US EPA Information Collection Rule

Base Analysis Document: GAC Studies

July 20, 2000

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2. Introduction

The *Base Analysis Document: GAC Studies* is part of the documentation package for the *ICR Treatment Study Database*. The term "base analysis" refers to the review, analysis and reduction of the raw data from each study to generate a standard set of data elements that are consistent across all GAC studies. For the majority of users, the output from the base analysis will be more relevant and useful than the raw data. Furthermore, the standard data elements developed during the base analysis are managed in a relational database which provides the user with a platform for more sophisticated analyses. For users that are interested in the raw data, the reviewed *Data Collection Spreadsheets* can be accessed through the *TS Data Library* module of the database (USEPA, 2000).

The *ICR Treatment Study Database* is a relational database designed to manage and organize the complex data sets generate by the 99 treatment studies conducted under the ICR. The raw data from these studies is managed in the *Treatment Study Data Library*, while the results from the base analysis are managed in either the *GAC Data Module* or the *Membrane Data Module*. These modules are described in more detail in the *User's Guide* for this database (USEPA, 2000).

The *GAC and Membrane Data Modules* are extremely powerful tools designed to support more sophisticated analyses by allowing users to sort and query the base analysis results in a variety of ways. These modules also perform calculations based on user defined breakthrough criteria, for GAC studies, or based on user defined blended water quality goals for membrane studies. To use this tool to its full potential, it is important to understand the assumptions and methodology used to conduct the base analysis.

The purpose of this document is to describe the base analysis approach used for GAC treatment studies. Section 3 provides some background on the GAC treatment studies, while Section 4 presents an overview of the analysis. Section 5 describes the review processes used to identify and correct erroneous data. Sections 6 through 8 present the details of the base analysis for GAC studies. The appendix contains the logic and variables used for the GAC calculation algorithm contained in the *ICR Treatment Study Database*.

3. Background

Sixty-three of the 99 studies conducted under the ICR, evaluated GAC technology. GAC treatment studies were conducted at bench-, pilot-, or full-scale in accordance with the procedures outlined in the *ICR Manual for Bench- and Pilot-Scale Treatment Studies* (USEPA, 1996a).

Bench-scale studies were performed using the rapid small-scale column test (RSSCT) a column test designed to maintain similitude to full-scale GAC adsorbers. The operation time of the RSSCT is typically 5 to 20 percent of that for a pilot-scale column, because the GAC used in the RSSCT is ground to a smaller size. The relationship between RSSCT and full-scale empty-bed contact time (EBCT), hydraulic loading rate, and operation time is proportional to the ratio of GAC particle sizes used. The standard experimental design for RSSCT studies included operating two columns, at full-scale equivalent EBCTs of 10 and 20 minutes, during each of four quarterly sessions designed to capture seasonal variability in water quality. Each column was typically operated until 70 percent total organic carbon (TOC) breakthrough was achieved, i.e., the effluent TOC concentration had met or exceeded 70 percent of the average GAC influent TOC concentration. Other criteria for column termination are described in the *ICR Manual for Bench- and Pilot-Scale Treatment Studies* (USEPA, 1996a).

Pilot-scale GAC study protocol involved testing at two EBCTs, 10 and 20 minutes. One pilot run at each EBCT was usually sufficient, however, a second pilot study at each EBCT was required if the initial study run length for the 20 minute EBCT contactor was shorter than 4,000 hours. One full-scale study, which examined a 15 minute EBCT, was accepted by USEPA.

The distribution of the 63 GAC studies by protocol and source water type is shown in Table 3-1. Eleven studies were conducted on groundwater sources and 52 on surface water sources. The 63 GAC studies included 44 bench-scale studies, 18 pilot-scale studies and 1 full-scale study.

Table 3-1. Distribution of ICR GAC treatment studies

Study Protocol	Total	Surface Water	Groundwater
RSSCT	44	36	8
Pilot-Scale	18	15	3
Full-Scale	1	1	0

Successful application of the RSSCT has been shown to yield breakthrough profiles similar to pilot-scale runs (USEPA, 1996a). Unlike a long-term pilot-scale GAC run, seasonal variability in water quality or treatment cannot impact a single RSSCT run, due to the use of a single batch

influent water. However, the impact of seasonal variability on GAC performance can be observed by conducting quarterly RSSCT runs, as required by the ICR.

Some source waters tested, such as ground waters, were shown to have limited seasonal variability. In these cases, some utilities chose to investigate other parameters, such as additional EBCTs, pretreatment impacts, or other GAC types. These non-standard study designs were usually performed using RSSCTs, although some pilot-scale studies also investigated additional parameters.

The data collected for each parameter during a single RSSCT or pilot-scale run yields a breakthrough profile. In this form, the data represents the relative performance of GAC for disinfection byproduct (DBP) precursor removal. Efficient full-scale GAC operation, however, is achieved by operating multiple GAC contactors in parallel, with staggered reactivation cycles, and blending the effluents of all contactors prior to disinfection. During this mode of operation, termed "blended contactor operation" or "effluent blending," individual contactors can be operated past the point at which the effluent they produce exceeds the treatment objective.

A runtime to a given treatment objective determined by a single contactor breakthrough curve will underestimate the runtime that can be achieved through blended contactor operation. However, the data produced by a single contactor study can be modeled to estimate runtimes under blended contactor operation. The *GAC Data Module* in the *ICR Treatment Study Database* allows for user queries based on blended contactor operation. This is explained in more detail in Section 8.

4. Overview of Data Analysis

Over the course of a GAC study, a significant amount of influent and effluent water quality data was collected. This data demonstrates the ability of GAC to remove DBP precursors as a function of operation time. In most cases, the data also provides a comparison of GAC performance at 10 and 20 minute EBCTs. Some studies evaluated the impact of pretreatment, GAC type, and influent pH on GAC performance.

The GAC base analysis included an analysis of influent water quality and effluent breakthrough data. Every water quality parameter measured during every GAC run yielded a breakthrough curve. In order to create a data set that can be easily queried based on runtime or treatment objective criteria, all breakthrough data was modeled and fit to a logistic function model. The standard form of the logistic function model results in a relationship between concentration and runtime. The inverse form of the equation was developed to provide a direct calculation of runtime as a function of concentration.

To provide a higher rate of successful curve fits, and to limit the impact of deviant observations on model results, an outlier identification procedure was performed, to statistically identify data outliers. These outliers were "winsorized," a procedure that involves replacing the datapoint value with a new value closer to the best-fit. By doing so, the impact of outlier data points on curve fits was reduced without removing the datapoints. Through an expert-level review, "extreme outliers" that would have adverse effects on the curve fit process were removed prior to curve fitting.

In practice, GAC contactors can be operated more efficiently by blending the effluent streams from multiple contactors operated in parallel, with staggered GAC replacement or reactivation intervals. This mode of operation is termed "effluent blending" or "blended contactor operation." Since the data generated by every treatment study performed resulted in breakthrough curves representing single GAC contactors, a model was utilized to estimate the integral breakthrough curve, a relationship between blended effluent water quality and contactor runtime. When operated in this mode, each contactor can be on-line past the point at which their individual effluents meet the treatment objective, since the treatment objective must be maintained in the blended effluent.

An important goal during data analysis was to determine the blended contactor breakthrough curve for every parameter analyzed during all GAC runs. Users of the *Treatment Study Database* can query the results of the studies to determine blended contactor runtime (the runtime of each individual contactor when operated as one of multiple contactors in parallel with staggered GAC replacement or reactivation intervals) based on a blended effluent water quality objective, or blended water quality at a given blended contactor runtime. This was accomplished using the surrogate correlation approach (SCA). The SCA method is based on using the total organic carbon (TOC) integral breakthrough curve, a relationship between single contactor runtime and blended contactor TOC. Data points on both the single contactor and integral breakthrough curves at a given TOC concentration are mapped, and all other water quality

parameters associated with the single contactor effluent data set at that TOC concentration are applied to the blended effluent curve. A detailed explanation of the SCA is given in Section 8.

5. Data Review

In order to ensure that the data used in this analysis was complete and accurate, the following review process was implemented: 1.) the raw data was reviewed upon receipt from the utility; 2.) the data was reviewed to identify outliers prior to analysis; 3.) the results of the base analysis were reviewed; and 4.) the data uploaded to the database was reviewed. Errors were identified and corrected through this multi-tiered review approach minimizing the propagation of errors and greatly improving the accuracy of the information in the database. The following section describes each of these review processes.

Utilities reported the data from their studies using standard *Data Collection Spreadsheets*, thus the data from all studies using the same testing protocol was submitted in the same format (USEPA, 1997). This facilitated the development of a spreadsheet tool that allowed the following checks to be performed on the raw data:

- Verify that the data has been reported in the proper tables in the *Data Collection Spreadsheets.*

- Verify that all calculations in the *Data Collection Spreadsheets* were performed correctly. Specific calculation checks include GAC particle size, GAC mass, and scaling calculations for RSSCTs, as well as THM and HAA class sums. GAC process design parameters were also reviewed.

- Review the reported test conditions for the simulated distribution system (SDS) procedure. Utilities were asked to verify SDS tests with reported conditions that were inconsistent with chlorination chemistry or that varied greatly from the target or average conditions. In cases where it was verified that the SDS test was not performed correctly, all disinfection byproduct (DBP) data associated with that test was rejected and not used in subsequent analyses. Furthermore, all DBP data associated with any SDS test for which a chlorine residual was reported below the minimum reporting level (MRL) was rejected.

- GAC influent and effluent water quality data was reviewed as time series plots (concentration against operation time) to help identify possible errors. This review included all water quality parameters, including DBP surrogates, DBP class sums, and DBP species. Utilities were asked to verify data that was flagged as potential outlier data during this review.

- Atypical breakthrough profiles were flagged and utilities were asked to verify data that yielded unusually-shaped breakthrough curves.

