# A REVIEW OF FATE, TREATABILITY AND ANALYSES OF EMERGING CONTAMINANTS IN WET WEATHER FLOWS

by

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A THESIS

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LIST OF ABBREVATIONS AND SYMBOLS

| | |
|---|---|
| CSOs | Combined Sewer Overflows |
| C.I. | Confidence interval |
| ECs | Emerging Contaminants |
| ECD | Electron Capture Detector |
| EPA | Environmental Protection Agency |
| ESI | Electron Spray Ionization |
| GC | Gas chromatography |
| gm | Gram |
| H | Henry's law constant |
| HPLC | High performance Liquid Chromatography |
| $K_{OC}$ | Soil-organic partition coefficient |
| $K_{OW}$ | Octanol-water partition coefficient |
| kg | Kilogram |
| L | Liter |
| LOD | Limit of Detection |
| LOQ | Limit of Quantification |
| Max | Maximum |
| Min | Minimum |
| mL | Milli liter |
| MS | Mass spectrophotometer |

| | |
|---|---|
| ng | Nanogram |
| OC | Organic content |
| PCPs | Personal Care Products |
| PPCPs | Pharmaceuticals and Personal Care Products |
| SIM | Selective Ion Monitoring |
| SPE | Solid Phase Extraction |
| SS | Suspended solids |
| SSOs | Separate Sewer Overflows |
| STP | Sewage Treatment Plant |
| WWFs | Wet Weather Flows |
| µg | Microgram |
| µL | Micro liter |
| % | Percent |
| < | Less than |
| > | Greater than |

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**ABSTRACT**

Emerging contaminants are of great concern because their presence in the environment at low concentrations (µg/L – ng/L) can be associated with significant health risks and, historically, most have not been regulated, especially considering their estrogenic properties. They have been detected in most of the nations' waters during recent years and many are not readily removed using conventional wastewater and water treatment methods. There is a long list of pollutants that are considered as emerging contaminants, but those that are most commonly studied include pharmaceuticals and personal care products (PCPs), and pesticides.

This thesis includes an extensive literature review of these emerging contaminants in wet weather flows (WWFs), specifically separate stormwater, CSOs, and SSOs, to document the presence of emerging contaminants and to summarize what is known about their treatability and fate. There is limited information regarding emerging contaminant presence in wet-weather flows. Therefore, information concerning wastewaters discharges and surface water observations was also reviewed. This thesis has focused on characterizing emerging contaminants, specifically their presence and magnitude, in wet weather flows. This thesis also compiled literature information on analytical methods that can be been used to quantify emerging contaminant concentrations in wet weather flows (especially the methods that have been successfully used for similar samples and that have the needed detection limits). The treatability information by unit process was

compiled and reviewed for its applicability to wet-weather flows. Fugacity modeling was conducted to identify the likely fate of these compounds after discharge to urban receiving waters. Subsurface fate modeling was performed using a factorial design and a vadose zone model, representing the expected range of conditions.

# CHAPTER I

# INTRODUCTION

Many reports have been published in the last two decades on the occurrence, detection, and treatability of pharmaceuticals and PCPs in water bodies throughout the world. The analytical methods used to quantify these materials are not commonly available in many laboratories. Special methods have been developed to detect these compounds at the extremely low levels of interest. Typically, High Performance Liquid Chromatography with Mass Spectrophotometer Detector (HPLC-MS), research grade Gas Chromatography with Mass Spectrophotometer Detector (GC-MS), and High Performance Liquid Chromatography with Electro Spray and Dual Mass Spectrophotometer Detectors (HPLC-ESI-MS-MS) have been used for the detection of these compounds. Although most methods show relatively good performance, special sample preparation steps often are needed, such as compound derivatization steps for GC/MS, and signal suppression and matrix effects associated with LC-ESI-MS-MS. Most of these methods are expensive and time consuming and are not viable for most commercial laboratories.

The effective treatability of emerging contaminants in wet weather flows (combined sewage, sanitary sewage overflows, and stormwaters) may require varying steps ranging from conventional processes such as screening and disinfection, to advanced treatment methods using nanofiltration and membranes. The advanced treatment methods can be expensive as they require high energy usage, amongst other consumable materials. Rather than using a single, expensive treatment technology, combinations of conventional wet weather treatment methods, such as sedimentation and filtration, may be a more cost-effective approach. Parameters such as particle size, settling properties, discharge rates, and retention times, however, need to be considered as major factors in the efficacy of these treatment methods. In order to obtain a better understanding of these issues, a full factorial experimental design was used to evaluate through modeling the factors affecting the partitioning and fate of the emerging contaminants in the environment.

During the literature review, the following ECs have been most commonly observed and studied:

1) Prescription medications
2) Over-the-counter drugs
3) Antibiotics
4) Hormones and steroids
5) Pesticides
6) Personal care products

Pesticides are frequently included as an emerging contaminant (Jacobsen et al 2005, Petrovic et al 2003) even though they have received some regulatory attention over the years. However, pesticide regulations often relate to their toxicity and not their possible other long-term estrogenic effects associated with low concentrations.

# CHAPTER II

# OCCURRENCES OF EMERGING CONTAMINANTS

## 2.1 Pharmaceuticals and personal care products

The most commonly occurring pharmaceuticals and personal care products are from several therauptic classes (Lee et al. 2003, Vanderford et al. 2003, and Castiglioni et al. 2003). Some of these medication classes, plus representative compounds in each class, are as follows:

Antibiotics: Erythromycin, Clarithromycin, Ciprofloxacin, Ofloxacin, Amoxycillin.

Analgesics: Ibuprofen, Naproxen, Ketoprofen, Fenoprofen, Indomethacin.

Estrogens: Estrone, 17β-estradiol.

Lipid Generators: Bezafibrate, Gemfibrozil.

Many of the publications during the last two decades have reported the occurrence of pharmaceuticals and personal care products in a wide variety of waters, but primarily in municipal wastewater treatment influents and effluents (Castiglioni et al. 2005, Miao etal. 2002, Lindqvist et al. 2005, Pedrouzo et al. 2007, Lee et al. 2005, Thomas et al. 2004), rivers (Lindqvist et al. 2005, Kosjek et al. 2005), other surface waters (Hao et al. 2006, Pedrouzo et al. 2007, Togola et al. 2007) and drinking waters (Kosjek et al. 2005). Representative occurrences of pharmaceuticals and PCPs, along with observed concentrations, are shown in Table 2.1.

Table 1.1 Observed Concentrations of Pharmaceuticals in different waters based on Individual study

| | Observed Concentrations (ng/L) | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **Compound** | **STP influent** | | | **STP effluent** | | | **River waters** | | | **Surface waters** | | | **Reference** |
| | Min | Max | Mean | Min | Max | Mean | Min | Max | Mean | Min | Max | Mean | |
| **Ibuprofen** | | | | nd | nd | nd | | | | | | | Castiglioni etal 2005 |
| **Ciproflaxin** | | | | 27 | 514 | | | | | | | | |
| **Clofibric acid** | | | | 0.5 | 82 | | | | | | | | |
| **Diazepam** | | | | nd | nd | | | | | | | | |
| **Carbamazepine** | | | | 33 | 1318 | | | | | | | | |
| **Bezafibrate** | | | | 0.3 | 117 | | | | | | | | |
| **Atenolol** | | | | 27 | 1168 | | | | | | | | |
| | | | | | | | | | | | | | |
| **Ibuprofen** | | | | 10 | 15 | | | | | | | | Miao etal 2002 |
| **Naproxen** | | | | 25 | 300 | | | | | | | | |
| **Bezafibrate** | | | | 20 | 65 | | | | | | | | |
| **Diclofenac** | | | | 25 | 65 | | | | | | | | |
| **Gemfibrozil** | | | | 30 | 60 | | | | | | | | |
| **Fenoprofen** | | | | 20 | 25 | | | | | | | | |
| | | | | | | | | | | | | | |
| **Carbamazepine** | 290 | 310 | | 380 | 470 | | 20 | 66 | | | | | Vieno etal 2006 |
| **Atenolol** | 510 | 800 | | 40 | 440 | | 12 | 25 | | | | | |
| **Metoprolol** | 980 | 1350 | | 910 | 1070 | | 20 | 116 | | | | | |
| | | | | | | | | | | | | | |
| **Diazepam** | | | nd | | | nd | | 33 | | | | | Ternes etal 2001 |
| **Caffeine** | | | 147000 | | | 190 | | 880 | | | | | |
| **Naproxen** | | | | | | | | | | | | 41 | Hao etal 2006 |

Continuation of above table

| | Observed Concentrations (ng/L) | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **Compound** | **STP influent** | | | **STP effluent** | | | **River waters** | | | **Surface waters** | | | **Reference** |
| | Min | Max | Mean | Min | Max | Mean | Min | Max | Mean | Min | Max | Mean | |
| **Carbamazepine** | | | | | | | | | | | | 1.5,4.2,16 | |
| **Gemfibrozil** | | | | | | | | | | | | 13 | |
| **Erythromycin** | | | | | | | | | | | | 1.9,6.9 | |
| | | | | | | | | | | | | | |
| **Ibuprofen** | | | 13100 | 80 | 3920 | | | | | | | | Lindqvist etal 2005 |
| **Naproxen** | | | 4900 | 160 | 1920 | | | | | | | | |
| **Bezafibrate** | | | 420 | 20 | 840 | | | | | | | | |
| **Diclofenac** | | | 350 | 160 | 360 | | | | | | | | |
| **Ketoprofen** | | | 2000 | 40 | 1280 | | | | | | | | |
| | | | | | | | | | | | | | |
| **Ibuprofen** | 1610 | 5990 | | 20 | 690 | | | | | 18 | 44 | | Pedrouzo etal 2007 |
| **Naproxen** | 340 | 8620 | | 20 | 450 | | | | | | | | |
| **Clofibric acid** | 30 | 2020 | | 10 | 120 | | | | | 11 | 14 | | |
| **Carbamazepine** | 60 | 480 | | 80 | 290 | | | | | 9 | 37 | | |
| **Bezafibrate** | Nd | nd | | 70 | 340 | | | | | | | | |
| **Diclofenac** | 120 | 550 | | 10 | 460 | | | | | 25 | 41 | | |
| **Caffeine** | 420 | 40120 | | 20 | 1010 | | | | | 106 | 240 | | |
| **Ibuprofen** | 2740 | 9210 | | 40 | 970 | | | | | | | | Lee etal 2003 |
| **Naproxen** | 1100 | 6060 | | 210 | 1110 | | | | | | | | |
| **Diclofenac** | 30 | 200 | | 20 | 210 | | | | | | | | |
| **Ketoprofen** | 30 | 700 | | 30 | 150 | | | | | | | | |

Continuation of above table

| | Observed Concentrations (ng/L) | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **Compound** | **STP influent** | | | **STP effluent** | | | **River waters** | | | **Surface waters** | | | **Reference** |
| | Min | Max | Mean | Min | Max | Mean | Min | Max | Mean | Min | Max | Mean | |
| **Gemfibrozil** | 100 | 750 | | 20 | 540 | | | | | | | | Lee et al 2003 |
| **Triclosan** | 370 | 3240 | | 30 | 740 | | | | | | | | |
| **Indomethacin** | 50 | 200 | | 30 | 240 | | | | | | | | |
| **Ibuprofen** | | | | 2.4 | 197.6 | | | | | 3 | 610.6 | | Togola etal 2007 |
| **Naproxen** | | | | 13.6 | 2666.8 | | | | | 2.6 | 274.6 | | |
| **Carbamazepine** | | | | 30.9 | 2519.3 | | | | | 1.8 | 82.7 | | |
| **Diclofenac** | | | | 26.3 | 918.6 | | | | | 7.1 | 172.5 | | |
| **Ketoprofen** | | | | 15.2 | 1136.5 | | | | | 4.4 | 33.2 | | |
| **Gemfibrozil** | | | | 4.3 | 108.8 | | | | | 2.7 | 85.8 | | |
| **Caffeine** | | | | 2.6 | 3257.2 | | | | | 3.5 | 159.8 | | |
| **Ibuprofen** | 4100 | 10210 | | 110 | 2170 | | | | | | | | Lee etal 2005 |
| **Naproxen** | 1730 | 6030 | | 360 | 2540 | | | | | | | | |
| **Diclofenac** | 50 | 2450 | | 70 | 250 | | | | | | | | |
| **Ketoprofen** | 60 | 150 | | 40 | 90 | | | | | | | | |
| **Gemfibrozil** | 120 | 36530 | | 80 | 2090 | | | | | | | | |
| **Triclosan** | 870 | 1830 | | 50 | 360 | | | | | | | | |
| **Estrone** | 8 | 52 | | <1 | 54 | | | | | | | | |
| **Indomethacin** | 30 | 430 | | 40 | 490 | | | | | | | | |
| **Ibuprofen** | | | | | | 18 | | | | | | | Thomas etal 2004 |
| **Naproxen** | | | | | | 31 | | | | | | | |
| **Diclofenac** | | | | | | nd | | | | | | | |
| **Ketoprofen** | | | | | | 23 | | | | | | | |
| **Triclosan** | | | | | | 72 | | | | | | | |
| **Caffeine** | | | | | | 36 | | | | | | | |

nd: not detected

## 2.2 Veterinary Pharmaceuticals

Because separate stormwater flows, unless contaminated through surface leakage of septic water or leaky sewers, are not likely to contain human pharmaceuticals, the scope of the research was extended to consider veterinary pharmaceuticals as a class of emerging contaminants. Specifically, this research hypothesized that dog feces are a likely source of these compounds in separate stormwater runoff since dogs do not bury their feces. However, there were no specific literature references available for these compounds. Interviews were held with local veterinarians (personal communications) to determine the most commonly used pet medicines, and their uses. Table 2.2 lists these pet pharmaceuticals, and their use.

Table 2.2 Veterinary pharmaceuticals and their usage

| Compound | Usage |
|---|---|
| Nystatin | Anti-infective |
| Thiabendazole | Anti-infective |
| Dexamethasone | Anti-infective |
| Metronidazole | Anti-infective |
| Clindamycin | Anti-infective |
| Permethrin | Flea preventative |
| Fipronil | Flea preventative |
| Imidacloprid | Flea preventative |
| Methoprene | Flea preventative |
| Prednisone | Anti Inflammatory |
| Betamethasone | Anti Inflammatory |
| Ketoconazole | Anti-fungal |
| Ivermectin | Heart worm preventative |
| Amoxicillin | Antibiotic |
| Tetracycline | Antibiotic |
| Gentamicin | Antibiotic |

## 2.3 Pesticides

As noted above, pesticides are another class of emerging contaminants and are frequently detected in wet weather flows. The usage of pesticides in urban areas is mostly for weed and insect control near houses, along roads and railway rights of way, parks, lawns and golf courses (Recke et al. 1993). Kunimatsu et al. (1992) found that the concentrations of pesticides varied for each monitored storm runoff event and no clear correlation was observed with precipitation. Instead, the loading rates depended on the length of period after application, drainage system, application method, volatilization, microorganisms and sunlight. Schiff et al. (2004) also identified first flush effects for pesticides. Pesticides commonly are analyzed using EPA Method 508, described in Chapter 3.

# CHAPTER III

# DETECTION of EMERGING CONTAMINANTS

Emerging contaminants, unlike the major pollutants associated with wet-weather and sewage flows, occur in extremely low levels and require special methods for their detection. The methods used for the detection of emerging contaminants are commonly not available in many laboratories, and some of the most commonly used analytical methods for their detection are High Performance Liquid Chromatography with Mass Spectrophotometer Detector (HPLC-MS), research grade Gas Chromatography with Mass Spectrophotometer Detector (GC-MS), and High Performance Liquid Chromatography with Electro Spray and Dual Mass Spectrophotometer Detectors (HPLC-ESI-MS-MS). The following section briefly describes these analytical methods, along with sample preparation methods.

## 3.1 Sample Extraction and Concentration

**Solid Phase Extraction**

Solid Phase Extraction (SPE) is used commonly to extract and concentrate the analytes from the water matrix. It involves different steps which include dilution, buffer addition, pH adjustment, and elution. SPE is considered to be the most effective extraction technique when compared with the traditional techniques for dissolved pollutants: liquid-liquid extraction, Soxhlet, automated Soxhlet, and steam distillation. Comparatively, it is accurate, reproducible, reliable, and capable of multi-analyte determination. However it is not suitable when analytes need to be extracted from particulates in the samples. Some of the most commonly used SPE cartridges include Oasis HLB, Oasis MCX, Strata-X, Lichrolut EN, and RP-$C_{18}$. At least one study has reported that Oasis HLB cartridges are efficient and resulted in high recoveries of the analytes investigated in the study (Zhang et al. 2007). Most of the acidic compounds are recovered better at pH < 3, and the neutral and basic compounds are recovered better at pH values between 7 and 10. These pH ranges result in better adsorption of analytes onto the SPE cartridges (Miao et al. 2002, Vieno et al. 2006, Ternes et al. 2001, Togola et al. 2007, and Gibson et al. 2007).

## 3.2 Analytical Methods for Detection of PPCPs

**HPLC-ESI-MS-MS (High Performance Liquid Chromatography with Electro Spray and Dual Mass Spectrophotometer Detectors)**

HPLC-ESI-MS-MS is effective for the detection of most of the emerging contaminants because of their polar nature, low volatility and thermal instability. Electrospray ionization often is used to convert the analyte into a sole ion which can be detected by a mass spectrometer. Tandem mass spectrometry involves multiple steps of mass selection for the detection of analyte ions. MS/MS involves the quantification of the ions in SIM (selective ion monitoring) and MRM (multiple reaction monitoring) modes which increases the specificity of detection. Some of the most commonly used HPLC equipment include the Waters 2690 HPLC equipped with a Genesis $C_{18}$ column, LC (Agilent 1100 system, which consists of a binary pump, a vacuum degasser, an autosampler, and a thermostated column), with a Waters 2695 HPLC separation module equipped with a Waters Symmetry $C_{18}$ column.

