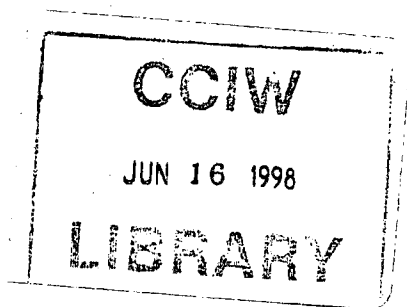
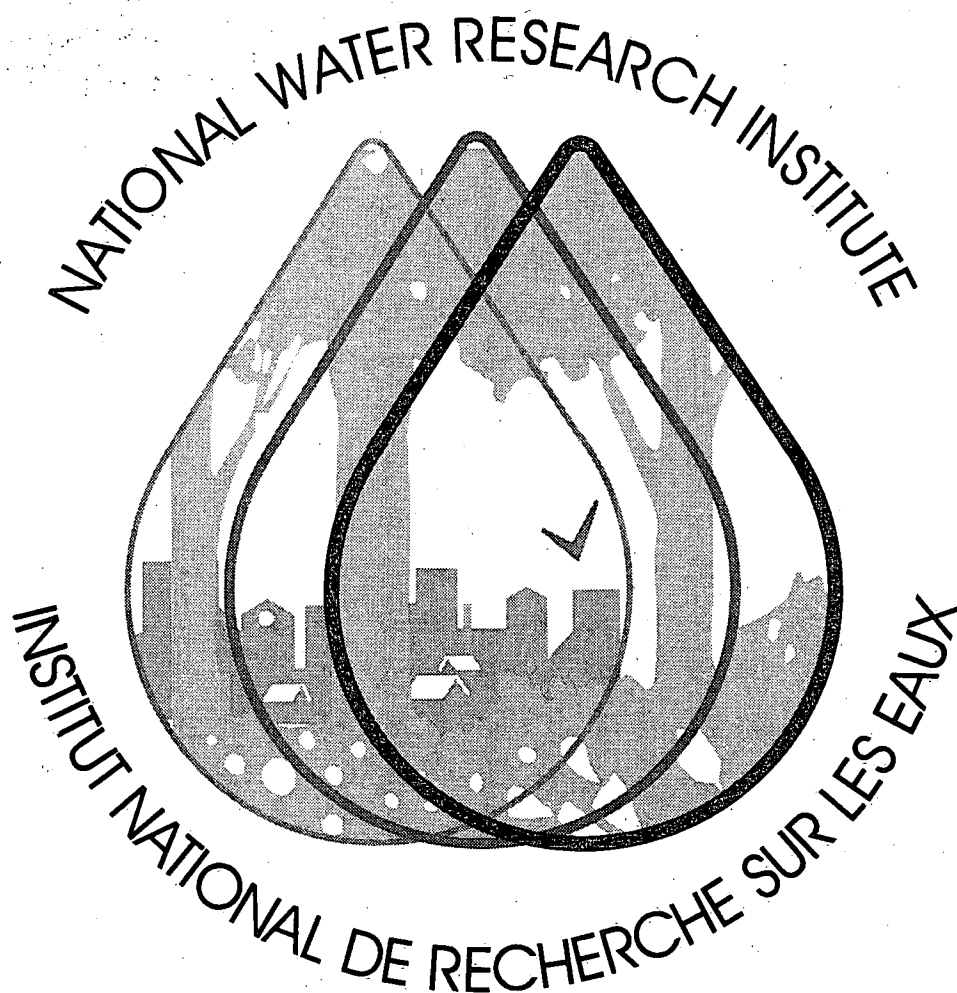


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**A TWO-DIMENSIONAL CONTAMINANT
FATE AND TRANSPORT MODEL FOR THE
LOWER ATHABASCA**

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MANAGEMENT PERSPECTIVE

This report describes a two-dimensional contaminant fate and transport model and its application to the lower Athabasca River. This is one of the major deliverables of a multi-year project funded by the Interdepartmental Panel on Energy R&D (PERD) and Environment Canada to study the aquatic impact of oil sands and heavy oil operations in northeastern Alberta. The Athabasca tar sands contain a substantial part of Canada's oil supply. A number of nitrogen-, and sulphur-PAC's (polycyclic aromatic compounds) as well as their alkyl derivatives have been identified in tar sands plants process streams and emissions. Some of these PAC's are known mutagens and carcinogens. The fate and persistence of these chemicals downstream of tar sands plants on the Athabasca River have been examined using a combination of field and laboratory data collection coupled with computer simulation modelling. The model, ATHMOD2, is expected to be used in future environmental impact assessments which are required as a result of industry expansion. It can easily be applied to other toxic substances and rivers to consider continuous and single spill discharges where incomplete mixing required two-dimensional analysis. It has been designed to operate within the Windows environment and has a user friendly input interface coupled with sophisticated model output visualization features.

SOMMAIRE À L'INTENTION DE LA DIRECTION

Le présent rapport décrit un modèle bidimensionnel de transport et de devenir d'un contaminant et son utilisation pour le bassin inférieur de la rivière Athabasca. Il s'agit là de l'un des principaux travaux d'un projet étalé sur plusieurs années et financé par le Groupe interministériel de recherche et d'exploitation énergétiques (GRDE) et Environnement Canada, projet qui vise à étudier l'impact de l'exploitation des sables bitumineux et des huiles lourdes sur le milieu aquatique dans le nord-est de l'Alberta. Les sables bitumineux de l'Athabasca représentent une fraction importante de l'approvisionnement en pétrole du Canada. Un certain nombre de CAP (composés aromatiques polycycliques) azotés et sulfurés, ainsi que leurs dérivés alkylés, ont été décelés dans les circuits et les émissions des procédés de traitement de ces sables. On sait que certains de ces composés sont mutagènes et cancérigènes. Le devenir et la persistance desdits composés en aval des usines de sables bitumineux sur la rivière Athabasca ont été examinés grâce à la collecte de données sur le terrain et en laboratoire, combinée à une simulation par modélisation sur ordinateur. On prévoit utiliser le modèle, ATHMOD2, pour de futures évaluations de l'impact environnemental, rendues nécessaires par l'expansion de l'industrie. Il peut facilement s'appliquer à d'autres substances toxiques et à d'autres rivières, pour évaluer les déversements continus et temporaires là où un mélange incomplet nécessite une analyse bidimensionnelle. Conçu pour fonctionner en Windows, le modèle présente une interface d'entrée conviviale, combinée à une visualisation sophistiquée à la sortie.

RÉSUMÉ

Le bassin inférieur de la rivière Athabasca traverse les gisements de sables bitumineux de l'Athabasca dans le nord de l'Alberta. Deux usines d'extraction et de traitement de ces sables sont exploitées près de la rivière, en aval de Fort McMurray. Les effluents de l'une des usines (Suncor) sont déversés dans la rivière et contiennent de faibles concentrations de composés aromatiques polycycliques (CAP). Par suite de l'expansion de l'industrie, il faudra procéder à plusieurs évaluations de l'impact environnemental. Pour obtenir un outil d'évaluation de ces CAP, on a élaboré un modèle bidimensionnel de devenir des contaminants et on l'a appliqué à une portion de 120 km de la rivière Athabasca, en aval de Fort McMurray. L'étalonnage hydraulique du modèle a été effectué à l'aide de sodium et de chlorure provenant d'un affluent majeur, utilisés comme traceurs. Deux groupes de composés ont été modélisés : 1) les CAP provenant de l'effluent de Suncor; 2) les CAP provenant de sources naturelles ou de base. Les concentrations de CAP étaient généralement $< 1 \text{ ng/L}$, nécessitant de grands volumes pour l'extraction et des méthodes d'analyse très sensibles. Les processus, comme le partage sédiments/eau et la biodégradation, ont été évalués à partir d'expériences sur le terrain utilisant l'eau et les sédiments en suspension de la rivière. La majeure partie des composés avaient des demi-vies d'environ 36 heures, ce qui présentait une bonne corrélation avec la cinétique de décomposition déterminée par étalonnage du modèle selon les concentrations mesurées dans la rivière.

A Two-Dimensional Contaminant Fate and Transport Model for the Lower Athabasca River

Booty, W.G., Brownlee, B.G., MacInnis, G.A., and Resler, O.

Abstract

The lower Athabasca River flows through the Athabasca Oil Sands deposits in northeastern Alberta. Two oil sands mining/extraction/upgrading plants operate near the river downstream of Fort McMurray. Effluents from one of the plants (Suncor) is discharged to the river and contains low concentrations of polycyclic aromatic compounds (PAC's). Several environmental impact assessments are required as a result of industry expansion. To provide an assessment tool for the PAC's, a two-dimensional contaminant fate model has been developed and applied to a 120 km portion of the Athabasca River downstream from Fort McMurray. Hydraulic calibration of the model was carried out using sodium and chloride from a major tributary as tracers. Two groups of compounds were modelled: (1) PAC's from the Suncor effluent, and (2) PAC's from natural/background sources. PAC concentrations in the river were typically < 1 ng/L, requiring large volume extractions and highly sensitive analytical methods of analysis. Processes such as sediment-water partitioning and biodegradation were determined from field experiments using river water and suspended sediment. The majority of the compounds showed half-lives of approximately 36 hours, which matched very well with decay kinetics determined through model calibration to measured river concentrations.

INTRODUCTION

The area in the lower Athabasca river watershed of northeastern Alberta contains an extensive oil sands deposit. A significant portion of Canada's petroleum production is derived from the extraction and upgrading operations that are carried out by Suncor, Inc. and Syncrude Canada Ltd. A multi-year project was started in 1989 to study the possible impact of these oil sands extraction and upgrading operations on aquatic ecosystems along the Athabasca River. The project is funded by the National Water Research Institute and the Interdepartmental Panel for Energy Research and Development (PERD). One of the goals of this project was to develop predictive models which can be used to examine the fate and transport of effluents from the oil sands extraction plants. These include polycyclic aromatic hydrocarbons (PAH's), which are naturally found in the area, as well as thiophenes and quinolines. PAH's may be acutely toxic or genotoxic, which is dependent upon the number and configuration of the fused benzene rings and the presence or absence of other chemicals (Heitkamp and Cerniglia 1989). Also, many of the metabolites of PAH's are known to be mutagenic, carcinogenic, or both (Bumpus 1989). Many of these chemicals appear on the CEPA (Canadian Environmental Protection Act) priority substance list and have been identified as persistent, bioaccumulative, and toxic substances. Chemicals that meet or exceed criteria for toxicity, bioaccumulation and persistence, which were detected in effluents in this study include fluoranthene, phenanthrene, acridine, and pyrene. Toxicity testing on 21 quinoline derivatives (Birkholz et al., 1990) demonstrated that all compounds are moderately toxic according to the Microtox assay.

Based upon the results of the first 2 years of reconnaissance work to characterize the Athabasca

River system, a preliminary, one dimensional chemical fate model was developed and tested (Booty et al., 1991) for phenols downstream of Ft. McMurray to the delta at Lake Athabasca. Subsequent field data indicated that the river does not mix well across its width (Bourbonniere, R.A., 1992). Consequently, a 2-dimensional model (ATHMOD2) was developed to simulate the distribution of chemicals within the river.

MODEL DESCRIPTION

ATHMOD2 is a two-dimensional model that considers contaminant concentrations along the longitudinal or downstream direction as well as the lateral or cross-stream direction. In this model it is assumed that there is no vertical concentration gradient. The model is a modified version of TWODIFIN (OMOE, 1988). TWODIFIN is an acronym for TWO-Dimensional FINite-time model. ATHMOD2 is designed to consider continuous and single spill discharge scenarios. It is also modified to incorporate additional in-river decay processes required to model toxic organic compounds such as PAH's. In addition, the model has been coupled with a new user interface and has been compiled using Visual Basic so that the original Fortran 77 code runs within the Windows environment. A description of the new interface is described in the next section.

The model is based upon a stream tube concept which was developed by Yotsukura and Cobb, 1972; Yotsukura and Sayre, 1976; Yotsukura and Sayre, 1977. In this model, the channel is divided into a number of strips called stream tubes so that the discharge within each stream tube is the same. The model uses a cumulative partial discharge, q , at a selected cross section instead of the actual lateral discharge, y , as the independent variable. In this case, the cross sectional concentration distributions $c(x, q)$ predicted by the model are functions of q . By knowing the relation between q and y at each transect, the distributions can be transformed into $c(x, y)$ distributions.

The 2-D convective-dispersion equation for a non-conservative material in the far field region of the mixing zone can be expressed in the form:

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = e_x \frac{\partial^2 c}{\partial x^2} + u D_y \frac{\partial^2 c}{\partial q^2} - K_d c$$

- where
- x = longitudinal coordinate (m)
 - y = lateral coordinate (m) from the reference bank
 - q = cumulative partial discharge (m^3/s)
 - t = time (s)
 - u = velocity of flow in the x direction (m/s)
 - e_x = longitudinal dispersion coefficient (m^2/s)
 - D_y = lateral diffusion factor (m^5/s^2)
 - K_d = first order decay rate coefficient (1/s)
 - c = concentration at point (x, q) at time (t)

The solution to equation (1) for a constant effluent discharge and concentration is:

$$C = \frac{u \exp \frac{ux}{(2e_x)}}{4\sqrt{\pi e_x e_q}} \sum_1^n \left\{ (\Delta w) \left[\frac{\exp(-2\sqrt{ab})}{(ab)^{1/4}} \left\{ \operatorname{erf} \left(\sqrt{\frac{a}{t-t_j}} - \sqrt{b(t-t_j)} \right) - \operatorname{erf} \left(\sqrt{\frac{a}{t-t_i}} - \sqrt{b(t-t_i)} \right) \right\} \right] \right\}$$

where $a = (x^2/4e_x) + ((q_s - q)^2/4e_q)$
 $b = (u^2/4e_x) + K_d$

and u = velocity of flow (m/s)
 x = distance downstream from the source (m)
 t = time (s)
 t_i = time of beginning of release (s)
 t_j = time of end of release (s)
 w = rate of release of mass (1/s)
 e_x = longitudinal dispersion coefficient (m²/s)
 e_q = transverse diffusion coefficient (m⁶/s³)

The transverse diffusion coefficient is calculated in the model using the relation:

$$e_q = \beta Q^2 u / b$$

where Q is the total discharge for a reach and β is a dimensionless factor which is calculated from tracer studies (Booty, 1994).

The river is divided longitudinally into reaches and stream tubes. Each reach is assumed to have reasonably constant hydrodynamic characteristics. The model allows for up to 15 reaches and 15 stream tubes. The important parameters having longitudinal variabilities of concern include width, depth, velocity, decay rate, and stream bed material. These variabilities are considered in equation 1 and in the ATHMOD2 model the decay term K_d has been expanded to include expressions for volatilization, biodegradation, photolysis, oxidation, and hydrolysis. To take into account the variation of the hydrodynamic parameters from reach to reach, moving averages are determined that approximate the effective values of river width, depth, and velocity of flow. In order to scale the depth, width, and velocity to different flow conditions, Leopold-Maddock relationships are used (Leopold and Maddock, 1953). The model uses Bansal's equation (Bansal, M.K., 1971) to compute the dispersion coefficients if they are not available from tracer studies.

ATHMOD2 USER INTERFACE

The interface consists of a number of windows which allow the user to create the input data set for the model, edit the input data, edit the views of the river including the placement of the transects, and select options for viewing the output data. By selecting the file menu the user can create a new input data file, open an existing input data file, or save the file.

Typically the first step in setting up the model is to select the positions of the transects that will

define the reaches along the river. The user interface provides a number of windows that allow the user to view the river at different scales. The Large Map Window is the top portion of the screen shown in Figure 1. It is a scrollable map of the Athabasca River. The user is given a view that is approximately 25 km wide by 9 km high. The Small Map Window, which is the bottom portion of the screen shown in Figure 1, gives the user the view of the entire portion of the river that is being modelled. A box that is proportional in scale to the Large Map Window can be used to scroll within the Large Map Window. The user can easily add a transect by clicking on the Add Transect button and dragging it onto the Athabasca River map. Once the transect icon has been placed on the map, the user can still modify the location of the transect by dragging the transect icon to the desired location. The user also has the ability to manually enter a transect by using the Edit Transect option. This allows the user to type in exactly how far down the river the transect is from the starting reference point. This menu option also allows the user to enter the transect data into a new transect created from the drag and drop Add Transect operation.

Selecting "Parameters" from the model menu activates the model setup window (Figure 2). This window allows the user to display and modify the:

- Title of the study
- Pollutant name
- Model resolution
- Days to run the model
- Number of stream tubes
- Fraction of flow between the bank and discharge pipe
- Delta value for estimating the number of bank images
- Tolerance level to determine degree of mixedness
- Background concentration of the pollutant
- Use of Leopold-Maddock relationship
- Use of longitudinal dispersion coefficient

Selecting "Edit Transect" from the model menu activates the window (Figure 3) which allows the user to view and modify the input data for each reach and associated transects. The parameters include:

- Distance from the outfall
- Longitudinal dispersion coefficient
- Transverse dispersion coefficient
- Leopold-Maddock constants (width, depth, and velocity)
- Reach design temperature and stream flow
- Reach length and channel geometry (width-depth profile)
- Flow velocity
- Decay rate

By selecting "Decay Rate" with the mouse, a new window appears (Figure 4), which allows the user to supply individual decay reaction rate values, which include:

- Volatilization
- Photolysis
- Oxidation
- Benthic biodegradation

Hydrolysis Metabolization

The final step involves entering the effluent discharge data. The parameters that may be modified within the Effluent Discharge window (Figure 5) are:

- Source data time interval

- Number of intervals

- For each time interval:

 - Time

 - Discharge rate

 - Concentration

When the input file has been created and saved the model may be run by selecting "Run model" from the Model menu. The results of the model run are then displayed directly on the Pollutant Concentration window view of the river, as shown in Figure 6. The x axis represents the distance down the river and the y axis represents the stream tubes. The vertical lines represent the transects at which water flow and chemistry are observed. By moving the mouse cursor to any point on the screen, the reach number, stream tube number, distance from the outfall, and concentration of the contaminant is shown.

The View Data Window (Figure 7) may be selected to display the model output data in tabular form. The user may also cut and paste the data into any Windows spreadsheet.

EXPERIMENTAL

Collection and Field Processing of Samples

A schematic of the sampling strategy is shown in Figure 8. Calibration of a two-dimensional model requires lateral data (transects) at a number of points upstream and downstream from the source (Suncor wastewater discharge to the Athabasca River). Seven transects were sampled at five points across the river at approximately 0.1, 0.3, 0.5, 0.7 and 0.9 of the distance from the left bank (Sites A, B, C, D, and E). These transects were upstream of the Horse River (only a four-point transect was sampled here), and at km 33.3, 40.2, 53.9, 60.0, 90.1, and 131.9 from the reference point for the model. The Suncor discharge is at km 37.8.

River water was pumped from 0.5 m depth through an Alfa-Laval MAB-103 continuous-flow centrifuge using PTFE-lined tubing. Centrifugate was collected and extracted (see below) and the suspended sediment was removed from the centrifuge bowls and frozen. In order to sample one transect per day and obtain sufficient suspended sediment, it was necessary to use two boats and three centrifuges.

Water (centrifugate) samples (20 L) were extracted onsite by stirring with dichloromethane (DCM) in a stainless vessel following appropriate pH adjustment (pH 12 for base/neutral extract followed

by pH 2 for acid extract). Diphenyl- d_{10} was added as a recovery standard. The method is described in more detail in Fox (1986) and in Brownlee et al. (1995). Suncor wastewater samples (4 L, collected by Suncor staff) were extracted in a separatory funnel at pH 12 with three portions of DCM, the pH adjusted to 2 and extracted with a further three portions of DCM. All extracts were shipped to the National Water Research Institute in Burlington for laboratory analysis.