- For pilot-scale studies, GAC effluent water quality data was also plotted on a normalized basis (percent of influent concentration) to provide another qualitative level of review. This

form of plotting the data is useful when influent water quality data is variable, as may occur during pilot runs.

- The total operation time of the 10 and 20 minute EBCT runs was compared to verify that the 20 minute EBCT run was approximately double that for the 10 minute EBCT run. In cases where this expected trend was not observed, utilities were asked to provide an explanation for this result.

- For RSSCT studies, GAC effluent water quality data (not including brominated DBP compounds) that exceeded the measured GAC influent data were flagged. Utilities were asked to verify these data.

- GAC run length was reviewed to determine if appropriate run termination criteria were utilized. If 70 percent TOC breakthrough, or the alternate run termination criteria, was not achieved, the utility was asked to explain the reason for early run termination.

These reviews generated checklists that were sent to the utility responsible for the study. The utility was asked to supply missing information and verify possible errors. The range of problems identified during this review varied greatly over the 63 studies. The review of some studies identified only a few minor problems, while other studies required multiple reviews to correct all deficiencies and verify all questionable data. During this process, many problems were corrected that would have otherwise gone undetected during subsequent data review and analysis.

5.1. Review of Study Data for Outliers

After the utilities made corrections to their raw data, the *Data Collection Spreadsheets* were finalized and electronically protected. However, in cases where utilities did not have a justification for removing questionable data, i.e., there were no known QC failures or experimental errors to justify removal of the data, outlier data still remained in the finalized spreadsheets. The second step of the review process focused on the identification and removal of these outlier data.

Using an automated spreadsheet tool, breakthrough curves were generated for all water quality data (including DBP surrogates, DBP class sums, and DBP species). The breakthrough curve sets for all studies were subjected to two levels of qualitative review. During the initial review, extreme outliers were identified. Outliers confirmed by a second level expert review were removed.

As described in Section 8, the breakthrough curve data generated for each parameter during each run was condensed by fitting it to a logistic function model. This procedure was performed by SAS software and included a systematic outlier determination procedure. Indiscriminate deletion

of deviant observations can cause goodness of fit measures (i.e., R^2) to be unrealistically high. Rather than deleting potential outliers, suspect observations were replaced by less extreme values by the following procedure (USEPA, 1999):

1. Fit the logistic function model to the observed data and determine approximate 95 percent prediction limits on the observations.

2. Observations that exceed the threshold "*Predicted* $\pm$ *(U95 - L95)*K*" were adjusted to "*Predicted* $\pm$ *(U95 - L95)*K*," where U95 is the upper 95 percent confidence limit and L95 is the lower 95 percent confidence limit. The constant K determines the magnitude of the adjustment, with larger values of K corresponding to fewer declared outliers and smaller adjustments to those that are detected. The value for the constant K was set to 1/3 based on simulation results that indicated a good balance between false alarms and power to identify substantial outliers (>3 standard deviations from the best-fit prediction). Approximately 2.5 percent of the data were identified as outliers and adjusted by this procedure.

3. Refit the logistic function model using the dataset containing adjusted values.

As a final level of review, all SAS curve fits were subjected to an expert-level review. This review step is necessary since it is possible to obtain convergence on a solution that does not accurately reflect the trend of the data. In some cases, this was caused by an outlier that has a strong impact on the best-fit of the data set. These outliers were removed so that the dataset could be re-fit successfully. A summary of the issues identified during the raw data and outlier reviews and a count of the outliers identified and removed prior to analysis for each study is documented in the *Graphical Summary File* in the *Treatment Study Data Library* (USEPA, 2000). Of the total number of data points, 0.14 percent were identified as outliers and removed. In a few cases, the entire breakthrough curve for one or more analytes was removed from further analysis and inclusion in the database after expert review: 1.5 percent of all breakthrough curves were rejected.

5.2. Review of Base Analysis Results

Upon completion of the GAC study base analysis, the results were reviewed with respect to accuracy and reasonableness. To ensure accuracy, the data extractions from the *Data Collection Spreadsheets* that were used in the base analysis were compared with the source data. In the case of discrepancies, the data extractions were corrected and the base analysis was repeated. An expert review of the base analysis output was performed to verify that the results were reasonable. During this expert review, the results of the base analysis were evaluated in the context of the expected performance of GAC treating water of a certain quality. DBP concentrations formed upon chlorination in the GAC influent and effluent were assessed with respect to the chlorination conditions and precursor levels in the waters. Finally, the results of the base analysis were compared with the results of analyses performed by the utility or

consultant that conducted the study. Any major discrepancies were documented in the *Graphical Summary File* in the *Treatment Study Data Library* (USEPA, 2000).

5.3. Review of Data Uploaded to the Database

The results of the base analysis were uploaded to the *ICR Treatment Study Database*. To ensure the accuracy of the upload process, the results in the database table were cross-checked against the upload files generated during the base analysis process. Spreadsheet tools were developed to assist in this review and resulted in a direct verification of most of the uploaded data.

6. Treatment Study Run Determination

One of the primary objectives of the base analysis was to reduce the large, complex data sets from each treatment study to data and information that could be managed in a database structure. The basic unit of structure is a treatment study run, and each run was assigned a corresponding treatment study run identification number (TSRunID). Typically, each individual GAC run was assigned a unique TSRunID. Most bench-scale GAC treatment studies are comprised of 8 TSRunIDs, while pilot-scale studies are typically comprised of 2 or 4 TSRunIDs. In isolated cases, two TSRunIDs were assigned to one GAC run. This was done when it was determined by expert-level review that GAC pretreatment conditions changed significantly after a point in the run, requiring that the data be divided into two separate TSRunIDs.

The treatment study run designations are critical elements of the base analysis since they defined the bounds over which data was analyzed and summarized. In the *Treatment Study Database*, the TSRunID is the field that links all of the data from a specific treatment study run, i.e., the TSRunID is the primary key in many database tables. The following sections summarize the analyses conducted on the GAC study data, and unless noted otherwise, all analyses were conducted on data within a given TSRunID.

7. Data Summaries for GAC Studies

7.1. Influent Water Quality

A statistical summary of the influent water quality data was generated for each TSRunID, including the average, standard deviation, and 25th, 50th and 75th percentiles for each parameter. If "null" records are displayed for an influent water quality parameter, either the parameter was not measured during the study, or the data for that parameter was removed during one of the reviews discussed in Section 5.

Statistics for the following influent water quality parameters are included in the Influent Water Quality table of the database: temperature, pH, alkalinity, total hardness, calcium hardness, ammonia, bromide, TOC, UV-254, TSUVA, SDS-chlorine demand, SDS-TOX, SDS-THM4, SDS-HAA5, SDS-HAA6, SDS-HAA9, SDS-CHCl3, SDS-BDCM, SDS-DBCM, SDS-CHBr3, SDS-MCAA, SDS-DCAA, SDS-TCAA, SDS-MBAA, SDS-DBAA, SDS-BCAA, SDS-TBAA, SDS-CDBAA, and SDS-DCBAA.

7.2. Summary of SDS Conditions

A statistical summary of the SDS chlorination conditions was generated for each TSRunID, including the average, standard deviation, and 25th, 50th and 75th percentiles for each parameter. If "null" records are displayed for a SDS parameter, either the parameter was not measured during the study, or the data for that parameter was removed during one of the reviews discussed in Section 5.

Statistics for the following SDS parameters are included in the Simulated Distribution System Conditions table of the database: SDS incubation time, SDS incubation temperature, SDS pH and SDS free chlorine residual.

The statistics reported in the database were calculated from all GAC influent and effluent SDS conditions reported during a specific TSRunID. The influent and effluent SDS data were combined in this manner since the same target SDS conditions were used for both influent and effluent samples.

Utilities were asked to report the measured chlorination conditions for each SDS test conducted; however, some utilities did not have this data available and reported the target SDS conditions instead. In the database, target SDS conditions will have a standard deviation equal to 0.00. However, the converse is not necessarily true: a standard deviation of 0.00 does not necessarily imply that target conditions were reported. For example, the use of a temperature incubator may allow all SDS tests to be conducted at the same temperature within the precision of temperature measurements.

7.3. Summary of GAC Pretreatment Process Information

Detailed information for the pretreatment processes used prior to GAC treatment was provided in the *Data Collection Spreadsheets.* However, standard nomenclature and abbreviations were not used, and this would limit a user's ability to query this information across studies in a meaningful manner. To correct this deficiency, the pretreatment data for each TSRunID was summarized using standard nomenclature.

The first step of this process was the extraction of the raw pretreatment information from the *Data Collection Spreadsheets.* The raw data was analyzed to determine standard process names, process chemicals, and dosing units for each process. Typically, the detailed process description was not modified during this analysis. A standard pretreatment code was also assigned to the entire process train used for each TSRunID. For example, the pretreatment code "CONV" was used as an abbreviation for conventional treatment: the combination of coagulation, flocculation, sedimentation and filtration processes.

Once the pretreatment information was standardized, the process name, process description, chemical name, chemical dose, chemical dose units and pretreatment code were uploaded to the Pretreatment Information table of the database. A concatenated (combined) version of the pretreatment information was also generated and uploaded to the GAC Study Design table of the database.

7.4. Summary of Field QA/QC Data

During the treatment studies, utilities were required to collect and analyze duplicate samples for all parameters monitored during the study. These duplicates are referred to as field duplicates. For each pair of field duplicate data (i.e., the primary and duplicate values), a relative percent error (RPE_FDup) was calculated according to Equation 7-1:

$$RPE\_FDup = (|C_1 - C_2| / C_1) \times 100\% \qquad \text{Equation 7-1}$$

where C_1 is the concentration of the primary sample and C_2 is the concentration of the duplicate sample.

RPEs for field duplicates were only calculated when values for both the primary and duplicate samples were reported and detected above the MRL. If either the primary or the duplicate sample or both were below the MRL, then the RPE_FDup was not calculated for the data set.