HPLC-ESI-MS-MS is effective in analyzing most of the pharmaceutical compounds with retention times ranging between 2 and 35 min (Castiglioni et al 2005, Miao et al. 2002, Vanderford et al. 2003, Vieno et al. 2006, Zhang et al. 2007). A few of the compounds had analytical difficulty because of the signal suppression during the ESI step. To overcome this, more efficient sample preparation (such as addition of surrogate standards) was required to achieve better recoveries of the analytes.

**GC-MS (Gas Chromatography with Mass Spectrophotometer Detector)**

Gas chromatography, although less selective when compared to HPLC, is less complex and more cost effective. It is used for the analysis of compounds that are volatile in nature and thermally stable. Gas chromatography often involves the conversion of analytes into derivatives, which reduces the molecule's polarity and increases its volatility. The most common derivatizing steps include using trimethylsilyl (TMS), N-Methyl-N-(trimethylsilyl) trifluoroacetamide (MSTFA), N-(t-butyldimethylsilyl)-N-methyltrifluoroacetamide (MTBSTFA) and pentafluorobenzyl bromide (PFBBr). The respective derivatives are analyzed then by GC-MS (Gibson et al. 2007, Lee et al. 2003, Reddersen et al. 2003, Thomas et al. 2004, and Togola et al. 2007). Recoveries for most of the compounds studied met the analytical requirements, although some poor recoveries were observed due to inefficient sample preparation and storage steps.

Recoveries and detection limits for some of the pharmaceuticals using the above listed analytical methods are summarized in Table 3.1.

Table 3.1 Analytical Methods and Extraction Recoveries of pharmaceuticals and personal care products

| Analyte | Extraction Method | Recovery (%) | Analytical Method | LOD(ng/L) | LOQ(ng/L) | Reference |
|---|---|---|---|---|---|---|
| **Ibuprofen** | SPE | 92±3.7[a] | HPLC-MS-MS | | 1.38[a] | Castiglioni et al 2005 |
| | SPE | 71[a] | HPLC-MS-MS | 5 | | Miao et al 2002 |
| | SPE | 96±15 | HPLC-MS-MS | 1 | | Vanderford et al 2003 |
| | SPE | 93±7[c],96±5[d],46±2[a],68±9[b] | HPLC-MS-MS | | 1[c,d],5[a,b] | Lindqvist et al 2005 |
| | SPE-Derivatization | 67[f],110[d] | GC-MS | 3.5 | | Sacher et al 2001 |
| | SPE-Derivatization | 97±3[g],92±6[a] | GC-MS | 10 | | Lee et al 2003 |
| | SPE-Derivatization | 87±4[g] | GC-MS | 10 | | Lee et al 2005 |
| | SPE-Derivatization | 108±5[g] | GC-MS | 10 | | Thomas et al 2004 |
| | SPE-Derivatization | 67±18 | GC-MS | 36 (full scan mode), 0.6 (SIM) | 104(full scan mode), 1.6 (SIM) | Koutsouba et al 2003 |
| | SPE-Derivatization | 86.4±11[g] | GC-MS | | 30 | Moldovan et al 2006 |
| | | | | | | |
| **Naproxen** | SPE | 68.4[a] | HPLC-MS-MS | | 10 | Castiglioni et al 2005 |
| | SPE | 91±9 | HPLC-MS-MS | 1 | | Vanderford et al 2003 |
| | SPE | 87±6[c],89±4[d],81±6[a],86±6[b] | HPLC-MS-MS | | 5[c,d],25[a,b] | Lindqvist et al 2005 |
| | SPE | 50±16[a],50±10[b],25[e] | HPLC-MS-MS | 15[e] | | Pedrouzo et al 2007 |
| | SPE-Derivatization | 101±4[g],93±5[a] | GC-MS | 10 | | Lee et al 2003 |
| | SPE-Derivatization | 101±3[g] | GC-MS | 10 | | Lee et al 2005 |
| | SPE-Derivatization | 101±4[g] | GC-MS | 9 | | Thomas et al 2004 |
| | | | | | | |
| **Clofibric acid** | SPE | 81±1.8[a] | HPLC-MS-MS | | 0.36[a] | Castiglioni et al 2005 |
| | SPE | 82.2 | HPLC-MS-MS | 10 | | Miao et al 2002 |
| | SPE | 54±20[a],33±20[b],61[e] | HPLC-MS-MS | 5[e] | | Pedrouzo et al 2007 |
| | SPE-Derivatization | 77[f],103[d] | GC-MS | 5.3 | | Sacher et al 2001 |

Continuation of above table

| Analyte | Extraction Method | Recovery (%) | Analytical Method | LOD(ng/L) | LOQ(ng/L) | Reference |
|---|---|---|---|---|---|---|
| | SPE-Derivatization | 99±2[g],95±5[a] | GC-MS | 10 | | Lee et al 2003 |
| | SPE-Derivatization | 90±15 | GC-MS | 244 (full scan mode),1.8 (SIM) | 714( full scan mode), 5 (SIM) | Koutsouba et al 2003 |
| | | | | | | |
| **Diazepam** | SPE | 96±5.1[a] | HPLC-MS-MS | | 1.08 | Castiglioni et al 2005 |
| | SPE | 80±19 | HPLC-MS-MS | 1 | | Vanderford et al 2003 |
| | SPE-Derivatization | 77[f],93[d] | GC-MS | 6.9 | | Sacher et al 2001 |
| | SPE-Derivatization | 78.9±5.4[g] | GC-MS | | 30 | Moldovan et al 2006 |
| | | | | | | |
| **Carbamazepine** | SPE | 98±7.2 | HPLC-MS-MS | | 1.3 | Castiglioni et al 2005 |
| | SPE | 67±10[a],34±26[b],101[e] | HPLC-MS-MS | 3[e] | | Pedrouzo et al 2007 |
| | SPE-Derivatization | 80[f],74[d] | GC-MS | 9.6 | | Sacher etal 2001 |
| | SPE-Derivatization | 103±5[f],99±7[c],108±10[e],79±2[a] | GC-MS | | 8 | Lin et al 2005 |
| | SPE-Derivatization | 109.7±16.4 | GC-MS | | 30 | Moldovan et al 2006 |
| | | | | | | |
| **Bezafibrate** | SPE | 76±2.6[a] | HPLC-MS-MS | | 0.1[a] | Castiglioni et al 2005 |
| | SPE | 67.1[a] | HPLC-MS-MS | 10 | | Miao et al 2002 |
| | SPE | 73±4[c],64±2[d],58±1[a],64±2[b] | HPLC-MS-MS | | 1[c,d],5[a,b] | Lindqvist et al 2005 |
| | SPE-Derivatization | 93[f],151[d] | GC-MS | 7.5 | | Sacher etal 2001 |
| | | | | | | |
| **Diclofenac** | SPE | 62.8[a] | HPLC-MS-MS | 10 | | Miao et al 2002 |
| | SPE | 83±11 | HPLC-MS-MS | 1 | | Vanderford et al 2003 |
| | SPE | 75±11[c],77±6[d],64±1[a],77±6[b] | HPLC-MS-MS | | 1[c,d],5[a,b] | Lindqvist et al 2005 |
| | SPE | 57±18[a],37±2[b],47[e] | HPLC-MS-MS | 5[e] | | Pedrouzo et al 2007 |

Continuation of above table

| Analyte | Extraction Method | Recovery (%) | Analytical Method | LOD(ng/L) | LOQ(ng/L) | Reference |
|---|---|---|---|---|---|---|
| | SPE-Derivatization | 70[f],70[d] | GC-MS | 8.7 | | Sacher et al 2001 |
| | SPE-Derivatization | 80±2[g] | GC-MS | 45 | | Thomas et al 2004 |
| | SPE-Derivatization | 80±9[f],81±9[c],63±4[e],54±7[a] | GC-MS | | 2 | Lin et al 2005 |
| | SPE-Derivatization | 76±9 | | 38(Full scan mode), 1(SIM) | 108(Full scan mode), 2(SIM) | Koutsouba et al 2003 |
| | | | | | | |
| **Ketoprofen** | SPE | 83.9 | HPLC-MS-MS | 20 | | Miao et al 2002 |
| | SPE | 95±6[c],83±5[d],69±2[a],83±5[b] | HPLC-MS-MS | | 5[c,d],25[a,b] | Lindqvist et al 2005 |
| | SPE-Derivatization | 102±4[g] | GC-MS | 10 | | Lee etal 2005 |
| | SPE-Derivatization | 50±6[f],59±5[c],77±7[e],83±2[a] | GC-MS | | 2 | Lin et al 2005 |
| | | | | | | |
| **Gemfibrozil** | SPE | 78.2[a] | HPLC-MS-MS | 5 | | Miao et al 2002 |
| | SPE | 94±10 | HPLC-MS-MS | 1 | | Vanderford et al 2003 |
| | SPE-Derivatization | 49[f],89[d] | GC-MS | 5.2 | | Sacher et al 2001 |
| | SPE-Derivatization | 100±3[g],98±6[a] | GC-MS | 10 | | Lee et al 2003 |
| | SPE-Derivatization | 99±4[g] | GC-MS | 10 | | Lee et al 2005 |
| | | | | | | |
| **Atenolol** | SPE | 106±6[a] | HPLC-MS-MS | | 1.07[a] | Castiglioni et al 2005 |
| | SPE | 81±3[c],90±6[d],101±4[a],108±10[b] | HPLC-MS-MS | | 6.5[c],11.8[d],21[a],49[b] | Vieno et al 2006 |
| | SPE | 86[f],67[d] | HPLC-MS-MS | 2.4 | | Sacher et al 2001 |
| | | | | | | |
| **Triclosan** | SPE | 79±17 | HPLC-MS-MS | 1 | | Vanderford et al 2003 |
| | SPE-Derivatization | 89±2[g],84±6[a] | GC-MS | 10 | | Lee et al 2003 |
| | SPE-Derivatization | 93±5[g] | GC-MS | 10 | | Lee et al 2005 |

Continuation of above table

| Analyte | Extraction Method | Recovery (%) | Analytical Method | LOD(ng/L) | LOQ(ng/L) | Reference |
|---|---|---|---|---|---|---|
| | SPE-Derivatization | 79.2±7.3 | GC-MS | | 30 | Moldovan etal 2006 |
| | | | | | | |
| **Fenoprofen** | SPE | 91.5 | HPLC-MS-MS | 10 | | Miao et al 2002 |
| | SPE-Derivatization | 71[f],99[d] | GC-MS | 3.3 | | Sacher et al 2001 |
| | SPE-Derivatization | 95±4[g],96±5[a] | GC-MS | 10 | | Lee et al 2003 |
| | SPE-Derivatization | 98±3[g] | GC-MS | 10 | | Lee et al 2005 |
| | | | | | | |
| **Caffeine** | SPE | 93±10 | HPLC-MS-MS | 1 | | Vanderford et al 2003 |
| | SPE | 84±7[a],50±1[b],45[e] | HPLC-MS-MS | 3[e] | | Pedrouzo et al 2007 |
| | SPE-Derivatization | 34±11[g] | GC-MS | 9 | | Thomas et al 2004 |
| | SPE-Derivatization | 64.1±6.5 | GC-MS | | 30 | Moldovan et al 2006 |
| | | | | | | |
| **Estrone** | SPE | 97±6.4[a] | HPLC-MS-MS | | 1.5[a] | Castiglioni et al 2005 |
| | SPE-Derivatization | 105±6[g] | GC-MS | 10 | | Lee et al 2005 |
| | | | | | | |
| **Erythromycin** | SPE | 50±5.1[a] | HPLC-MS-MS | | 0.4[a] | Castiglioni et al 2005 |
| | SPE | 71±10 | HPLC-MS-MS | 1 | | Vanderford et al 2003 |
| | | | | | | |
| **Indomethacin** | SPE | 58.5±10 | HPLC-MS-MS | 10 | | Miao et al 2002 |
| | SPE-Derivatization | 86[f],114[d] | GC-MS | 5.4 | | Sacher et al 2001 |
| | SPE-Derivatization | 93±4[g],83±7[a] | GC-MS | 10 | | Lee et al 2003 |
| | SPE-Derivatization | 107±5[g] | GC-MS | 10 | | Lee et al 2005 |

a: spiked with STP effluent, b: spiked with STP influent, c: spiked with ground water, d: spiked with surface water, e: spiked with river water, f: spiked with tap water, g: spiked with distilled water

### 3.3 Detection of Pesticides (EPA Method 508)

In EPA Method 508, the analytes of interest are extracted manually or by an auto extraction technique and then analyzed in a gas chromatograph with an electron capture detector (GC/ECD). Methylene chloride is used as the extracting solvent. As in all very low level analyses, interferences and matrix effects are of concern. Recovery values and method detection limits for the targeted pesticides are shown in Table 3.2.

Table 3.2 Single laboratory Accuracy, Precision, Method Detection Limits (MDLs) for Analytes from Reagent Water (NATIONAL EXPOSURE RESEARCH LABORATORY OFFICE OF RESEARCH AND DEVELOPMENT U.S. ENVIRONMENTAL PROTECTION AGENCY, CINCINNATI, OHIO, 1995)

| Analyte | Fortified Conc (µg/L) | N[a] | Recovery (%) | RSD % | MDL (µg/L) |
|---|---|---|---|---|---|
| Aldrin | 0.075 | 7 | 66 | 9 | 0.014 |
| Chlordane-alpha | 0.015 | 7 | 117 | 8 | 0.0041 |
| Chlordane-gamma | 0.015 | 7 | 109 | 3 | 0.0016 |
| Chloroneb | 0.5 | 7 | 47 | 34 | 0.25 |
| Chlorobenzilate | 5 | 8 | 99 | 5 | 2.2 |
| Chlorothalonil | 0.025 | 7 | 119 | 12 | 0.011 |
| DCPA | 0.025 | 7 | 112 | 4 | 0.0032 |
| 4,4'-DDD | 0.025 | 7 | 115 | 5 | 0.0044 |
| 4,4'-DDE | 0.01 | 7 | 127 | 6 | 0.0025 |
| 4,4'-DDT | 0.06 | 7 | 87 | 23 | 0.039 |
| Dieldrin | 0.02 | 7 | 77 | 22 | 0.011 |
| Endosulfan I | 0.015 | 7 | 78 | 25 | 0.0092 |
| Endosulfan Sulfate | 0.015 | 7 | 129 | 4 | 0.0024 |
| Endrin | 0.015 | 7 | 72 | 18 | 0.0062 |
| Endrin Aldehyde | 0.025 | 7 | 95 | 15 | 0.011 |
| Endosulfan II | 0.015 | 7 | 148 | 35 | 0.024 |
| Etridiazole | 0.025 | 7 | 96 | 17 | 0.013 |
| HCH-alpha | 0.025 | 8 | 94 | 8 | 0.0053 |
| HCH-beta | 0.01 | 7 | 95 | 12 | 0.0036 |
| HCH-delta | 0.01 | 7 | 84 | 7 | 0.002 |

Continuation of above table

| Analyte | Fortified Conc (µg/L) | N[a] | Recovery (%) | RSD % | MDL (µg/L) |
|---|---|---|---|---|---|
| HCH-gamma | 0.015 | 7 | 80 | 16 | 0.006 |
| Heptachlor | 0.01 | 7 | 67 | 7 | 0.0015 |
| Heptachlor Epoxide | 0.015 | 7 | 71 | 18 | 0.0059 |
| Hexachlorobenzene | 0.005 | 7 | 115 | 43 | 0.0077 |
| Methoxychlor | 0.05 | 7 | 120 | 11 | 0.022 |
| cis-Permethrin | 5 | 7 | 64 | 24 | 0.25 |
| trans-Permethrin | 5 | 7 | 122 | 9 | 0.18 |
| Propachlor | 5 | 7 | 90 | 18 | 0.25 |
| Trifluralin | 0.025 | 7 | 108 | 3 | 0.0026 |

[a]N = Number of sample replicates.

RSD: Relative Standard Deviation (absolute value of the coefficient of variation expressed as a percentage).

MDL: Method Detection Limit (minimum amount of substance that can be detected with a given confidence).

# CHAPTER IV
# TREATABILITY OF EMERGING CONTAMINANTS

## 4.1 Pharmaceuticals and personal care products

Many reports have been published in the last two decades describing the effectiveness of different treatment methods for removing these emerging contaminants, mostly based on the treatment of municipal wastewaters. The treatment methods examined included sedimentation, flocculation, coagulation, rapid sand filtration, ozonation, adsorption, activated sludge, membrane bioreactors, nano- and ultra filtration, and ultraviolet (UV) light and chlorine disinfection.

Primary sedimentation and flocculation processes at municipal treatment plants were not very effective at removing the pharmaceutical compounds, with most removal rates < 40% (Thomas et al. 2005, Carballa et al. 2004). Sedimentation after ferric chloride coagulation followed by rapid sand filtration (Vieno et al. 2007) also was ineffective, with removal rates of about 10% for the pharmaceuticals studied. Ozonation, according to many researchers, has been much more effective at removing most of the compounds. Several studies (Vieno et al. 2007, Snyder et al. 2006, and Jasim et al. 2006) reported removal rates for most of the compounds between 60 and 99% using ozone. Increasing the ozone dosage and the addition of $H_2O_2$ improved the removal rates for some of the compounds (Snyder et al. 2006). Reaction time, amount of ozone dosage, alkalinity of the water, and the reactivity of the compounds towards ozone, are reported to be important factors affecting the increase of removal rates.