Laboratory Analyses -- Quantitation of Base/Neutral Compounds

Water was separated from the DCM extracts, the extracts dried by passing through combusted (450°C) sodium sulfate and concentrated on a rotary evaporator. The extracts were then transferred to graduated 15 mL tubes and further evaporated under an argon stream. A portion was solvent-exchanged into toluene and chrysene- d_{12} was added as an internal standard. The extract was then analyzed by gas chromatography-mass spectrometry (GC-MS) in the single ion mode (SIM). Each sample was injected five times using a different method for each injection depending on the target compound(s) being quantitated. The different groups quantitated were: polycyclic aromatic hydrocarbons (PAHs), alkylated PAHs, benzothiophenes, quinolines, and miscellaneous (aromatic amines, phenanthrene, diphenyl- d_{10}). For the river water samples results were corrected based on diphenyl- d_{10} recoveries.

The instrument used was a Hewlett-Packard model 5890 gas chromatograph connected to a Hewlett-Packard model 5791 mass selective detector operating in electron impact mode at 70 eV. The column was a 30 m x 0.25 mm capillary coated with 0.25 μm of DB-5ms, helium carrier at ca. 35 cm/s (constant flow mode). The temperature program was $80\text{--}245^{\circ}\text{C}$ at $3^{\circ}\text{C}/\text{min}$ to 245°C , then at $4^{\circ}\text{C}/\text{min}$ to 280°C with ten minute hold. A 1 μL sample was injected by splitless injection.

Average relative standard deviation for sampling and analysis was 15% ($n=30$), based on results for eight of the compounds in duplicate samples collected at four of the transects.

Laboratory Analyses -- Identification of Base/Neutral Compounds

Prior to establishing the target list of base/neutral compounds to quantitate, Suncor wastewater base/neutral extracts were examined qualitatively by GC-MS. Several compounds could be identified by comparison of retention times and spectra with authentic materials available at the time. In other cases, we had to rely on comparison with library spectra and estimates of likely retention times. In one case (2,4-dimethylbenzothiophene) authentic material was only obtained after the quantitation had been completed. The mass spectra for the 2,4-DMBTP in the effluent and for the standard are shown in Figures 9 and 10 respectively. The qualitative results for all of the compounds are summarized in Table 1.

Table 1. Information available for identification of compounds quantitated in Suncor effluent and Athabasca River, May, 1993.

| Compound | | Std. ^a | RT Match TIC ^b | RT Match XIC ^c | Spec. Match | RI Exp. ^d | RI Lit. ^e |
|---------------------------------|----------------|-------------------|---------------------------------|---------------------------------|----------------|-------------------------|-------------------------|
| 7-Methylquinoline | | Y | Y | Y | Y | 227.47 | 231.37 ^f |
| 2,4-Dimethylquinoline | | Y | Y | Y | Y | 242.69 | |
| Trimethylquinoline Isomer (1st) | N | | | Y ^f | | | |
| Trimethylquinoline Isomer (2nd) | N | | | Y ^f | | | |
| Acridine | | Y | Y | Y | Y | 303.71 | 304.04 ^f |
| Benzoquinoline Isomer | | N | | | Y ^g | 307.56 | 307.94 ^f |
| 3/4-Methylbenzothiophene | Y | Y | Y | Y | 220.06 | | 220.55 ² |
| 2,4-Dimethylbenzothiophene | N ^h | Y | Y | Y | 238.02 | | 238.39 ² |
| Naphthalene ⁱ | Y | Y | | | | | |
| Phenanthrene ⁱ | Y | Y | | | | | |
| Fluoranthene ⁱ | Y | Y | | | | | |
| Pyrene ⁱ | | Y | Y | | | | |

^a Authentic material available (Y)/unavailable (N) for quantitation.

^b Retention time match with standard for the Total Ion Chromatogram.

^c Retention time match with standard for 3-4 ions in Extracted Ion Chromatogram.

^d Experimental Retention Index.

^e Literature Retention Index; Ref. 1 Vassilaros et al. (1982); Ref 2 Andersson (1986).

^f Assigned on the basis of *m/z* 171 ion and match with library spectrum.

^g Retention Index and library spectrum match for benzo[f]quinoline or phenanthridine.

^h Authentic material was available for identification.

ⁱ Assigned on basis of quantitation ion and retention time.

The concentrations of the organic compounds in the Suncor wastewater and the Athabasca River collected during May of 1993 for the sites shown in Figure 8 are presented in Appendix A.

Water Column Disappearance Experiments

To 2 L amber glass wide mouth bottles were added 400 mL of Athabasca River sediment and 2000 mL of unfiltered Athabasca River water followed by 100 mL of an aqueous solution of the test compounds 7-methylquinoline, 2,4-dimethylquinoline, 3-methylbenzothiophene, acridine and pyrene to give a nominal initial concentration of 500 ng/L of each test compound. The jars were closed with caps that were drilled with holes to accomodate stirring paddles. The bottle contents were stirred gently at room temperature with a mechanical stirrer motor. At 0, 1, 2, 4 and 7 days, the

water from one bottle was extracted with DCM (3 x 100 mL). The extracts were worked up and analyzed in the laboratory in the same manner as the large volume extracts except that diphenylamine (1 µg/mL) was used as the internal standard. The results are shown in Figure 11.

MODEL APPLICATION and CALIBRATION

Data collected during the 1993 sampling year was used to calibrate the model. Major ion chemistry and flow data were used to determine the transverse mixing characteristics of the river reaches (Booty, 1994). Daily loadings for the Suncor effluent were available for the period of May 25-31. As seen in Appendix A for the Suncor wastewater, the daily loadings are not constant as both discharge rates and concentrations of the chemicals vary. Due to sampling logistics, the sampling of river concentrations were carried out at different transects on different days as the crews moved downstream. Consequently, model outputs have been selected which most closely match the measured values with respect to time of travel in the river. Model predicted vs measured results are also examined with and without decay reaction kinetics.

2,4-Dimethylbenzothiophene

2,4-DMBTP is one of the compounds in the Suncor wastestream that does not occur naturally in the river. This is seen in Appendix A where 2,4-DMBTP is a non-detect (ND) at the u/s Horse River site and at transect 1 (km 33.5), both of which are upstream of the Suncor wastestream discharge. The background value for the model runs was set to 0.0 ng/L. An error analysis was carried out using the results of replicate analyses of river water samples for each compound. The overall average residual standard deviation of 15% was used for the determination of the error bars which are shown in all of the following figures for the observed data.

At transect 2 (km 40.2), as shown in Figure 12, the model significantly underestimates the concentration in the first 2 stream tubes. The Suncor wastestream enters the river close to the left bank, and in the model it is equally input to the 1st and second stream tubes. The model predicted concentrations in the other 8 stream tubes match the observed data almost exactly. This is a result of the fact that there is very little lateral mixing between the discharge point at km 37.8 and transect 2 at km 40.2. In the model, it is assumed that the effluent is at the same temperature and has the same buoyancy as the river water. However, this was determined well after the sampling had been completed to not be the case. The effluent is much warmer than the river water and more buoyant. Early exploratory sampling for major ions indicated that the river was vertically mixed and so subsequent sampling was not carried out at different depths, but only in the top 0.5 metres. Consequently, we believe that the higher measured concentrations than those predicted by the model are due to incomplete vertical mixing of the effluent.

At transect 3 (53.9 km) (Figure 12), the pollutant still does not appear to be completely vertically mixed. However, the effect of lateral diffusion is obvious from the measured data and is well predicted by the model.

At transect 4 (60.0 km) (Figure 13) the model predicted and measured concentrations match extremely well. By this point it appears that the chemical is vertically mixed within the river. By transect 5 (90.1 km) (Figure 13) the model begins to overpredict the concentrations on the left side of the river. The higher measured concentration at 0.9 from the left bank must be due to analytical error or contamination as there is no source of 2,4-DMBTP to account for such an anomaly.

At transect 6 (131.9 km) (Figure 14) the model overpredicts the concentrations across the entire river. This is assumed to be due to the decay of the chemical in the system with time.

No experimental decay data were available for this compound so the overall decay rate ($t_{1/2} = 36$ hrs) was determined through calibration of the model with the observed data. However, this value is close to that found for 3-methylbenzothiophene ($t_{1/2} = 32$ hrs) through experimental studies (Figure 11).

As expected, the model predictions at transects 2 and 3 (Figure 15) are virtually identical to those simulated with the decay set to zero (Figure 12). The model predicted concentrations at transect 4 (Figure 16) with decay are not quite as close of a match to the measured data as they are for decay set to zero. However, at transect 5 (Figure 16) the model predicted concentrations across the river match the measured data extremely well as compared to those without decay kinetics (Figure 13). The model predicted concentrations across the river at transect 6 (Figure 17) match the measured data much more closely than those in Figure (14) with no decay. It is also interesting to note that after 98 kms of travel the 2,4-DMBTP has still not completely mixed laterally across the river. It is also apparent that for the model to more accurately simulate the decay of 2,4-DMBTP between transects 5 and 6 needs to be higher than it is in the previous reaches. The model was run again with $t_{1/2} = 36$ hrs for the reaches upstream of transect 5 and the value of $t_{1/2}$ downstream was calibrated to give the best fit to the data at transect 6. A value of $t_{1/2} = 12$ hrs was found to give the best fit to the observed data (Figure 18). Further experimental work in this reach of the river is required to determine if this is a reasonable rate of decay.

7-Methylquinoline

This compound was only found in one sample (Appendix A; Site B, u/s Horse River) at a very low concentration (0.273 ng/L) upstream of the Suncor wastestream discharge. It is therefore not considered to have a significant natural source. The background concentration for the modelling was set at 0.1 ng/l (detection limit).

As is the case with the 2,4-DMBTP, the measured concentrations of 7-methylquinoline on the left bank of the river at transects 2 and 3 (Figure 19) are substantially higher than the model predicted values due to incomplete vertical mixing of the Suncor wastestream in the river. At transects 3 and 4 (Figure 20) the model predicted concentrations match the measured values within the range of uncertainty of the analytical methods. However, at transect 6 (Figure 21) with the decay term set to zero, the model overpredicts the measured concentrations.

The model was run again with the decay term set to the measured value of $t_{1/2} = 36$ hrs. For transects 2 and 3 (Figure 22) the model results are virtually the same as for no decay (Figure 19). At transect 4 (Figure 23) the model predicts a minor decrease in the concentrations in the first 2 stream tubes only as compared to the run with no decay (Figure 20). However, at transect 5 (Figure 23) the predicted concentrations are substantially lower than those determined with zero decay (Figure 20).

At transect 6 (Figure 24) the predicted concentrations give a much better fit to the measured data than for the model run with zero decay (Figure 21).

2,4-Dimethylquinoline

As seen in Appendix A, this compound is found at significant concentrations at both transects upstream of the Suncor wastewater stream discharge and is one of the major components in the wastewater stream.

Running the model with decay set to zero, at transect 2 (Figure 25), as was the case for the other compounds, the model underpredicts the concentration measured at the left side of the river due to the lack of vertical mixing of the effluent. However, by transect 3 (Figure 25), the model predicted and observed concentrations are beginning to approach one another. An even better match is seen at transect 4 (Figure 26). The model predicted versus observed data also match very well at transect 5 (Figure 26). The trend of the observed data at transect 6 (Figure 27) do not match the model predicted trend and indicate that there may be an additional source or sources of 2,4-dimethylquinoline along this stretch of the river. This is also obvious in that the water column disappearance kinetics studies (Figure 11) indicated that 2,4-dimethylquinoline should have a decay rate of $t_{1/2} = 48$ hrs. If this was used the model would greatly underestimate the measured river concentrations at the different transects. Unfortunately tributary loads of this compound downstream of the Suncor wastestream discharge are not known.

Pyrene

Pyrene is a minor component of the Suncor effluent (Appendix A) and is actually found at lower concentrations in the Athabasca River below the Suncor effluent discharge than upstream (Appendix A). Consequently, as a compound with natural sources along the river, the mixing of the Suncor effluent in the river is masked and can not be simulated with the model without the tributary loadings (Figures 28-30).

Benzoquinoline Isomer

This compound was not present in detectable quantities at the u/s Horse River transect (Appendix A). However, at mile 20.8 (km 33.3) it was detected at all sites except A. There is no known source of this compound between these two transects to explain the increase in concentration.

Benzoquinoline is also a significant component of the Suncor waste stream (Appendix A). The model predicted (decay set to zero) versus observed concentrations downstream of the effluent discharge are shown in Figures 31-33. Again due to incomplete vertical mixing of the effluent within the river, the model predicted concentrations on the left bank of the river are significantly less than the observed values. However, by transect 6 (Figure 33) the model overpredicts the observed concentrations, indicating that there had been loss of the compound between transects 5 and 6. No experimental water column disappearance kinetics data were obtained for this compound. A

decay value of $t_{1/2} = 36$ hrs was determined through calibration of the model with the observed concentrations. The results are shown in Figures 34-36.

CONCLUSIONS

- 1) The Suncor effluent remains incompletely vertically mixed in the Athabasca River for a distance of 16 to 22 km downstream of the discharge point for the various compounds. All of the compounds studied were found to be incompletely mixed across the river for at least 100 km downstream of the Suncor discharge.
- 2) 2,4-Dimethylbenzothiophene, 2,4-Dimethylquinoline and 7-Methylquinoline were found to be the best tracers of the Suncor effluent. They had no significant natural sources along the river and were major components of the Suncor wastestream.
- 3) The two-dimensional transport and fate model ATHMOD2 was successfully used to simulate the lateral mixing and decay of most of the Suncor wastestream compounds along the 120 km stretch of river downstream of Ft. McMurray. The experimental water column disappearance rates determined for the compounds were confirmed to be correct through calibration of the model with the observed data.
- 4) For those compounds with natural sources along the river and which were not major components of the Suncor wastestream, the downstream concentrations could not be accurately predicted by the model. Samples from the major tributaries have been collected but have not yet been analyzed for the compounds with natural sources. This data could be used as input to the model in order to more accurately simulate their transport and fate in the river. Further calibration and verification of the model requires another complete set of data collected during different flow conditions and effluent loadings.

ACKNOWLEDGEMENTS

We thank S.B. Smith and R. Neureuther, Technical Operations, National Water Research Institute, for providing field support. The contribution of S.B. Smith is especially appreciated for organizing the complex field logistics required in order to sample one transect per day. We also thank J. Lussenburg and the other Suncor staff who provided the daily samples of Suncor wastewater for us. Finally, we gratefully acknowledge the financial support from PERD.

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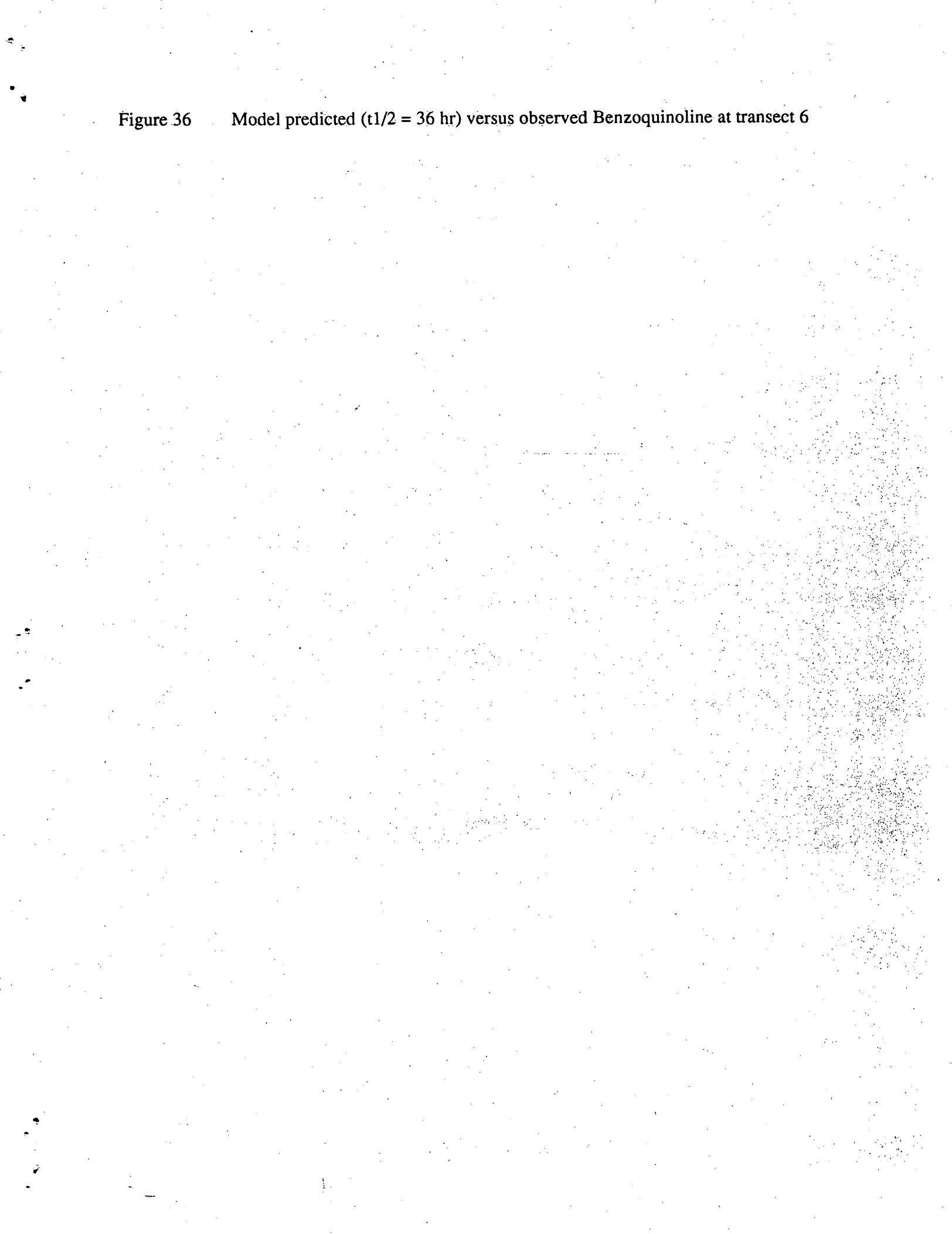
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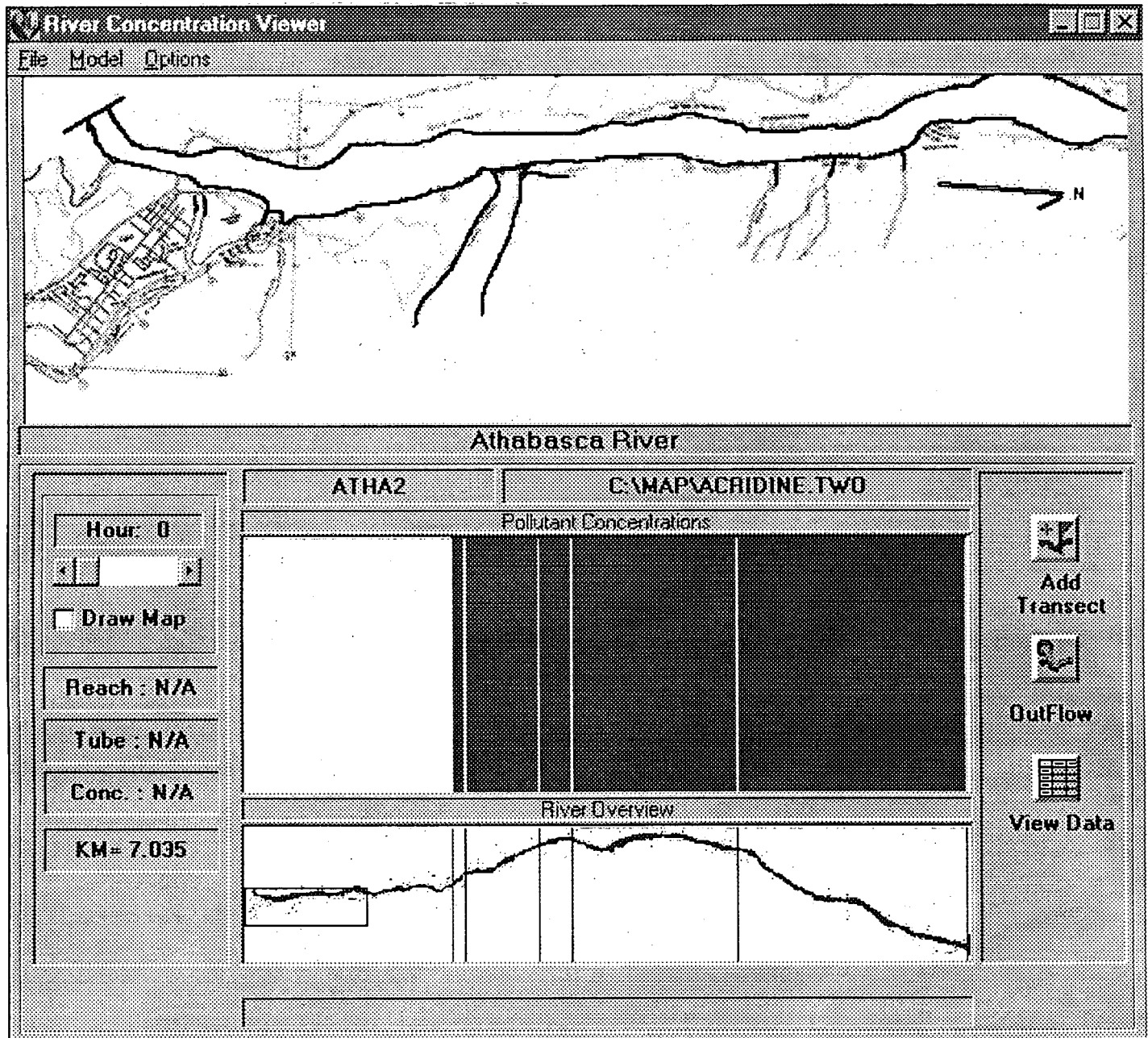


Figure 1

Transect

Transect # 2

Downstream distance of transect from
river zero (0) reference (km)

40.200

Longitudinal dispersion coefficient (m²/s)

0

Transverse dispersion factor

.00039

Leopold-Maddock Exponents

Width

.05

Depth

.5

Velocity

.45

Reach Design

Temperature (C)

20

Stream Flow
(m³/s)

766

Reach Reference Data

Temperature (C)

20

Stream Flow (m³/s)

766

Channel Width (m)

330

Channel Depth (m)

1.73

Channel Velocity (m/s)

1.36

Decay Rate (s⁻¹)

.0005628

Adsorption (?)