A statistical summary of the field duplicate RPE data was generated for each water quality parameter for each study. The statistical summary includes the count, average, standard deviation, and 25^{th}, 50^{th} and 75^{th} percentiles for each parameter. A record for a given parameter in a study may be "null" for any one of the following reasons: 1) the parameter was not measured during the study; 2) data for that parameter was removed during the review process; 3) duplicate

analyses were not performed for that parameter; or 4) no values were measured above the MRL for that parameter.

The statistics reported in the database were calculated from all influent and effluent field duplicate RPE data collected for a given water quality parameter. Unlike other parameters that are summarized over a TSRunID, the field duplicate RPE data is summarized over the entire study. The protocol for bench-scale GAC studies required taking several influent samples evenly-spaced over the course of the study. The RPE data includes these samples treated as field duplicates since they were taken from a batch influent. Field duplicates were taken at evenly-spaced intervals in the effluent to bench-scale studies. For pilot- and full-scale studies, field duplicates were taken at evenly-spaced intervals in both the influent and effluent to the GAC contactor.

Statistics for RPE field duplicate data are included in the Field Duplicate QA/QC Data table of the database for the following water quality parameters: alkalinity, ammonia, bromide, calcium hardness, HAA5, HAA6, HAA9, pH, SDS-BCAA, SDS-BDCM, SDS-CDBAA, SDS-CHBr3, SDS-CHCl3, SDS-Cl2 Residual, SDS-DBAA, SDS-DBCM, SDS-DCAA, SDS-DCBAA, SDS-MBAA, SDS-MCAA, SDS-TBAA, SDS-TCAA, SDS-TOX, temperature, THM4, TOC, total hardness, turbidity and UV_{254}.

7.5. Summary of Analytical QA/QC Data

Laboratories performing analyses in support of the ICR treatment studies were required to perform QC analyses on many of the parameters monitored during the studies (USEPA, 1996b). Specifically, laboratories were required to analyze analytical duplicates, laboratory fortified matrix spike samples, and performance evaluation (PE) samples. Analytical duplicates were performed by conducting a primary and a duplicate analysis on a single sample, and calculating the relative percent error (RPE_ADup) according to Equation 7-2:

$$RPE\_ADup = (|C_1 - C_2| / C_{Avg}) \times 100\% \qquad \text{Equation 7-2}$$

where C_1 is the result from the primary analysis, C_2 is the result from the duplicate analysis, and C_{Avg} is the average of C_1 and C_2.

Laboratory fortified matrix spikes were conducted by adding a know quantity of the method analyte to a sample and measuring the concentrations of the analyte in both the fortified and unfortified samples. The difference between the concentrations of these two samples is the measured fortifying concentration. The percent recovery for laboratory fortified matrix spike samples (PR_LMS) was calculated according to Equation 7-3:

$$PR\_LMS = (C_M / C_T) \times 100\% \qquad \text{Equation 7-3}$$

where C_M is the measured fortifying concentration and C_T is the true fortifying concentration.

PE samples were supplied by a third party (typically USEPA for the ICR treatment studies), and the concentration of these samples was unknown to the laboratory. The PE samples were analyzed, and the measured concentration was reported to the third party. The percent recovery for the PE samples (PR_PE) was calculated according to Equation 7-4:

$$PR\_PE = (C_M / C_T) \times 100\% \qquad \text{Equation 7-4}$$

where C_M is the measured concentration of the PE sample and C_T is the true concentration of the PE sample.

Values for all of these QA/QC parameters were only calculated when the analyte was measured above the MRL. Results below the MRL typically only occurred for analytical duplicates, and if either the primary or the duplicate sample or both were below the MRL, then the RPE_ADup was not calculated for the data set.

Laboratories reported a statistical summary for each QA/QC parameter for each analyte that was measured. Normally, the QA/QC information was summarized over each study that the laboratory supported. However, four laboratories, CA013, FL029, OR001, and VA001, reported statistics summarizing the QA/QC data over all studies that the laboratory supported.

For any study, the QA/QC data for a specific water quality parameter is associated with one laboratory, one analytical method and one MRL. When more than one laboratory, method or MRL was used for an analyte during a study, multiple sets of QA/QC data are reported for that analyte.

The statistical summary includes the count, average, standard deviation, and 25^{th}, 50^{th} and 75^{th} percentiles for each QA/QC parameter. A record for a given parameter in a study may be "null" for any one of the following reasons: 1) the parameter was not measured during the study; 2) the QA/QC analysis was not performed for that parameter; 3) the QA/QC data was not available for that parameter, or 4) no values were measured above the MRL for that parameter. Additionally, percentiles were not reported for records in which the count was less than six, and the standard deviation was not reported for records in which the count was less than two.

Statistics for QA/QC data are included in the database for the following water quality parameters: bromide, HAA5, HAA6, HAA9, SDS-BCAA, SDS-BDCM, SDS-CDBAA, SDS-CHBr3, SDS-CHCl3, SDS-DBAA, SDS-DBCM, SDS-DCAA, SDS-DCBAA, SDS-MBAA, SDS-MCAA, SDS-TBAA, SDS-TCAA, SDS-TOX, THM4, TOC, and UV-254.

8. GAC Breakthrough Curve Fitting: Logistic Function Model

8.1. Overview and Background of GAC Breakthrough Curve Modeling Approach

To effectively condense the large amount of data generated during each GAC run, breakthrough curve profiles were modeled using a modified version of the logistic function. The logistic function has previously been used to model GAC breakthrough curves and is a suitable model due to the characteristic 'S' shape of most breakthrough curves. Modifications to the logistic function were developed to improve its performance for modeling single contactor data. Curve fitting involved determining which model was applicable based on characteristics of the breakthrough curve, and applying the appropriate model to the breakthrough curve for each parameter. The values determined for the logistic function model coefficients were uploaded to the treatment studies database. These enhanced forms of the logistic function model were able to successfully fit single contactor breakthrough curve data for all parameters, including DBP surrogates, DBP sum class parameters, and individual DBP species. A method was also employed to detect outlier data points and to limit the influence of these deviant observations on the parameter estimates (USEPA, 1999).

A thorough evaluation of the modeling approach used for the GAC treatment studies data is contained in *Analysis of GAC Effluent Blending during the ICR Treatment Studies* (USEPA, 1999). This report describes in detail the background, approach, methods used, results, and specific results obtained on application of the logistic function model to GAC breakthrough data.

Chowdhury et al. (1996) and Summers et al. (1998) applied the following form of the logistic function to model experimental GAC breakthrough data:

$$C(t) = \frac{A_f}{1 + Be^{-Dt}} \qquad \text{Equation 8-1}$$

where $C(t)$ is the effluent concentration at single contactor runtime, t. The values for A_f, B, and D are determined experimentally by a best-fit to the breakthrough data. The parameter A_f represents the level to which the function approaches asymptotically. Parameters B and D affect the shape of the curve. Equation 8-1 was found to adequately fit GAC breakthrough curves for three water sources and the parameters TOC and formed total THM. With a few modifications, as described in Section 8.2 below, Equation 8-1 served as a basis for modeling of the ICR GAC treatment study single contactor breakthrough curves.

8.1.1. Modeling Approach to Simulate Multiple Contactors Operated in Parallel-Staggered Mode

When GAC contactors are utilized for DBP precursor control, multiple contactors can be used more efficiently when operated in parallel with staggered GAC replacement cycles (parallel-staggered operation mode), whereby the effluents of all contactors are blended prior to disinfection. By doing so, individual contactors can be operated past a point at which their effluent meets a given treatment objective, because the treatment objective must only be maintained in the blended effluent of all contactors.

In modeling the operation of multiple contactors operated in parallel-staggered mode, the goal is not to simulate the actual blended effluent water quality during normal operation, but to derive the integral breakthrough curve. The integral breakthrough curve is a tool used to determine the GAC replacement frequency for each individual contactor that will maintain the blended effluent below the treatment objective: *it is a curve that relates single contactor runtime to blended contactor effluent water quality.* Multiple contactor throughput to a treatment objective can be estimated from the integral breakthrough curve by determining the operation time when the curve intersects the treatment objective, as is done with single contactor breakthrough curves.

The *GAC Data Module* of the *ICR Treatment Study Database* includes the capability of calculating blended contactor runtimes based on a user-defined parameter and concentration, or calculating blended contactor water quality given a user-defined blended contactor runtime.

A time-averaged mathematical integration of the function that describes the breakthrough curve yields the integral breakthrough curve, as it describes the average value of the function at any point in time. Estimating blended contactor runtimes by integration of the single contactor breakthrough curve is termed the direct integration (DI) approach. See the *GAC Effluent Blending Report* (USEPA, 1999) for more details on the procedures and assumptions of this approach.

Theoretically, the direct integration approach is a reliable method for estimating blended effluent water quality. However, during development of the analysis approach for the ICR GAC treatment study data, the treatment study technical work group (TS-TWG) determined that it would be computationally intensive to apply the DI approach to the large number of breakthrough curves (7,700) comprising the ICR treatment study data set. Furthermore, the DI approach may be less reliable for breakthrough curves that do not follow the typical "S" pattern, such as "peak" curves or sharp "S" shaped curves followed by a plateau. For these reasons, another approach for estimating blended effluent water quality from single contactor data was developed for analysis of the ICR treatment study GAC data, as described in the Section 8.1.2.

8.1.2. Surrogate Correlation Approach

The surrogate correlation approach (SCA) was developed by the TS-TWG as an alternative to the direct integration approach for developing the integral breakthrough curve. This approach

simplifies and reduces the amount of computations necessary to estimate DBP formation in the effluent of blended GAC contactors. The SCA method is based on the assumption that the relationship between TOC and all other parameters (UV_{254} and SDS-DBPs) in the single contactor effluent is maintained in the blended effluent. In other words, the concentration and speciation of DBPs formed after chlorination of the blended effluent of multiple contactors with a given TOC concentration is the same as that formed after chlorination of the single contactor effluent with the same TOC concentration.