Conventional activated sludge treatment also was studied (Radjenovic et al. 2006, Lishman et al. 2006, Nakada et al. 2006) for its effectiveness on these compounds. For most of the compounds examined, the removal rates were greater than 60%. The two mechanisms associated with the reduction of the EC compounds were sorption/desorption from the sludge itself and biodegradation by the microorganisms in the sludge (Carballa et al. 2004, Radjenovic et al. 2006). For some of the compounds examined, the removal rates increased with an increase of SRT (sludge retention time), but the effect was not consistent for all compounds. Several researchers suggested that the effect of different SRTs and temperatures were areas for future research to enhance EC treatment.

Table 4.1 Removal rates of pharmaceuticals and PCPs with respect to different treatment processes

| Contaminant | Type of water | Unit processes examined | Removal (%) | Influent conc.(µg/L) | Effluent conc.(µg/L) | Reference |
|---|---|---|---|---|---|---|
| Carbamazepine | River water | Ferric coag+sed+ rapid sand filtration | 7 | | | Vieno et al 2007 |
| Carbamazepine | River water | Ozonation alone after ( Ferric coag+sed+ rapid sand filtration) | >99 | | | Vieno et al 2007 |
| Carbamazepine | Sanitary waste water | Primary+ Activated sludge | 0 | | | Castiglioni et al 2006 |
| Carbamazepine | Sewage sludge | Anaerobic digestion | 0 | | | Carballa et al 2007 |
| Carbamazepine | Sanitary waste water | Membrane bioreactor | 0 | 0.24(median) | 0.3(median) | Radjenovic et al 2006 |
| Carbamazepine | Sanitary waste water | Conventional Activated Sludge | 0 | 0.24(median) | 0.25(median) | Radjenovic et al 2006 |
| Carbamazepine | Sanitary waste water | Primary+ Activated sludge | upto 78 | 15-350 | 15-160 | Nakada et al 2006 |
| Caffeine | Sanitary waste water | Primary+ Activated Sludge+ (Alum+ Gravity Filtration+ Disinfection) | 17,99.9 | | | Thomas et al 2005 |
| Caffeine | Distilled water | Floc/Sed+ Dual Media Filtration+ Disinfection | 3.4-12.7 | | | Bundy et al 2007 |
| Caffeine | Distilled water | Floc/Sed+ Dual Media Filtration+GAC Disinfection | >94 | | | Bundy et al 2007 |
| Ibuprofen | Sanitary waste water | Activated Sludge | 95 | 8.45(mean) | 0.384(mean) | Lishman et al 2006 |
| Ibuprofen | Sanitary waste water | primary+ biological reactor | 63 | | | Carballa et al 2004 |

Continuation of above table

| Contaminant | Type of water | Unit processes examined | Removal (%) | Influent conc.(μg/L) | Effluent conc.(μg/L) | Reference |
|---|---|---|---|---|---|---|
| Ibuprofen | River water | ozonation alone after ( Ferric coag+sed+ rapid sand filtration) | 92 | | | Vieno et al 2007 |
| Ibuprofen | Sanitary waste water | Primary+ Activated sludge | 38[d],93[e] | | | Castiglioni et al 2006 |
| Ibuprofen | Sewage sludge | Anaerobic digestion | 41±15 | | | Carballa et al 2007 |
| Ibuprofen | Sanitary waste water | Membrane bioreactor | 99.8±0.386 | 17(median) | 0(median) | Radjenovic et al 2006 |
| Ibuprofen | Sanitary waste water | Conventional Activated Sludge | 82.5±15.8 | 17(median) | 2(median) | Radjenovic et al 2006 |
| Ibuprofen | Sanitary waste water | Primary+ Activated Sludge | 83-99 | 300-1200 | 1-110 | Nakada et al 2006 |
| Naproxen | Sanitary waste water | Activated Sludge | 93 | 5.58(mean) | 0.452(mean) | Lishman et al 2006 |
| Naproxen | Sanitary waste water | primary + biological reactor | 48 | | | Carballa et al 2004 |
| Naproxen | River water | Ferric coag+sed+ rapid sand filtration | 10 | | | Vieno et al 2007 |
| Naproxen | River water | ozonation alone after ( Ferric coag+sed+ rapid sand filtration) | 75 | | | Vieno et al 2007 |
| Naproxen | Sanitary waste water | Primary+ Activated Sludge+ (Alum+ Gravity Filtration+ Disinfection) | 3[a],99.8[b] | | | Thomas et al 2005 |

Continuation of above table

| Contaminant | Type of water | Unit processes examined | Removal (%) | Influent conc.(µg/L) | Effluent conc.(µg/L) | Reference |
|---|---|---|---|---|---|---|
| Naproxen | Sanitary waste water | Membrane Bioreactor | 99.3±1.52 | 11.6(median) | 0(median) | Radjenovic et al 2006 |
| Naproxen | Sanitary waste water | Conventional Activated Sludge | 85.1±11.4 | 11.6(median) | 3(median) | Radjenovic et al 2006 |
| Naproxen | Sanitary waste water | Primary+ Activated Sludge | upto 82 | 30-250 | 11-150 | Nakada et al 2006 |
| Diazepam | Sewage sludge | Anaerobic Digestion | 50±16 | | | Carballa et al 2007 |
| Diclofenac | River water | Ferric coag+sed+ rapid sand filtration | 8 | | | Vieno et al 2007 |
| Diclofenac | River water | ozonation alone after ( Ferric coag+sed+ rapid sand filtration) | >94 | | | Vieno et al 2007 |
| Diclofenac | Sanitary waste water | Primary+ Activated Sludge+ (Alum+ Gravity Filtration+ Disinfection) | 14[a],89[b],100[c] | | | Thomas et al 2005 |
| Diclofenac | Sewage sludge | Anaerobic Digestion | 69±10 | | | Carballa et al 2007 |
| Diclofenac | Sanitary waste water | Membrane bioreactor | 87.4±14.1 | 2.8(median) | 0.2(median) | Radjenovic et al 2006 |
| Diclofenac | Sanitary waste water | Conventional Activated Sludge | 50.1±20.1 | 2.8(median) | 1.2(median) | Radjenovic et al 2006 |
| Gemfibrozil | Sanitary waste water | Activated sludge | 66 | | | Lishman et al 2006 |
| Gemfibrozil | Sanitary waste water | Membrane bioreactor | 89.6±23.3 | 3.8(median) | 0(median) | Radjenovic et al 2006 |
| Gemfibrozil | Sanitary waste water | Conventional Activated Sludge | 38.8±16.9 | 3.8(median) | 2.5(median) | Radjenovic et al 2006 |

Continuation of above table

| Contaminant | Type of water | Unit processes examined | Removal (%) | Influent conc.(μg/L) | Effluent conc.(μg/L) | Reference |
|---|---|---|---|---|---|---|
| Acetaminophen | Sanitary waste water | Membrane bioreactor | 99.6±0.299 | 18(median) | 0(median) | Radjenovic et al 2006 |
| Acetaminophen | Sanitary waste water | Conventional Activated Sludge | 98.4±1.72 | 18(median) | 0.1(median) | Radjenovic et al 2006 |
| | | | | | | |
| Iopromide | Sewage sludge | Anaerobic Digestion | 22±11 | | | Carballa et al 2007 |
| Estrone | Sanitary waste water | Lagoon | 86 | 0.0295(mean) | 0.0076(mean) | Lishman et al 2006 |
| Estrone | Sanitary waste water | Primary+ Activated sludge | 0 | | | Castiglioni et al 2006 |
| Estrone | Sewage sludge | Anaerobic Digestion | 88±6 | | | Carballa et al 2007 |
| Estrone | Sanitary waste water | Primary+ Activated sludge | 83-90 | 25-200 | 3-110 | Nakada et al 2006 |
| Bezafibrate | River water | Ferric coag+sed+ rapid sand filtration | 27 | | | Vieno et al 2007 |
| Bezafibrate | River water | ozonation alone after ( Ferric coag+sed+ rapid sand filtration) | >77 | | | Vieno et al 2007 |
| Bezafibrate | Sanitary waste water | Primary+ Activated sludge | 15[d],87[e] | | | Castiglioni et al 2006 |
| Bezafibrate | Sanitary waste water | Membrane bioreactor | 95.8±8.66 | 1.75(median) | 0.1(median) | Radjenovic et al 2006 |
| Bezafibrate | Sanitary waste water | Conventional Activated Sludge | 48.4±33.8 | 1.75(median) | 0.75(median) | Radjenovic et al 2006 |
| Triclosan | Sanitary waste water | Activated Sludge | 93 | 1.93(mean) | 0.108(mean) | Lishman et al 2006 |

Continuation of above table

| Contaminant | Type of water | Unit processes examined | Removal (%) | Influent conc.(µg/L) | Effluent conc.(µg/L) | Reference |
|---|---|---|---|---|---|---|
| Triclosan | Sanitary waste water | Activated sludge + filtration | 95 | | | Lishman et al 2006 |
| Triclosan | Sanitary waste water | Primary+ Activated Sludge+ (Alum+ Gravity Filtration+ Disinfection) | 26[a],98.4[b] | | | Thomas et al 2005 |
| Triclosan | Sanitary waste water | Primary+ Activated Sludge | 46-92 | 200-1000 | 20-200 | Nakada et al 2006 |
| Ketoprofen | Sanitary waste water | Activated sludge | 44 | | | Lishman et al 2006 |
| Ketoprofen | Sanitary waste water | Primary+ Activated Sludge+ (Alum+ Gravity Filtration+ Disinfection) | 7[a],94[b],98.9[c] | | | Thomas et al 2005 |
| Ketoprofen | River water | Ferric coag+sed+ rapid sand filtration | 13 | | | Vieno et al 2007 |
| Ketoprofen | River water | Ozonation alone after ( Ferric coag+sed+ rapid sand filtration) | >62 | | | Vieno et al 2007 |
| Ketoprofen | Sanitary waste water | Membrane bioreactor | 91.9±6.55 | 1.8(median) | 0.2(median) | Radjenovic et al 2006 |
| Ketoprofen | Sanitary waste water | Conventional Activated Sludge | 51.5±22.9 | 1.8(median) | 0.75(median) | Radjenovic et al 2006 |
| Ketoprofen | Sanitary waste water | Primary+ Activated Sludge | 15-68 | 100-400 | 50-200 | Nakada et al 2006 |
| Clofibric Acid | Sanitary waste water | Primary+ Activated sludge | 30[d], <0.36[e] | | | Castiglioni et al 2006 |
| Clofibric Acid | Sanitary waste water | Membrane bioreactor | 71.8±30.9 | 0.11(median) | 0.02(median) | Radjenovic et al 2006 |

Continuation of above table

| Contaminant | Type of water | Unit processes examined | Removal (%) | Influent conc.(μg/L) | Effluent conc.(μg/L) | Reference |
|---|---|---|---|---|---|---|
| Atenolol | River water | Ferric coag+sed+ rapid sand filtration | 12 | | | Vieno et al 2007 |
| Atenolol | River water | Ozonation alone after ( Ferric coag+sed+ rapid sand filtration) | >73 | | | Vieno et al 2007 |
| Atenolol | Sanitary waste water | Primary+ Activated sludge | 10[d],55[e] | | | Castiglioni et al 2006 |
| Atenolol | Sanitary waste water | Membrane bioreactor | 65.5±36.2 | 1.5(median) | 0.5(median) | Radjenovic et al 2006 |
| Ciprofloxacin | River water | Ferric coag+sed+ rapid sand filtration | 35 | | | Vieno et al 2007 |
| Ciprofloxacin | River water | Ozonation alone after ( Ferric coag+sed+ rapid sand filtration) | 16 | | | Vieno et al 2007 |
| Ciprofloxacin | Sanitary waste water | Primary+ Activated sludge | 60[d],63[e] | | | Castiglioni et al 2006 |
| Ofloxacin | Sanitary waste water | Primary+ Activated sludge | 43,57 | | | Castiglioni et al 2006 |
| Ofloxacin | Sanitary waste water | Membrane bioreactor | 94±6.51 | 0.44(median) | 0.04(median) | Radjenovic et al 2006 |
| Ofloxacin | Sanitary waste water | Conventional Activated Sludge | 23.8±23.5 | 0.44(median) | 0.3(median) | Radjenovic et al 2006 |
| Erythromycin | Sanitary waste water | Primary+ Activated sludge | 0 | | | Castiglioni et al 2006 |
| Erythromycin | Sanitary waste water | Membrane bioreactor | 67.3±16.1 | 0.15(median) | 0.05(median) | Radjenovic et al 2006 |
| Erythromycin | Sanitary waste water | Conventional Activated Sludge | 23.8±29.2 | 0.15(median) | 0.08(median) | Radjenovic et al 2006 |

Continuation of above table

| Contaminant | Type of water | Unit processes examined | Removal (%) | Influent conc.(µg/L) | Effluent conc.(µg/L) | Reference |
|---|---|---|---|---|---|---|
| Fenoprofen | Sanitary waste water | Primary+ Activated Sludge | 65-97 | 15-90 | 2--9 | Nakada et al 2006 |
| Indomethacin | Sanitary waste water | Activated sludge | 23 | 0.23(mean) | 0.19(mean) | Lishman et al 2006 |
| Indomethacin | Sanitary waste water | Membrane bioreactor | 46.6±23.2 | 0.11(median) | 0.06(median) | Radjenovic et al 2006 |
| Indomethacin | Sanitary waste water | Conventional Activated Sludge | 23.4±22.3 | 0.11(median) | 0.085(median) | Radjenovic et al 2006 |
| Metoprolol | River water | Ferric coag+sed+ rapid sand filtration | 11 | | | Vieno et al 2007 |
| Metoprolol | River water | Ozonation alone after ( Ferric coag+sed+ rapid sand filtration) | >95 | | | Vieno et al 2007 |
| Metoprolol | Sanitary waste water | Membrane bioreactor | 58.7±72.8 | 0.3(median) | 0.1(median) | Radjenovic et al 2006 |
| Metoprolol | Sanitary waste water | Conventional Activated Sludge | <10 | 0.3(median) | 0.27(median) | Radjenovic et al 2006 |

a: mean reduction after primary treatment, b: mean reduction after secondary treatment, c: mean reduction after advanced treatment, d: median reduction rate in winter, e: median reduction rate in summer

The addition of an adsorption step (GAC, granular activated carbon, or PAC, powdered activated carbon) in most of the studied processes (Bundy et al. 2007, Snyder etal 2007, and Vieno et al. 2007) significantly increased the removal of the pharmaceuticals and PCPs, resulting in removal rates close to 90%. The amount of the powdered activated carbon used, the nature of the compound, and the reaction times, must be taken into consideration when optimizing EC removal from wastewater and potentially from stormwaters.

The membrane processes using RO (reverse osmosis) or nano- and ultra filtration, proved to be very effective in the treatment of pharmaceuticals and PCPs, with removal rates greater than 90% for most of the compounds (Snyder et al. 2007, Yoon et al. 2007). The removal is likely due to the retention of the compounds onto the membranes as a result of the hydrophobic nature of the compounds. The adsorption increased with increasing Kow values of the EC, indicating increasing hydrophobicity. In addition, ion exchange processes may influence this removal.

Most of the veterinary pharmaceuticals behave similarly to compounds in the general PPCP listing. Therefore, the treatability expectations discussed above can also be used as general guidance for their reduction.

## 4.2 Pesticides

The most effective treatment of most pesticides usually involves carbon adsorption using activated carbon. This treatment technology is employed already in several stormwater treatment devices that include a filtration unit.

Pesticide removals can occur in vegetated filter strips during stormwater infiltration. The pesticide removals were associated with sorption to soil and vegetation

(Arora et al. 1996). The addition of vegetation in the stormwater flow path increased the microbial activity, leading to some pesticide degradation (Staddon et al. 2001). These researchers found that soil type, slope, length, vegetation density, and vegetation type influenced the efficiency of microbial degradation of pesticides.

# CHAPTER V

# FATE OF EMERGING CONTAMINANTS IN SURFACE WATERS

Any compound released into the environment will partition between solid, liquid and gaseous phases. The partitioning of a compound into different phases depends on the physical and chemical properties of the phases and of the compound itself. Typically, pollutants with high Koc and Kow values tend to adsorb onto the solid phase. Those with lower Koc and Kow values (and if polar) associate with the liquid phase. A fugacity model developed by Mackay, et al. (1992) was used to predict the partitioning of these emerging pollutants into the three phases. The modeling approach is described in the following section

## 5.1 Fugacity Approach for Predicting the Partitioning of PPCPs and Pesticides with Different Phases

Fugacity literally means the "tendency to flee." Fugacity modeling is based on chemical equilibrium and is used to determine the relative concentrations of a chemical in air, water, and soil phases. The Level I Fugacity model (Mackay, et al., 1992) was used to calculate the likely fate of representative emerging compounds. These calculations were based on pre-specified control volumes for each media compartment. A Level I Fugacity model assumes the equilibrium distribution of a fixed quantity of conserved chemical, in a closed environment at equilibrium. It does not account for degradation reactions, advective processes, or other intermediate transport processes. The characteristics of different compartments used in these calculations are shown in Table 5.1.