Next

Previous

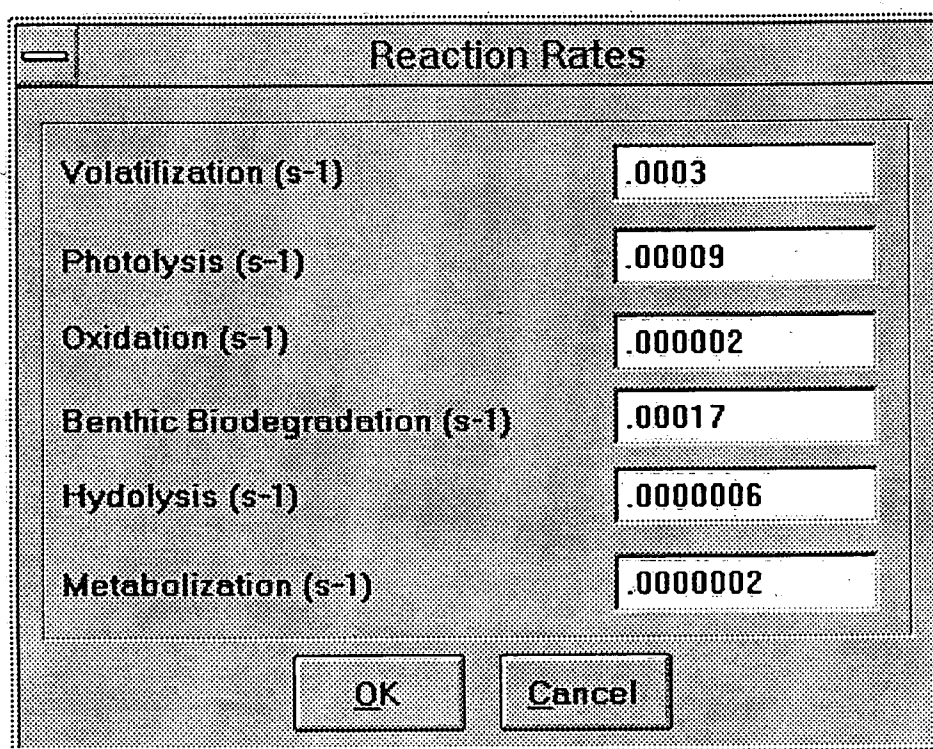
New

Delete

Save

Exit

Figure 3



A screenshot of a software dialog box titled "Reaction Rates". The dialog box has a standard Windows-style title bar with a minimize button. Inside, there is a list of six reaction processes, each with a corresponding numerical value in a text input field. The processes are: Volatilization (s-1) with a value of .0003, Photolysis (s-1) with .00009, Oxidation (s-1) with .000002, Benthic Biodegradation (s-1) with .00017, Hydrolysis (s-1) with .0000006, and Metabolization (s-1) with .0000002. At the bottom of the dialog are two buttons: "OK" and "Cancel".

| Reaction Process | Rate (s-1) |
|------------------------|------------|
| Volatilization | .0003 |
| Photolysis | .00009 |
| Oxidation | .000002 |
| Benthic Biodegradation | .00017 |
| Hydrolysis | .0000006 |
| Metabolization | .0000002 |

Figure 4

Outflow

Source Data Time Interval 24

Number of Time Intervals 15

| | Time Interval | Discharge Rate | Concentration | |
|----|---------------|----------------|---------------|---|
| 1 | 0 | .395 | 260 | ↑ |
| 2 | 24 | .5 | 195 | |
| 3 | 48 | .386 | 210 | |
| 4 | 72 | .395 | 273 | |
| 5 | 96 | .415 | 196 | |
| 6 | 120 | .414 | 228 | |
| 7 | 144 | .413 | 263 | |
| 8 | 168 | .462 | 260 | |
| 9 | 192 | .491 | 260 | |
| 10 | 216 | .45 | 260 | |
| 11 | 240 | .45 | 260 | ↓ |

OK Cancel

Figure 5

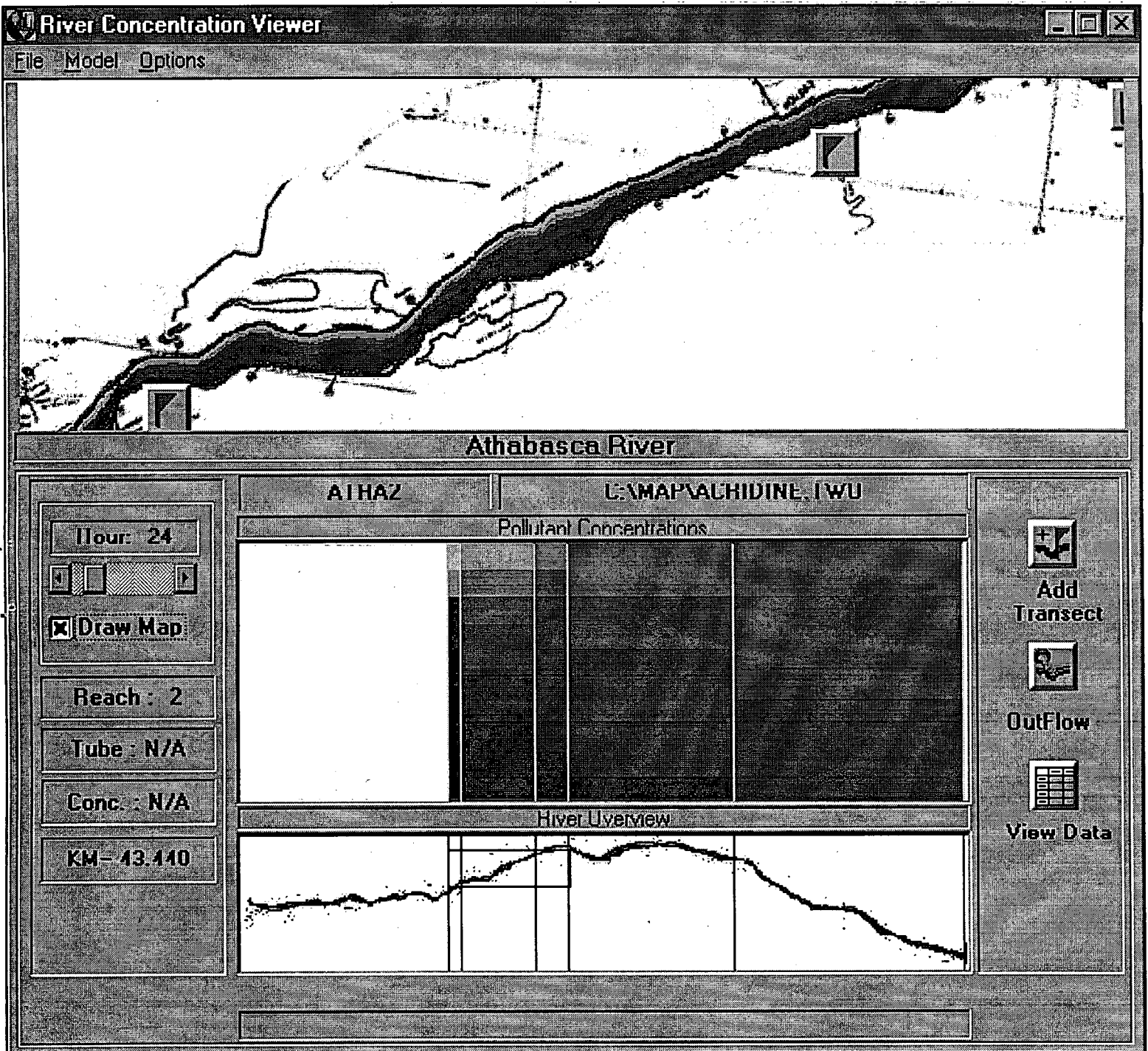


Figure 6

| ATHA2 Data | | | | | | ▼ | ▲ |
|------------|------|--------|--------|--------|--------|---|---|
| Transect | Hour | Tube 6 | Tube 7 | Tube 8 | Tube | ↑ | |
| | | | | | | | |
| | | | | | | | |
| 1 | 0 | 0.0800 | 0.0800 | 0.0800 | 0.0800 | | |
| 1 | 6 | 0.0800 | 0.0805 | 0.1020 | 5.6025 | | |
| 1 | 12 | 0.0800 | 0.0805 | 0.1020 | 5.5785 | | |
| 1 | 18 | 0.0800 | 0.0805 | 0.1015 | 5.5085 | | |
| 1 | 24 | 0.0800 | 0.0805 | 0.1010 | 5.3925 | | |
| 1 | 30 | 0.0800 | 0.0805 | 0.1005 | 5.2215 | | |
| 1 | 36 | 0.0800 | 0.0805 | 0.0995 | 5.0120 | | |
| 1 | 42 | 0.0800 | 0.0805 | 0.0990 | 4.7910 | | |
| 1 | 48 | 0.0800 | 0.0805 | 0.0980 | 4.5585 | | |
| 1 | 54 | 0.0800 | 0.0805 | 0.0980 | 4.6165 | | |
| 1 | 60 | 0.0800 | 0.0805 | 0.0995 | 4.9725 | | |
| 1 | 66 | 0.0800 | 0.0805 | 0.1010 | 5.3325 | | |
| 1 | 72 | 0.0800 | 0.0805 | 0.1025 | 5.6965 | | |
| 1 | 78 | 0.0800 | 0.0805 | 0.1025 | 5.7090 | | |
| 1 | 84 | 0.0800 | 0.0805 | 0.1010 | 5.3630 | | |
| 1 | 90 | 0.0800 | 0.0805 | 0.0995 | 5.0065 | | |
| 1 | 96 | 0.0800 | 0.0805 | 0.0980 | 4.6400 | | |
| 1 | 102 | 0.0800 | 0.0805 | 0.0980 | 4.5425 | | |
| | | | | | | ↓ | |
| ← | | | | | | → | |

