78E-07	6.87E-12	1.503
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
0	0	2	1	1	0	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	1	



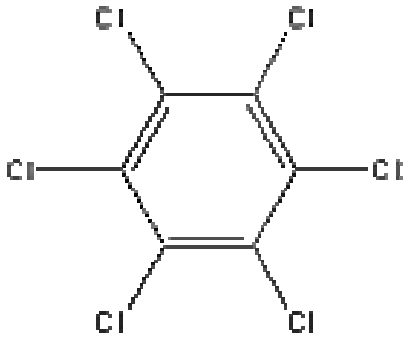
Heptachlor

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
373.32	95.5	0.1800	6.10	4.00E-04	0.000294	6.11E-11	1.580
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
1	0	0	0	0	0	2	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	0	



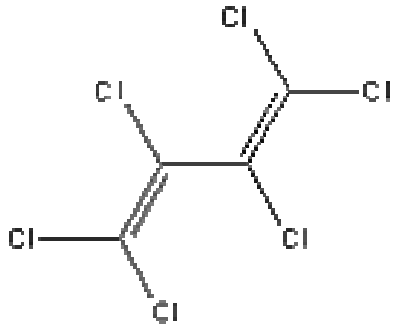
Hepatchlor epoxide

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
389.32	160.0	0.2000	4.98	1.95E-05	2.10E-05	5.17E-12	1.580
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
1	0	0	0	0	0	2	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	0	



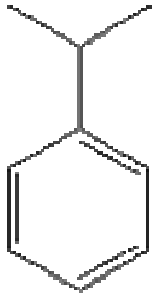
Hexachlorobenzene

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
284.78	231.8	0.0062	5.73	1.80E-05	0.0017	2.70E-14	2.044
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
3	0	0	1	0	1	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	0	



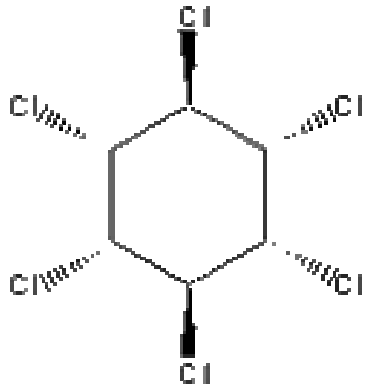
Hexachlorobutadiene

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
260.76	-21.0	3.2000	4.78	2.20E-01	0.0103	3.00E-14	1.680
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
2	0	0	0	0	0	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	0	



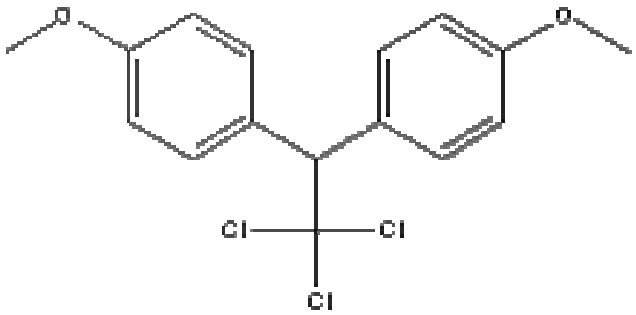
Isopropylbenzene

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
120.20	-96.0	61.3000	3.66	4.50E+00	0.0115	6.50E-12	0.862
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
3	0	0	1	0	1	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	2	



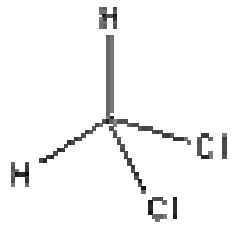
Lindane

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
290.83	112.5	7.3000	3.72	4.20E-05	5.14E-06	1.90E-13	1.870
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
0	0	0	0	0	0	1	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	0	



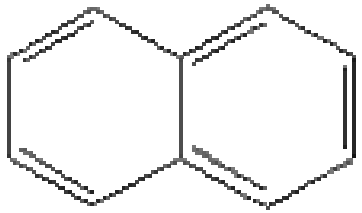
Methoxychlor

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
345.66	87.0	0.1000	5.08	2.58E-06	2.03E-07	5.35E-11	1.410
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
6	0	0	2	0	2	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	2	



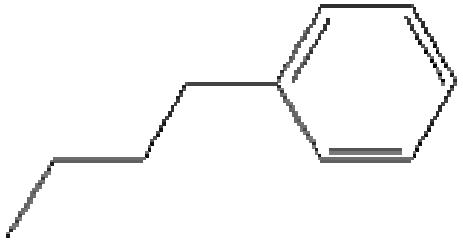
Methylene chloride

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
84.93	-95.1	13000.0000	1.25	4.35E+02	0.00325	1.42E-13	1.326
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
0	0	0	0	0	0	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	0	