Table 5.1 Level 1 Fugacity Parameters for Emerging Contaminants (Mackay Method)

| Compartment | Air | Water | Soil | Sediment | Suspended sediment | Fish |
|---|---|---|---|---|---|---|
| Volume, V ($m^3$) | 1E+14 | 2E+11 | 9E+09 | 1E+08 | 1E+06 | 2E+05 |
| Depth, h (m) | 1000 | 20 | 0.1 | 0.01 | | |
| Area, A ($m^2$) | 1E+11 | 1.E+10 | 9E+11 | 1E+10 | | |
| Fraction OC | | | 0.02 | 0.04 | 0.2 | |
| Density, ρ ($kg/m^3$) | 1.2 | 1000 | 2400 | 2400 | 1500 | 1000 |
| Adv. Residence time, T (hrs) | 100 | 100 | | 5E+04 | | |
| Adv. Flow, G | 1E+12 | 2E+09 | | 2000 | | |

The fugacity of a compound is calculated as $f = M/\Sigma V_i Z_i$ (eq. 5.1)

Where M is the total amount of chemical (mol)

$V_i$ is the medium volume ($m^3$)

$Z_i$ is the corresponding fugacity capacity for the chemical in each medium

The number of moles partitioned into each respective phase is in turn calculated as:

$M= f^*\Sigma V_i Z_i$

The equations for phase Z values used in Level I calculations are as shown below:

Air: $$Z_1 = \frac{1}{RT}$$ (eq. 5.2)

Water: $$Z_2 = \frac{1}{H}$$ (eq. 5.3)

Sediment: $$Z_3 = Z_2 * \mathrm{P}_3 * \phi_3 * \frac{K_{OC}}{1000}$$ (eq. 5.4)

Suspended Sediment: $$Z_4 = Z_2 * \mathrm{P}_4 * \phi_4 * \frac{K_{OC}}{1000}$$ (eq. 5.5)

Fish: $$Z_5 = Z_2 * \mathrm{P}_5 * L * \frac{K_{OW}}{1000}$$ (eq. 5.6)

Where:

R = gas constant (8.314 J/mol K)

T = absolute temperature (K)

H = Henry's law constant (atm*$m^3$/mol)

Kow = Octanol-water partition coefficient

Koc = Organic-carbon partition coefficient

$\rho_i$ = density of phase i (kg/$m^3$)

$\varphi_i$ = mass fraction of organic fraction in phase i (g/g)

L= lipid content of fish

The physical and chemical properties of the compounds included in this modeling study are shown in Tables 5.2 and 5.3.

Table 5.2 Physical and Chemical Properties of PPCPs examined in the study

| Compound | Log Kow | Koc | Henrys constant (atm $m^3$/mole) |
|---|---|---|---|
| Nystatin | 7.08 | 170 | 2E-07 |
| Dexamethasone | 1.83 | 240 | 7.2E-08 |
| Methoprene | 5.5 | 23000 | 6.9E-06 |
| Prednisone | 1.46 | 150 | 2.8E-10 |
| Metronidazole | -0.02 | 23 | 1.7E-11 |
| Clindamycin | 2.16 | 360 | 2.9E-22 |
| Ketoconazole | 4.34 | 8970 | 5.6E-20 |
| Carbamazepine | 2.45 | 510 | 1.1E-10 |
| Caffeine | -0.07 | 22 | 3.6E-11 |
| Ibuprofen | 3.97 | 3400 | 1.5E-07 |
| Diclofenac | 4.51 | 830 | 4.7E-12 |
| Acetaminophen | 0.46 | 42 | 6.4E-13 |
| Triclosan | 4.76 | 9200 | 1.5E-07 |
| Ciprofloxacin | 0.28 | 61000 | 5.1E-19 |
| Metoprolol | 1.88 | 62 | 2.1E-11 |
| Salicylic acid | 2.62 | 65,104 | 7.34E-09 |
| Dioxin | 6.8 | 24000000 | 5.0E-05 |

Table 5.3 Physical and Chemical Properties of PPCPs examined in the Fugacity study

| Compound | Log Kow | Koc | Henrys constant (atm-$m^3$/mole) |
|---|---|---|---|
| Aldrin | 7.08 | 22909 | 4.4E-05 |
| Chloroneb | 2.47 | 1260 | 1.0E-04 |
| Chlorothalonil | 1.83 | 1800 | 2.5E-07 |
| DDD | 6.5 | 724436 | 6.6E-06 |
| DDE | 4 | 50118 | 4.2E-05 |
| DDT | 5.5 | 239883 | 8.3E-06 |
| Dieldrin | 1.46 | 8730 | 1.0E-05 |
| Endosulfan | -0.02 | 2884 | 6.6E-05 |
| Endrin | 2.16 | 10000 | 6.4E-06 |
| Etridiazole | 4.34 | 1000 | 3.0E-05 |
| HCH-α | 2.45 | 2089 | 6.7E-06 |
| HCH-β | -0.07 | 9550 | 4.4E-07 |
| HCH-δ | 3.97 | 661 | 4.3E-07 |
| HCH-γ | 4.51 | 1071 | 5.1E-06 |
| Heptachlor | 0.46 | 23988 | 2.9E-04 |
| Heptachlor epoxide | 4.76 | 7800 | 3.2E-05 |
| Methoxychlor | 0.28 | 80000 | 2.0E-07 |
| Permethrin | 1.88 | 10715 | 1.9E-06 |
| Propachlor | 2.62 | 79 | 3.6E-07 |
| Trifluralin | 6.8 | 7943 | 1.0E-04 |
| Aroclor 1016 | 7.08 | 17783 | 1.3E-04 |
| Aroclor 1221 | 2.47 | 5754 | 2.3E-04 |
| Aroclor 1232 | 1.83 | 7079 | 3.1E-04 |
| Aroclor 1242 | 6.5 | 66070 | 3.4E-04 |
| Aroclor 1248 | 4 | 275423 | 4.4E-04 |
| Aroclor 1254 | 5.5 | 1000000 | 2.8E-04 |
| Aroclor 1260 | 1.46 | 6760830 | 3.4E-04 |
| Toxaphene | -0.02 | 7244 | 6.0E-06 |
| Chlordane | 2.16 | 21380 | 4.9E-05 |

These fugacity calculations assumed that 100,000 kg of each compound was released into the environment and the percentage partitions into different phases were as shown in Table 5.4 and 5.5

Table 5.4 Partitioning of PPCPs into different phases

| | | Partitioning into different phases | | | | |
|---|---|---|---|---|---|---|
| Compound | Fugacity | % in air | % in water | % in sediment | % in suspended sediment | % in fish |
| Nystatin | 6.7E-14 | 0.25 | 61.97 | 0.51 | 0.02 | 37.25 |
| Dexamethasone | 9.1E-14 | 0.15 | 98.68 | 1.14 | 0.04 | 0.00 |
| Methoprene | 4.8E-12 | 6.14 | 43.57 | 48.10 | 1.50 | 0.69 |
| Prednisone | 3.9E-16 | 0.00 | 99.26 | 0.71 | 0.02 | 0.00 |
| Metronidazole | 5.0E-17 | 0.00 | 99.89 | 0.11 | 0.00 | 0.00 |
| Clindamycin | 3.4E-28 | 0.00 | 98.25 | 1.70 | 0.05 | 0.00 |
| ketoconazole | 3.6E-26 | 0.00 | 69.20 | 29.79 | 0.93 | 0.08 |
| Carbamazepine | 2.3E-16 | 0.00 | 97.54 | 2.39 | 0.07 | 0.00 |
| Caffeine | 9.3E-17 | 0.00 | 99.89 | 0.11 | 0.00 | 0.00 |
| Ibuprofen | 3.1E-13 | 0.26 | 85.34 | 13.93 | 0.44 | 0.04 |
| Diclofenac | 7.6E-18 | 0.00 | 95.90 | 3.82 | 0.12 | 0.16 |
| Acetaminophen | 2.1E-18 | 0.00 | 99.79 | 0.20 | 0.01 | 0.00 |
| Triclosan | 1.8E-13 | 0.21 | 68.43 | 30.22 | 0.94 | 0.20 |
| Ciprofloxacin | 1.9E-25 | 0.00 | 24.88 | 72.84 | 2.28 | 0.00 |
| Metoprolol | 3.9E-17 | 0.00 | 99.69 | 0.30 | 0.01 | 0.00 |
| Salicylic acid | 6.3E-15 | 0.00 | 23.68 | 74.00 | 2.31 | 0.00 |
| Dioxin | 6.5E-14 | 0.09 | 0.08 | 96.78 | 3.02 | 0.03 |

Table 5.5 Partitioning of pesticides into different phases

| | | Partition into different phases | | | | |
|---|---|---|---|---|---|---|
| Compound | Fugacity | % in air | % in water | % in sediment | % in suspended sediment | % in fish |
| Aldrin | 1.9E-11 | 28.18 | 31.33 | 34.46 | 1.08 | 4.95 |
| Chloroneb | 7.8E-11 | 66.24 | 31.78 | 1.92 | 0.06 | 0.00 |
| Chlorothalonil | 4.3E-13 | 0.47 | 91.39 | 7.90 | 0.25 | 0.00 |
| DDD | 2.8E-13 | 0.36 | 2.70 | 93.78 | 2.93 | 0.22 |
| DDE | 1.4E-11 | 17.76 | 20.89 | 50.25 | 1.57 | 9.53 |
| DDT | 8.7E-13 | 1.26 | 7.43 | 85.61 | 2.68 | 3.02 |
| Dieldrin | 8.0E-12 | 12.43 | 60.81 | 25.48 | 0.80 | 0.48 |
| Endosulfan | 3.3E-11 | 54.13 | 40.13 | 5.56 | 0.17 | 0.01 |
| Endrin | 5.1E-12 | 7.96 | 61.24 | 29.40 | 0.92 | 0.49 |
| Etridiazole | 3.6E-11 | 36.88 | 60.15 | 2.89 | 0.09 | 0.00 |
| HCH-α | 9.3E-12 | 11.01 | 80.63 | 8.08 | 0.25 | 0.03 |
| HCH-β | 5.1E-13 | 0.61 | 67.48 | 30.93 | 0.97 | 0.02 |
| HCH-δ | 7.1E-13 | 0.84 | 95.95 | 3.04 | 0.10 | 0.07 |
| HCH-γ | 7.6E-12 | 9.07 | 86.33 | 4.44 | 0.14 | 0.02 |
| Heptachlor | 4.8E-11 | 73.23 | 12.19 | 14.03 | 0.44 | 0.11 |
| Heptachlor epoxide | 2.0E-11 | 31.86 | 48.72 | 18.24 | 0.57 | 0.61 |
| Methoxychlor | 5.9E-14 | 0.08 | 20.12 | 77.26 | 2.41 | 0.12 |
| Permethrin | 1.4E-12 | 2.21 | 57.91 | 29.79 | 0.93 | 9.16 |
| Propachlor | 8.4E-13 | 0.73 | 98.89 | 0.37 | 0.01 | 0.00 |
| Trifluralin | 4.4E-11 | 59.99 | 28.50 | 10.87 | 0.34 | 0.31 |
| Aroclor 1016 | 5.6E-11 | 58.54 | 22.03 | 18.81 | 0.59 | 0.03 |
| Aroclor 1221 | 1.0E-10 | 78.53 | 16.71 | 4.61 | 0.14 | 0.01 |
| Aroclor 1232 | 9.1E-11 | 82.41 | 13.01 | 4.42 | 0.14 | 0.02 |
| Aroclor 1242 | 5.8E-11 | 62.14 | 8.86 | 28.11 | 0.88 | 0.01 |
| Aroclor 1248 | 3.2E-11 | 37.93 | 4.22 | 55.77 | 1.74 | 0.33 |
| Aroclor 1254 | 7.7E-12 | 10.26 | 1.77 | 85.13 | 2.66 | 0.18 |
| Aroclor 1260 | 1.3E-12 | 2.03 | 0.29 | 94.63 | 2.96 | 0.09 |
| Toxaphene | 4.8E-12 | 8.19 | 66.80 | 23.23 | 0.73 | 1.06 |
| Chlordane | 1.9E-11 | 31.80 | 32.01 | 32.85 | 1.03 | 2.31 |

These fugacity calculations show that the compounds are predominantly partitioned into either the water or sediment phases, with only a few compounds primarily partitioning into the air phase. The concentrations of compounds associated with particulates likely can be reduced substantially using traditional sediment practices, either in wastewater treatment plants, or in stormwater detention ponds. However, the effectiveness of sedimentation will depend on the size of the particles with which these compounds are associated. Sedimentation basins are designed to provide close to 100% treatment of a specific particle size, and larger. If the compounds associate with smaller particles than this critical particle size, sedimentation will be less efficient. Media filtration may reduce the compounds predominantly found both in the water and particulate-associated phases, especially with suitable selection of media (activated carbon). Media filtration's critical particle size limit is determined by the pore size of the media itself and it has been shown to be effective at removing particles < 10 µm from stormwater runoff. The addition of sorption media, such as activated carbon, allows the media to remove both particulate and dissolved pollutants provided that there is sufficient contact time for the chemical- or physical-sorption to occur. The modeling showed substantial partitioning into the water phase, indicating that wet-weather treatment technologies may require "filtration" (ion exchange or sorption unit processes) to be incorporated in the treatment train.

## 5.2 Studying the Effects of Environmental Factors on PPCP and Pesticide Associations with different Phases using Fugacity Calculations

The effects of different environmental factors on the partitioning of emerging contaminants into different media were studied using a full $2^3$ factorial design. The number of runs and possible interactions of the factors were shown in Table 5.6. The high value of a factor is shown by a '+' and the low value by a '-'sign. The high and low values of the factors are based on the available literature.

Table 5.6 $2^3$ Factorial Design showing Experimental Conditions for Eight Runs (Box et al 1978)

| Run | A | B | C | AB | AC | BC | ABC |
|---|---|---|---|---|---|---|---|
| 1 | + | + | + | + | + | + | + |
| 2 | + | + | - | + | - | - | - |
| 3 | + | - | + | - | + | - | - |
| 4 | + | - | - | - | - | + | + |
| 5 | - | + | + | - | - | + | - |
| 6 | - | + | - | - | + | - | + |
| 7 | - | - | + | + | - | - | + |
| 8 | - | - | - | + | + | + | - |

A: Concentration of Contaminant
B: Concentration of Suspended Sediment
C: Organic Fraction of Suspended Sediment

The high and low values of the factors considered in the design are shown in Tables 5.7 and 5.8.

Table 5.7 $2^3$ Full Factorial Design Variable Data for PPCPs

| Variable | Low value | High value |
|---|---|---|
| Concentration of Carbamazepine (A), μg/L | 0.002 | 0.083 |
| Concentration of Caffeine (A), μg/L | 0.004 | 0.24 |
| Concentration of Ibuprofen (A), μg/L | 0.003 | 0.6 |
| Concentration of Diclofenac (A), μg/L | 0.007 | 0.18 |
| Concentration of Acetaminophen (A), μg/L | 0.012 | 0.03 |
| Concentration of Triclosan (A), μg/L | 0.03 | 0.74 |
| Concentration of Ciprofloxacin (A), μg/L | 0.027 | 0.5 |
| Concentration of Metoprolol (A), μg/L | 0.02 | 0.12 |
| Concentration of Salicylic acid (A), μg/L | 0.013 | 0.22 |
| Concentration of Dioxin (A), μg/L | 0.004 | 0.071 |
| Concentration of Nystatin(A), μg/L | 0.002 | 0.74 |
| Concentration of Dexamethasone(A), μg/L | 0.002 | 0.74 |
| Concentration of methoprene(A), μg/L | 0.002 | 0.74 |
| Concentration of prednisone (A), μg/L | 0.002 | 0.74 |
| Concentration of Metronidazole (A), μg/L | 0.002 | 0.74 |
| Concentration of Clindamycin (A), μg/L | 0.002 | 0.74 |
| Concentration of Ketoconazole(A), μg/L | 0.002 | 0.74 |
| Concentration of Suspended solids (B), mg/L | 10 | 500 |
| Organic Fraction of Suspended Solids ( C) | 0.05 | 0.2 |

Table 5.7 $2^3$ Full Factorial Design Variable Data for Pesticides

| Variable | Low value | High value |
|---|---|---|
| Concentration of Contaminant (A), µg/L | 0.002 | 0.083 |
| Concentration of Suspended solids (B), mg/L | 10 | 500 |
| Organic Fraction of Suspended Solids ( C) | 0.05 | 0.2 |

The effects of selected factors on partitioning of emerging contaminants into water, sediment and suspended sediment were analyzed and the results were shown in Appendices A and B. As an example, the results of the nystatin and chloroneb analyses are shown below.