This method of estimating blended effluent water quality from single contactor data requires that an integral breakthrough curve be developed from the single contactor TOC breakthrough curve only. Once this curve is known, along with a relationship between TOC and all other parameters in the single contactor effluent, integral breakthrough curves are estimated for all other parameters. This approach not only allows for the evaluation of blended contactor runtimes to various breakthrough criteria, but also for the occurrence of other DBPs at that runtime. For example, this would allow for the assessment of whether or not regulating one DBP or DBP group can effectively control the occurrence of other DBPs or DBP groups.

An example of the SCA procedure is described in the steps below and summarized graphically in Figure 8-1.

1. Select a treatment objective (e.g., THM4 = 32 µg/L).

2. Use the single contactor breakthrough curve for the parameter of interest and determine the single contactor runtime (RT_{SC}) at which the treatment objective is exceeded.

3. Use the RT_{SC} from Step 2 to determine the concentrations of all other parameters from the single contactor breakthrough curves. (In this step, the single contactor effluent concentrations of all parameters are "linked" through the single contactor runtime, RT_{SC}).

4. Use the RT_{SC} from Step 2 to determine the single contactor effluent TOC concentration that corresponds to the treatment objective.

5. From the integral TOC breakthrough curve, calculated by the DI approach, determine the blended contactor runtime (RT_{BL}) to reach the TOC concentration calculated in step 4. This is the only point in the analysis where it is necessary to apply the DI method to establish an integral breakthrough curve, and only the TOC integral breakthrough curve is required. Extrapolation of the TOC integral breakthrough curve to 150 percent of t_{ub}, the upper bound on single contactor runtime, allows more of the single contactor information to be used when evaluating blended contactor breakthrough criteria.

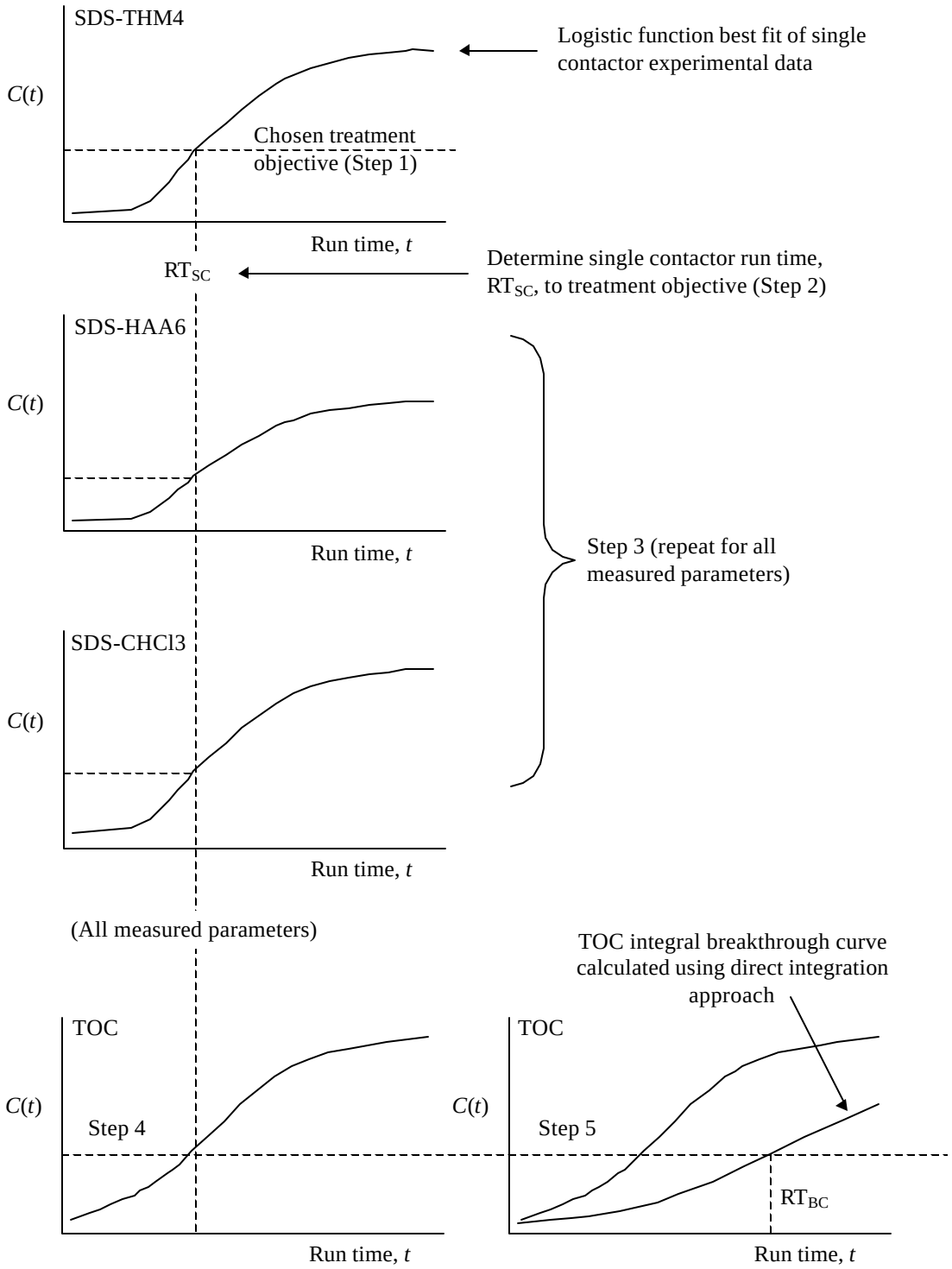


Figure 8-1. Graphical summary of SCA procedure used for base analysis of GAC treatment studies

This analysis makes the following assumptions:

1. The logistic function model can accurately describe the breakthrough of DBP precursors and DBP precursor surrogates.

2. The relationship between TOC and DBP precursors (concentration and speciation) observed in the single contactor effluent is maintained in the blended effluent.

3. The TOC breakthrough curve can be extrapolated by 150 percent with reasonable results.

4. The TOC integral breakthrough curve accurately predicts the blended water quality of an infinite number of multiple contactors operated in parallel-staggered mode. Furthermore, the TOC integral breakthrough curve based on an infinite number of contactors is a reasonable approximation to a finite numbers of contactors.

The *GAC Effluent Blending Report* (USEPA, 1999) includes verification of these four assumptions.

8.2. Logistic Function Model

For every curve fit performed, Table 8-1 describes the parameters that are uploaded to the curve fit parameter table of the database.

Table 8-1. Curve fit parameters contained in the database

Parameter	Description
TSRunID	Treatment study run identification number
Chem	Measured parameter
CoefA0	Value for logistic function model parameter A_0 for a single contactor breakthrough curve
CoefAf	Value for logistic function model parameter A_f for a single contactor breakthrough curve
CoefB	Value for logistic function model parameter *B* for a single contactor breakthrough curve
CoefD	Value for logistic function model parameter *D* for a single contactor breakthrough curve
t_lb	Lower bound on time of single contactor breakthrough curve
t_ub	Upper bound on time of single contactor breakthrough curve
t_{max}	Time at which maximum GAC effluent concentration (C_{max}) occurs for a single contactor breakthrough curve
t_0	Point at which breakthrough curve exceeds a concentration of zero.
S	Slope of linear portion of the logistic function model. The value of S is always zero or negative. If zero, the linear decreasing portion of the curve is not applied.
Flag1	Default value for flag 1 ("No").
Flag2	Default value for flag 2 ("No").
Flag3	Default value for flag 3 ("No").
Flag4	Default value for flag 4 ("No").
BL_B	Value for logistic function model parameter *B* for blended contactor breakthrough curve
BL_D	Value for logistic function model parameter *D* for blended contactor breakthrough curve
BL_lb	Lower bound on time of blended contactor breakthrough curve
BL_ub	Upper bound on time of blended contactor breakthrough curve

The parameters listed in Table 8-1 are used with closed form equations to calculate both single and blended contactor effluent concentrations, and both single and blended contactor runtime, based on a user defined breakthrough criteria. The treatment study database contains a dynamic system of equations that allows the user to evaluate any breakthrough criteria for maximum flexibility.

The equations contained in the database are based on the following three functions, which allow every breakthrough dataset contained in the database to be modeled for dynamic output.

$$C(t) = 0 \qquad t_{lb} \le t < t_0 \qquad \text{Equation 8-2}$$

$$C(t) = \frac{A_f}{1 + Be^{-Dt}} + A_0 \qquad t_0 \le t \le t_{max} \qquad \text{Equation 8-3}$$

$$C(t) = C_{\max} + S(t - t_0) \qquad t_{max} < t \le t_{ub} \qquad \text{Equation 8-4}$$

where A_0, A_f, B, and D are the logistic function parameters, $C(t)$ is the single contactor effluent concentration at time t, t_{lb} is the lower bound on runtime, t_{ub} is the upper bound on runtime, t_0 is the point at which the equation result is greater than zero, t_{max} is the point of maximum concentration, C_{max}, and S is the slope of the linear equation.

Equations 8-2, 8-3, and 8-4 comprise the step-lag-peak logistic function model. A detailed description of this model is contained in *GAC Effluent Blending Report* (USEPA, 1999). Depending on the values of t_0 and t_{max} relative to t_{lb} and t_{ub}, the step-lag-peak logistic function model simplifies to the step-lag logistic function model or the step logistic function model. For example, if $t_{max} = t_{ub}$ for a given parameter, Equation 8-4 does not apply, as there is never a point on the breakthrough curve when the value for the runtime, t, is between t_{max} and t_{ub}. Therefore, the model employed to describe the breakthrough curve would be the step-lag logistic function model, comprised of Equations 8-2 and 8-3.