Figure 7

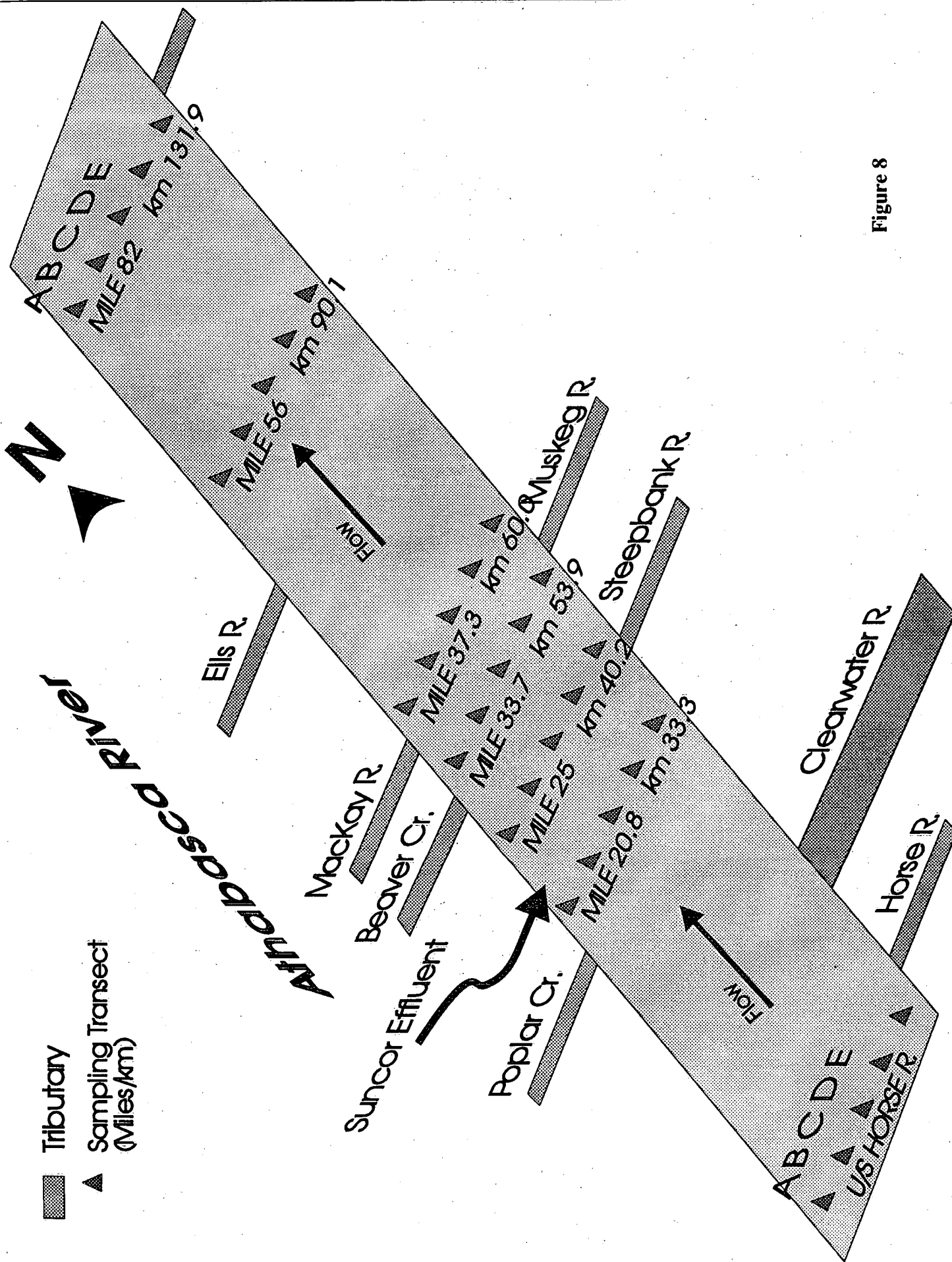


Figure 8

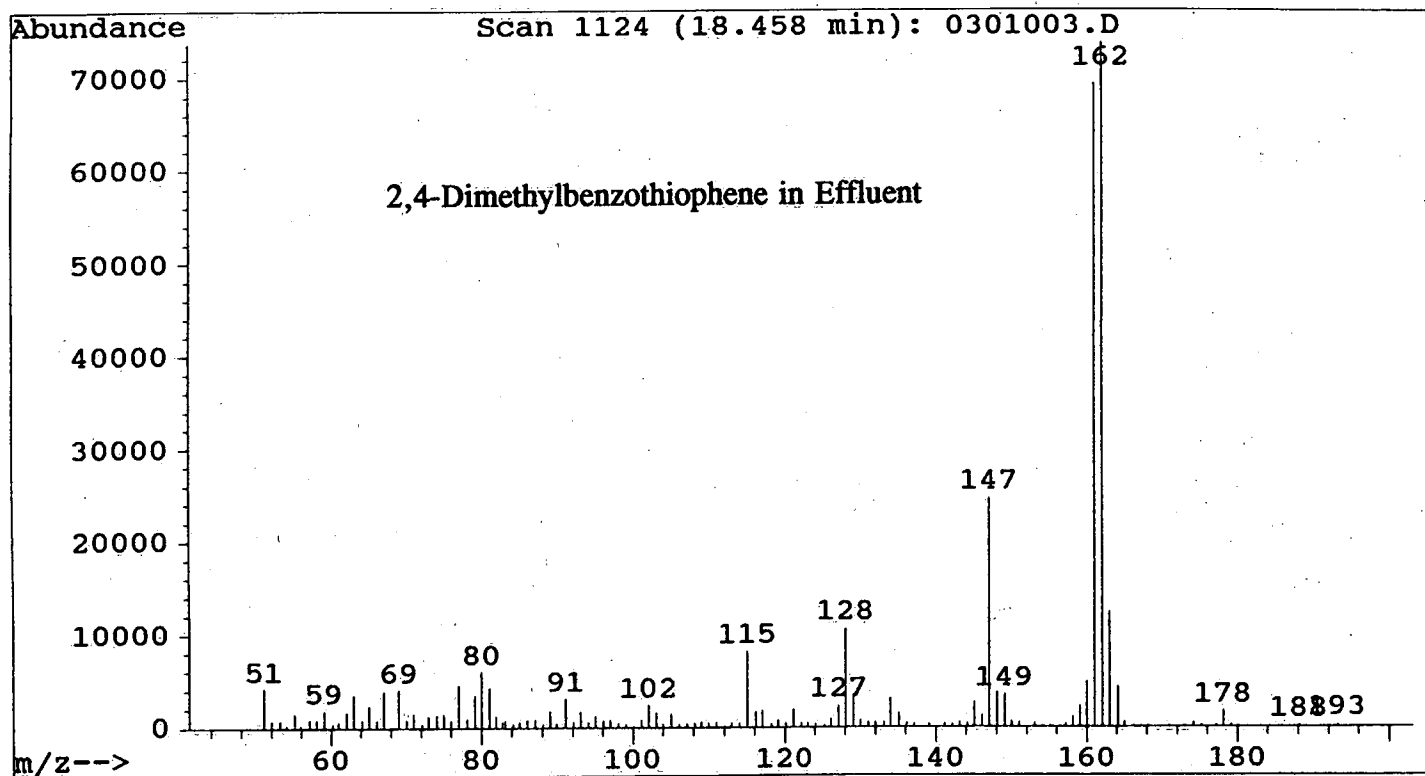


Figure 9

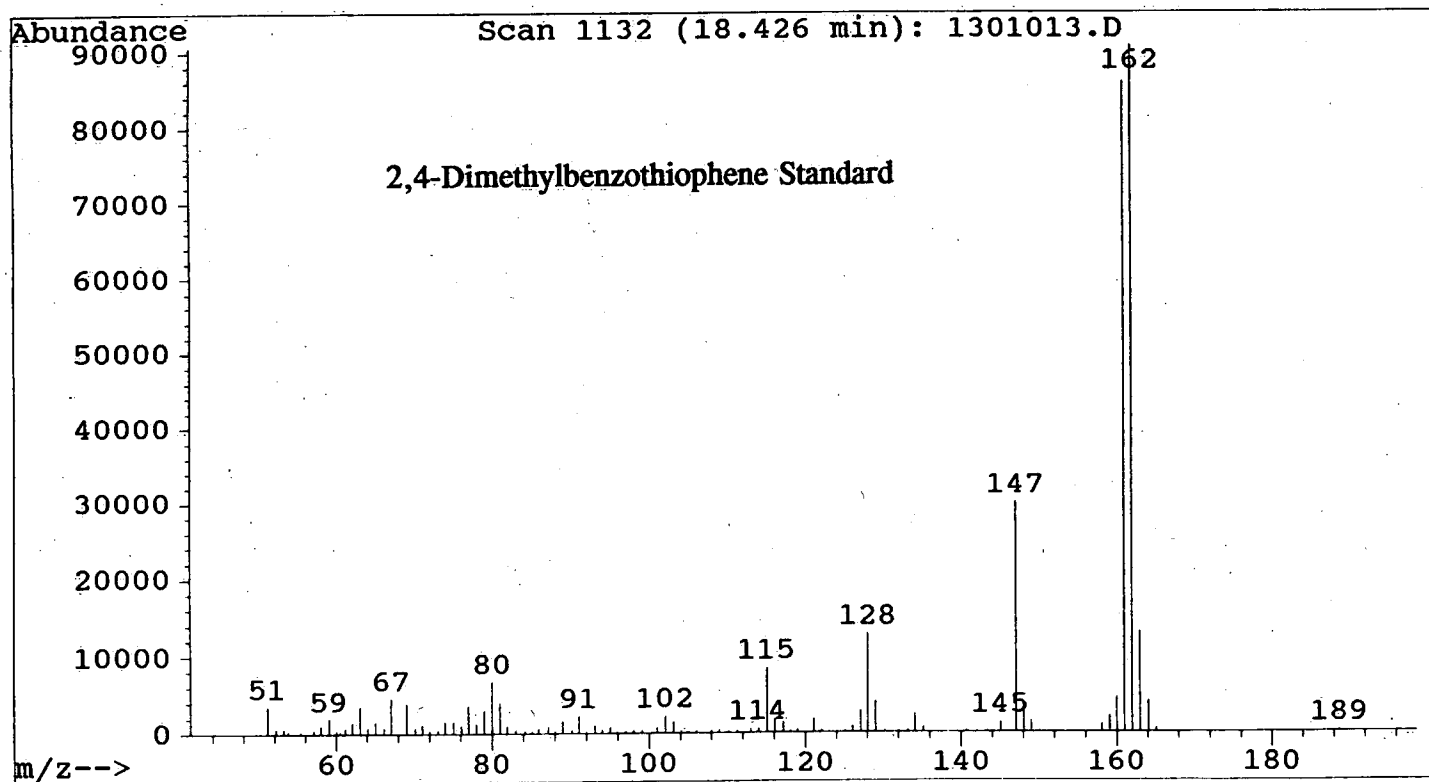


Figure 10

Water Column Disappearance Kinetics

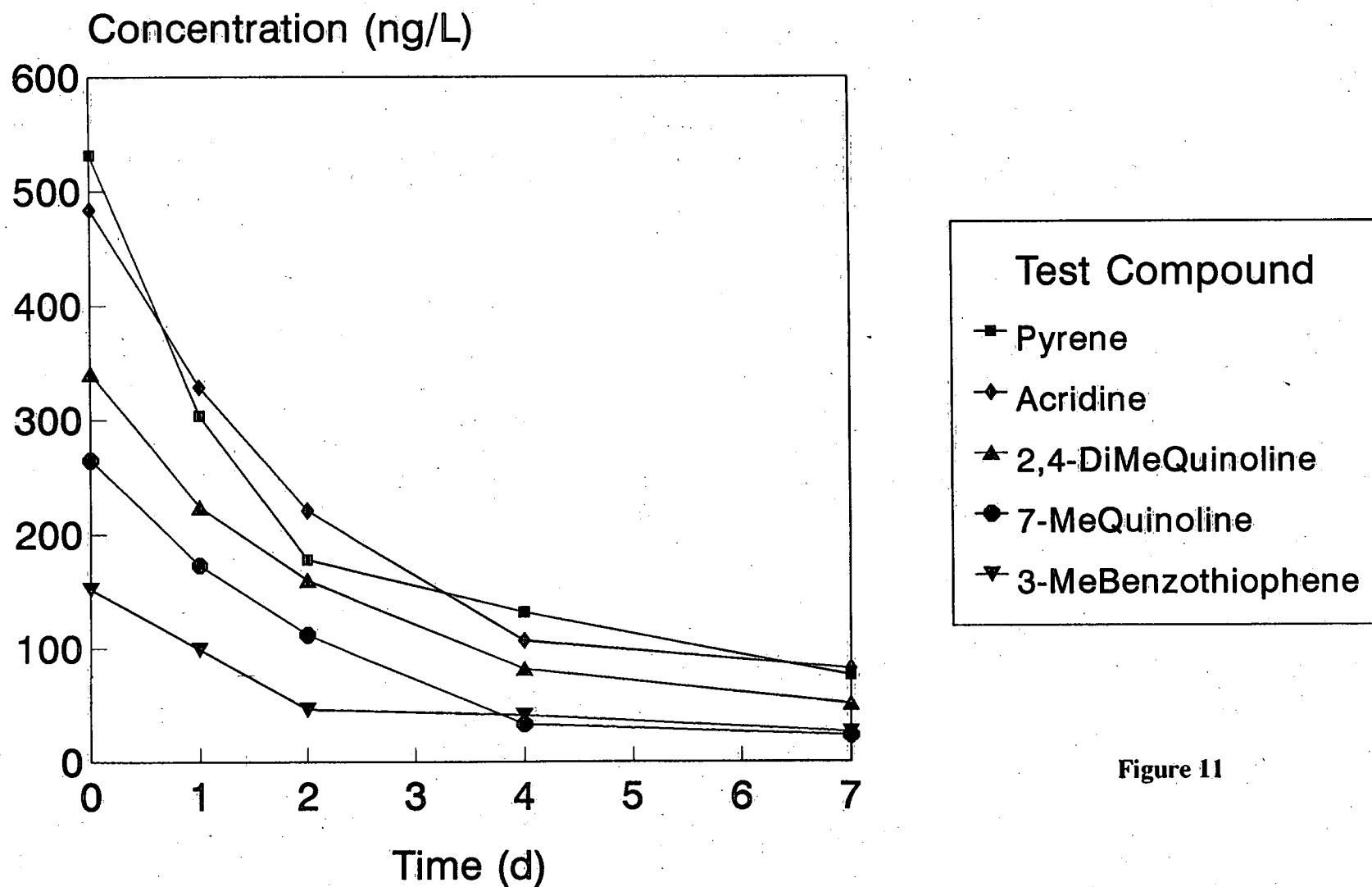
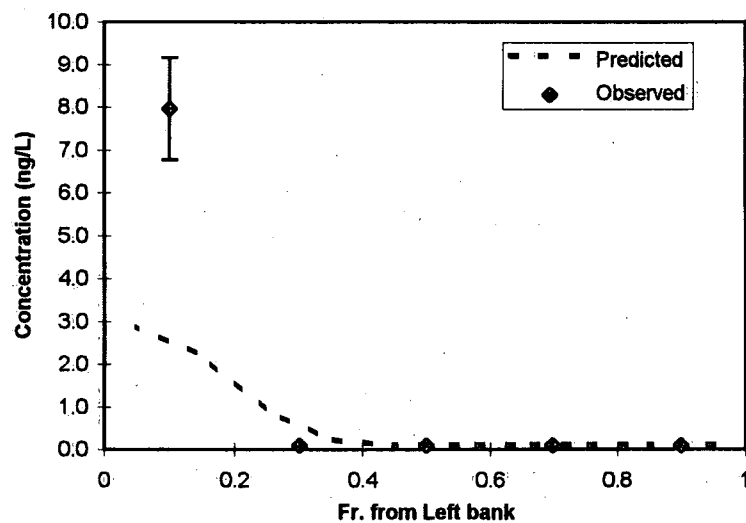


Figure 11

Figure 12

| 2,4-Dimethylbenzothiophene Output; T=15°C | | | | | | | | | | | | | | | | |
|---|----------|--------|--------|--------|--------|--------|--------|--------|--------|--------|---------|--------|--------|--------|--------|--------|
| Fr. from Left Bank | | 0.95 | 0.85 | 0.75 | 0.65 | 0.55 | 0.45 | 0.35 | 0.25 | 0.15 | 0.05 | 0.1 | 0.3 | 0.5 | 0.7 | 0.9 |
| Transect | Time (h) | Tube 1 | Tube 2 | Tube 3 | Tube 4 | Tube 5 | Tube 6 | Tube 7 | Tube 8 | Tube 9 | Tube 10 | Site A | Site B | Site C | Site D | Site E |
| 2 | 24 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1005 | 0.1115 | 0.2355 | 0.92 | 2.2115 | 2.885 | 7.97 | 0.1 | 0.1 | 0.1 | 0.1 |
| 3 | 48 | 0.1 | 0.101 | 0.106 | 0.1255 | 0.1905 | 0.3595 | 0.695 | 1.1945 | 1.728 | 2.0775 | 3.92 | 1.43 | 1.27 | 0.1 | 0.1 |

2,4-DMBTP at Transect 2



2,4-DMBTP at Transect 3

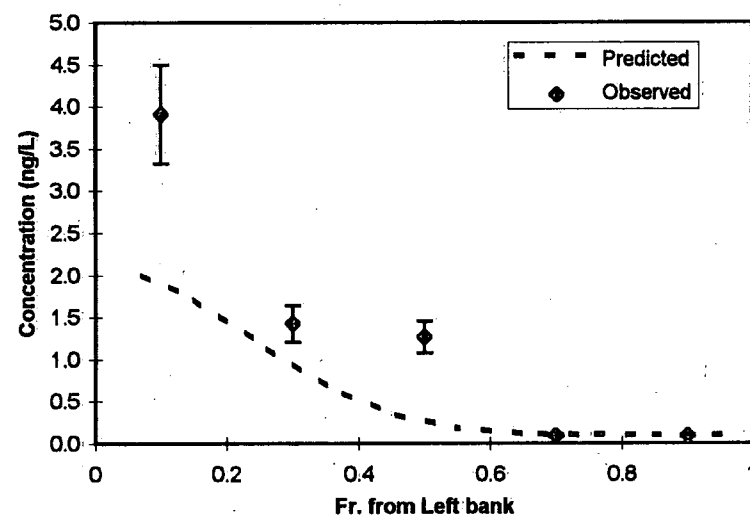
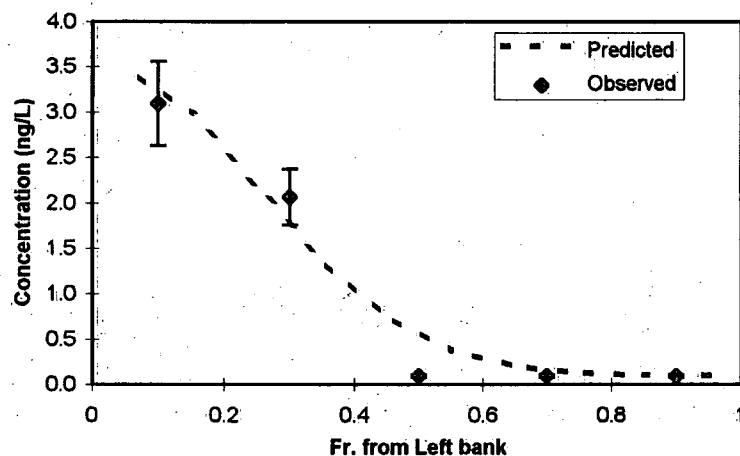


Figure 13

Organic compounds in Atha. R. May/93

| 2,4-Dimethylbenzothiophene Output; T=15°C | | | | | | | | | | | | | | | | |
|---|----------|--------|--------|--------|--------|--------|--------|--------|--------|--------|---------|--------|--------|--------|--------|--------|
| Fr. from Left Bank | | 0.95 | 0.85 | 0.75 | 0.65 | 0.55 | 0.45 | 0.35 | 0.25 | 0.15 | 0.05 | 0.1 | 0.3 | 0.5 | 0.7 | 0.9 |
| Transect | Time (h) | Tube 1 | Tube 2 | Tube 3 | Tube 4 | Tube 5 | Tube 6 | Tube 7 | Tube 8 | Tube 9 | Tube 10 | Site A | Site B | Site C | Site D | Site E |
| 4 | 96 | 0.102 | 0.108 | 0.1315 | 0.203 | 0.383 | 0.7545 | 1.3735 | 2.1875 | 2.9915 | 3.499 | 3.1 | 2.07 | 0.1 | 0.1 | 0.1 |
| 5 | 114 | 0.1965 | 0.2525 | 0.3755 | 0.584 | 0.892 | 1.296 | 1.764 | 2.232 | 2.615 | 2.8315 | 1.77 | 1.61 | 0.936 | 0.626 | 1.27 |

2,4-DMBTP at Transect 4



2,4-DMBTP at Transect 5

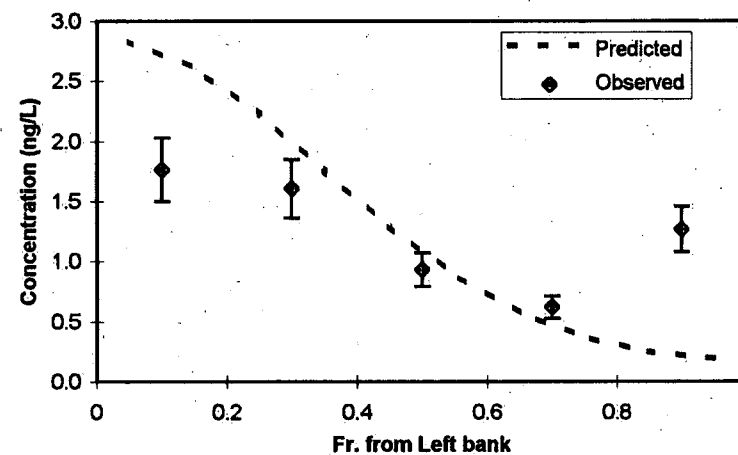


Figure 14

Organic compounds in Atha. R. May/93

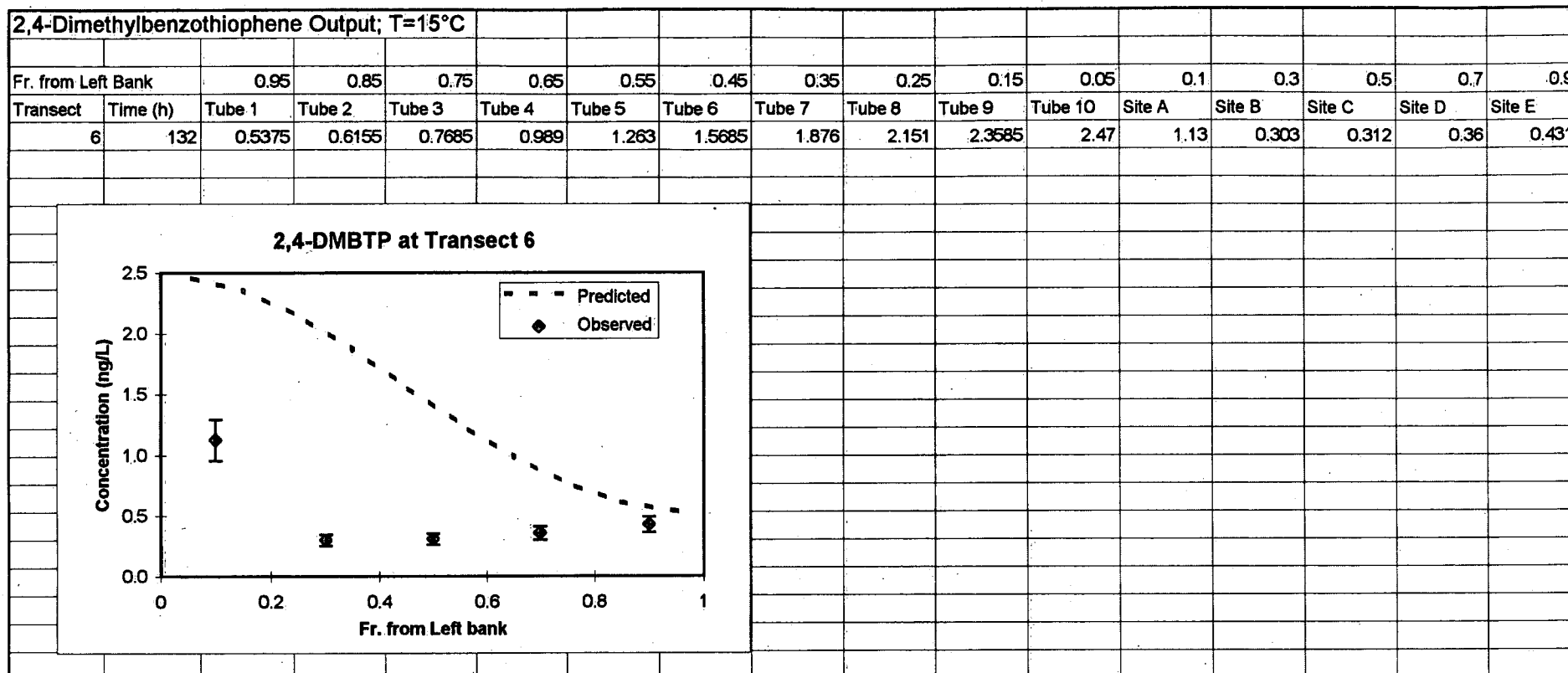


Figure 15

2,4-Dimethylbenzothiophene Output with $t_{1/2}=36$ hours; $T=15^{\circ}\text{C}$

| Fr. from Left Bank | | 0.95 | 0.85 | 0.75 | 0.65 | 0.55 | 0.45 | 0.35 | 0.25 | 0.15 | 0.05 | 0.1 | 0.3 | 0.5 | 0.7 | 0.9 |
|--------------------|----------|--------|--------|--------|--------|--------|--------|--------|--------|--------|---------|--------|--------|--------|--------|--------|
| Transect | Time (h) | Tube 1 | Tube 2 | Tube 3 | Tube 4 | Tube 5 | Tube 6 | Tube 7 | Tube 8 | Tube 9 | Tube 10 | Site A | Site B | Site C | Site D | Site E |
| 2 | 24 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1005 | 0.1115 | 0.234 | 0.91 | 2.1865 | 2.852 | 7.97 | 0.1 | 0.1 | 0.1 | 0.1 |
| 3 | 48 | 0.1 | 0.101 | 0.1055 | 0.123 | 0.1825 | 0.3375 | 0.6455 | 1.105 | 1.5955 | 1.9165 | 3.92 | 1.43 | 1.27 | 0.1 | 0.1 |