Table 5.8 Model Predicted Portioning of Nystatin with $2^3$ Factorial Design Variables

| **Factor Value** | | | **Moles of Analyte Partitioned Into** | | |
|---|---|---|---|---|---|
| **A** | **B** | **C** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 5.0E+07 | 4.0E+05 | 4.2E+03 |
| + | + | - | 5.0E+07 | 4.0E+05 | 1.1E+03 |
| + | - | + | 5.0E+07 | 4.0E+05 | 8.4E+01 |
| + | - | - | 5.0E+07 | 4.0E+05 | 2.1E+01 |
| - | + | + | 1.3E+05 | 1.1E+03 | 2.8E+00 |
| - | + | - | 1.3E+05 | 1.1E+03 | 2.8E+00 |
| - | - | + | 1.3E+05 | 1.1E+03 | 2.3E-01 |
| - | - | - | 1.3E+05 | 1.1E+03 | 5.7E-02 |

Table 5.9 Calculated Effects of Factors and their Interactions on the Associations of Nystatin with Different Media

| **Factors/Interactions** | **Effect** | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 2.0E+08 | 1.6E+06 | 5.4E+03 |
| B | -3.2E+03 | -2.6E+01 | 5.2E+03 |
| C | -2.0E+03 | -1.6E+01 | 3.2E+03 |
| AB | -3.2E+03 | -2.6E+01 | 5.2E+03 |
| AC | -2.0E+03 | -1.6E+01 | 3.2E+03 |
| BC | -1.9E+03 | -1.6E+01 | 3.1E+03 |
| ABC | -1.9E+03 | -1.6E+01 | 3.1E+03 |

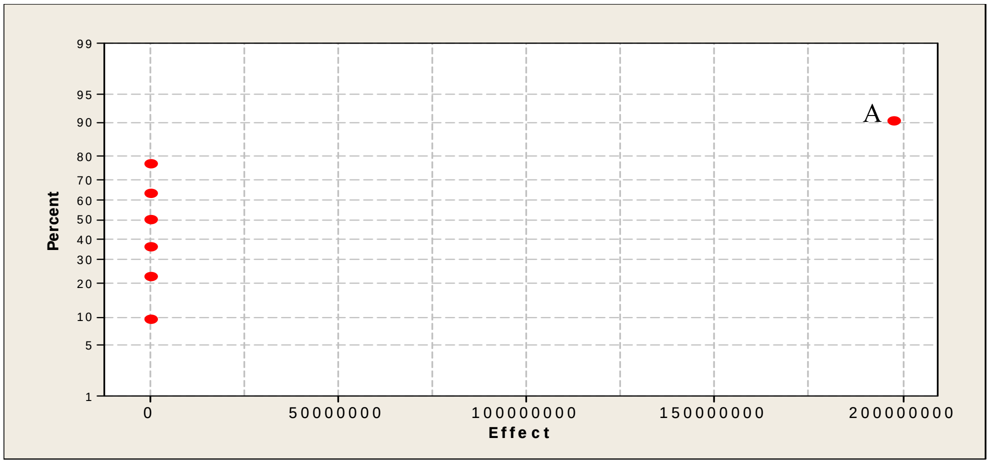



Figure 5.1 Probability plot of effects of partitioning of Nystatin with water

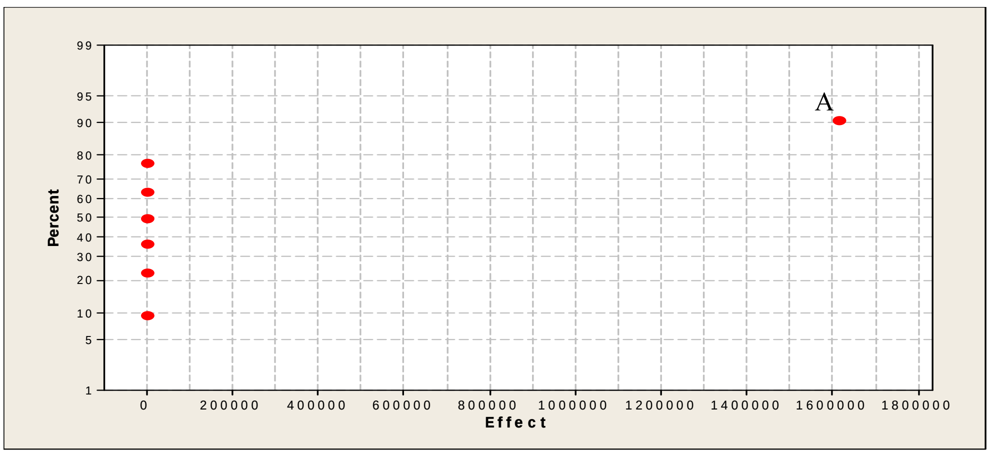



Figure 5.2 Probability plot of effects of partitioning of Nystatin with sediment

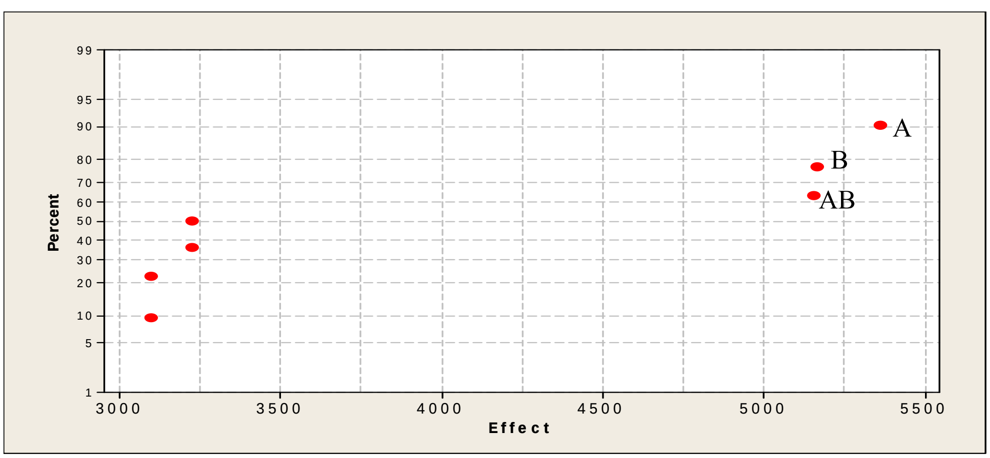



Figure 5.3 Probability plot of effects of partitioning of Nystatin with suspended sediment

Table 5.10 Model Predicted Portioning of Chloroneb with $2^3$ Factorial Design Variables

| **Factor Value** | | | **Moles of Analyte Partitioned Into** | | |
|---|---|---|---|---|---|
| **A** | **B** | **C** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 1.5E+09 | 9.3E+07 | 9.7E+05 |
| + | + | - | 1.5E+09 | 9.3E+07 | 2.4E+05 |
| + | - | + | 1.5E+09 | 9.3E+07 | 1.9E+04 |
| + | - | - | 1.5E+09 | 9.3E+07 | 4.8E+03 |
| - | + | + | 1.5E+07 | 9.3E+05 | 9.7E+03 |
| - | + | - | 1.5E+07 | 9.3E+05 | 2.4E+03 |
| - | - | + | 1.5E+07 | 9.3E+05 | 1.9E+02 |
| - | - | - | 1.5E+07 | 9.3E+05 | 4.8E+01 |

Table 5.11 Calculated Effects of Factors and their Interactions on the Associations of Chloroneb with Different Media

| **Factors/Interactions** | **Effect** | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 6.1E+09 | 3.7E+08 | 1.2E+06 |
| B | -3.8E+05 | -2.3E+04 | 1.2E+06 |
| C | -2.4E+05 | -1.4E+04 | 7.5E+05 |
| AB | -3.7E+05 | -2.3E+04 | 1.2E+06 |
| AC | -2.3E+05 | -1.4E+04 | 7.3E+05 |
| BC | -2.3E+05 | -1.4E+04 | 7.2E+05 |
| ABC | -2.2E+05 | -1.4E+04 | 7.0E+05 |

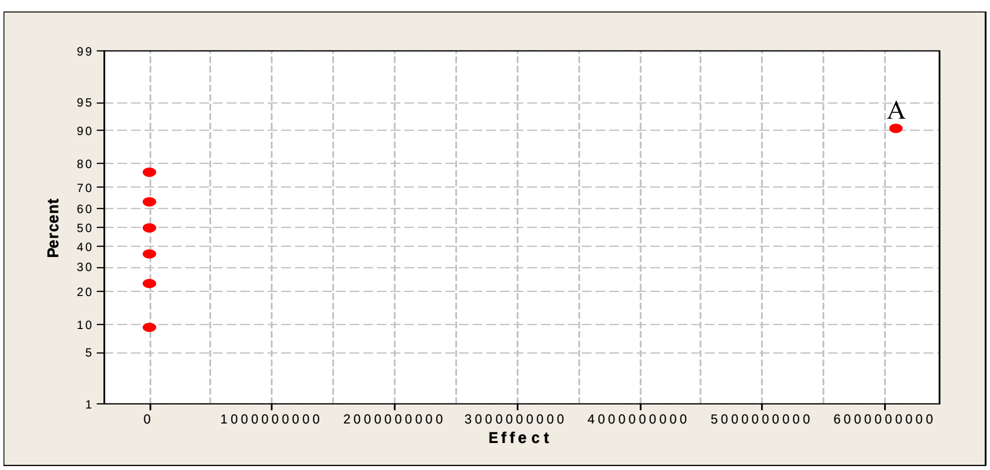



Figure 5.4 Probability plot of effects of partitioning of Chloroneb with water

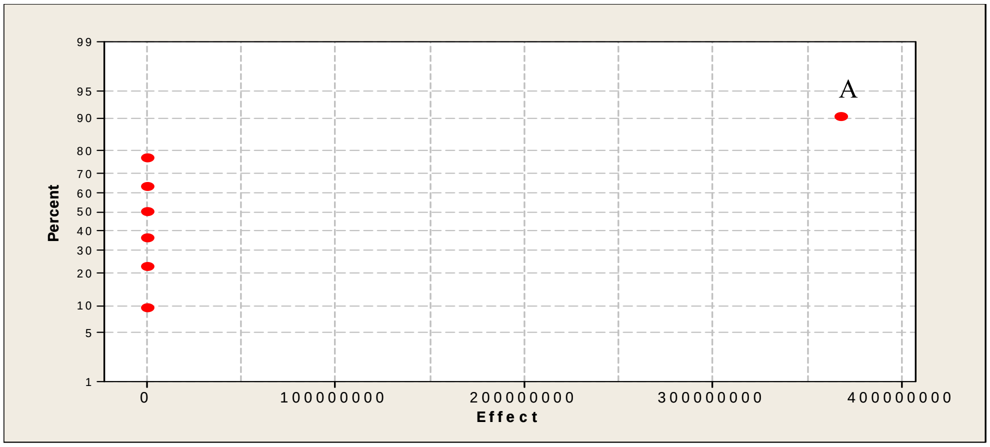



Figure 5.5 Probability plot of effects of partitioning of Chloroneb with sediment

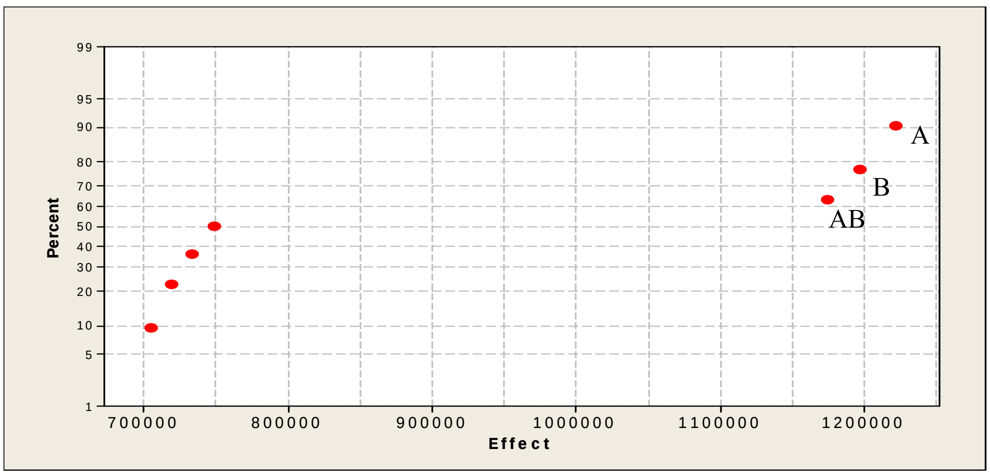



Figure 5.6 Probability plot of effects of partitioning of Chloroneb with suspended sediment

Tables 5.8 and 5.10 show the predicted portioned moles of nystatin and chloroneb into water, sediment and suspended sediment under the different combinations of the factors, based on the $2^3$ factorial design. Tables 5.9 and 5.11 show the calculated effects of the factors and their interactions on the partitioning of nystatin and chloroneb with water, sediment and suspended sediment. Figures 5.1 – 5.6 are probability plots of the effects of the factors and their interactions on partitioning of nystatin and chloroneb into the three main phases and illustrate the significant factors affecting the partitioning. The probability plots for the water and sediment phases (Figures 5.1, 5.2, 5.4, 5.5) indicate that the concentrations of the contaminant (A) in the system significantly (and positively) affected the partitioning of the compounds. In the case of partitioning to the suspended sediment phase (Figures 5.3, 5.6), the concentrations of the contaminant (A), concentrations of the suspended sediment (B), and their interaction (AB) had the greatest effects on partitioning. Similar results were found when the results of the factorial analyses and Fugacity modeling were compared for all the other PPCPs and pesticides, as shown in Appendices A and B.

# CHAPTER VI

# FATE OF EMERGING CONTAMINANTS IN THE VADOSE ZONE

Stormwater infiltration as a designed engineering practice may facilitate transport of ECs to the groundwater. In the recent years, there have been extensive studies on the fate and transport of various organic and inorganic pollutants in the saturated and unsaturated layers of the soil. Various computer models have been developed to determine the movement of the pollutants in the sub surfaces of the soil. SESOIL (Waterloo Hydrogeologic Inc) was selected as a suitable model to evaluate the processes and predict the fate of these contaminants as a result of wet-weather flow infiltration.

## 6.1 An Overview on SESOIL

The Seasonal Soil Compartment Model (SESOIL) is an integrated screening-level soil compartment model, which is used to model the water transport, sediment transport and the fate of the pollutants in the subsurface. It simulates contaminant transport and fate based on diffusion, adsorption, volatilization, biodegradation, and hydrolysis. Arthur D. Little, Inc (ADL), developed the model for EPA's Office of Water and the Office of Toxic Substances (OTS) in 1981, and, in 1984, a fourth soil compartment was added to enhance the existing three. During the end of the 1980s, it was integrated with the Graphical Exposure Modeling System for the PC (PCGEMS) that was later named RISKPRO.

## 6.2 Modeling Capabilities

SESOIL was developed as a screening-level model, using soil, chemical, and meteorological values as input information. The data requirements for SESOIL were generally less than needed for most other similar models. As it accepts time varying pollutant loading, it has a capability of simulating chemical releases into soil from various sources such as landfill sites, accidental leaks, agricultural applications, leaking underground storage tanks, or deposition from the atmosphere.

## 6.3 Methodology

The various processes modeled by SESOIL are subdivided into three cycles – the hydrologic cycle, the sediment cycle and the pollutant fate cycle. The hydrologic cycle focuses on moisture movement, the sediment cycle deals with runoff from the soil surface, and the pollutant fate cycle deals with the movement of the pollutant through the soil.

Hydrologic Cycle

The hydrologic cycle simulates the movement of the moisture through the soil compartment. Only vertical movement is considered here. The hydrology of the site is obtained from the output of this module. These results are passed then onto the sediment washload cycle. This submodel is based on the adaptation of the water balance dynamics theory of Eagleson (1978). The water balance equations used by Eagleson are:

$$P - E - MR = S + G - Y \qquad \text{(eq. 6.1)}$$

$$I = P - S \qquad \text{(eq. 6.2)}$$

where the yield (Y) is equal to the sum of the surface runoff (S) and groundwater recharge (G). Yield is also a function of the total precipitation (P), evapotranspiration (E), and moisture retention (MR). And infiltration (I) equals to the difference of total precipitation and the surface runoff.

Sediment Washload Cycle

This submodel is used to estimate the erosion and sediment yield on watersheds. This model uses the runoff results from the hydrologic cycle to estimate the sediment transport. This erosion model is comprised of the three basic processes of soil detachment, transport, and deposition. The Universal Soil Loss Equation (USLE) is employed in the detachment process. The USLE is used to predict the annual sediment erosion which was subjected to sheet and rill erosion. The various parameters involved in the USLE are rainfall factor (R), soil erodibility (K), slope length (L), slope degree factor (S), crop practice factor (C), and the conservation practice factor (P).

Pollutant Fate Cycle

The pollutant fate cycle uses the output obtained from the hydrologic and sediment washload cycles and stimulates the fate and transport of the specified pollutants. This model is based on the following mass balance equation.

$$O(t-1) + I(t) = T(t) + R(t) + M(t) \qquad \text{(eq. 6.3)}$$

Where

O (t-1) = the amount of pollutant originally in the soil compartment at time t-1($\mu g/cm^2$),

I (t) = the amount of pollutant entering the soil compartment during a time step ($\mu g/cm^2$),

T (t) = the amount of pollutant transformed within the soil compartment during the time step ($\mu g/cm^2$),

R (t) = the amount of pollutant remaining in the soil compartment at time t ($\mu g/cm^2$),

M (t) = the amount of pollutant migrating out of the soil compartment during the time step ($\mu g/cm^2$)

The fate of the pollutant consists of the movement of the pollutant, as well as the potential transformation reactions involving the pollutant. These transformations involve the partitioning of the component across the three phases: soil air, soil moisture and soil solids. It also may include biodegradation through microbial activity, photodegradation, and hydrolysis. The concentration of the component in one phase is used to calculate the concentrations in the other two phases as equilibrium exists between all three phases. The concentration in the soil air is calculated via the modified Henry's law:

$$C_{sa} = cH/R\ (T + 273) \quad \text{(eq. 6.4)}$$

Where

$C_{sa}$ = pollutant concentration in soil air (μg/ml); c = pollutant concentration in soil water (μg/ml); H = Henry's law constant ($m^3$atm/mol); R = Universal gas constant; T = soil temperature ($^oC$).

The concentration adsorbed to the soil is estimated using the Freundlich isotherm:

$$s = K_d c^{1/n} \quad \text{(eq. 6.5)}$$

Where,

s = pollutant adsorbed concentration (μg/g); n = Freundlich exponent; $K_d$ = pollutant partitioning coefficient (μg/g)/ (μg/ml); c = pollutant concentration in soil water (μg/ml)

The total concentration of the pollutant in the soil is computed as:

$$C_o = f_a * C_{sa} + \theta * C + \rho_b S \quad \text{(eq. 6.6)}$$

Where,

$C_o$ = overall (total) pollutant concentration (μg/$cm^3$);

$f_a = f - \theta$ = the air-filled porosity (mL/mL); f = soil porosity (mL/mL),

$\theta$ = soil water content (mL/mL); $\rho_b$= soil bulk density (g/$cm^3$).