Through the *GAC Data Module*, the user is able to perform runtime and concentration based queries. For a single contactor concentration based query, the user can either input a value or request the maximum concentration for a given parameter. There are lower and upper runtime bounds associated with every breakthrough curve, and it is important that the user understand the impact of these bounds (when they are exceeded) on the output of database calculations. For the purposes of this discussion, "target parameter" is the parameter for which the query is being performed, and "selected parameter" is any other parameter (selected by the user) for which data calculation results will also be provided. Various flags can be tripped after a query, and a description of these flags is contained in the Appendix to the *ICR Treatment Study Database User's Guide*. An abbreviated discussion of flags is contained in the appendix to this document, and in the *GAC Data Module* of the *ICR Treatment Study Database.*

When the runtime queried for a target parameter is less than the lower bound on runtime, t_{lb}, or greater than the upper bound on runtime, t_{ub}, the runtime bound value will be returned. For example, if the value of t_{lb} for TOC is 5 days, and queried runtime is 3 days, a value of 5 days will be returned, as well as the TOC concentration at 5 days. Once the runtime is determined for the target parameter within each TSRunID (based on a runtime or concentration query), this runtime is used to provide data for the selected parameters. If this runtime is outside the bound set for a selected parameter, a value of 99999 is returned for the selected parameter. Thus, there is an important distinction in how the database handles runtimes out of bounds for the target and selected parameters.

The bounds for concentration are determined by the calculated values of C_{min}, the minimum concentration, and C_{max}, the maximum concentration, for each breakthrough curve. When the target concentration is greater than C_{max}, the concentration at C_{max} is returned, along with the runtime at the maximum concentration, t_{max}. For some curve fit types, the maximum concentration occurs prior to the end of the breakthrough curve, so the runtime returned in this case will not always necessarily be equal to t_{ub}. The user may also query by the maximum concentration. The value of C_{max} and runtime t_{max} for the target parameter will be returned.

Within the *Blended Breakthrough Criteria Module,* blended contactor queries can be based on blended contactor runtime or concentration. The upper bound on runtime for the blended contactor breakthrough curve, RTbl_max, is 150 percent of t_{ub}. When the blended contactor runtime queried or the blended contactor runtime determined based on the concentration queried is greater than RTbl_max, a flag is tripped and the runtime returned is equal to RTbl_max. The concentrations of selected water quality parameters are determined based on the single contactor runtime corresponding to RTbl_max.

Within the *Single Contactor Breakthrough Criteria Module*, the blended contactor runtime can be selected for output. When the blended contactor runtime corresponding the single contactor runtime exceeds RTbl_max, a runtime value is not returned. Instead, a value of 88888.88 is returned to warn the user of this condition.

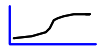
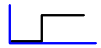
Due to the presence of peak curves, with increasing followed by decreasing concentrations, a runtime query could result in a calculated concentration that occurs after the peak. Therefore, the maximum concentration reached during the run already occurred. To warn the user that this has occurred, a flag is tripped under this condition. For a concentration based criteria, the database will return the runtime at the first occurrence of the target parameter. However, once the runtime is determined, it may fall on the decreasing leg of a peak function representing a selected parameter. When this occurs, the flag is tripped.

Further information on equation bounds, how these bounds impact database calculations, and the conditions under which flags are tripped can be found in the Appendix to this document and in the *Treatment Study Database User's Guide* (USEPA, 2000).

The following sections describe the eight curve fit types utilized for GAC breakthrough curves in the *ICR Treatment Study Database*. A summary of the eight curve fit types is included in Table 8-2. The robustness of the logistic function model described in Equations 8-2, 8-3, and 8-4 allowed for a variety of curve fit types, including standard logistic function fits, peak curves, and step functions, as described below.

In all cases, a best-fit of the logistic function model to the data was generated by least squares minimization approach. The coefficient of determination, R^2, was computed for all best-fits. The logistic function models were fit by non-linear least-squares using PROC NLIN in version

Table 8-2 Summary of logistic function model curve fit types

CFT	Name	Description	A_0	A_f	B	D	S	t_0	t_{max}	Percent of curve fits	Example
1	Standard Logistic Function Fit	Standard logistic function fit.	Any value	≥0	>0	>0	=0	≥0	$=t_{ub}$	63%	
2	Step-Lag-Peak Logistic Function Fit	Logistic function fit with decreasing linear fit after peak.	Any value	≥0	>0	>0	<0	≥0	$<t_{ub}$	9%	
3	Step Function	Step function, concentration = 0 until t_0, concentration = A_f after t_0.	0	>0	0	0	0	≥0	$=t_{ub}$	2%	
4	Step Function Followed by Decreasing Function	Step function followed by a plateau and then a linear decrease. Step begins at t_0. Linear decrease begins at t_{max}.	0	>0	0	0	<0	≥0	$>t_0$ and $<t_{ub}$	<1%	
5	Instantaneous Peak Followed by Decreasing Function	Step function followed immediately by a linear decrease. Step begins at t_0, $t_{max} = t_0 + 0.01$, and linear decrease begins at this point.	0	>0	0	0	<0	>0	$=t_0 + 0.01$	<1%	
6	Zero Fit	Flat line at concentration of zero.	0	0	0	0	0	0	$=t_{ub}$	14%	
7	Decreasing Linear Function	Decreasing linear function.	0	>0	0	0	<0	$<t_{lb}$	$=t_{lb}$	<1%	
8	Null Fit	No curve fit performed due to insufficient data reported, or insufficient data accepted for data analysis.	Null	Null	Null	Null	0	0	Null	11%	

6.12 of the SAS system (Littell et al., 1996). Additional details and SAS code are included in Appendix B of the *GAC Effluent Blending Report* (USEPA, 1999).

8.2.1. Curve Fit Type 1: Standard Logistic Function Fit

Curve Fit Type 1 (CFT1) is the standard logistic function fit, including the step and step-lag logistic function models. For CFT1, parameter $S = 0$ and $t_{max} = t_{ub}$, and therefore the linear portion of the model is not invoked. The maximum concentration, C_{max}, occurs at t_{max}. If $A_0 < 0$, then the curve may begin at a negative concentration. However, until t exceeds the value of t_0, the output is zero. The majority (63 percent) of GAC breakthrough curves were modeled utilizing CFT1.

8.2.2. Curve Fit Type 2: Step-Lag-Peak Logistic Function Fit

Many GAC breakthrough curves, especially those for brominated DBP species, are characterized by increasing and then decreasing concentrations. During data analysis, these breakthrough curves were fit using the step-lag-peak logistic function model: the step-lag logistic function captured the increasing portion of the curve, while a simple linear function (with slope S) captured the decreasing portion of the curve located after the peak concentration. In some cases, the linear portion of the curve yielded concentrations below zero. In these cases, negative concentrations were replaced with a value of zero. The point of maximum concentration, C_{max}, occurs at t_{max}, and $t_{max} < t_{ub}$. Three criteria were utilized during SAS curve fitting to identify peak curves:

1. The measured peak concentration, C_{max}, is at least 20 percent greater than the concentration at the last observed data point.

2. The runtime t_{max} is less than 80 percent of the upper bound on runtime, t_{ub}.

3. The data point corresponding to t_{max} is located prior to the penultimate observed data point.

These criteria were needed to decrease the number of false positive peak curve designations. Nine percent of the GAC breakthrough curves were classified and fit as CFT2 curves.

8.2.3. Curve Fit Type 3: Step Function

Many breakthrough curves, especially those for a parameter measured near its minimum reporting level (MRL), are characterized by several points with a concentration of zero (those reported below the MRL) followed by several points at a fairly constant value typically near the MRL. These curves were best captured by a step function model. The step function model was derived from the logistic function model by setting A_0, B, and D equal to zero. Equation 8-2 remains the same, while Equation 8-3 simplifies to:

$$C(t) = A_f \qquad t_0 \le t \le t_{max} \qquad \text{Equation 8-5}$$

For CFT3 curves, $S = 0$ and $t_{max} = t_{ub}$, so the decreasing linear function is not invoked. The step begins at $t = t_0$. Two percent of the GAC breakthrough curves were classified and fit as CFT3 curves. For the special case where $t_0 \le t_{lb}$, a constant value is returned for any runtime.

8.2.4. Curve Fit Type 4: Step Function Followed by Decreasing Function

In a few cases, a limited number of datapoints were measured above the MRL for a breakthrough curve, and these points were located in the middle of the dataset. Therefore, the data measured above the MRL were preceded and followed by data reported below the MRL. These instances were treated as a type of "peak" curve, but due to the "step" nature of the data and the limited number of points, a step function was used to fit a portion of the data, while a linear function with negative slope was used to fit the remainder of the dataset. As with CFT2 curves, the portion of the decreasing linear function that decreases below zero is reported as a concentration of zero. As with CFT3 curves, the step begins when $t = t_0$. Furthermore, $S < 0$, $t_{max} > t_0$, and $t_{max} < t_{ub}$. The decreasing portion of the curve begins at t_{max}. Less than 1 percent of all curve fits were classified as CFT4.

8.2.5. Curve Fit Type 5: Instantaneous Peak Followed by Decreasing Function

CFT5 is very similar to CFT4 except that $t_0 = t_{max}$. Thus, at the point at which the step function begins, there is no plateau, and the concentration immediately begins to decrease from this peak value. As with CFT4, $S < 0$ and $t_{max} < t_{ub}$. Less than 1 percent of all curve fits were classified as CFT5. Note, t_{max} was adjusted to a value slightly higher than t_0 (i.e., $t_{max} = t_0 + 0.01$) so that this special curve fit type would be compatible with the calculation logic.

8.2.6. Curve Fit Type 6: Zero Fit

For 14 percent of the curve fits, all data in the breakthrough curve were reported as below the MRL. This occurred most often for some DBP species, particularly MCAA and MBAA. In these cases, the logistic function model was required to return a concentration of zero for any value of t. This was achieved using the logistic function model by setting A_0, A_f, B, and D to zero. Values for S and t_0 were also set to zero, and $t_{max} = t_{ub}$.