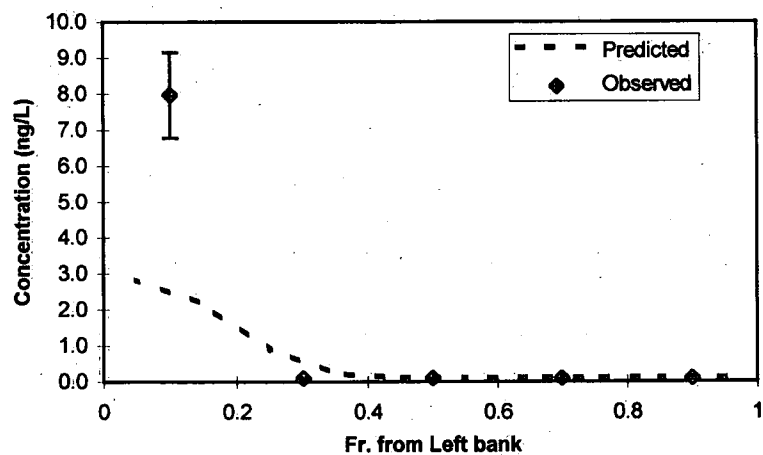
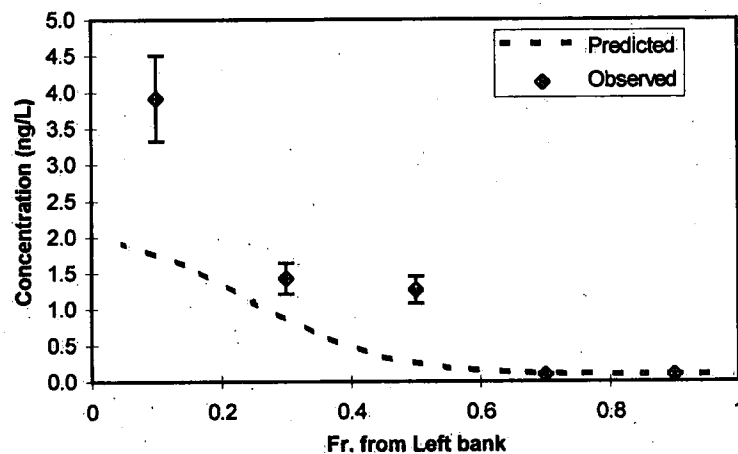
2,4-DMBTP at Transect 2 -- $t_{1/2}=36$ h2,4-DMBTP at Transect 3 -- $t_{1/2}=36$ h

Figure 16

2,4-Dimethylbenzothiophene Output with $t_{1/2}=36$ hours; $T=15^{\circ}\text{C}$

| Fr. from Left Bank | | 0.95 | 0.85 | 0.75 | 0.65 | 0.55 | 0.45 | 0.35 | 0.25 | 0.15 | 0.05 | 0.1 | 0.3 | 0.5 | 0.7 | 0.9 |
|--------------------|----------|--------|--------|--------|--------|--------|--------|--------|--------|--------|---------|--------|--------|--------|--------|--------|
| Transect | Time (h) | Tube 1 | Tube 2 | Tube 3 | Tube 4 | Tube 5 | Tube 6 | Tube 7 | Tube 8 | Tube 9 | Tube 10 | Site A | Site B | Site C | Site D | Site E |
| 4 | 96 | 0.102 | 0.1075 | 0.1275 | 0.1895 | 0.3475 | 0.674 | 1.2185 | 1.935 | 2.643 | 3.0895 | 3.1 | 2.07 | 0.1 | 0.1 | 0.1 |
| 5 | 114 | 0.167 | 0.206 | 0.2925 | 0.4385 | 0.6545 | 0.9385 | 1.2675 | 1.597 | 1.867 | 2.0195 | 1.77 | 1.61 | 0.936 | 0.626 | 1.27 |

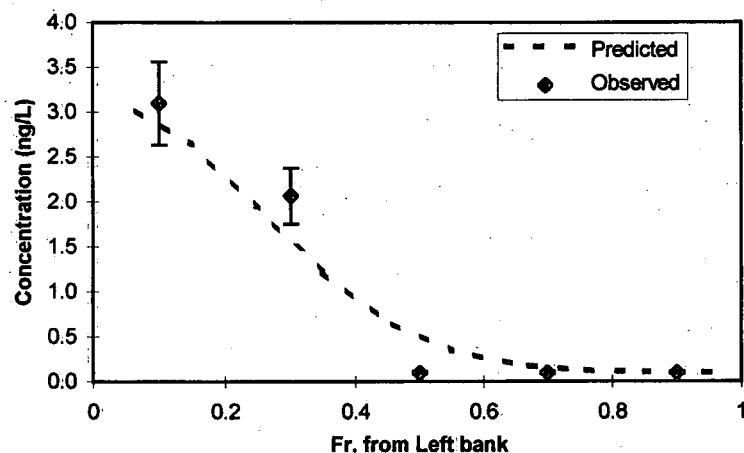
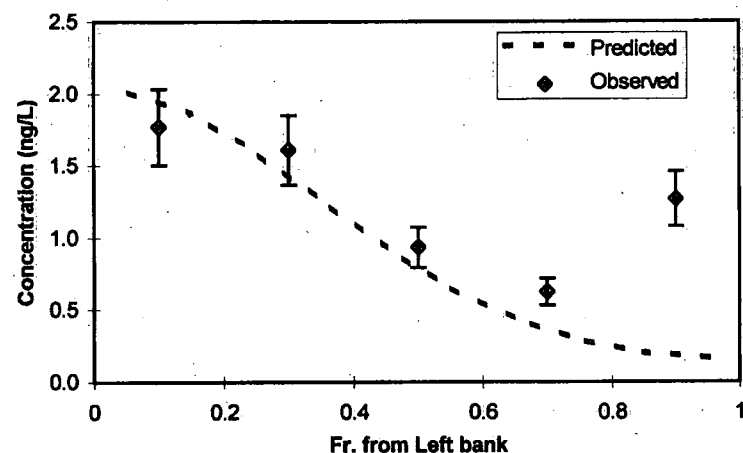
2,4-DMBTP at Transect 4 -- $t_{1/2}=36$ h2,4-DMBTP at Transect 5 -- $t_{1/2}=36$ h

Figure 17

Organic compounds in Atha. R. May/93

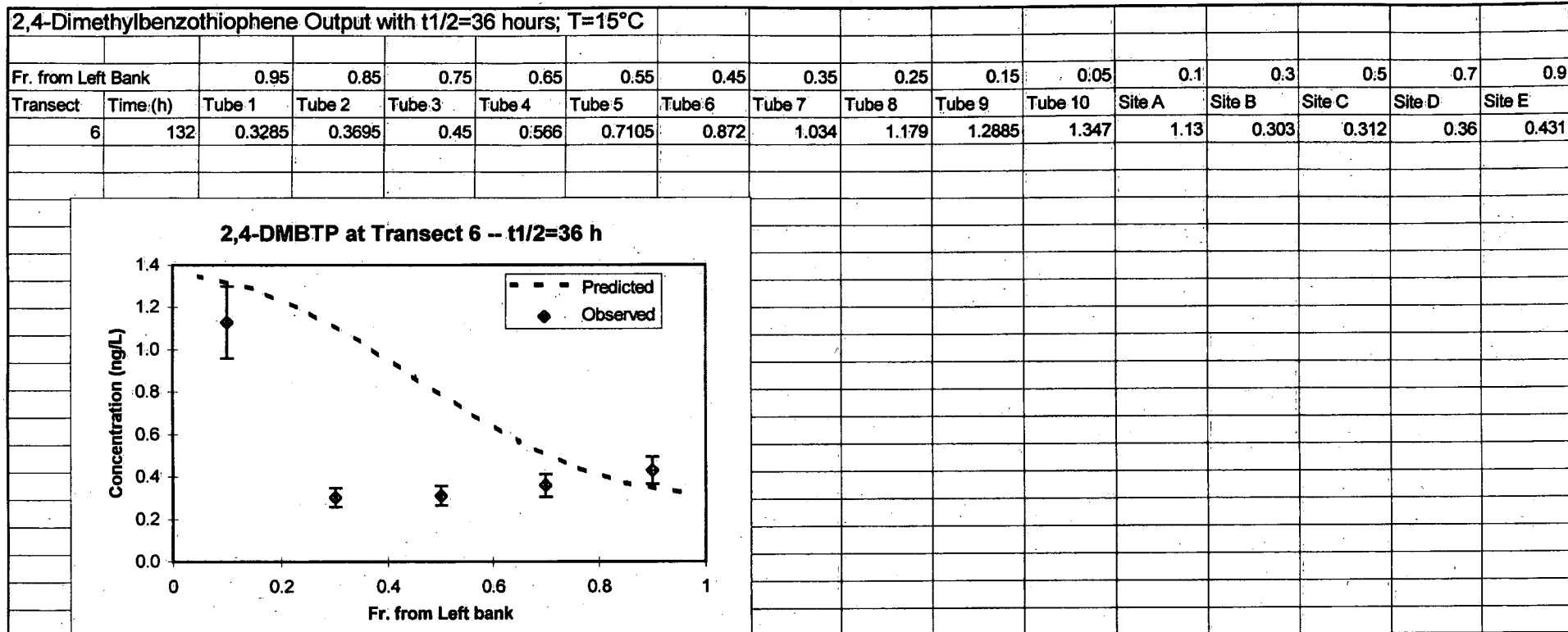


Figure 18

Organic compounds in Atha. R. May/93

2,4-Dimethylbenzothiophene Output with variable $t_{1/2}$ (36 and 12 hours); $T=15^{\circ}\text{C}$

| Fr. from Left Bank | | 0.95 | 0.85 | 0.75 | 0.65 | 0.55 | 0.45 | 0.35 | 0.25 | 0.15 | 0.05 | 0.1 | 0.3 | 0.5 | 0.7 | 0.9 |
|--------------------|----------|--------|--------|--------|--------|--------|--------|--------|--------|--------|---------|--------|--------|--------|--------|--------|
| Transect | Time (h) | Tube 1 | Tube 2 | Tube 3 | Tube 4 | Tube 5 | Tube 6 | Tube 7 | Tube 8 | Tube 9 | Tube 10 | Site A | Site B | Site C | Site D | Site E |
| 6 | 132 | 0.226 | 0.249 | 0.2935 | 0.358 | 0.4385 | 0.528 | 0.618 | 0.699 | 0.76 | 0.7925 | 1.13 | 0.303 | 0.312 | 0.36 | 0.431 |

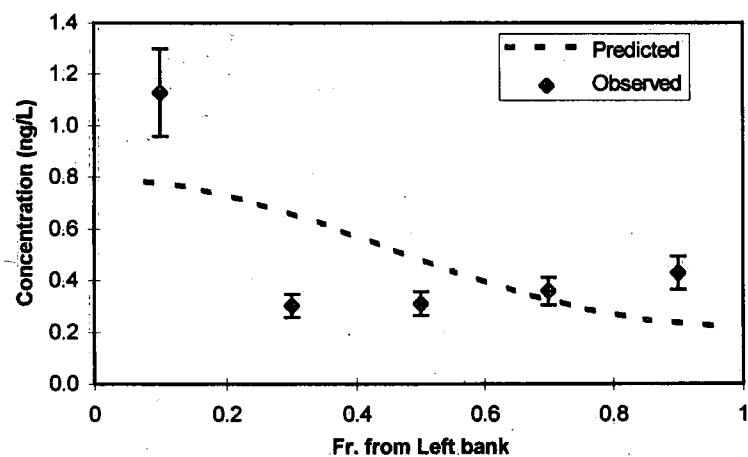
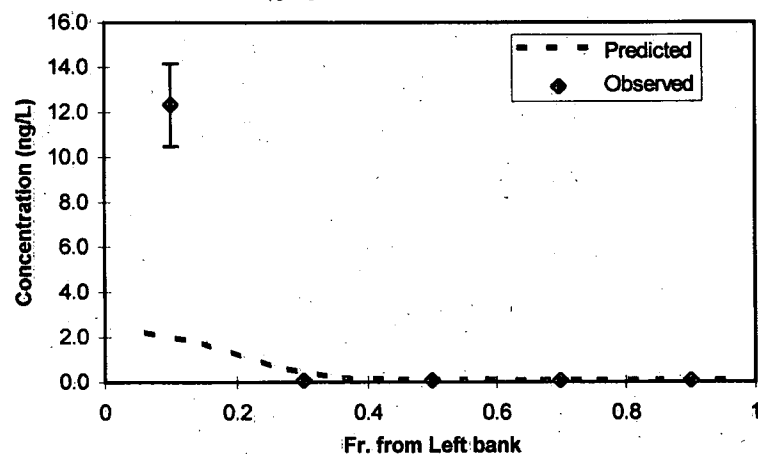
2,4-DMBTP at Transect 6 -- $t_{1/2}=12$ h

Figure 19

| 7-Methylquinoline Output; T=15°C | | | | | | | | | | | | | | | | |
|----------------------------------|----------|--------|--------|--------|--------|--------|--------|--------|--------|--------|---------|--------|--------|--------|--------|--------|
| Fr. from Left Bank | | 0.95 | 0.85 | 0.75 | 0.65 | 0.55 | 0.45 | 0.35 | 0.25 | 0.15 | 0.05 | 0.1 | 0.3 | 0.5 | 0.7 | 0.9 |
| Transect | Time (h) | Tube 1 | Tube 2 | Tube 3 | Tube 4 | Tube 5 | Tube 6 | Tube 7 | Tube 8 | Tube 9 | Tube 10 | Site A | Site B | Site C | Site D | Site E |
| 2 | 24 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1005 | 0.1095 | 0.2065 | 0.7425 | 1.7545 | 2.282 | 12.33 | 0.1 | 0.1 | 0.1 | 0.1 |
| 3 | 48 | 0.1 | 0.1005 | 0.104 | 0.1185 | 0.1665 | 0.291 | 0.539 | 0.908 | 1.301 | 1.5585 | 2.28 | 2.05 | 0.1 | 0.1 | 0.1 |

7-Methylquinoline at Transect 2



7-Methylquinoline at Transect 3

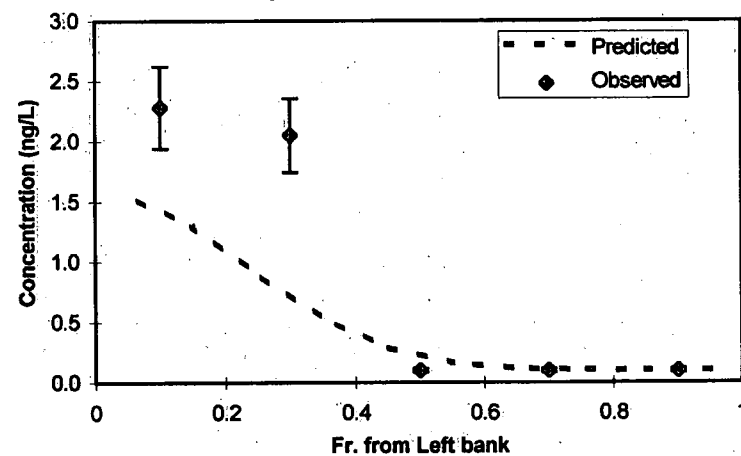


Figure 20

| 7-Methylquinoline Output; T=15°C | | | | | | | | | | | | | | | | |
|----------------------------------|----------|--------|--------|--------|--------|--------|--------|--------|--------|--------|---------|--------|--------|--------|--------|--------|
| Fr. from Left Bank | | 0.95 | 0.85 | 0.75 | 0.65 | 0.55 | 0.45 | 0.35 | 0.25 | 0.15 | 0.05 | 0.1 | 0.3 | 0.5 | 0.7 | 0.9 |
| Transect | Time (h) | Tube 1 | Tube 2 | Tube 3 | Tube 4 | Tube 5 | Tube 6 | Tube 7 | Tube 8 | Tube 9 | Tube 10 | Site A | Site B | Site C | Site D | Site E |
| 4 | 96 | 0.1005 | 0.103 | 0.111 | 0.1355 | 0.197 | 0.3225 | 0.531 | 0.8045 | 1.074 | 1.244 | 0.818 | 1.17 | 0.1 | 0.1 | 0.1 |
| 5 | 114 | 0.1265 | 0.1415 | 0.175 | 0.232 | 0.3155 | 0.425 | 0.552 | 0.6785 | 0.782 | 0.8405 | 0.693 | 0.783 | 0.1 | 0.1 | 0.1 |

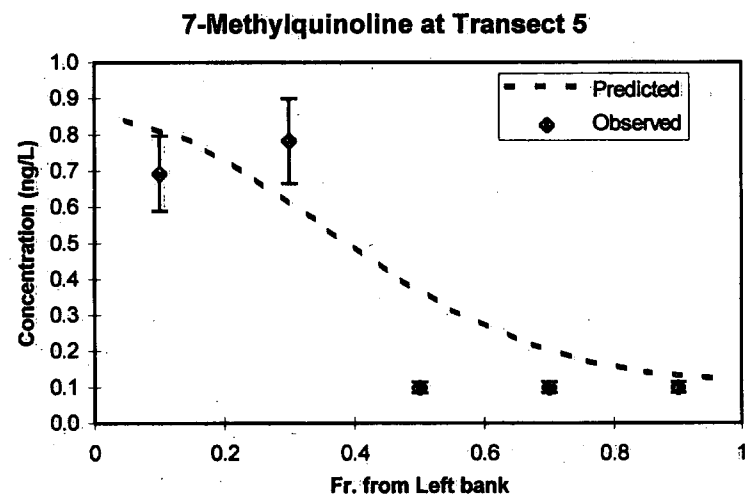
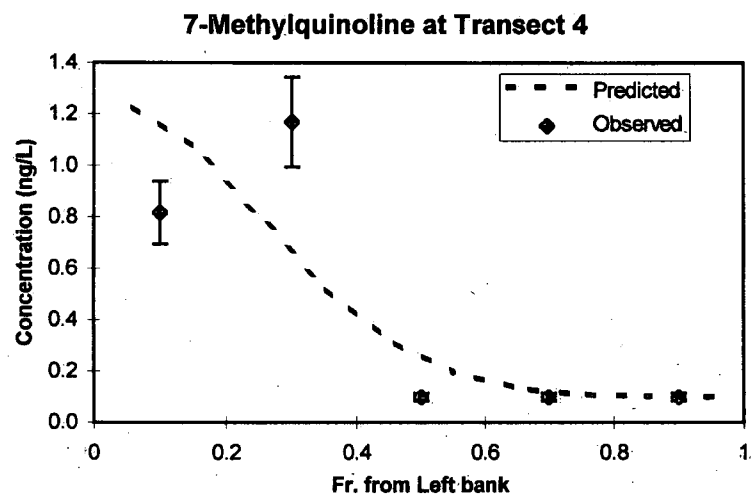


Figure 21

Organic compounds in Atha. R. May/93

7-Methylquinoline Output; T=15°C

| | | | | | | | | | | | | | | | | |
|--------------------|----------|--------|--------|--------|--------|--------|--------|--------|--------|--------|---------|--------|--------|--------|--------|--------|
| | | | | | | | | | | | | | | | | |
| Fr. from Left Bank | | 0.95 | 0.85 | 0.75 | 0.65 | 0.55 | 0.45 | 0.35 | 0.25 | 0.15 | 0.05 | 0.1 | 0.3 | 0.5 | 0.7 | 0.9 |
| Transect | Time (h) | Tube 1 | Tube 2 | Tube 3 | Tube 4 | Tube 5 | Tube 6 | Tube 7 | Tube 8 | Tube 9 | Tube 10 | Site A | Site B | Site C | Site D | Site E |
| 6 | 132 | 0.2055 | 0.224 | 0.2605 | 0.313 | 0.3785 | 0.4515 | 0.5245 | 0.5895 | 0.639 | 0.666 | 0.1 | 0.1 | 0.213 | 0.1 | 0.1 |
| | | | | | | | | | | | | | | | | |
| | | | | | | | | | | | | | | | | |
| | | | | | | | | | | | | | | | | |