### 6.4 Fate of Pharmaceuticals and Personal Care Products in the Unsaturated Zone

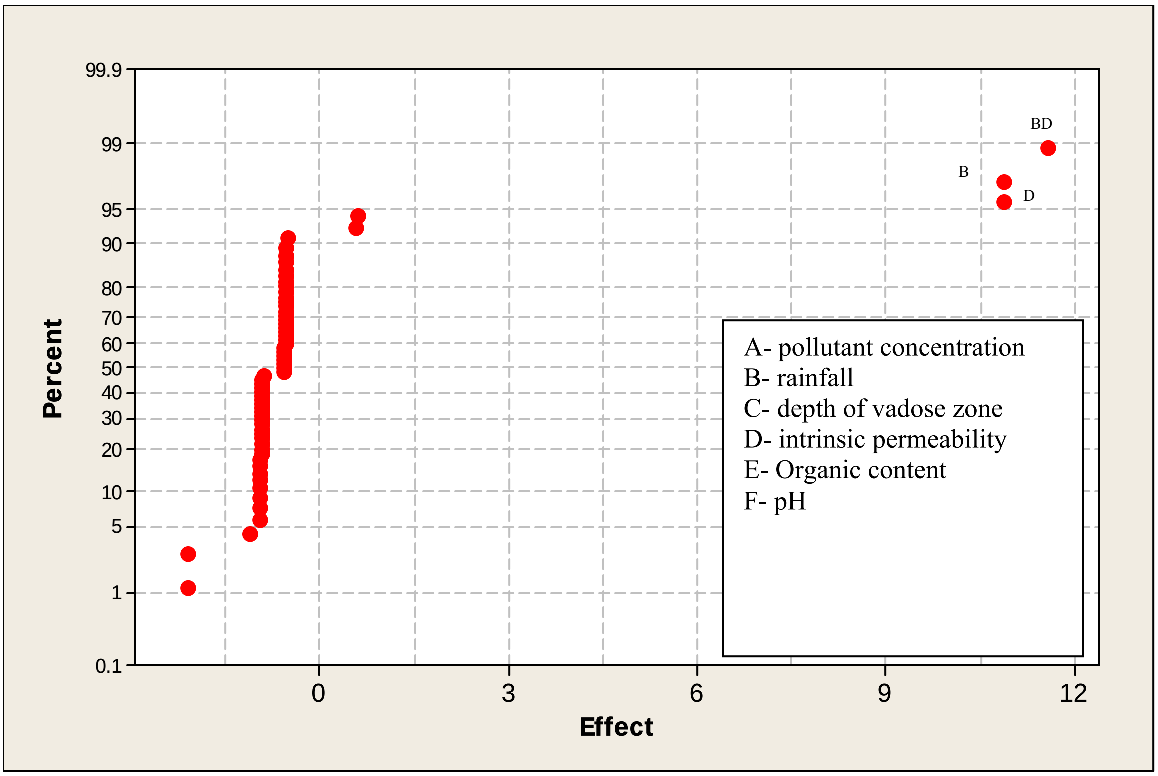
The fate of PPCPs in the unsaturated soil profile was studied using the SESOIL software (Waterloo Hydrogeologic Inc). A full $2^6$ factorial design was used to determine the factors and their interactions effecting the pollutant movement in the vadose zone. Pollutant concentrations, rainfall, vadose zone thickness, intrinsic permeability, organic content and pH, were chosen as the possible factors and their effects were evaluated. The high and low values of the factors, except for the pollutant concentrations, used in this project, were identical to those used in a similar work (Mikula, et al. 2005) that investigated the potential movement of a representative metal, major cation and major ion in the vadose zone.

Table 6.1 High and low values of controlling factors (Mikula et al 2005)

| Factor | High | Low |
|---|---|---|
| Concentration of Nystatin (μg/L) | 0.74 | 0.002 |
| Concentration of Dexamethasone (μg/L) | 0.74 | 0.002 |
| Concentration of Methoprene (μg/L) | 0.74 | 0.002 |
| Concentration of Prednisone (μg/L) | 0.74 | 0.002 |
| Concentration of Metronidazole (μg/L) | 0.74 | 0.002 |
| Concentration of Clindamycin (μg/L) | 0.74 | 0.002 |
| Concentration of Ketconazole (μg/L) | 0.74 | 0.002 |
| Concentration of Carbamazepine (μg/L) | 0.083 | 0.002 |
| Concentration of Caffeine (μg/L) | 0.24 | 0.004 |
| Concentration of Ibuprofen (μg/L) | 0.6 | 0.003 |
| Concentration of Diclofanac (μg/L) | 0.18 | 0.007 |
| Concentration of Acetaminophen (μg/L) | 0.03 | 0.012 |
| Concentration of Triclosan (μg/L) | 0.74 | 0.03 |
| Concentration of Ciprofloxacin (μg/L) | 0.5 | 0.027 |
| Concentration of Metoprolol (μg/L) | 0.12 | 0.02 |
| Concentration of Salicylic acid (μg/L) | 0.22 | 0.013 |
| Rainfall Location and Depth (cm) | West Palm Beach | Phoenix |
| | 154 | 6.7 |
| Vadose zone thickness (cm) | 1200 | 300 |
| Intrinsic permeability ($cm^2$) | 1.00E-07 | 1.00E-10 |
| Organic content (%) | 3 | 0.5 |
| pH | 7.2-8.0 | 4.3-5.0 |

The simulation run time was chosen to be 10 years and the rainfall and soil types were chosen from the SESOIL database. Besides the controlling factors being examined, other factors (soil and pollutant chemical parameters) which were needed to predict pollutant movement are shown for each simulation in Appendix C. A total of 64 runs were conducted for each pollutant and the effects of different factors on the pollutant movement were evaluated by generating normal probability plots as shown in Appendix C. As an example, the results of the pollutant migration analyses for nystatin are shown in Figure 6.1.

Figure 6.1 Estimated main effects and effect interactions on nystatin migration in vadose zone




It can be seen from Figure 6.1 that rainfall and intrinsic permeability, plus their interaction, were the significant factors affecting the migration of nystatin in the vadose zone. Similar results were observed for all the studied compounds, as shown in Appendix C.

The results generated by the SESOIL showed that most of the studied PPCPs moved along with the infiltrating stormwater and did not sorb to the soils. Higher rainfall amounts, therefore, naturally allowed them to migrate deeply into the vadose zone. The effect of intrinsic permeability was also identified as being significant, since the combination of increased rainfall and increased permeability encourages rapid transport of the water, plus any water-soluble pollutants, in the vadose zone and eventually to the groundwater..

The retardation factors for the PPCPs are calculated to predict the movement of these compounds with respect to water movement. The retardation factors were calculated as the ratio of the saturated hydraulic conductivity of the soils to the pollutant migration rates. The minimum and maximum migration rates of the pollutants along with their retardation factors were shown in Table 6.2

Table 6.2 Retardation factors for the PPCPs in saturated zone

| | Max. Sat. Hydraulic Conductivity | | Min. Sat. Hydraulic Conductivity | |
|---|---|---|---|---|
| | 0.634 m/hr | | 0.000462 m/hr | |
| Compound | Max. Migration Rate (m/hr) | Retardation Factor | Min. Migration Rate (m/hr) | Retardation Factor |
| Nystatin | 3.05E-04 | 3279 | 7.54E-06 | 61 |
| Dexamethasone | 3.39E-04 | 2953 | 8.33E-06 | 55 |
| Methoprene | 8.98E-05 | 11142 | 2.23E-06 | 208 |
| Prednisone | 5.87E-04 | 1704 | 1.46E-05 | 32 |
| Metronidazole | 6.42E-04 | 1558 | 1.59E-05 | 29 |
| Clindamycin | 3.66E-04 | 2733 | 9.08E-06 | 51 |
| ketoconazole | 4.35E-04 | 2299 | 1.08E-05 | 43 |
| Carbamazepine | 4.07E-04 | 2455 | 1.01E-05 | 46 |
| Caffeine | 7.18E-04 | 1393 | 1.78E-05 | 26 |
| Ibuprofen | 1.52E-04 | 6585 | 3.77E-06 | 123 |
| Diclofenac | 2.76E-04 | 3622 | 6.85E-06 | 67 |
| Acetaminophen | 7.46E-04 | 1341 | 1.85E-05 | 25 |
| Triclosan | 1.10E-04 | 9054 | 2.74E-06 | 169 |
| Ciprofloxacin | 1.31E-04 | 7624 | 3.26E-06 | 142 |
| Metoprolol | 6.14E-04 | 1628 | 1.52E-05 | 30 |
| Salicylic acid | 3.11E-04 | 3219 | 7.71E-06 | 60 |

It can be seen from Table 6.2 that the retardation factors of pollutants in the saturated zone were in the range of 25 to more than 11000, indicating potentially very slow movement rates in the saturated zone.

The disposal of pesticide contaminated stormwater to the subsurface should receive special attention. Pitt, et al. (1995) identified pesticides as having moderate to high groundwater contamination potentials due to their mobility through the vadose zone in areas having sandy soils, with little soil attenuation and the difficulty of treatment before discharge.

Several studies have investigated pesticide movement through soil and it was found out that the mobility depends on several significant factors including soil texture, pesticide persistence, total organic carbon content, depth of the water table (Shirmohammadi etal 1989), solubility, and adsorption rates (Bucheli etal 2007). Usually, pesticides with low water solubility and high $K_{ow}$, especially in organic rich soils, are less mobile. Biological degradation can be an effective mechanism for the decomposition of some pesticides retained in the soil (Takemetsu etal 1985), although most are resistant to degradation.

# CHAPTER VII

# CONCLUSIONS

Emerging contaminants, due to their health effects and potential to interfere with normal biochemical processes in the human body, their very low concentrations, and their general lack of regulation at these low environmental concentrations, are of great concern. Their fate and movement in the environment needs to be studied in a thorough manner and treatment technologies may need to be developed, or existing ones enhanced, to remove them before they enter the receiving waters and eventually the drinking water supply. These compounds are also a challenge because they require special analytical methods to detect and quantify these contaminants in environmental samples. Costly analytical methods are needed, such as HPLC-ESI-MS-MS and GC-MS and GC-ECD, to achieve good recoveries. The literature highlighted the concerns associated with inefficient sample extraction and concentration.

The fate analyses of the emerging contaminants showed their associations were mostly with the water phase, with fewer associated with the sediment phases. This was not surprising since many pharmaceuticals are designed to be transported in the bloodstream, which is mostly water. Stronger associations with the sediment phase may be associated with whether a compound is designed to travel freely in the bloodstream or whether it requires lipids/fats for sorption. Compounds that partition to the solid phase may be treatable through sedimentation. However, sedimentation will not be effective if the compounds partition preferentially to very small solids (< 5 – 10 µm) since the critical particle size used in wet weather flow sedimentation basin design may be larger than these sizes. The preferential partitioning into the water phase indicates that common physical treatment technologies used for many wet weather flow may not be as effective. This is supported by the literature that shows that removals are poor in the clarifier/sedimentation basins at wastewater treatment plants. Media filtration may be required in order to have the chemical reactions required to remove these compounds from stormwater. As the literature has shown, media filtration can remove a wide variety of pollutants, with varying degrees of effectiveness. The effectiveness is associated with providing sufficient contact time for pollutant removal. The calculated retardation factors for groundwater movement indicate that, while media filters may not provide permanent retention of these pollutants, it may be effective for many compounds for several years. Media filtration as a unit operation is associated with stormwater filters for biofiltration practices (for ion exchange and sorption), in-line filtration devices. This research shows that suitable selection of media is necessary. Other advanced treatment technologies that typically are not employed in wet-weather flow treatment, such as oxidation and microfiltration, may be cost-effective for these compounds, particularly if the regulations change to require large removals of these compounds from stormwater.

SESOIL was shown to be a suitable model for predicting the migration depths of emerging contaminants in sub-surface environment. SESOIL noted that the rainfall and the intrinsic permeability of the soil were the primary factors affecting the pollutant migration. The SESOIL output was used to calculate subsurface retardation factors for these emerging contaminants. The modeling activity presented herein is limited because the site data used were only for two typical soils and can not represent all possible conditions. The model simulation also requires several simplifications to the processes known to be occurring in the field. In addition, for several compounds, the amount of information available in the literature was small and the modeling coefficients could only be estimated within 1 – 2 orders of magnitude.

Potential future research could effectively focus on properly estimating the chemical properties of these emerging contaminants. In addition, analyzing real time samples to estimate the fate and persistence of these compounds in the environment effectively is needed.

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## APPENDIX A

## PROPERTIES AND FATE MODELING OF PPCPs

Table A.1 Model Predicted Portioning of Nystatin with $2^3$ Factorial Design Variables

| **Factor Value** | | | **Moles of Analyte Partitioned Into** | | |
|---|---|---|---|---|---|
| **Conc of Nystatin (A)** | **Conc. Of S.S.(B)** | **Organic fraction of S.S(C)** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 5.0E+07 | 4.0E+05 | 4.2E+03 |
| + | + | - | 5.0E+07 | 4.0E+05 | 1.1E+03 |
| + | - | + | 5.0E+07 | 4.0E+05 | 8.4E+01 |
| + | - | - | 5.0E+07 | 4.0E+05 | 2.1E+01 |
| - | + | + | 1.3E+05 | 1.1E+03 | 2.8E+00 |
| - | + | - | 1.3E+05 | 1.1E+03 | 2.8E+00 |
| - | - | + | 1.3E+05 | 1.1E+03 | 2.3E-01 |
| - | - | - | 1.3E+05 | 1.1E+03 | 5.7E-02 |

Table A.2 Calculated Effects of Factors and their Interactions on the Associations of Nystatin with Different Media

| **Factors/Interactions** | **Effect** | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 2.0E+08 | 1.6E+06 | 5.4E+03 |
| B | -3.2E+03 | -2.6E+01 | 5.2E+03 |
| C | -2.0E+03 | -1.6E+01 | 3.2E+03 |
| AB | -3.2E+03 | -2.6E+01 | 5.2E+03 |
| AC | -2.0E+03 | -1.6E+01 | 3.2E+03 |
| BC | -1.9E+03 | -1.6E+01 | 3.1E+03 |
| ABC | -1.9E+03 | -1.6E+01 | 3.1E+03 |

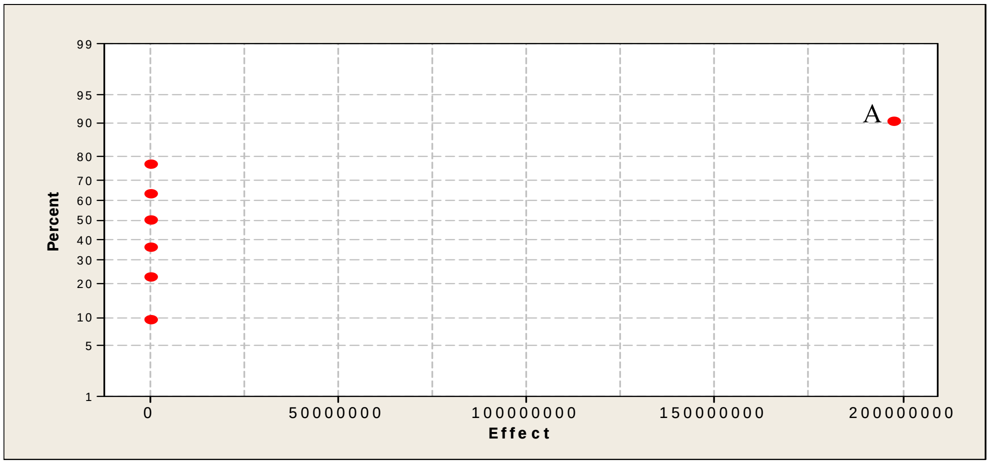


Figure A.1 Probability plot of effects of partitioning of Nystatin with water

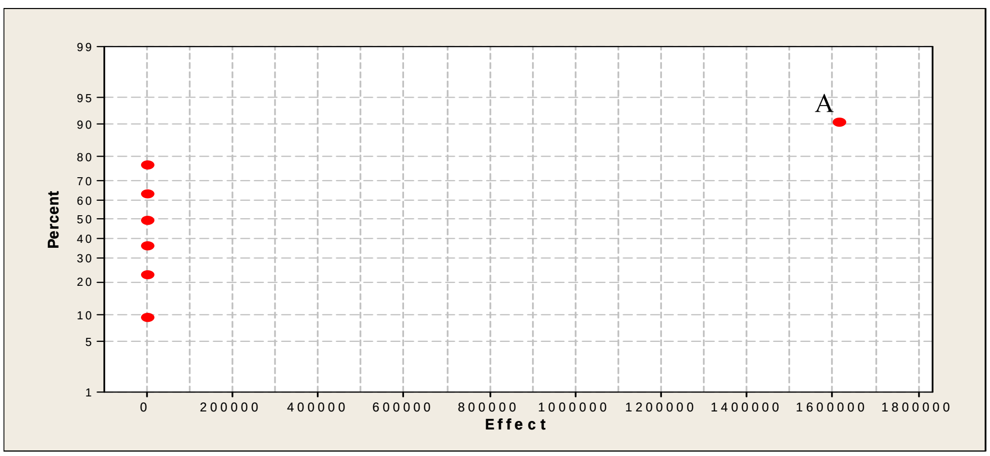


Figure A.2 Probability plot of effects of partitioning of Nystatin with sediment

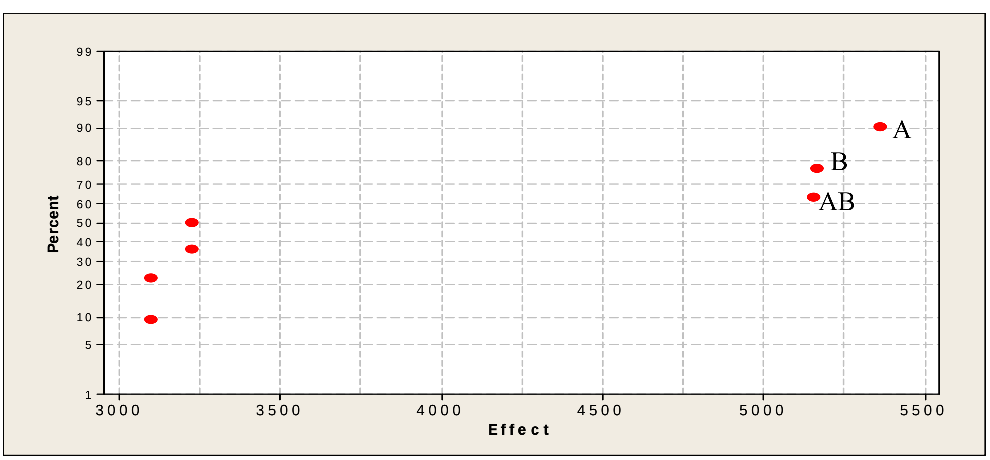


Figure A.3 Probability plot of effects of partitioning of Nystatin with suspended sediment