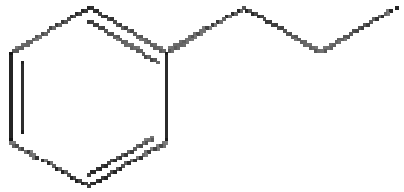
Naphthalene

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
128.18	80.2	31.0000	3.30	8.50E-02	0.00044	2.16E-11	0.997
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
5	0	0	2	0	2	0	2
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	0	



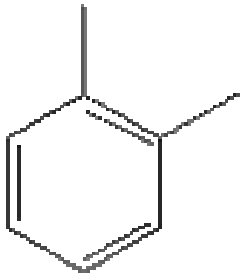
N-Butylbenzene

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
134.22	-87.9	11.8000	4.38	1.06E+00	0.0159	8.72E-12	0.860
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
3	0	0	1	0	1	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	1	



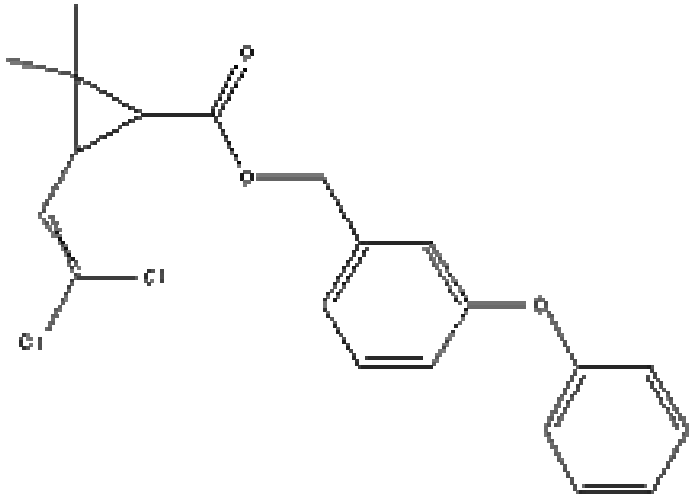
N-Propylbenzene

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
120.20	-99.5	52.2000	3.69	3.42E+00	0.0105	6.00E-12	0.862
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
3	0	0	1	0	1	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	1	



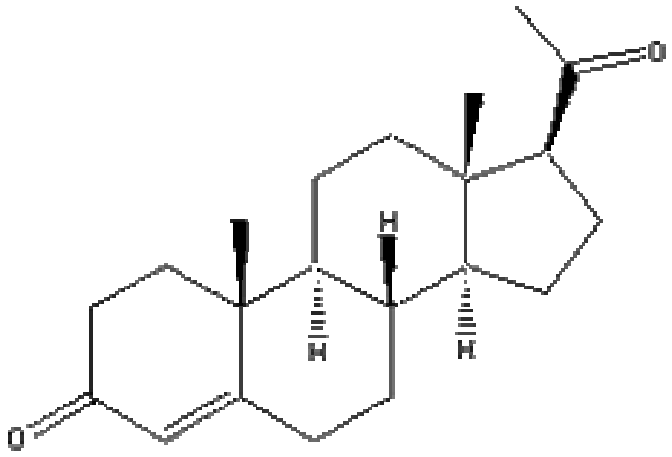
O-Xylene

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
106.17	-25.2	178.0000	3.12	6.61E+00	0.00518	1.37E-11	0.897
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
3	0	0	1	0	1	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	2	



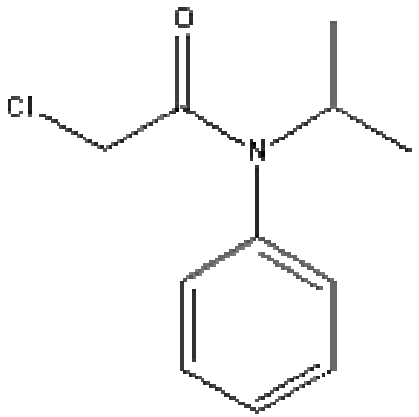
Permethrin

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
391.30	34.0	0.0060	6.50	2.18E-08	1.87E-06	3.90E-11	1.190
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
6	1	0	2	0	2	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
1	0	0	0	0	0	3	



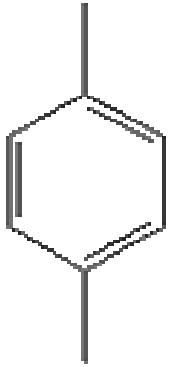
Progesterone

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
314.47	121.0	8.8100	3.87	1.30E-06	6.49E-08	1.04E-10	1.166
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
1	2	0	0	0	0	4	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	3	



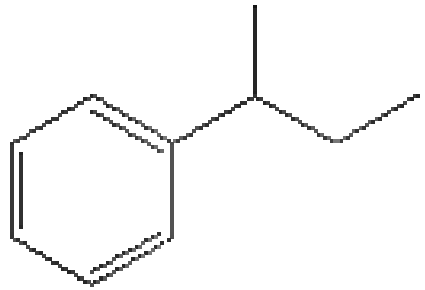
Propachlor

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
211.69	77.0	700.0000	2.18	2.30E-04	9.15E-08	2.10E-11	1.242
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
3	1	0	1	0	1	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	2	