7-Methylquinoline at Transect 6

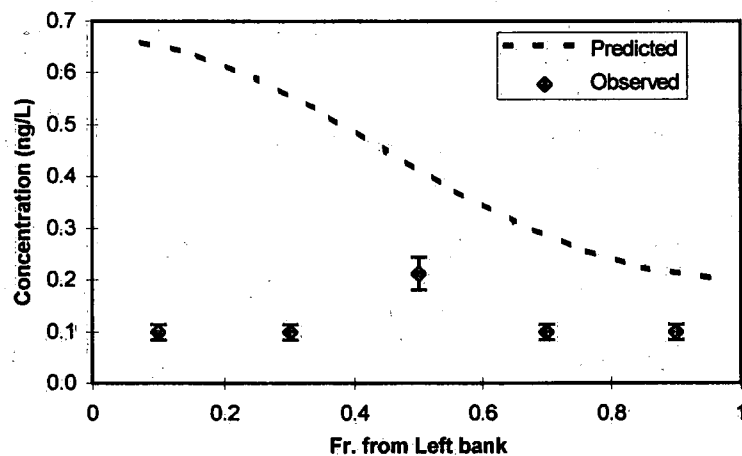


Figure 22

| 7-Methylquinoline Output with $t_{1/2}=36$ hours; $T=15^{\circ}\text{C}$ | | | | | | | | | | | | | | | | |
|--|----------|--------|--------|--------|--------|--------|--------|--------|--------|--------|---------|--------|--------|--------|--------|--------|
| Fr. from Left Bank | | 0.95 | 0.85 | 0.75 | 0.65 | 0.55 | 0.45 | 0.35 | 0.25 | 0.15 | 0.05 | 0.1 | 0.3 | 0.5 | 0.7 | 0.9 |
| Transect | Time (h) | Tube 1 | Tube 2 | Tube 3 | Tube 4 | Tube 5 | Tube 6 | Tube 7 | Tube 8 | Tube 9 | Tube 10 | Site A | Site B | Site C | Site D | Site E |
| 2 | 24 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1005 | 0.109 | 0.205 | 0.735 | 1.735 | 2.256 | 12.33 | 0.1 | 0.1 | 0.1 | 0.1 |
| 3 | 48 | 0.1 | 0.1005 | 0.1035 | 0.117 | 0.161 | 0.275 | 0.5025 | 0.8415 | 1.203 | 1.44 | 2.28 | 2.05 | 0.1 | 0.1 | 0.1 |

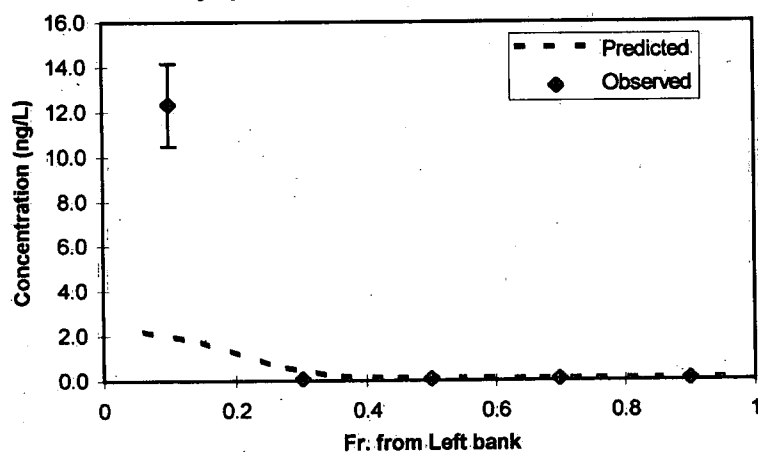
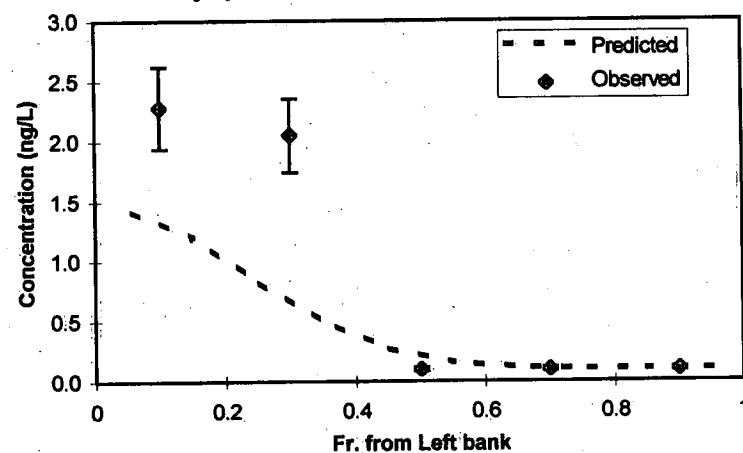
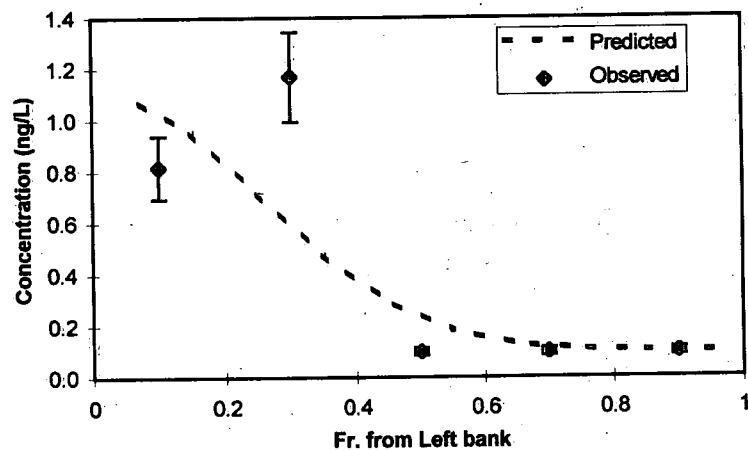
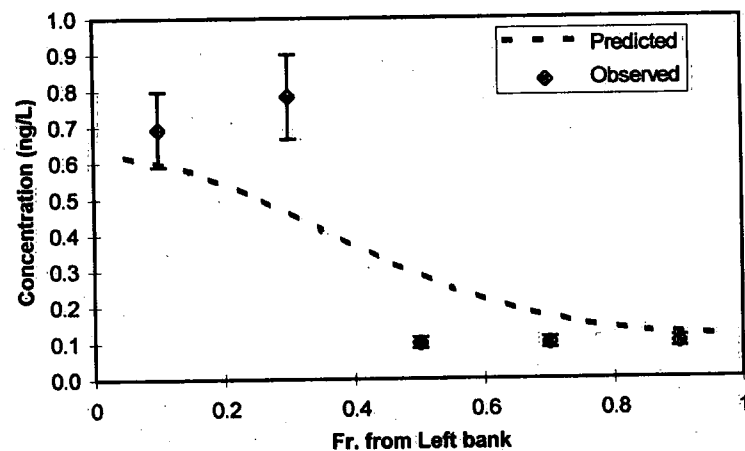
7-Methylquinoline at Transect 2 -- $t_{1/2}=36$ h7-Methylquinoline at Transect 3 -- $t_{1/2}=36$ h

Figure 23

| 7-Methylquinoline Output with $t_{1/2}=36$ hours; $T=15^{\circ}\text{C}$ | | | | | | | | | | | | | | | | |
|--|----------|--------|--------|--------|--------|--------|--------|--------|--------|--------|---------|--------|--------|--------|--------|--------|
| Fr. from Left Bank | | 0.95 | 0.85 | 0.75 | 0.65 | 0.55 | 0.45 | 0.35 | 0.25 | 0.15 | 0.05 | 0.1 | 0.3 | 0.5 | 0.7 | 0.9 |
| Transect | Time (h) | Tube 1 | Tube 2 | Tube 3 | Tube 4 | Tube 5 | Tube 6 | Tube 7 | Tube 8 | Tube 9 | Tube 10 | Site A | Site B | Site C | Site D | Site E |
| 4 | 96 | 0.1005 | 0.1025 | 0.1095 | 0.131 | 0.1845 | 0.295 | 0.4785 | 0.7185 | 0.956 | 1.106 | 0.818 | 1.17 | 0.1 | 0.1 | 0.1 |
| 5 | 114 | 0.1185 | 0.129 | 0.1525 | 0.192 | 0.2505 | 0.3275 | 0.4165 | 0.5055 | 0.578 | 0.619 | 0.693 | 0.783 | 0.1 | 0.1 | 0.1 |

7-Methylquinoline at Transect 4 – $t_{1/2}=36$ h7-Methylquinoline at Transect 5 – $t_{1/2}=36$ h

7-Methylquinoline at Transect 6 -- $t_{1/2}=36$ h

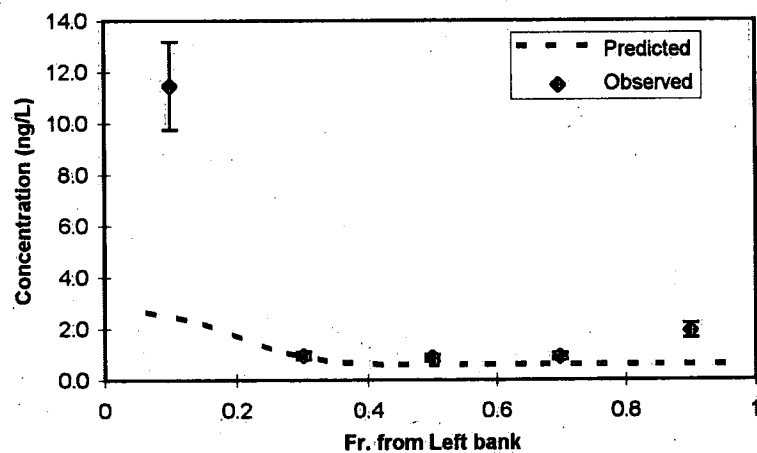
This graph plots the concentration of 7-Methylquinoline (ng/L) against the distance from the left bank (Fr. from Left bank). The y-axis ranges from 0.00 to 0.40 ng/L, and the x-axis ranges from 0 to 1. A dashed line represents the predicted concentration, which decreases from approximately 0.39 ng/L at distance 0 to 0.16 ng/L at distance 1. Observed data points are shown as diamonds with vertical error bars. The observed concentrations are relatively low, ranging from approximately 0.10 to 0.22 ng/L.

| Fr. from Left bank | Predicted Concentration (ng/L) | Observed Concentration (ng/L) |
|--------------------|--------------------------------|-------------------------------|
| 0.1 | 0.38 | 0.10 |
| 0.3 | 0.35 | 0.10 |
| 0.5 | 0.28 | 0.22 |
| 0.7 | 0.20 | 0.10 |
| 0.9 | 0.17 | 0.10 |

Figure 25

| 2,4-Dimethylquinoline Output; T=15°C | | | | | | | | | | | | | | | | |
|--------------------------------------|----------|--------|--------|--------|--------|--------|--------|--------|--------|--------|---------|--------|--------|--------|--------|--------|
| Fr. from Left Bank | | 0.95 | 0.85 | 0.75 | 0.65 | 0.55 | 0.45 | 0.35 | 0.25 | 0.15 | 0.05 | 0.1 | 0.3 | 0.5 | 0.7 | 0.9 |
| Transect | Time:(h) | Tube 1 | Tube 2 | Tube 3 | Tube 4 | Tube 5 | Tube 6 | Tube 7 | Tube 8 | Tube 9 | Tube 10 | Site A | Site B | Site C | Site D | Site E |
| 2 | 24 | 0.6 | 0.6 | 0.6 | 0.6 | 0.6005 | 0.609 | 0.7055 | 1.238 | 2.242 | 2.7655 | 11.48 | 0.981 | 0.892 | 0.934 | 1.93 |
| 3 | 48 | 0.6 | 0.6005 | 0.604 | 0.6185 | 0.6655 | 0.7875 | 1.031 | 1.3935 | 1.7795 | 2.0325 | 2.23 | 1.77 | 1.04 | 0.1 | 0.1 |

2,4-Dimethylquinoline at Transect 2



2,4-Dimethylquinoline at Transect 3

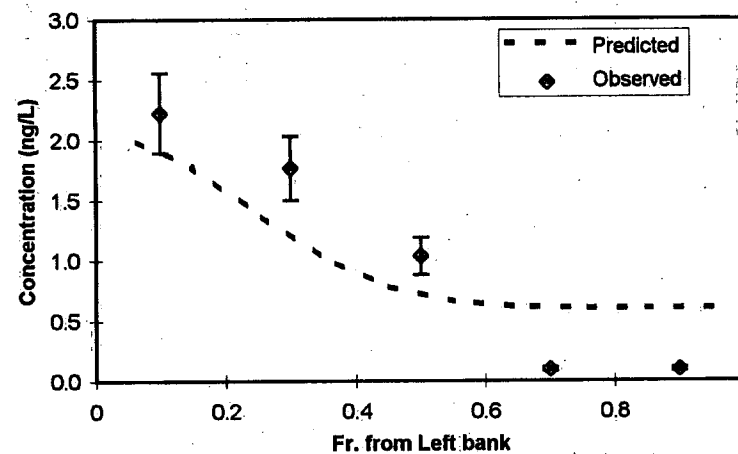


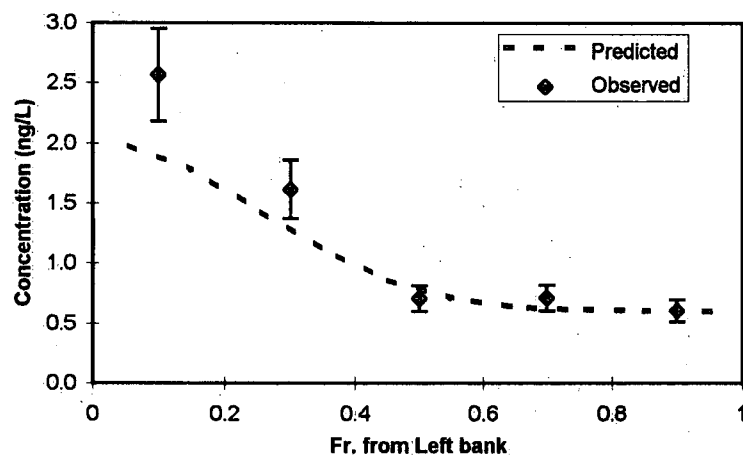
Figure 26

Organic compounds in Atha. R. May/93

2,4-Dimethylquinoline Output; T=15°C

| Fr. from Left Bank | | 0.95 | 0.85 | 0.75 | 0.65 | 0.55 | 0.45 | 0.35 | 0.25 | 0.15 | 0.05 | 0.1 | 0.3 | 0.5 | 0.7 | 0.9 |
|--------------------|----------|--------|--------|--------|--------|--------|--------|--------|--------|--------|---------|--------|--------|--------|--------|--------|
| Transect | Time (h) | Tube 1 | Tube 2 | Tube 3 | Tube 4 | Tube 5 | Tube 6 | Tube 7 | Tube 8 | Tube 9 | Tube 10 | Site A | Site B | Site C | Site D | Site E |
| 4 | 96 | 0.601 | 0.6035 | 0.6135 | 0.643 | 0.717 | 0.87 | 1.124 | 1.457 | 1.786 | 1.993 | 2.57 | 1.62 | 0.711 | 0.717 | 0.61 |
| 5 | 114 | 0.6335 | 0.6525 | 0.695 | 0.7665 | 0.8715 | 1.01 | 1.17 | 1.3295 | 1.4605 | 1.5345 | 2.31 | 1.54 | 0.796 | 0.578 | 0.982 |

2,4-Dimethylquinoline at Transect 4



2,4-Dimethylquinoline at Transect 5

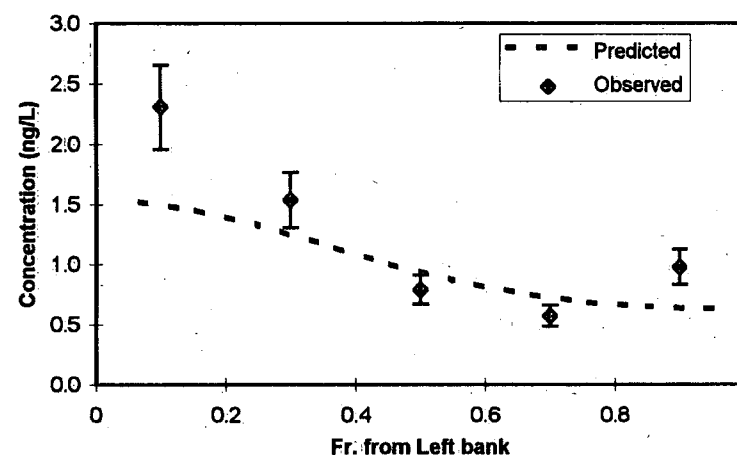


Figure 27

Organic compounds in Atha. R. May/93

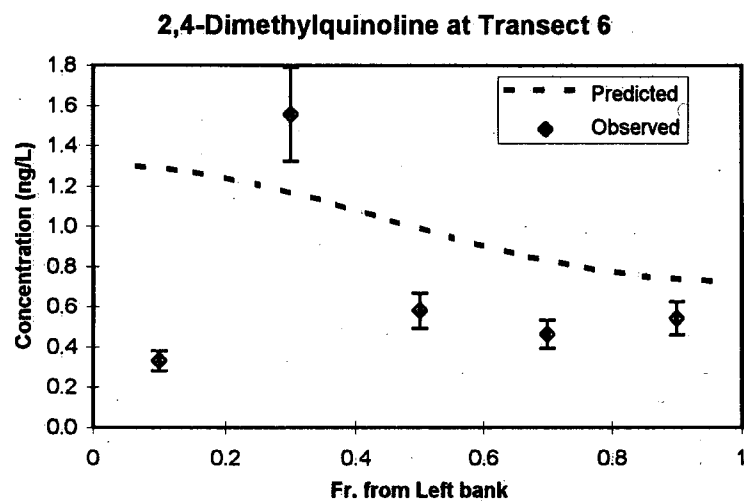
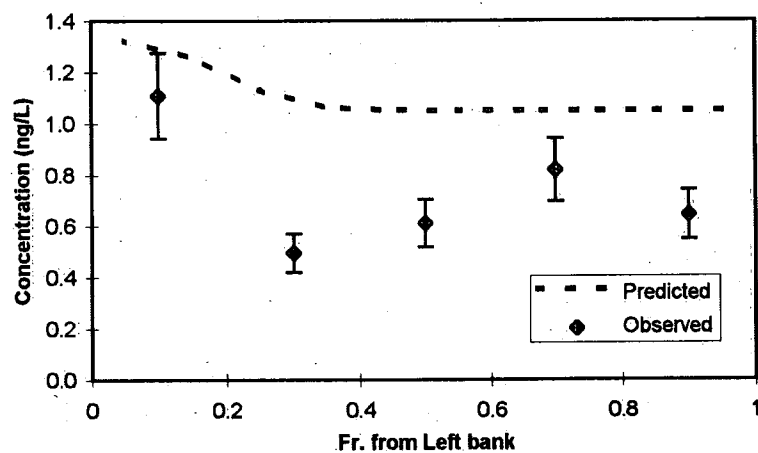
[illegible]

Figure 28

| Pyrene Output; T=15°C | | | | | | | | | | | | | | | | |
|-----------------------|----------|--------|--------|--------|--------|--------|--------|--------|--------|--------|---------|--------|--------|--------|--------|--------|
| Fr. from Left Bank | | 0.95 | 0.85 | 0.75 | 0.65 | 0.55 | 0.45 | 0.35 | 0.25 | 0.15 | 0.05 | 0.1 | 0.3 | 0.5 | 0.7 | 0.9 |
| Transect | Time (h) | Tube 1 | Tube 2 | Tube 3 | Tube 4 | Tube 5 | Tube 6 | Tube 7 | Tube 8 | Tube 9 | Tube 10 | Site A | Site B | Site C | Site D | Site E |
| 2 | 24 | 1.05 | 1.05 | 1.05 | 1.05 | 1.05 | 1.051 | 1.0635 | 1.1315 | 1.2595 | 1.326 | 1.11 | 0.498 | 0.614 | 0.822 | 0.647 |
| 3 | 48 | 1.05 | 1.05 | 1.0505 | 1.052 | 1.0565 | 1.068 | 1.091 | 1.126 | 1.163 | 1.187 | 0.782 | 1.07 | 0.374 | 0.521 | 0.784 |