Table A.3 Model Predicted Portioning of Dexamethasone with $2^3$ Factorial Design Variables

| **Factor Value** | | | **Moles of Analyte Partitioned Into** | | |
|---|---|---|---|---|---|
| **Conc of Dexamethasone (A)** | **Conc of S.S. (B)** | **Organic fraction of S.S (C)** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 1.9E+08 | 2.1E+06 | 2.2E+04 |
| + | + | - | 1.9E+08 | 2.1E+06 | 5.6E+03 |
| + | - | + | 1.9E+08 | 2.1E+06 | 4.5E+02 |
| + | - | - | 1.9E+08 | 2.1E+06 | 1.1E+02 |
| - | + | + | 5.0E+05 | 5.8E+03 | 6.0E+01 |
| - | + | - | 5.0E+05 | 5.8E+03 | 1.5E+01 |
| - | - | + | 5.0E+05 | 5.8E+03 | 1.2E+00 |
| - | - | - | 5.0E+05 | 5.8E+03 | 3.0E-01 |

Table A.4 Calculated Effects of Factors and their Interactions on the Associations of Dexamethasone with Different Media

| **Factors/Interactions** | **Effect** | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 7.4E+08 | 8.6E+06 | 2.8E+04 |
| B | -2.7E+04 | -3.1E+02 | 2.7E+04 |
| C | -1.7E+04 | -1.9E+02 | 1.7E+04 |
| AB | -2.7E+04 | -3.1E+02 | 2.7E+04 |
| AC | -1.7E+04 | -1.9E+02 | 1.7E+04 |
| BC | -1.6E+04 | -1.9E+02 | 1.6E+04 |
| ABC | -1.6E+04 | -1.9E+02 | 1.6E+04 |

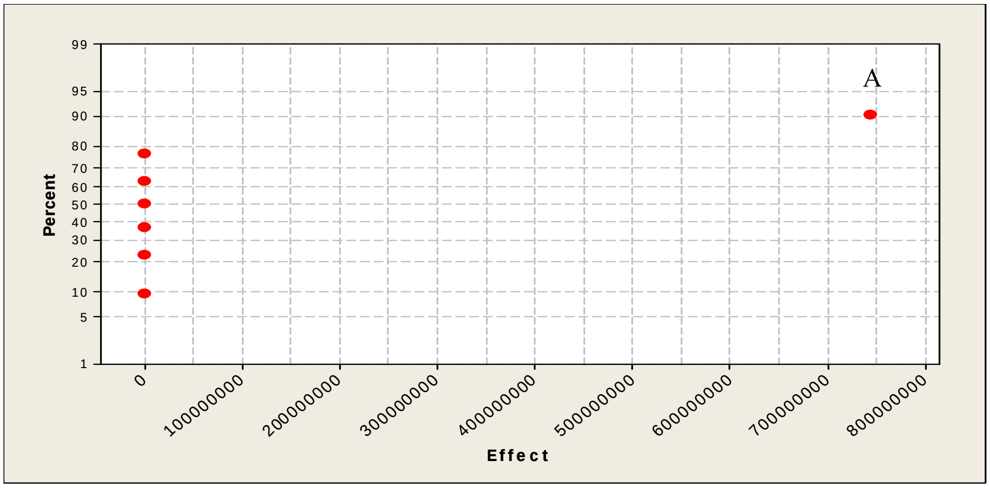


Figure A.4Probability plot of effects of partitioning of Dexamethasone with water

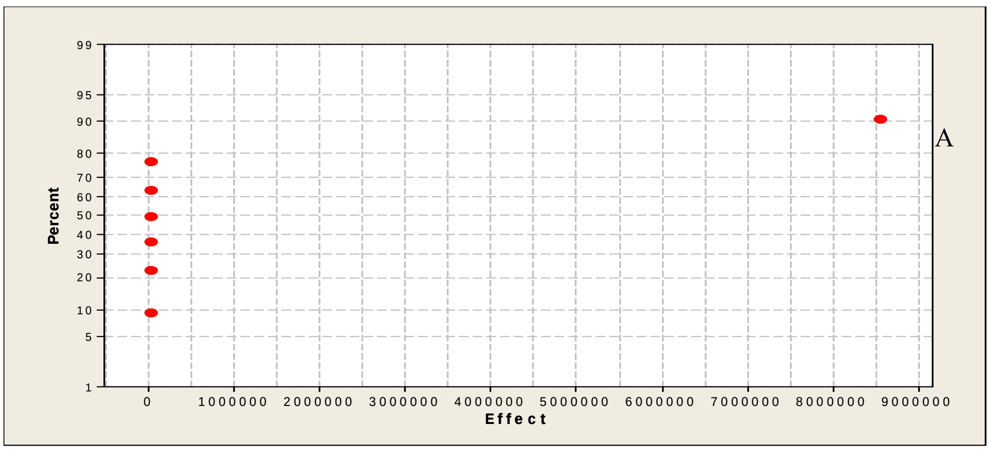


Figure A.5Probability plot of effects of partitioning of Dexamethasone with sediment

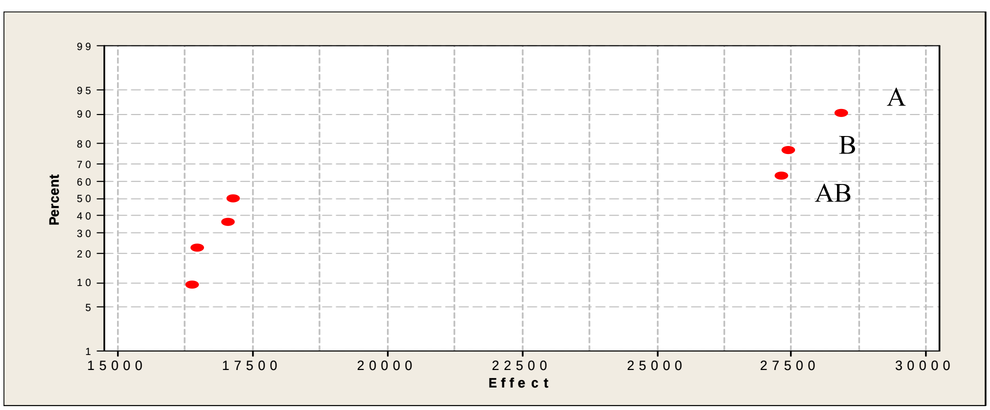


Figure A.6Probability plot of effects of partitioning of Dexamethasone with suspended sediment

Table A.5 Model Predicted Portioning of Methoprene with $2^3$ Factorial Design Variables

| Factor Value | | | Moles of Analyte Partitioned Into | | |
|---|---|---|---|---|---|
| Conc of Methoprene(A) | Conc of S.S.(B) | Organic fraction of S.S(C) | Water | Sediment | Suspended Sediment |
| + | + | + | 1.0E+08 | 1.2E+08 | 1.2E+06 |
| + | + | - | 1.1E+08 | 1.2E+08 | 3.0E+05 |
| + | - | + | 1.1E+08 | 1.2E+08 | 2.4E+04 |
| + | - | - | 1.1E+08 | 1.2E+08 | 6.1E+03 |
| - | + | + | 2.8E+05 | 3.1E+05 | 3.3E+03 |
| - | + | - | 2.8E+05 | 3.1E+05 | 8.2E+02 |
| - | - | + | 2.8E+05 | 3.1E+05 | 6.6E+01 |
| - | - | - | 2.8E+05 | 3.1E+05 | 1.6E+01 |

Table A.6 Calculated Effects of Factors and their Interactions on the Associations of Methoprene with Different Media

| Factors/Interactions | Effect | | |
|---|---|---|---|
| | Water | Sediment | Suspended Sediment |
| A | 4.2E+08 | 4.6E+08 | 1.5E+06 |
| B | -6.6E+05 | -7.2E+05 | 1.5E+06 |
| C | -4.1E+05 | -4.5E+05 | 9.2E+05 |
| AB | -6.5E+05 | -7.2E+05 | 1.5E+06 |
| AC | -4.1E+05 | -4.5E+05 | 9.2E+05 |
| BC | -3.9E+05 | -4.3E+05 | 8.9E+05 |
| ABC | -3.9E+05 | -4.3E+05 | 8.8E+05 |

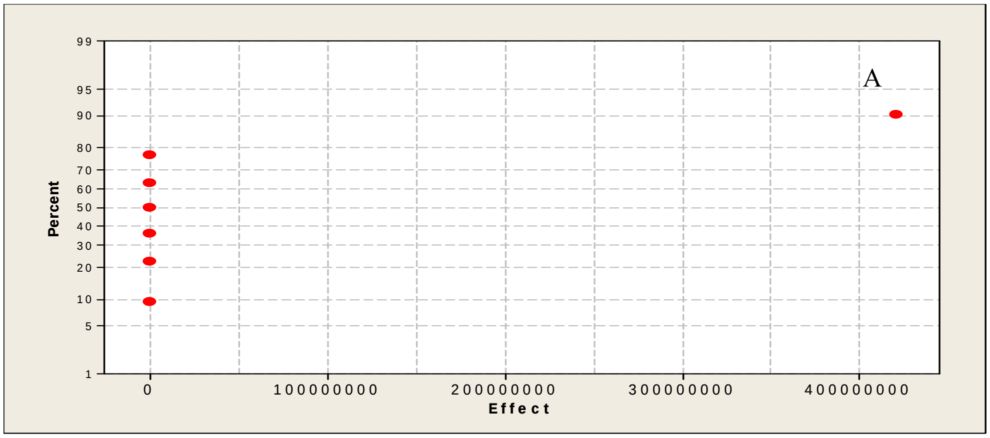


Figure A.7Probability plot of effects of partitioning of Methoprene with water

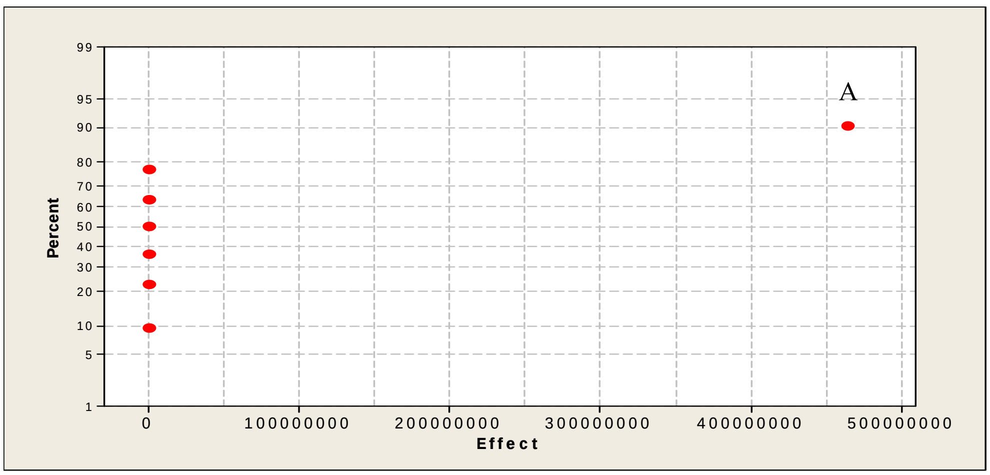


Figure A.8Probability plot of effects of partitioning of Methoprene with sediment

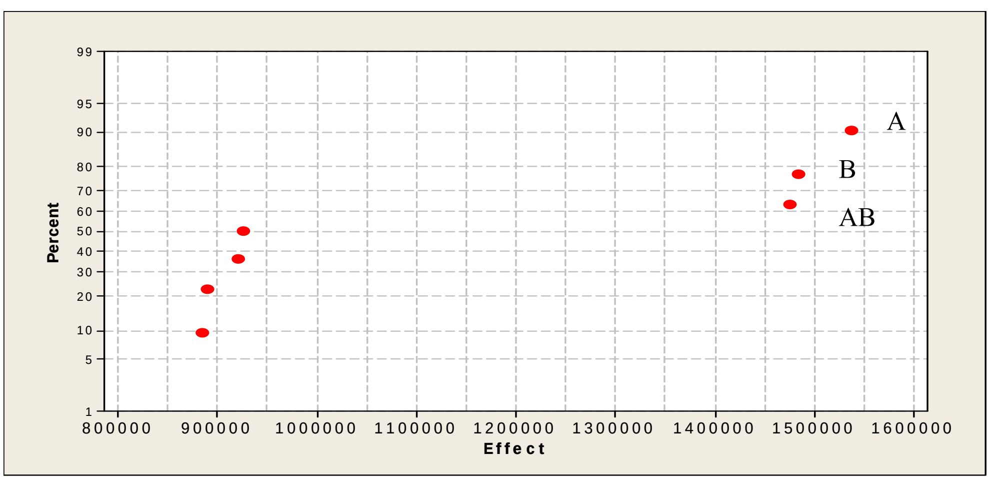


Figure A.9Probability plot of effects of partitioning of Methoprene with suspended sediment

Table A.7 Model Predicted Portioning of Prednisone with $2^3$ Factorial Design Variables

| **Factor Value** | | | **Moles of Analyte Partitioned Into** | | |
|---|---|---|---|---|---|
| **Conc of Prednisone(A)** | **Conc of S.S.(B)** | **Organic fraction of S.S.(C)** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 2.0E+08 | 1.5E+06 | 1.5E+04 |
| + | + | - | 2.0E+08 | 1.5E+06 | 3.8E+03 |
| + | - | + | 2.0E+08 | 1.5E+06 | 3.1E+02 |
| + | - | - | 2.0E+08 | 1.5E+06 | 7.7E+01 |
| - | + | + | 5.5E+05 | 4.0E+03 | 4.2E+01 |
| - | + | - | 5.5E+05 | 4.0E+03 | 1.0E+01 |
| - | - | + | 5.5E+05 | 4.0E+03 | 8.3E-01 |
| - | - | - | 5.5E+05 | 4.0E+03 | 2.1E-01 |

Table A.8 Calculated Effects of Factors and their Interactions on the Associations of Prednisone with Different Media

| **Factors/Interactions** | **Effect** | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 8.2E+08 | 5.9E+06 | 2.0E+04 |
| B | -1.9E+04 | -1.3E+02 | 1.9E+04 |
| C | -1.2E+04 | -8.4E+01 | 1.2E+04 |
| AB | -1.9E+04 | -1.3E+02 | 1.9E+04 |
| AC | -1.2E+04 | -8.4E+01 | 1.2E+04 |
| BC | -1.1E+04 | -8.1E+01 | 1.1E+04 |
| ABC | -1.1E+04 | -8.1E+01 | 1.1E+04 |

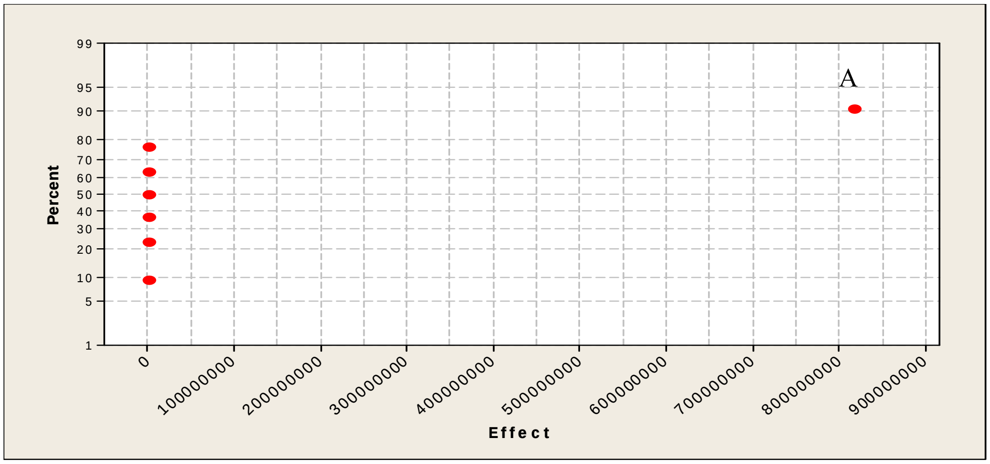


Figure A.10Probability plot of effects of partitioning of Prednisone with water

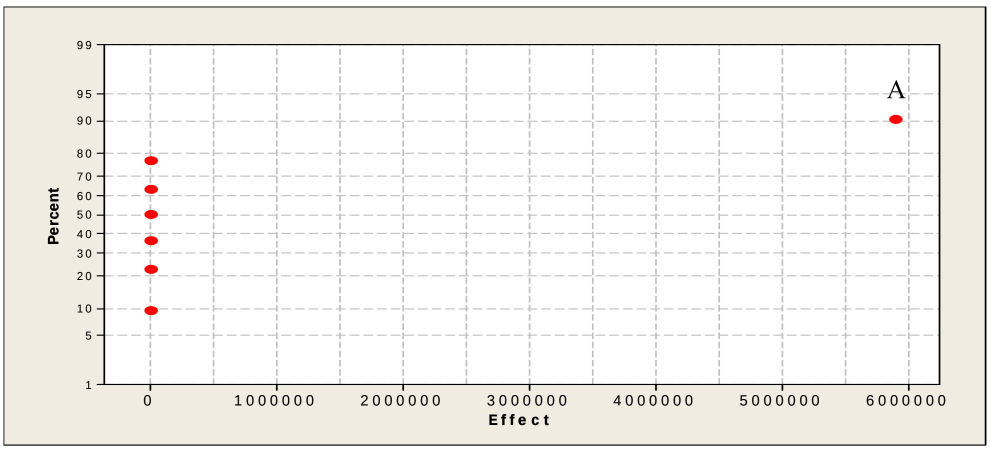


Figure A.11Probability plot of effects of partitioning of Prednisone with sediment