8.2.7. Curve Fit Type 7: Decreasing Linear Function

On rare occasions, the highest measured value for a data set occurred at t_{lb}, the first measured value. For these cases, t_{lb} and t_{max} were set equal to the same value. The value for S was negative and equal to the slope of the best-fit linear function capturing the decreasing data. The value for t_0 was always less than t_{lb}, and usually equal to zero. As stated earlier for other curve fit types, when the result of the decreasing linear function becomes negative, the database outputs a value of zero. Less than 1 percent of all curve fits were classified as CFT7.

8.2.8. Curve Fit Type 8: Null Fit

For 11 percent of the data sets, data were either not analyzed for a parameter or not reportable due to quality control issues. For example, the analysis of CDBAA, DCBAA, and TBAA were not required, and therefore many studies did not report values for these parameters. In these cases, blank entries were entered for A_0, A_f, B, D, t_{lb}, t_{ub}, and t_{max}. The database will return null (blank) concentrations for these parameters.

8.2.9. Inverted Form of Logistic Function Model

Through the *GAC Data Module* of the *ICR Treatment Study Database*, the user can input a target effluent concentration, and receive as output the GAC single contactor runtime to that target concentration. The inverted form of the logistic function model is used to accomplish this, and is described in the Appendix.

8.3. Blended Contactor Model

The assumptions underlying the blended contactor model used in the database are described in detail in *GAC Effluent Blending Report* (USEPA, 1999). A critical assumption that database users should be aware of is that the blended contactor model assumes an infinite number of contactors on-line, operated in parallel with staggered reactivation cycles. In practical terms, the model is adequate (accurate within 10 percent) for a minimum number of 13 contactors. For 10 contactors on-line, the model is accurate within 12 percent. In both cases, the runtime determined by the model will be greater than the actual runtime for a finite number of contactors. The *GAC Effluent Blending Report* (USEPA, 1999) contains an analysis of the impact of number of contactors on model accuracy.

As described in Section 8.1.2, the SCA requires that an integral breakthrough curve be determined for TOC only. The step logistic function model was applied to all TOC breakthrough curves. Therefore, for TOC, $t_0 = 0$ and $t_{max} = t_{ub}$. The integral breakthrough curve for a step function is:

$$\overline{C}(t) = A_0 + A_f + \frac{A_f}{Dt}\ln\left(\frac{1+Be^{-Dt}}{1+B}\right) \qquad \text{Equation 8-6}$$

Further information on the derivation of this function is contained in *GAC Effluent Blending Report* (USEPA, 1999).

Typically, a linear or second order polynomial relationship exists between GAC effluent TOC concentration and any other parameter. The SCA method does not determine or use these correlations directly but instead assumes they exist and are constant in both the single contactor effluent and blended effluent. This relationship is exploited by linking the concentration of all water quality parameters at a common single contactor runtime (see Figure 8-1). Thus, once a single contactor runtime is defined for one parameter, the runtime can be used to determine the

corresponding concentrations of all other parameters. Using Equation 8-6, the integral breakthrough curve is calculated for the TOC single contactor breakthrough curve only. Then the single contactor TOC concentration is applied to the integral TOC breakthrough curve to determine the blended runtime at which an equivalent TOC concentration is reached.

In many cases, the blended contactor breakthrough curve for TOC must be extrapolated beyond t_{ub} in order to calculate a blended runtime to achieve a specific regulatory target. Extrapolation was accomplished simply by designating the upper bound on blended contactor runtime, RTbl_max, as 150 percent of t_{ub} for the single contactor TOC breakthrough curve. During the expert review process, all single contactor breakthrough curves for TOC were reviewed to ensure that extrapolation of the blended contactor breakthrough curve would be acceptable based on the shape of the single contactor breakthrough curve.

8.4. Data Modeling and Review Approach

8.4.1. SAS Output

After the initial review of the data was complete, as described in Section 5, the breakthrough curve datasets were ready to be modeled. The best-fit of the logistic function model to the data was generated by least squares minimization approach. The coefficient of determination, R^2, was computed for all best-fits. The logistic function models were fit by non-linear least-squares using PROC NLIN in version 6.12 of the SAS system (Littell et al., 1996). Additional details and SAS code are included in Appendix B of the *GAC Effluent Blending Report* (USEPA, 1999).

Due to the variety of breakthrough patterns observed, the following steps were incorporated into the SAS algorithm:

1. Count the number of observed datapoints. If the dataset contained fewer than 6 points with reported concentrations above the MRL, no curve fit was performed. SAS returned values of zero for A_0, A_f, B, D, t_0, and S.

2. Determine if a peak curve condition was true (see Section 8.2.2). If so, determine the best-fit using the step-lag-peak logistic function model. If not, determine the best-fit using step-lag logistic function model. All TOC breakthrough curves were by default fit to the step logistic function model.

3. Identify and winsorize outliers (see Section 8.4.2). If any data was winsorized, refit the dataset.

4. Output values for A_0, A_f, B, D, S, and t_0. The output also included standard deviations for theses coefficients, as well as the coefficient of correlation, R^2, a variable indicating whether convergence was achieved, and number of outliers winsorized.

8.4.2. Winsorization

The large amount of data processed during ICR treatment studies data analysis required the use of automated curve fitting procedures. To ensure that the fitted models were robust to extreme values, an outlier adjustment methodology that used all experimental data points, but limited the influence of deviant observations on the parameter estimates, was developed and used for this analysis.

Indiscriminate deletion of deviant observations can cause goodness of fit measures (i.e., R^2) to be unrealistically high. Rather than deleting potential outliers, suspect observations were replaced by less extreme values (winsorized) by the following procedure:

1. Fit the logistic function model to the observed data and determine approximate 95 percent prediction limits on the observations.

2. Observations that exceed the threshold "*Predicted $\pm$ (U95 - L95)*K*" were adjusted to "*Predicted $\pm$ (U95 - L95)*K*," where U95 is the upper 95 percent confidence limit and L95 is the lower 95 percent confidence limit. The constant K determines the magnitude of the adjustment, with larger values of K corresponding to fewer declared outliers and smaller adjustments to those that are detected. The value for the constant K was set to 1/3 based on simulation results that indicated a good balance between false alarms and power to identify substantial outliers (>3 standard deviations from the best-fit prediction). Approximately 2.5 percent of the data were identified as outliers and adjusted by this procedure.

3. Refit the logistic function model using the dataset containing adjusted values.

8.4.3. SAS Output Review

All SAS curve fits were subjected to an expert-level review. A spreadsheet tool was developed that allowed for a visual inspection of the SAS-determined curve fit in comparison to the breakthrough curve data. The spreadsheet tool also included flags that highlighted various conditions that warranted a check of SAS output (e.g., a change in curve fit type, etc.).

The following steps were included in the expert-level review of the curve fits:

- Every curve fit was reviewed, since it is possible to obtain convergence on a solution that does not accurately reflect the trend of the data. In some cases, this was caused by an outlier that had a strong impact on the best-fit of the data set. These outliers were removed so that the data-set could be re-fit successfully.

- Some peak curve fits (CFT2) were reclassified as standard logistic function model fits (CFT1) and re-fit. This was typically caused by a false-positive determination of the data set

as a peak curve. In many cases, the SAS output for the value of *S* was zero, indicating a poor peak curve fit, or the need to reclassify the dataset as CFT1.

- Data sets with fewer than 6 points measured above the MRL resulted in a zero fit (CFT6) by SAS. The review determined whether the curve fit should stay as is, or should be refit to another curve fit type. Many of these curves were refit using a step function or logistic function model.

- The TOC breakthrough curves were examined to ensure that extrapolation of the blended contactor curve to 150 percent of t_{ub} would yield acceptable results.

- Due to quality control failures, outlier removal, or data not analyzed, parameters within a single TSRunID sometimes had different bounds, i.e., different values for the parameters t_{lb} and t_{ub}. The curve fits with more restrictive bounds were reviewed to determine if the bound could be widened so that a constant bound would apply to all parameters within a TSRunID. Whenever possible, the bounds on curve fits with more restrictive bounds were widened to yield consistent bounds across all parameters for a TSRunID.

A summary of the issues identified during the raw data and outlier reviews and a count of the outliers identified and removed prior to analysis for each study is documented in the *Graphical Summary File* in the *Treatment Study Data Library* (USEPA, 2000). Of the total number of data points, 0.14% were identified as outliers and removed. In a few cases (1.5 percent of all breakthrough curves), the entire breakthrough curve for one or more analytes was removed from further analysis and inclusion in the database after expert review.

9. References

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Appendix: GAC Breakthrough Calculation Logic

The ICR database calculates the breakthrough data for selected water quality parameters (WQPs) for each treatment study run (TSRunID). The logic and the variables used in this calculation algorithm are described in this appendix.