Pyrene at Transect 2



Pyrene at Transect 3

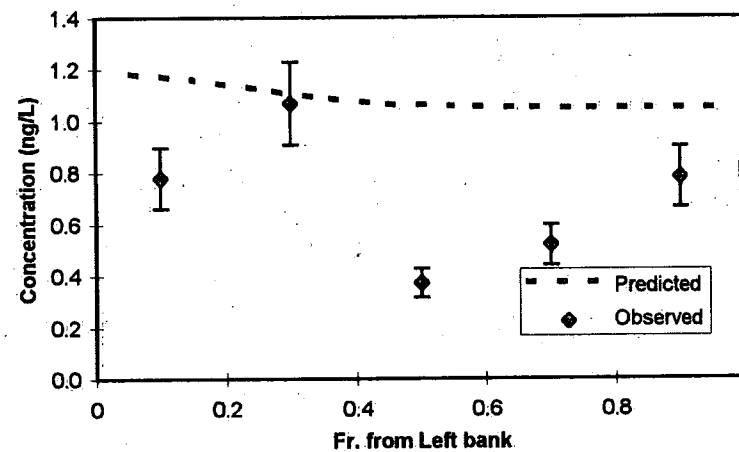
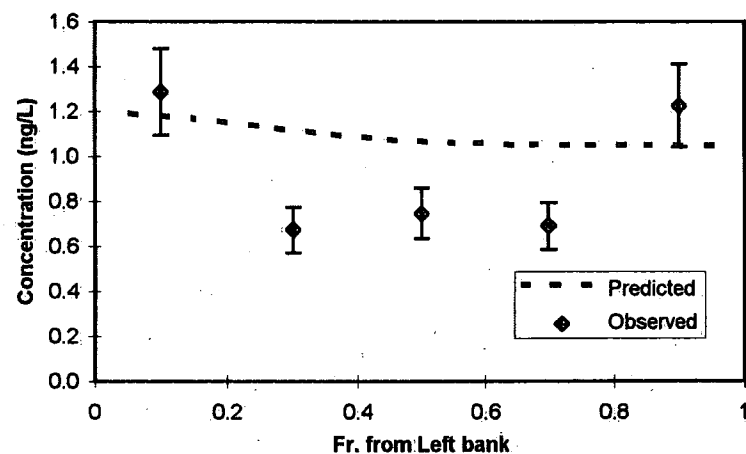


Figure 29

| Pyrene Output; T=15°C | | | | | | | | | | | | | | | | |
|-----------------------|----------|--------|--------|--------|--------|--------|--------|--------|--------|--------|---------|--------|--------|--------|--------|--------|
| Fr. from Left Bank | | 0.95 | 0.85 | 0.75 | 0.65 | 0.55 | 0.45 | 0.35 | 0.25 | 0.15 | 0.05 | 0.1 | 0.3 | 0.5 | 0.7 | 0.9 |
| Transect | Time (h) | Tube 1 | Tube 2 | Tube 3 | Tube 4 | Tube 5 | Tube 6 | Tube 7 | Tube 8 | Tube 9 | Tube 10 | Site A | Site B | Site C | Site D | Site E |
| 4 | 96 | 1.05 | 1.0505 | 1.0515 | 1.0545 | 1.0625 | 1.078 | 1.104 | 1.1385 | 1.1725 | 1.194 | 1.29 | 0.677 | 0.75 | 0.694 | 1.23 |
| 5 | 114 | 1.0535 | 1.0555 | 1.06 | 1.0675 | 1.0785 | 1.093 | 1.11 | 1.127 | 1.1405 | 1.148 | 1.33 | 0.809 | 0.644 | 0.648 | 1.47 |

Pyrene at Transect 4



Pyrene at Transect 5

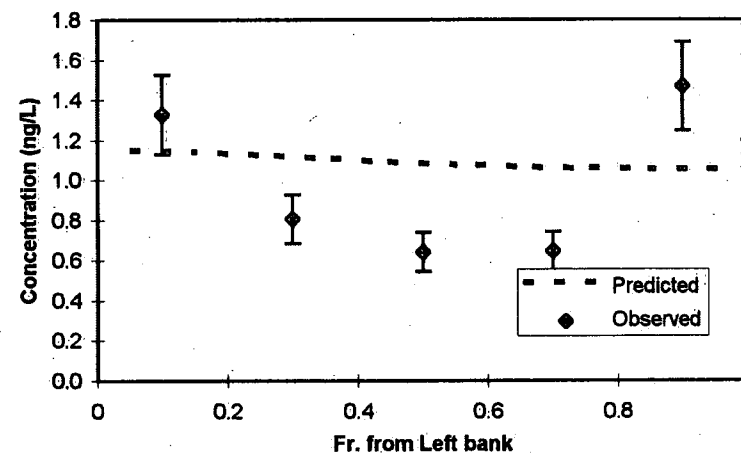


Figure 30

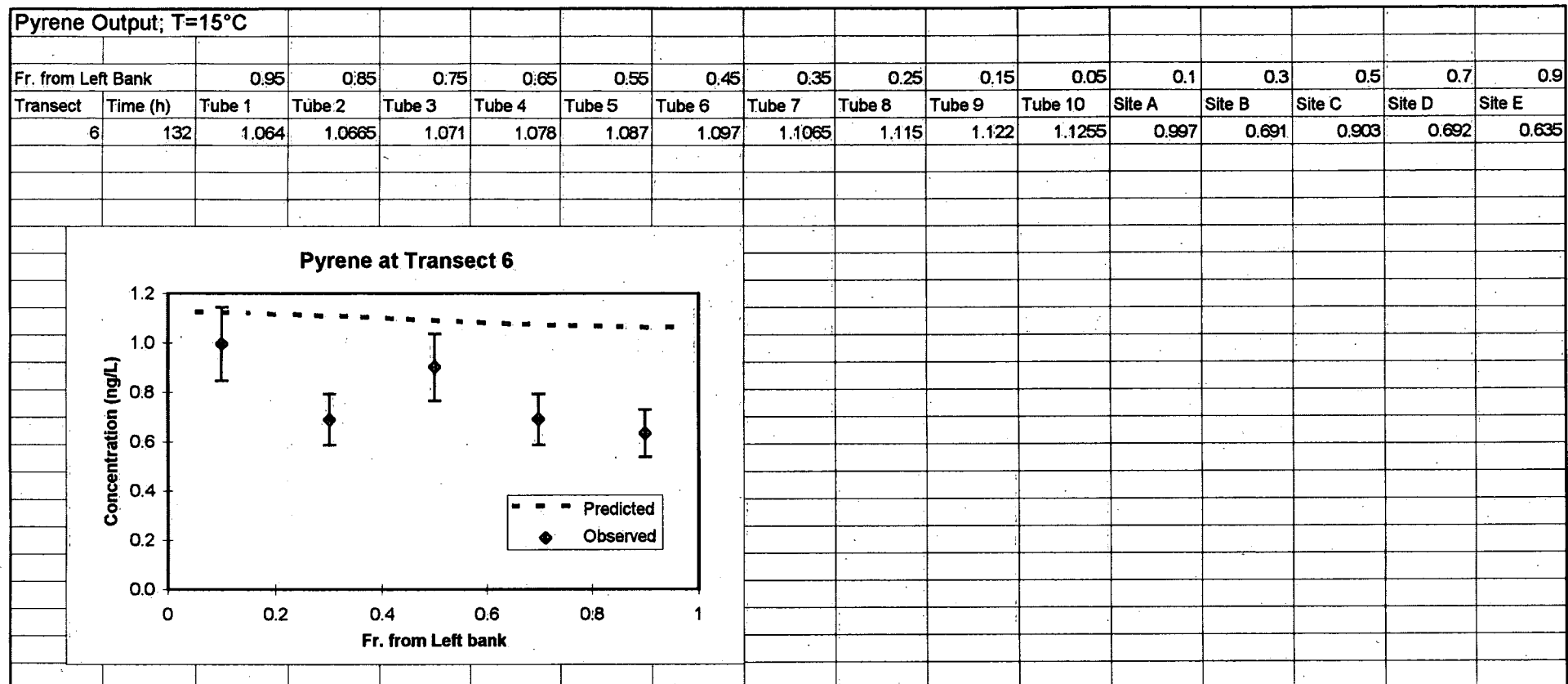
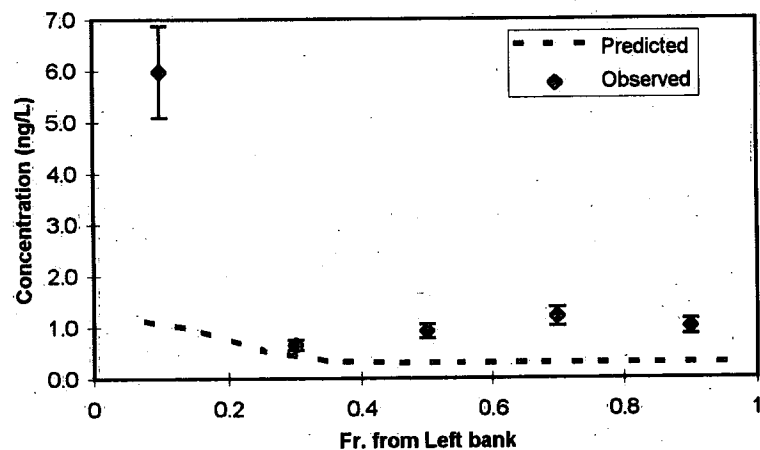


Figure 31

| Benzoquinoline Output; T=15°C | | | | | | | | | | | | | | | | | |
|-------------------------------|----------|--------|--------|--------|--------|--------|--------|--------|--------|--------|---------|--------|--------|--------|--------|--------|--|
| Fr. from Left Bank | | 0.95 | 0.85 | 0.75 | 0.65 | 0.55 | 0.45 | 0.35 | 0.25 | 0.15 | 0.05 | 0.1 | 0.3 | 0.5 | 0.7 | 0.9 | |
| Transect | Time (h) | Tube 1 | Tube 2 | Tube 3 | Tube 4 | Tube 5 | Tube 6 | Tube 7 | Tube 8 | Tube 9 | Tube 10 | Site A | Site B | Site C | Site D | Site E | |
| 2 | 24 | 0.3 | 0.3 | 0.3 | 0.3 | 0.3 | 0.3035 | 0.3435 | 0.5635 | 0.9785 | 1.195 | 5.99 | 0.667 | 0.921 | 1.21 | 1.01 | |
| 3 | 48 | 0.3 | 0.3005 | 0.302 | 0.308 | 0.3285 | 0.381 | 0.4855 | 0.641 | 0.807 | 0.916 | 1.54 | 1.21 | 1.29 | 0.1 | 0.1 | |

Benzoquinoline at Transect 2



Benzoquinoline at Transect 3

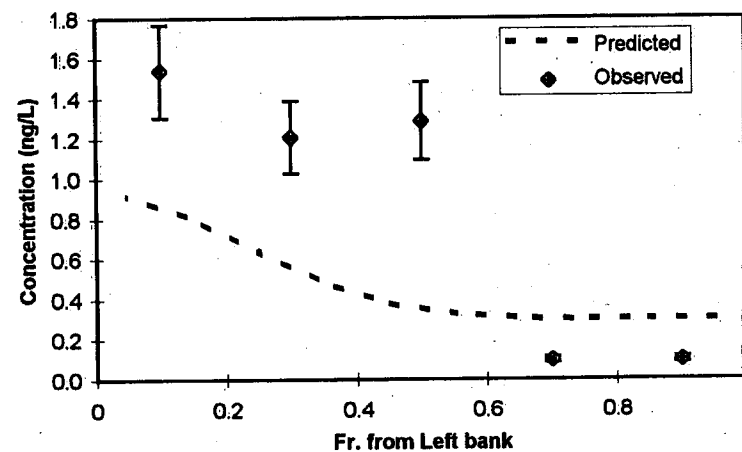
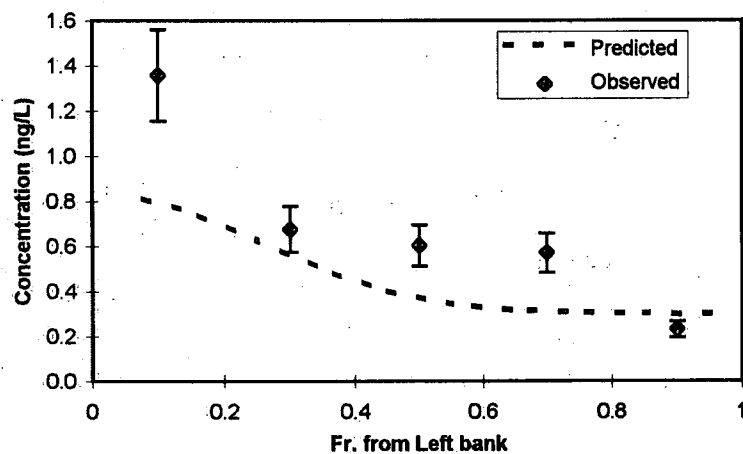


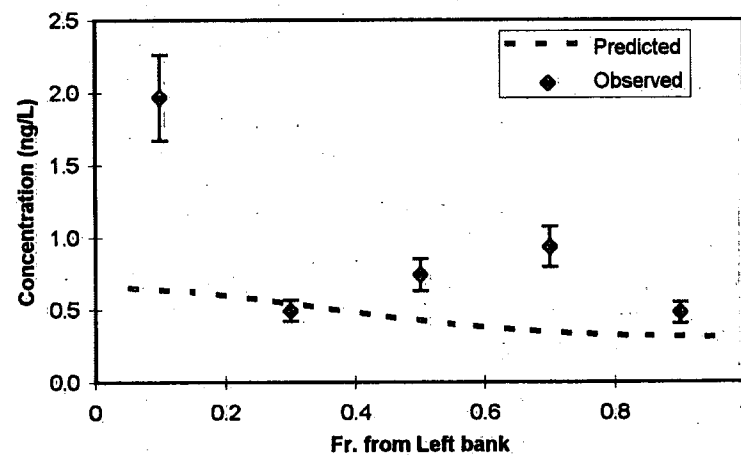
Figure 32

| Benzoquinoline Output; T=15°C | | | | | | | | | | | | | | | | |
|-------------------------------|----------|--------|--------|--------|--------|--------|--------|--------|--------|--------|---------|--------|--------|--------|--------|--------|
| Fr. from Left Bank | | 0.95 | 0.85 | 0.75 | 0.65 | 0.55 | 0.45 | 0.35 | 0.25 | 0.15 | 0.05 | 0.1 | 0.3 | 0.5 | 0.7 | 0.9 |
| Transect | Time (h) | Tube 1 | Tube 2 | Tube 3 | Tube 4 | Tube 5 | Tube 6 | Tube 7 | Tube 8 | Tube 9 | Tube 10 | Site A | Site B | Site C | Site D | Site E |
| 4 | 96 | 0.3005 | 0.3015 | 0.305 | 0.3165 | 0.345 | 0.4035 | 0.5005 | 0.628 | 0.754 | 0.833 | 1.36 | 0.678 | 0.606 | 0.573 | 0.233 |
| 5 | 114 | 0.3125 | 0.32 | 0.3365 | 0.3635 | 0.4035 | 0.4565 | 0.5175 | 0.5785 | 0.6285 | 0.6565 | 1.97 | 0.499 | 0.746 | 0.939 | 0.482 |

Benzoquinoline at Transect 4



Benzoquinoline at Transect 5



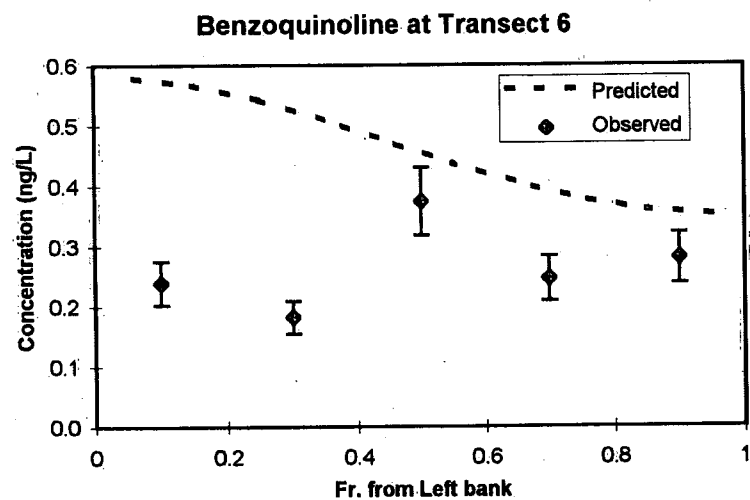
[illegible]

Figure 34

Organic compounds in Atha. R. May/93

| Benzoquinoline Output with $t_{1/2}=36$ hours; $T=15^{\circ}\text{C}$ | | | | | | | | | | | | | | | | |
|---|----------|--------|--------|--------|--------|--------|--------|--------|--------|--------|---------|--------|--------|--------|--------|--------|
| Fr. from Left Bank | | 0.95 | 0.85 | 0.75 | 0.65 | 0.55 | 0.45 | 0.35 | 0.25 | 0.15 | 0.05 | 0.1 | 0.3 | 0.5 | 0.7 | 0.9 |
| Transect | Time (h) | Tube 1 | Tube 2 | Tube 3 | Tube 4 | Tube 5 | Tube 6 | Tube 7 | Tube 8 | Tube 9 | Tube 10 | Site A | Site B | Site C | Site D | Site E |
| 2 | 24 | 0.3 | 0.3 | 0.3 | 0.3 | 0.3 | 0.3035 | 0.343 | 0.5605 | 0.971 | 1.185 | 5.99 | 0.667 | 0.921 | 1.21 | 1.01 |
| 3 | 48 | 0.3 | 0.3005 | 0.302 | 0.3075 | 0.326 | 0.374 | 0.47 | 0.613 | 0.7655 | 0.8655 | 1.54 | 1.21 | 1.29 | 0.1 | 0.1 |

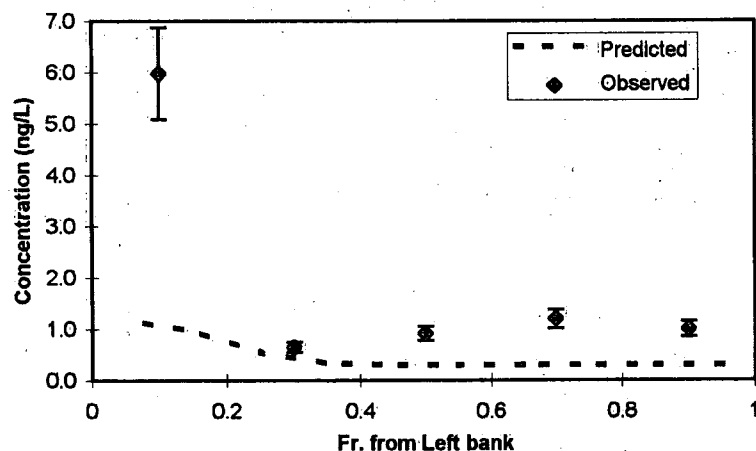
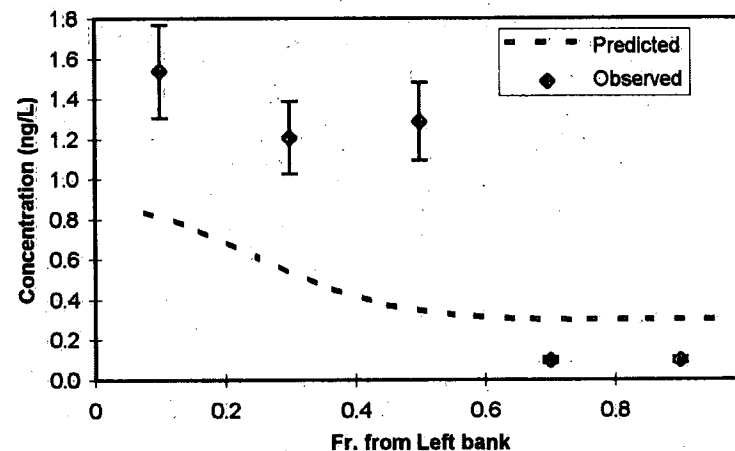
Benzoquinoline at Transect 2 – $t_{1/2}=36$ hBenzoquinoline at Transect 3 – $t_{1/2}=36$ h