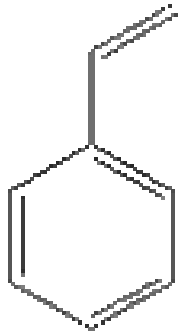
P-Xylene

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
106.17	13.2	162.0000	3.15	8.84E+00	0.0069	1.43E-11	0.861
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
3	0	0	1	0	1	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	2	



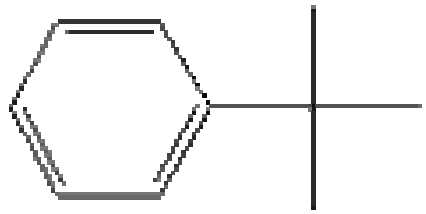
Sec-Butylbenzene

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
134.22	-82.7	17.6000	4.57	1.75E+00	0.0176	8.50E-12	0.862
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
3	0	0	1	0	1	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	2	



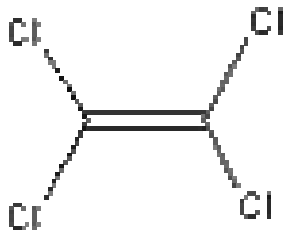
Styrene

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
104.15	-31.0	310.0000	2.95	6.40E+00	0.00275	5.80E-11	0.905
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
4	0	0	1	0	1	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	1	0	0	0	



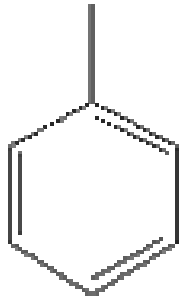
T-Butylbenzene

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
134.22	-57.8	29.5000	4.11	2.20E+00	0.0132	4.60E-12	0.867
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
3	0	0	1	0	1	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	3	



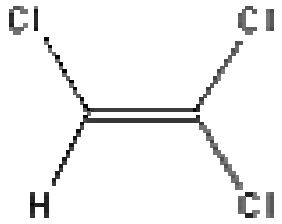
Tetrachloroethene

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
165.83	-22.3	206.0000	3.40	1.85E+01	0.0177	1.67E-13	1.623
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
1	0	0	0	0	0	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	1	0	0	0	



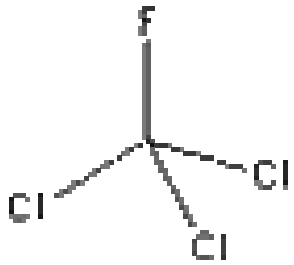
Toluene

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
92.14	-94.9	526.0000	2.73	2.84E+01	0.00664	5.96E-12	0.867
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
3	0	0	1	0	1	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	1	



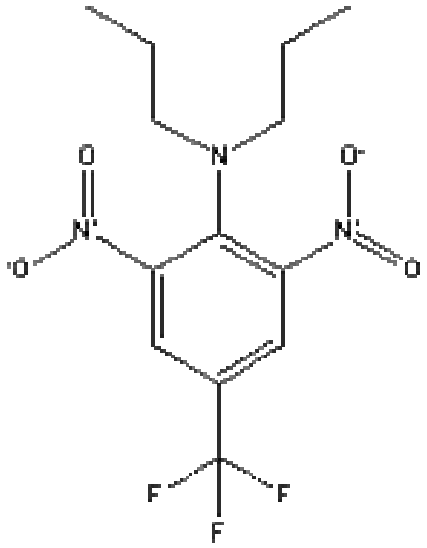
Trichloroethene

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
131.39	-84.7	1280.0000	2.42	6.90E+01	0.00985	2.36E-12	1.462
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
1	0	0	0	0	0	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	1	0	0	0	



Trichlorofluoromethane

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
137.37	-111.1	1100.0000	2.53	8.03E+02	0.097	5.00E-16	1.494
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
0	0	0	0	0	0	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	0	0	0	



Trifluralin

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
335.29	49.0	0.1840	5.34	4.58E-05	0.000103	2.40E-11	1.294
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
3	0	0	1	0	1	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	0	2	0	2	

Vinylchloride

Mol Weight	MP(°C)	H2O Solub (mg/L)	Log P	Vap Press (mm Hg)	Henry's Law K (atm-m^3/mole)	Atmosph. OH Rate K (cm^3/molecule-sec)	Density (g/cc)
62.50	-153.7	8800.0000	1.62	2.98E+03	0.0278	6.96E-12	0.911
C=C	**C=O**	**C=N**	**# Aromatic Rings**	**# 5-member Arom. Rings**	**# 6-member Arom. Rings**	**# Aliphatic Rings**	**# Conjugated Rings**
1	0	0	0	0	0	0	0
# Carboxilic Acid Groups	**# Hydroxyl Groups**	**# Alkane Groups**	**# Alkene Groups**	**# Nitrate Groups**	**# Nitrile Groups**	**# Methyl Groups**	
0	0	0	1	0	0	0	