User Input Variables:
RT_{bld} = Blended Runtime
RT_{sc} = Single Contactor Runtime
WQP = Water Quality Parameter
C_{input} = Target Concentration of a WQP (user can also specify Maximum Concentration)

Hard-coded Variables:
t_{ub} = Upper bound for runtime of a Single Contactor Breakthrough Curve
t_{lb} = Lower bound for runtime of a Single Contactor Breakthrough Curve
t_{max} = Time at which Maximum Effluent Concentration (C_{max}) occurs for a Single Contactor Breakthrough Curve (note: $t_{max} = t_{ub}$ for increasing logistic function)
A_0, A, B, and D are the coefficients representing the breakthrough curve (F1) for a specific TSRunID and WQP
S is the slope of the decreasing leg of a "peak" breakthrough curve (F2)

Variables Calculated by Database Algorithm:
C_{min} = Minimum concentration @ t_{lb}
C_{max} = Maximum concentration @ t_{max}
$RT_{bld-max}$ = The maximum blended runtime for a TSRunID ($1.5*t_{ub}$ for TOC curve). (note: the blended concentration at $RT_{bld-max}$ will be less than C_{max})
$RT_{bld-min}$ = The minimum blended runtime for a TSRunID (t_{lb} for TOC curve)
t_{ub-t2} = Single Contactor Runtime corresponding to $RT_{bld-max}$
t_{lb-t2} = Single Contactor Runtime corresponding to $RT_{bld-min}$

Equations Bounds for Numerical Solution to Integrated Logistic Function:
$t_1 = (3/D) * LN[(2*B/(1+sqr(1+4*B)))]$
$t_2 = (2/D) * LN(B)$
$t_3 = (3/D) * LN[(2/(sqr(1+4/B)-1))]$
$\lambda = LN(B/2)/(D*t_1)$

Additional Nomenclature:
t2 = Single Contactor Runtime (RT_{sc}) vs. Blended Runtime (RT_{bld}) curve
F1 = Upward trend logistic function
F2 = Downward trend linear function (for decreasing leg of peak curve)

FLAG 1: "$RT_{bld} = RT_{bld-max}$?" = YES/NO. The blended runtime corresponding to the breakthrough criteria entered by the user exceeded the maximum blended runtime for the treatment study run. As a result, the value displayed for the blended runtime is the maximum blended runtime. Furthermore, the single

contactor runtime (RTsc) corresponding to RTbl_max was used to calculate the concentrations of water quality parameters selected by user.

FLAG 2: "$RT_{sc} = t_{ub}$?" = YES/NO. The single contactor runtime entered by the user exceeds the maximum single contactor runtime for the specified water quality parameter and for the treatment study run. As a result, the value displayed for the single contactor runtime is the maximum single contactor runtime. Furthermore, the maximum runtime was used to calculate the concentrations of all other water quality parameters selected by the user.

FLAG 3: "$C_{input} \geq C_{max}$?" = YES/NO. The concentration for the water quality parameter entered by the user is equal to exceeds the maximum concentration during the treatment study run. If Flag 3 = YES and FLAG 1=NO, then the single contactor runtime corresponding to the maximum concentration was used to calculate the concentrations of the water quality parameters selected by the user. If Flag 3 = YES and Flag 1 = YES, then the single contactor runtime corresponding to the maximum blended contactor runtime was used to calculate the concentrations of the water quality parameters selected by the user.

FLAG 4: "Any C_{max} Exceeded?" = YES/NO. The maximum concentration for one or more parameters occurred before the displayed runtime. The breakthrough curve for that water quality parameter has an increasing and then decreasing curve (i.e., a peak curve), and Flag 4 indicates that the displayed concentration falls on the decreasing leg of the curve.

FLAG 88888: Blended runtime could not be calculated. The blended runtime could not be calculated because RT_{sc} exceeded the single contactor runtime corresponding to RT_{bld_max}.

FLAG 99999: Concentration could not be calculated. Data could not be reported for the specified water quality parameter since the single contactor runtime used in the calculations exceeded the upper or lower bound of the equation describing the breakthrough curve for that water quality parameter.

BLANK FLAG: The selected water quality parameter was not analyzed or reported.

Equations used in the breakthrough calculation:
The GAC base analysis module of the ICR database uses the four-parameter logistic equation, and the coefficients for this equation are generated by a statistical data analysis package (SAS). Peak curves are fit by a logistic function followed by a linear function.

The Single Contactor Concentration (C_s) as a function of Runtime (RT_{sc}) is shown in Equation 1.

$C_s\ (RT_{sc}) = 0$	for $t < t_0$
$C_s\ (RT_{sc}) = A_0 + A/(1 + B*EXP(–D*RT_{sc}))$	for $t \geq t_0$, $B > 0$, and $D > 0$

---------- **Equation 1**

The Runtime (RT_{sc}) as a function of Single Contactor Concentration (C_s) is shown in Equation 2.

$RT_{sc}\ (C_s) = 0$	for $A_0 + A/(1+B) \leq 0$ and $C_s \leq A_0 + A/(1+B)$
$RT_{sc}\ (C_s) = (1/D)*LN((B*(C_s - A_0))/(A + A_0 – C_s))$	for $A_0 + A/(1+B) \leq C_s < A + A_0$

---------- **Equation 2**

The Blended Runtime (RT_{bld}) as a function of the Single Contactor Runtime (RT_{sc}) is shown in Equation 3.

$RT_{bld}\ (RT_{sc}) = RT_{sc} / \lambda$	for $0 < RT_{sc} \leq \lambda*t_1$
$RT_{bld}\ (RT_{sc}) = t_1 + [6/(1 + B*EXP(-D*RT_{sc})) – 2]*(t_2 - t_1)$	for $\lambda*t_1 < RT_{sc} \leq t_2/2$
$RT_{bld}\ (RT_{sc}) = =(t_2*t_3)/[4*t_3 –3*t_2 – 6*(t_3 – t_2)/(1+B*EXP(-D*RT_{sc}))]$	for $t_2/2 < RT_{sc} \leq LN(2B)/D$
$RT_{bld}\ (RT_{sc}) = (t_3/3)*[1 + 1/(B*EXP(-D*RT_{sc}))]$	for $LN(2B)/D < RT_{sc} \leq \infty$

----------**Equation 3**

The Single Contactor Runtime as a function of the Blended Runtime is shown using Equation 4.

$RT_{sc}\ (RT_{bld}) = \lambda * RT_{bld}$	for $0 < RT_{bld} \leq t_1$
$RT_{sc}\ (RT_{bld}) = (1/D)*LN[B*(((2+(RT_{bld} - t_1)/(t_2 - t_1))/((4-(RT_{bld} - t_1)/(t_2 - t_1)))]$	for $t_1 < RT_{bld} \leq t_2$
$RT_{sc}\ (RT_{bld}) = (1/D)*LN[B*((RT_{bld}*(4*t_3 – 3*t_2) - (t_2*t_3))/((RT_{bld}\ (2*t_3 –3*t_2)+(t_2*t_3)))]$	for $t_2 < RT_{bld} \leq t_3$
$RT_{sc}\ (RT_{bld}) = (1/D)*LN[B*((3*RT_{bld}/t_3) - 1)]$	for $t_3 < RT_{bld} \leq \infty$

----------**Equation 4**

I. Blended Breakthrough Criteria:

Based on the assumption that there is a relationship between TOC and DBP concentrations in the effluent from a GAC contactor, Blended Contactor Runtimes can be determined for any DBP using the appropriate correlation and the blended breakthrough curve for TOC.

In the GAC base analysis calculation, the blended breakthrough curve for TOC was extrapolated to 150% of the upper bound for the single contactor runtime (t_{ub}). This allowed more of the single contactor information to be used when evaluating blended contactor breakthrough criteria.

I (a). Blended Contactor Runtime (RT_{bld}) Breakthrough Criteria

10 Select a TSRunID

Select a WQP: TOC
Calculate t_1, t_2, t_3, λ

Calculate $RT_{bld\text{-}min} = t_{lb}/\lambda$

Calculate $RT_{bld\text{-}max} = (t_{ub} * 1.5)$

Calculate $t_{ub\text{-}t2}$ @ $RT_{bld\text{-}max}$ using Equation 4

GOTO 400 AND Run Procedure 3

Calculate $t_{lb\text{-}t2} = t_{lb}$

Case 1: $RT_{bld} \geq RT_{bld\text{-}max}$

Case 2: $RT_{bld\text{-}min} < RT_{bld} < RT_{bld\text{-}max}$

Case 3: $RT_{bld} \leq RT_{bld\text{-}min}$

20 Select
Case 1: $RT_{bld} = RT_{bld\text{-}max}$ **AND**
$RT_{sc} = t_{ub\text{-}t2}$ **AND**
SET FLAG1 = "YES"
Case 2: Calculate RT_{sc} @ RT_{bld} using Equation 4
GOTO 400 AND Run Procedure 3
Case 3: $RT_{bld} = RT_{bld\text{-}min}$ **AND**
$RT_{sc} = t_{lb\text{-}t2}$
END 20

30 GOTO 200 AND RUN Procedure 1
Repeat 30 for all selected WQPs in TSRUNID

Repeat 10 for all TSRunIDs

I (b). Blended Concentration (C_{input}) Breakthrough Criteria

40 Select a TSRunID

Select a WQP: Target WQP

Case 1: A_0, A, B, D = NULL

Case 2: A_0, A, B, D = VALUES

Case 1: **RT_{sc} =** NULL **AND**
RT_{bld} = NULL **AND**
Concentration = NULL **AND**
GOTO 65

Case 2: **GOTO NEXT**

Select a WQP: TOC
Calculate $RT_{bld\text{-}min} = t_{lb} / \lambda$

Calculate $RT_{bld\text{-}max} = (t_{ub} * 1.5)$

Calculate $t_{ub\text{-}t2}$ @ $RT_{bld\text{-}max}$ using Equation 4

GOTO 400 AND Run Procedure 3

Calculate $t_{lb\text{-}t2} = t_{lb}$

Select a WQP: Target WQP

Calculate C_{max} @ t_{max} using Equation 1

Calculate C_{min} @ t_{lb} using Equation 1

Case 3: $C_{input} \geq C_{max}$

Case 4: $C_{min} < C_{input} < C_{max}$

Case 5: $C_{input} \leq C_{min}$

50 Select

Case 3: $RT_{sc} = t_{max}$ **AND**
SET FLAG3 = "YES"

Case 4: **IF Coefficient D = 0, THEN**
RTsc =t_0 ,
ELSE
Calculate RT_{sc} @ C_{input} using Equation 2

Case 5: $RT_{sc} = t_{lb}$

END 50

Case 6: $RT_{sc} \geq t_{ub\text{-}t2}$

Case 7: $t_{lb\text{-}t2} < RT_{sc} < t_{ub\text{-}t2}$

Case 8: $RT_{sc} \leq t_{lb\text{-}t2}$

60 Select

Case 6: $RT_{sc} = t_{ub\text{-}t2}$**AND**
RT_{bld} **=** $RT_{bld\text{-}max}$ **AND**
SET FLAG 1 = "YES"

Case 7: RT_{sc} **=** RT_{sc} **AND**
Calculate RT_{bld} @ RT_{sc} using Equation 3
GOTO 300 AND Run Procedure 2

Case 8: RT_{sc} **=** $t_{lb\text{-}t2}$ **AND**
RT_{bld} **=** $RT_{bld\text{-}min}$

END 60

65 GOTO 200 AND RUN Procedure 1
Repeat 65 for all selected WQPs in TSRunID

Repeat 40 for all TSRunIDs

II. Single Contactor Breakthrough Criteria:

In this option, the user can select a WQP and: 1.) enter a target concentration, 2.) enter a target single contactor runtime, 3.) or select the maximum concentration option. The algorithm for single contactor breakthrough criteria is described below.