Figure 35

| Benzoquinoline Output with $t_{1/2}=36$ hours; $T=15^{\circ}\text{C}$ | | | | | | | | | | | | | | | | |
|---|----------|--------|--------|--------|--------|--------|--------|--------|--------|--------|---------|--------|--------|--------|--------|--------|
| Fr. from Left Bank | | 0.95 | 0.85 | 0.75 | 0.65 | 0.55 | 0.45 | 0.35 | 0.25 | 0.15 | 0.05 | 0.1 | 0.3 | 0.5 | 0.7 | 0.9 |
| Transect | Time (h) | Tube 1 | Tube 2 | Tube 3 | Tube 4 | Tube 5 | Tube 6 | Tube 7 | Tube 8 | Tube 9 | Tube 10 | Site A | Site B | Site C | Site D | Site E |
| 4 | 96 | 0.3 | 0.301 | 0.3045 | 0.3145 | 0.3395 | 0.391 | 0.4765 | 0.5885 | 0.699 | 0.7685 | 1.36 | 0.678 | 0.606 | 0.573 | 0.233 |
| 5 | 114 | 0.309 | 0.314 | 0.3255 | 0.3445 | 0.3725 | 0.4095 | 0.4525 | 0.4955 | 0.5305 | 0.5505 | 1.97 | 0.499 | 0.746 | 0.939 | 0.482 |

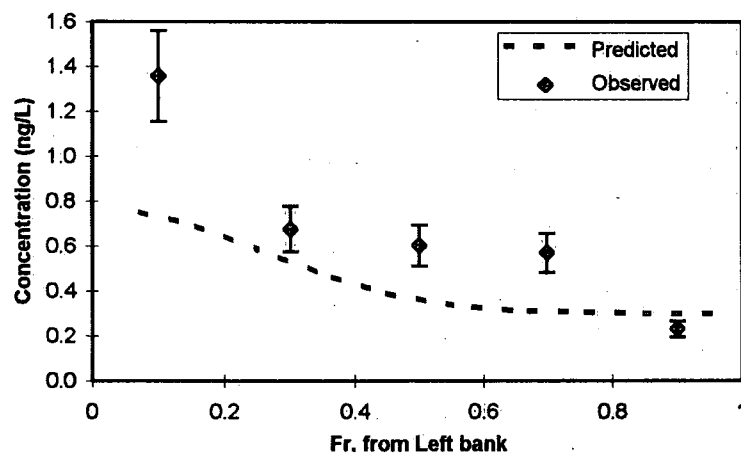
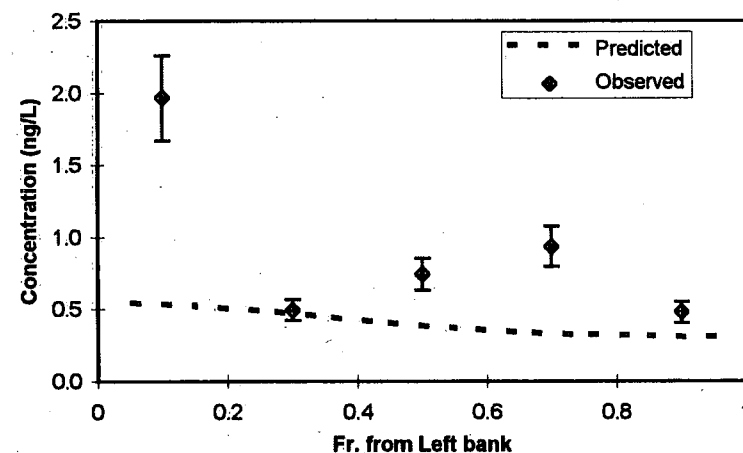
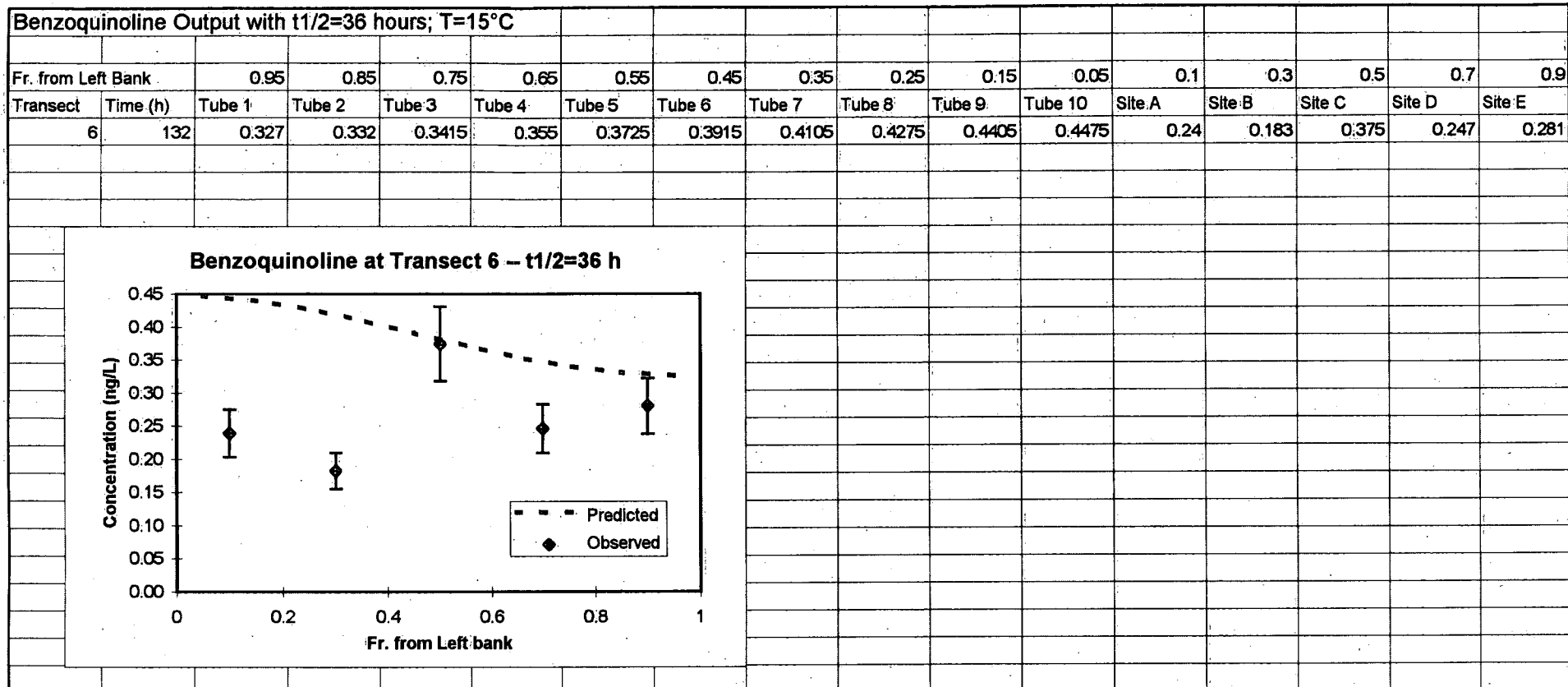
Benzoquinoline at Transect 4 -- $t_{1/2}=36$ hBenzoquinoline at Transect 5 -- $t_{1/2}=36$ h

Figure 36



APPENDIX A

May 1993 Athabasca River Sampling Data

Organic compounds in Atha. R. May/93

| Filename "ARMAY93" Created March 20, 1996 | | | | | | | |
|--|---|--------|--------|--------|--------|--------|--------|
| Organic compound concentrations for Suncor Wastewater and the Athabasca River May/93 | | | | | | | |
| Compound Name | Concentration in Suncor Wastewater (ng/L) | | | | | | |
| | 25-May | 26-May | 27-May | 28-May | 29-May | 30-May | 31-May |
| 7-Methylquinoline | 863 | 694 | 815 | 918 | 596 | 611 | 659 |
| 2,4-Dimethylquinoline | 833 | 692 | 799 | 1007 | 761 | 725 | 775 |
| Trimethylquinoline Isomer (1st) | 391 | 292 | 336 | 445 | 337 | 326 | 360 |
| Trimethylquinoline Isomer (2nd) | 246 | 196 | 225 | 300 | 234 | 219 | 249 |
| Acridine | 260 | 195 | 210 | 273 | 196 | 228 | 263 |
| Benzoquinoline Isomer | 295 | 293 | 344 | 414 | 282 | 339 | 490 |
| 3/4-Methylbenzothiophene | 495 | 429 | 471 | 602 | 414 | 597 | 633 |
| 2,4-Dimethylbenzothiophene | 855 | 920 | 1108 | 1873 | 2043 | 3726 | 4460 |
| Naphthalene | ND | 13.7 | 11.3 | 10.8 | 8.2 | 15.9 | 24.8 |
| Phenanthrene | ND | 4.3 | 3.4 | 6.5 | 4.2 | 7.9 | 8.8 |
| Fluoranthene | ND | 2.7 | 3.4 | 4.7 | 2.5 | 4.2 | 16.6 |
| Pyrene | 187 | 77 | 75.3 | 104 | 79.1 | 83 | 111 |
| Discharge (m3/day) | 34140 | 43192 | 33337 | 34120 | 35878 | 35738 | 35655 |
| Concentration (ng/L) u/s Horse R. May 22/93 | | | | | | | |
| | Site A (a) | Site B | Site C | Site D | | | |
| 7-Methylquinoline | ND | 0.273 | ND | ND | | | |
| 2,4-Dimethylquinoline | 1.84 | 2.34 | 1.52 | 4.07 | | | |
| Trimethylquinoline Isomer (1st) | ND | ND | ND | ND | | | |
| Trimethylquinoline Isomer (2nd) | ND | ND | ND | ND | | | |
| Acridine | ND | ND | ND | ND | | | |
| Benzoquinoline Isomer | ND | ND | ND | ND | | | |
| 3/4-Methylbenzothiophene | 0.364 | 0.345 | 0.51 | 0.435 | | | |
| 2,4-Dimethylbenzothiophene | ND | ND | ND | ND | | | |
| Naphthalene | 7.22 | 7.77 | 12.27 | 10.49 | | | |
| Phenanthrene | 1.78 | 1.48 | 1.38 | 1.29 | | | |
| Fluoranthene | 0.718 | 0.448 | 0.509 | 0.446 | | | |
| Pyrene | 3.14 | 1.18 | 1.28 | 1.21 | | | |
| Concentration (ng/L) at Mile 20.8 (km 33.3) May 24/93 | | | | | | | |
| | Site A | Site B | Site C | Site D | Site E | | |
| 7-Methylquinoline | ND | ND | ND | ND | ND | | |
| 2,4-Dimethylquinoline | 0.666 | 0.659 | 0.622 | 0.548 | 0.385 | | |
| Trimethylquinoline Isomer (1st) | ND | ND | ND | ND | ND | | |
| Trimethylquinoline Isomer (2nd) | ND | ND | ND | ND | ND | | |
| Acridine | ND | ND | ND | ND | ND | | |
| Benzoquinoline Isomer | ND | 0.233 | 0.255 | 0.563 | 0.388 | | |
| 3/4-Methylbenzothiophene | 0.604 | 1.03 | ND | ND | ND | | |
| 2,4-Dimethylbenzothiophene | ND | ND | ND | ND | ND | | |
| Naphthalene | 27.65 | 46.96 | 8.94 | 7.4 | 5.86 | | |
| Phenanthrene | 1.48 | 2.08 | 1.66 | 1.61 | 1.23 | | |
| Fluoranthene | 0.561 | 0.864 | 0.564 | 0.73 | 0.944 | | |
| Pyrene | 0.97 | 1.11 | 1.15 | 1.05 | 0.953 | | |

Organic compounds in Atha. R. May/93

| | Concentration (ng/L) at Mile 25 (km 40.2) May 26/93 | | | | |
|---------------------------------|---|--------|----------|--------|--------|
| | Site A | Site B | Site C-U | Site D | Site E |
| 7-Methylquinoline | 12.33 | ND | ND | ND | ND |
| 2,4-Dimethylquinoline | 11.48 | 0.981 | 0.892 | 0.934 | 1.93 |
| Trimethylquinoline Isomer (1st) | 2.99 | ND | ND | ND | ND |
| Trimethylquinoline Isomer (2nd) | 1.3 | 0.268 | 0.161 | ND | ND |
| Acridine | 2.94 | ND | ND | ND | ND |
| Benzoquinoline Isomer | 5.99 | 0.667 | 0.921 | 1.21 | 1.01 |
| 3/4-Methylbenzothiophene | 3.93 | 0.407 | 0.403 | 0.412 | 0.57 |
| 2,4-Dimethylbenzothiophene | 7.97 | ND | ND | ND | ND |
| Naphthalene | 5.51 | 3.54 | 12.2 | 13.67 | 19.1 |
| Phenanthrene | 0.951 | 1.03 | 1.43 | 1.25 | 1.25 |
| Fluoranthene | 0.381 | 0.326 | 0.465 | 0.604 | 0.396 |
| Pyrene | 1.11 | 0.498 | 0.614 | 0.822 | 0.647 |
| | | | | | |
| | | | | | |
| | | | | | |
| | Concentration (ng/L) at Mile 33.7 (km 53.9) May 27/93 | | | | |
| | Site A | Site B | Site C-U | Site D | Site E |
| 7-Methylquinoline | 2.28 | 2.05 | ND | ND | ND |
| 2,4-Dimethylquinoline | 2.23 | 1.77 | 1.04 | ND | ND |
| Trimethylquinoline Isomer (1st) | ND | ND | ND | ND | ND |
| Trimethylquinoline Isomer (2nd) | ND | ND | ND | ND | ND |
| Acridine | 0.782 | 0.661 | ND | ND | ND |
| Benzoquinoline Isomer | 1.54 | 1.21 | 1.29 | ND | ND |
| 3/4-Methylbenzothiophene | 1.78 | 1.8 | 1.02 | ND | ND |
| 2,4-Dimethylbenzothiophene | 3.92 | 1.43 | 1.27 | ND | ND |
| Naphthalene | 3.79 | 8.67 | 16.94 | 3.5 | 5.1 |
| Phenanthrene | 0.821 | 1.31 | 1.39 | 0.779 | 0.928 |
| Fluoranthene | 0.416 | 0.64 | 0.387 | 0.296 | 0.397 |
| Pyrene | 0.782 | 1.07 | 0.374 | 0.521 | 0.784 |
| | | | | | |
| | | | | | |
| | | | | | |
| | Concentration (ng/L) at Mile 37.3 (km 60.0) May 29/93 | | | | |
| | Site A | Site B | Site C-U | Site D | Site E |
| 7-Methylquinoline | 0.818 | 1.17 | ND | ND | ND |
| 2,4-Dimethylquinoline | 2.57 | 1.62 | 0.711 | 0.717 | 0.61 |
| Trimethylquinoline Isomer (1st) | ND | ND | ND | ND | ND |
| Trimethylquinoline Isomer (2nd) | ND | ND | ND | ND | ND |
| Acridine | 0.418 | ND | ND | ND | ND |
| Benzoquinoline Isomer | 1.36 | 0.678 | 0.606 | 0.573 | 0.233 |
| 3/4-Methylbenzothiophene | 1.4 | 0.737 | 0.511 | 0.332 | 0.702 |
| 2,4-Dimethylbenzothiophene | 3.1 | 2.07 | ND | ND | ND |
| Naphthalene | 21.36 | 7.6 | 17.12 | 10.17 | 27 |
| Phenanthrene | 2.04 | 1.08 | 1.23 | 0.997 | 1.28 |
| Fluoranthene | 0.744 | 0.444 | 0.411 | 0.374 | 0.509 |
| Pyrene | 1.29 | 0.677 | 0.75 | 0.694 | 1.23 |
| | | | | | |
| | | | | | |
| | | | | | |

Organic compounds in Atha. R. May/93

| | Concentration (ng/L) at Mile 56 (km 90.1) May 30/93 | | | | |
|---|--|-------------------|--------------------|----------|--------|
| | Site A | Site B | Site C | Site D | Site E |
| 7-Methylquinoline | 0.693 | 0.783 | ND | ND | ND |
| 2,4-Dimethylquinoline | 2.31 | 1.54 | 0.796 | 0.578 | 0.982 |
| Trimethylquinoline Isomer (1st) | ND | ND | ND | ND | ND |
| Trimethylquinoline Isomer (2nd) | ND | ND | ND | ND | ND |
| Acridine | ND | ND | ND | ND | ND |
| Benzoquinoline Isomer | 1.97 | 0.499 | 0.746 | 0.939 | 0.482 |
| 3/4-Methylbenzothiophene | 1.28 | 0.768 | 0.579 | 0.507 | 0.969 |
| 2,4-Dimethylbenzothiophene | 1.77 | 1.61 | 0.936 | 0.626 | 1.27 |
| Naphthalene | 30.07 | 9.94 | 7.82 | 7.47 | 21.77 |
| Phenanthrene | 1.5 | 0.965 | 0.791 | 0.959 | 1.55 |
| Fluoranthene | 0.756 | 0.372 | 0.435 | 0.43 | 0.762 |
| Pyrene | 1.33 | 0.809 | 0.644 | 0.648 | 1.47 |
| | | | | | |
| | Concentration (ng/L) at Mile 82 (km 131.9) May 31/93 | | | | |
| | Site A | Site B | Site C | Site D-U | Site E |
| 7-Methylquinoline | ND | ND | 0.213 | ND | ND |
| 2,4-Dimethylquinoline | 0.335 | 1.56 | 0.584 | 0.468 | 0.547 |
| Trimethylquinoline Isomer (1st) | ND | ND | ND | ND | ND |
| Trimethylquinoline Isomer (2nd) | ND | ND | ND | ND | ND |
| Acridine | ND | ND | ND | ND | ND |
| Benzoquinoline Isomer | 0.24 | 0.183 | 0.375 | 0.247 | 0.281 |
| 3/4-Methylbenzothiophene | 0.576 | 0.538 | 0.48 | 0.532 | 0.422 |
| 2,4-Dimethylbenzothiophene | 1.13 | 0.303 | 0.312 | 0.36 | 0.431 |
| Naphthalene | 7.23 | 10.6 | 6.64 | 10.67 | 6.96 |
| Phenanthrene | 0.958 | 0.794 | 2.16 | 1.09 | 0.708 |
| Fluoranthene | 0.398 | 0.343 | 0.736 | 0.368 | 0.275 |
| Pyrene | 0.997 | 0.691 | 0.903 | 0.692 | 0.635 |
| | | | | | |
| Compound | Ret. Time minutes | Quant. Ion m/z | Quant. Std. (b) | | |
| 7-Methylquinoline | 16.15 | 143 | Y | | |
| 2,4-Dimethylquinoline | 19.35 | 157 | Y | | |
| Trimethylquinoline Isomer (1st) | 23.56 | 171 | N | | |
| Trimethylquinoline Isomer (2nd) | 23.79 | 171 | N | | |
| Acridine | 32.58 | 179 | Y | | |
| Benzoquinoline Isomer (c) | 33.36 | 179 | N | | |
| 3/4-Methylbenzothiophene (d) | 14.41 | 148 | Y | | |
| 2,4-Dimethylbenzothiophene | 18.33 | 162 | N | | |
| Naphthalene | 10.12 | 128 | Y | | |
| Phenanthrene | 31.86 | 178 | Y | | |
| Fluoranthene | 40.91 | 202 | Y | | |
| Pyrene | 42.48 | 202 | Y | | |
| | | | | | |
| Footnotes: | | | | | |
| a. Site A=left bank; Site C= centre; Site E=right bank of river. U=upper sample of an upper/lower depth pair. | | | | | |
| b. Where standard was not available for quantitation, response for parent compound or isomer was used. | | | | | |
| c. Formerly assigned as phenanthridine on the basis of mass spectral library match. | | | | | |
| d. 3- and 4-Isomers have nearly identical retention times. Quantitation uncertain due to interfering peak. | | | | | |

11 AUG 2003

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