II (a). Single Contactor Concentration (C_{input}) Breakthrough Criteria

70 Select a TSRunID

Select a WQP: Target WQP

Case 1: A_0, A, B, D = NULL

Case 2: A_0, A, B, D = VALUES

Case 1: **RT_{sc} =** NULL **AND**
RT_{bld} = NULL **AND**
Concentration = NULL **AND**
GOTO 95

Case 2: **GOTO NEXT**

Select a WQP: TOC
Calculate $RT_{bld\text{-}min} = t_{lb} / \lambda$

Calculate $RT_{bld\text{-}max} = (t_{ub} * 1.5)$

Calculate $t_{ub\text{-}t2}$ @ $RT_{bld\text{-}max}$ using Equation 4

GOTO 400 AND Run Procedure 3

Calculate $t_{lb\text{-}t2} = t_{lb}$

Select a WQP: Target WQP

Calculate C_{max} @ t_{max} using Equation 1

Calculate C_{min} @ t_{lb} using Equation 1

Case 3: $C_{input} \geq C_{max}$

Case 4: $C_{min} < C_{input} < C_{max}$

Case 5: $C_{input} \leq C_{min}$

80 Select
Case 3: $RT_{sc} = t_{max}$ **AND**
SET FLAG3 = "YES"
Case 4: **IF Coefficient D = 0, THEN**
RTsc =t_0 ,
ELSE
Calculate RT_{sc} @ C_{input} using Equation 2
Case 5: $RT_{sc} = t_{lb}$
END 80

Case 6: $RT_{sc} \geq t_{ub\text{-}t2}$

Case 7: $t_{lb\text{-}t2} < RT_{sc} < t_{ub\text{-}t2}$

Case 8: $RT_{sc} \leq t_{lb\text{-}t2}$

90 Select
Case 6: RT_{bld} =**FLAG** "88888"
Case 7: **Calculate** RT_{bld} @ RT_{sc} using Equation 3
GOTO 300 AND Run Procedure 2
Case 8: RT_{bld} **=** $RT_{bld\text{-}min}$
END 90

95 GOTO 200 AND RUN Procedure 1
Repeat 95 for all selected WQPs in TSRunID

Repeat 70 for all TSRunIDs

II (b). Maximum Single Contactor Concentration (C_{max}) Breakthrough Criteria

100 Select a TSRunID

Select a WQP: Target WQP

Case 1: A_0, A, B, D = NULL

Case 2: A_0, A, B, D = VALUES

Case 1: **RT_{sc} =** NULL **AND**
RT_{bld} = NULL **AND**
Concentration = NULL **AND**
GOTO 115

Case 2: **$RT_{sc} = t_{max}$ AND**
GOTO NEXT

Select a WQP: TOC
Calculate $RT_{bld\text{-}min} = t_{lb} / \lambda$

Calculate $RT_{bld\text{-}max} = (t_{ub} * 1.5)$

Calculate $t_{ub\text{-}t2}$ @ $RT_{bld\text{-}max}$ using Equation 4

GOTO 400 AND Run Procedure 3

Calculate $t_{lb\text{-}t2} = t_{lb}$

Case 3: $RT_{sc} \geq t_{ub\text{-}t2}$

Case 4: $t_{lb\text{-}t2} < RT_{sc} < t_{ub\text{-}t2}$

Case 5: $RT_{sc} \leq t_{lb\text{-}t2}$

110 Select
Case 3: RT_{bld} =**FLAG** "88888"
Case 4: **Calculate** RT_{bld} @ RT_{sc} using Equation 3
GOTO 300 AND Run Procedure 2
Case 5: RT_{bld} **=** $RT_{bld\text{-}min}$
END 110

115 GOTO 200 AND RUN Procedure 1
Repeat 115 for all selected WQPs in TSRunID

Repeat 100 for all TSRunIDs

II (c). Single Contactor Runtime (RT_{sc}) Breakthrough Criteria

120 Select a TSRunID

Select a WQP: Target WQP

Case 1: A_0, A, B, D = NULL

Case 2: A_0, A, B, D = VALUES

Case 1: **RT_{sc} =** NULL **AND**
RT_{bld} = NULL **AND**
Concentration = NULL **AND**
GOTO 100

Case 2: **RT_{sc} = RT_{sc}** (Input Value) **AND**
GOTO NEXT

Select a WQP: TOC
Calculate $RT_{bld\text{-}min} = t_{lb} / \lambda$

Calculate $RT_{bld\text{-}max} = (t_{ub} * 1.5)$

Calculate $t_{ub\text{-}t2}$ @ $RT_{bld\text{-}max}$ using Equation 4

GOTO 400 AND Run Procedure 3

Calculate $t_{lb\text{-}t2} = t_{lb}$

Case 3: $RT_{sc} \geq t_{ub}$

Case 4: $t_{lb} < RT_{sc} < t_{ub}$

Case 5: $RT_{sc} \leq t_{lb}$

130 Select
Case 3: $RT_{sc} = t_{ub}$ **AND**
SET FLAG 2 = "YES"
Case 4: $RT_{sc} = RT_{sc}$ (Input Value)
Case 5: $RT_{sc} = t_{lb}$
END 130

Case 6: $RT_{sc} \geq t_{ub\text{-}t2}$

Case 7: $t_{lb\text{-}t2} < RT_{sc} < t_{ub\text{-}t2}$

Case 8: $RT_{sc} \leq t_{lb\text{-}t2}$

140 Select
Case 6: RT_{bld} =**FLAG** "88888"
Case 7: **Calculate** RT_{bld} @ RT_{sc} using Equation 3
GOTO 300 AND Run Procedure 2
Case 8: $RT_{bld} = RT_{bld\text{-}min}$
END 140

145 GOTO 200 AND RUN Procedure 1
Repeat 145 for all selected WQPs in TSRunID

Repeat 120 for all TSRunIDs

200 Procedure 1

Select a WQP: WQP
Case 1: A_0, A, B, D = NULL

Case 2: RT_{sc} = NULL

Case 3: $RT_{sc} < t_{lb}$

Case 4: $RT_{sc} < t_0$

Case 5: $t_0 \leq RT_{sc} \leq t_{max}$

Case 6: $t_{max} < RT_{sc} \leq t_{ub}$

Case 7: $RT_{sc} > t_{ub}$

210 Select

Case 1: **Concentration =** NULL

Case 2: **Concentration =** NULL

Case 3: **Concentration = FLAG** "99999"

Case 4: **Concentration =** 0

Case 5: **Calculate Concentration** @ RT_{sc} using Single Contactor breakthrough curve F1: $C_s (RT_{sc}) = A_0 + A / (1 + B*EXP(-D*RT_{sc}))$
IF $C_s (RT_{sc}) < 0$ **THEN Concentration = 0**

Case 6: **Calculate Concentration** @ RT_{sc} using Single Contactor breakthrough curve F2: $C_s (RT_{sc}) = C_{max} + S*(RT_{sc} - t_{max})$
AND SET FLAG 4 = "YES"
IF $C_s (RT_{sc}) < 0$ **THEN Concentration = 0**

Case 7: **Concentration = FLAG** "99999"

END 210

END 200
RETURN

300 Procedure 2

Select a WQP: TOC

Case 1: $RT_{sc} \leq (\lambda*t_1)$

Case 2: $\lambda*t_1 < RT_{sc} \leq t_2 /2$

Case 3: $t_2 /2 < RT_{sc} \leq LN(2B)/D$

Case 4: $LN(2B)/D < RT_{sc} < \infty$

310 Select

Case 1: $RT_{bld} = RT_{sc}/\lambda$

Case 2: $RT_{bld} = t_1 + [6/(1*B*EXP(-D*RT_{sc}))-2)]*(t_2 - t_1)$

Case 3: $RT_{bld} = (t_2*t_3)/[4*t_3 -3*t_2 - 6(t_3 - t_2)/(1 + B*EXP(-D*RT_{sc}))]$

Case 4: $RT_{bld} = (t_3/3) * [1 + 1 / (B*EXP(-D*RT_{sc}))]$

END 310

END 300
RETURN

400 Procedure 3

Select a WQP: TOC
Case 1: $RT_{bld} \leq t_1$

Case 2: $t_1 < RT_{bld} \leq t_2$

Case 3: $t_2 < RT_{bld} \leq t_3$

Case 4: $t_3 < RT_{bld} < \infty$

410 Select

Case 1: $RT_{sc} = \lambda * RT_{bld}$

Case 2: $RT_{sc} = (1/D)*LN[B(((2+(RT_{bld} - t_1)/(t_2 - t_1))/((4-(RT_{bld} - t_1)/(t_2 - t_1)))]$

Case 3: $RT_{sc} = (1/D)*LN[B*((RT_{bld}(4*t_3 - 3*t_2)-(t_2*t_3))/((RT_{bld}*(2*t_3 -3*t_2)+(t_2*t_3)))]$

Case 4: $RT_{sc} = (1/D)*LN[B*((3*RT_{bld}/t_3) - 1)]$

END 410

END 400
RETURN