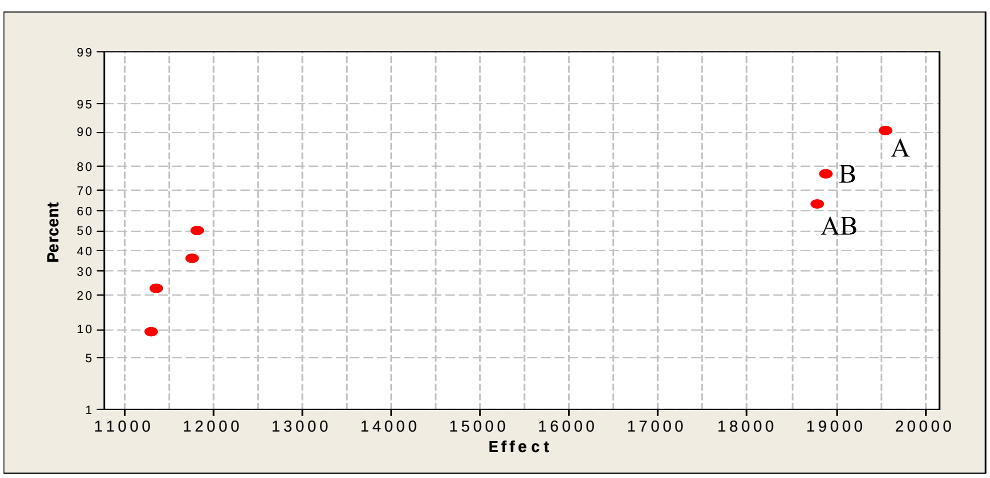


Figure A.12Probability plot of effects of partitioning of Prednisone with suspended sediment

Table A.9 Model Predicted Portioning of Metronidazole with $2^3$ Factorial Design Variables

| Factor Value | | | Moles of Analyte Partitioned Into | | |
|---|---|---|---|---|---|
| Conc of Metronidazole(A) | Conc of S.S(B) | Organic fraction of S.S(C) | Water | Sediment | Suspended Sediment |
| + | + | + | 4.3E+08 | 4.8E+05 | 5.0E+03 |
| + | + | - | 4.3E+08 | 4.8E+05 | 1.2E+03 |
| + | - | + | 4.3E+08 | 4.8E+05 | 9.9E+01 |
| + | - | - | 4.3E+08 | 4.8E+05 | 2.5E+01 |
| - | + | + | 1.2E+06 | 1.3E+03 | 1.3E+01 |
| - | + | - | 1.2E+06 | 1.3E+03 | 3.4E+00 |
| - | - | + | 1.2E+06 | 1.3E+03 | 2.7E-01 |
| - | - | - | 1.2E+06 | 1.3E+03 | 6.7E-02 |

Table A.10 Calculated Effects of Factors and their Interactions on the Associations of Metronidazole with Different Media

| Factors/Interactions | Effect | | |
|---|---|---|---|
| | Water | Sediment | Suspended Sediment |
| A | 1.7E+09 | 1.9E+06 | 6.3E+03 |
| B | -6.1E+03 | -6.7E+00 | 6.1E+03 |
| C | -3.8E+03 | -4.2E+00 | 3.8E+03 |
| AB | -6.1E+03 | -6.7E+00 | 6.1E+03 |
| AC | -3.8E+03 | -4.2E+00 | 3.8E+03 |
| BC | -3.7E+03 | -4.0E+00 | 3.7E+03 |
| ABC | -3.6E+03 | -4.0E+00 | 3.6E+03 |

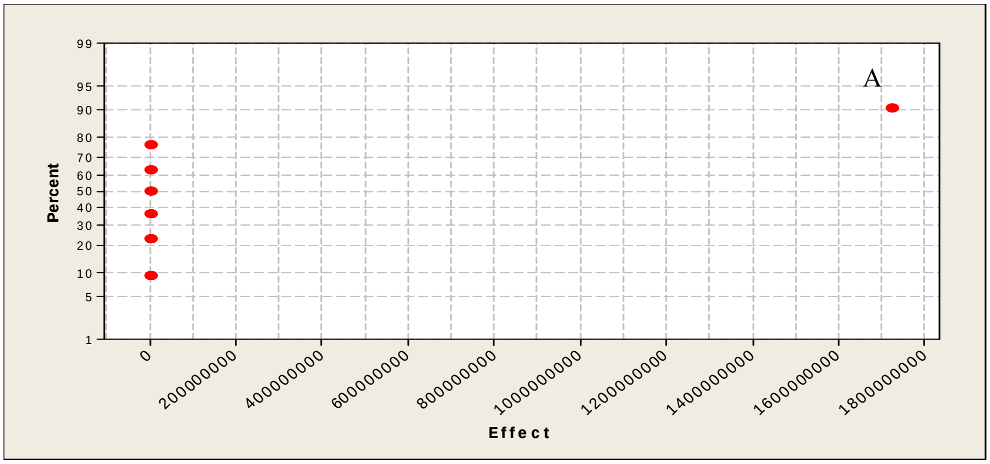


Figure A.13Probability plot of effects of partitioning of Metronidazole with water

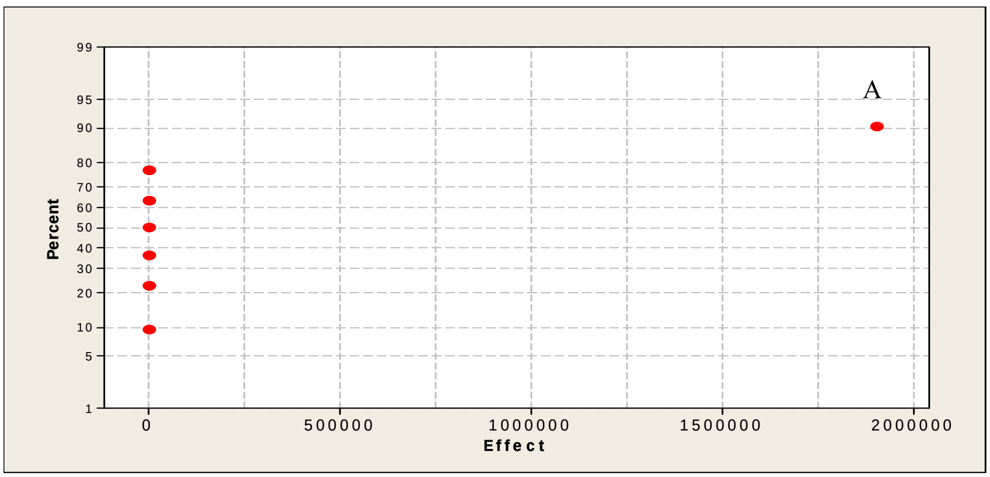


Figure A.14Probability plot of effects of partitioning of Metronidazole with sediment

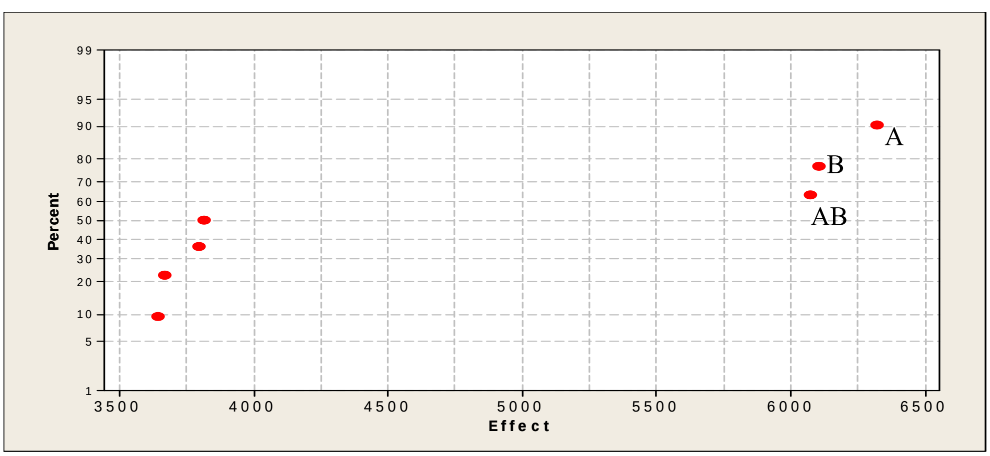


Figure A.15Probability plot of effects of partitioning of Metronidazole with suspended sediment

Table A.11 Model Predicted Portioning of Clindamycin with $2^3$ Factorial Design Variables

| **Factor Value** | | | **Moles of Analyte Partitioned Into** | | |
|---|---|---|---|---|---|
| **Conc of Clindamycin(A)** | **Conc of S.S(B)** | **Organic fraction of S.S(C)** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 1.7E+08 | 3.0E+06 | 3.1E+04 |
| + | + | - | 1.7E+08 | 3.0E+06 | 7.7E+03 |
| + | - | + | 1.7E+08 | 3.0E+06 | 6.2E+02 |
| + | - | - | 1.7E+08 | 3.0E+06 | 1.5E+02 |
| - | + | + | 4.6E+05 | 8.0E+03 | 8.3E+01 |
| - | + | - | 4.6E+05 | 8.0E+03 | 2.1E+01 |
| - | - | + | 4.6E+05 | 8.0E+03 | 1.7E+00 |
| - | - | - | 4.6E+05 | 8.0E+03 | 4.2E-01 |

Table A.12 Calculated Effects of Factors and their Interactions on the Associations of Clindamycin with Different Media

| **Factors/Interactions** | **Effect** | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 6.8E+08 | 1.2E+07 | 3.9E+04 |
| B | -3.7E+04 | -6.4E+02 | 3.8E+04 |
| C | -2.3E+04 | -4.0E+02 | 2.4E+04 |
| AB | -3.7E+04 | -6.4E+02 | 3.8E+04 |
| AC | -2.3E+04 | -4.0E+02 | 2.4E+04 |
| BC | -2.2E+04 | -3.9E+02 | 2.3E+04 |
| ABC | -2.2E+04 | -3.8E+02 | 2.3E+04 |

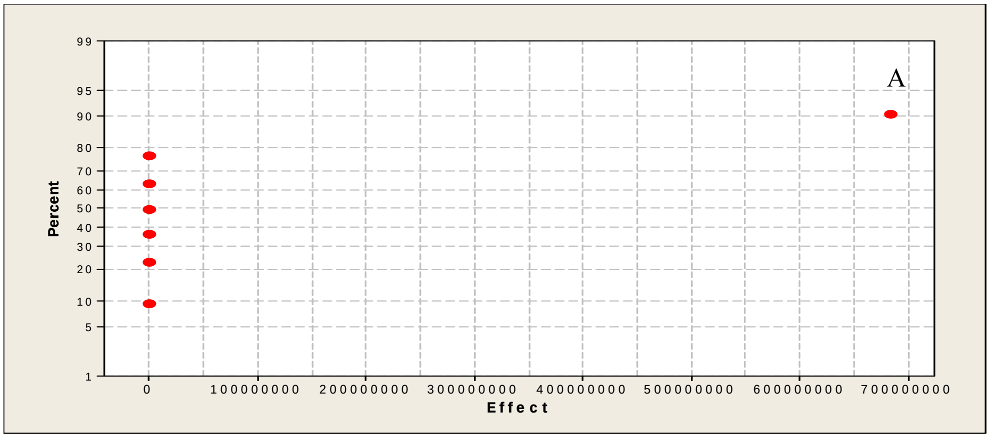


Figure A.16Probability plot of effects of partitioning of Clindamycin with water

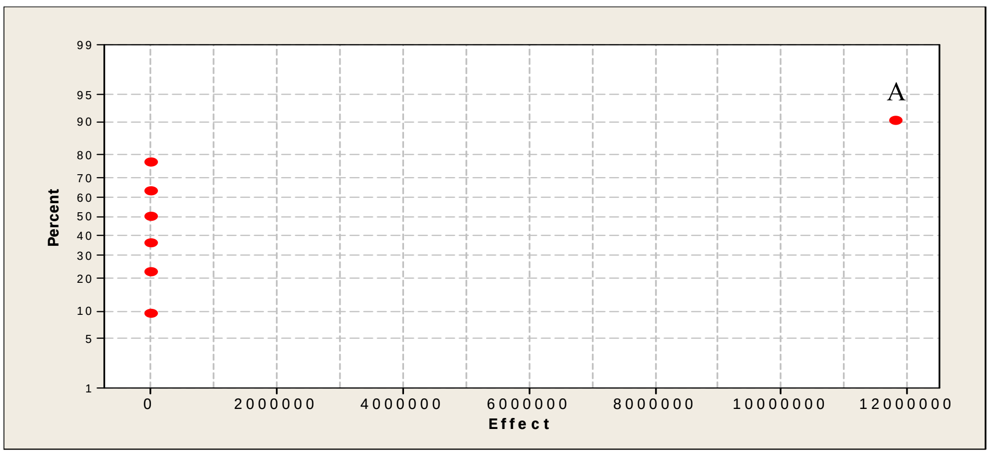


Figure A.17Probability plot of effects of partitioning of Clindamycin with sediment

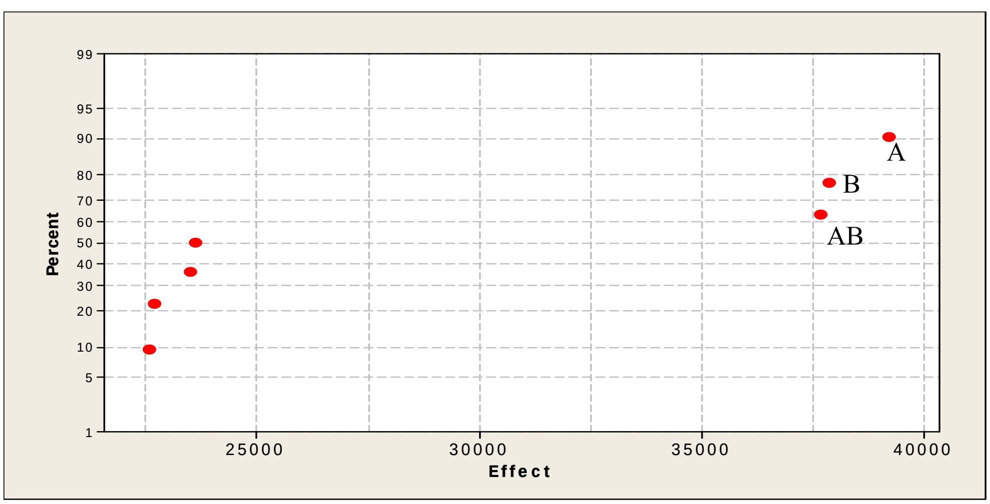


Figure A.18Probability plot of effects of partitioning of Clindamycin with suspended sediment

Table A.13 Model Predicted Portioning of Ketoconazole with $2^3$ Factorial Design Variables

| Factor Value | | | Moles of Analyte Partitioned Into | | |
|---|---|---|---|---|---|
| Conc of Ketoconazole(A) | Conc of S.S(B) | Organic fraction of S.S(C) | Water | Sediment | Suspended Sediment |
| + | + | + | 9.7E+07 | 4.2E+07 | 4.3E+05 |
| + | + | - | 9.7E+07 | 4.2E+07 | 1.1E+05 |
| + | - | + | 9.7E+07 | 4.2E+07 | 8.7E+03 |
| + | - | - | 9.7E+07 | 4.2E+07 | 2.2E+03 |
| - | + | + | 2.6E+05 | 1.1E+05 | 1.2E+03 |
| - | + | - | 2.6E+05 | 1.1E+05 | 2.9E+02 |
| - | - | + | 2.6E+05 | 1.1E+05 | 2.4E+01 |
| - | - | - | 2.6E+05 | 1.1E+05 | 5.9E+00 |

Table A.14 Calculated Effects of Factors and their Interactions on the Associations of Ketoconazole with Different Media

| Factors/Interactions | Effect | | |
|---|---|---|---|
| | Water | Sediment | Suspended Sediment |
| A | 3.9E+08 | 1.7E+08 | 5.5E+05 |
| B | -3.7E+05 | -1.6E+05 | 5.3E+05 |
| C | -2.3E+05 | -1.0E+05 | 3.3E+05 |
| AB | -3.7E+05 | -1.6E+05 | 5.3E+05 |
| AC | -2.3E+05 | -1.0E+05 | 3.3E+05 |
| BC | -2.2E+05 | -9.6E+04 | 3.2E+05 |
| ABC | -2.2E+05 | -9.6E+04 | 3.2E+05 |

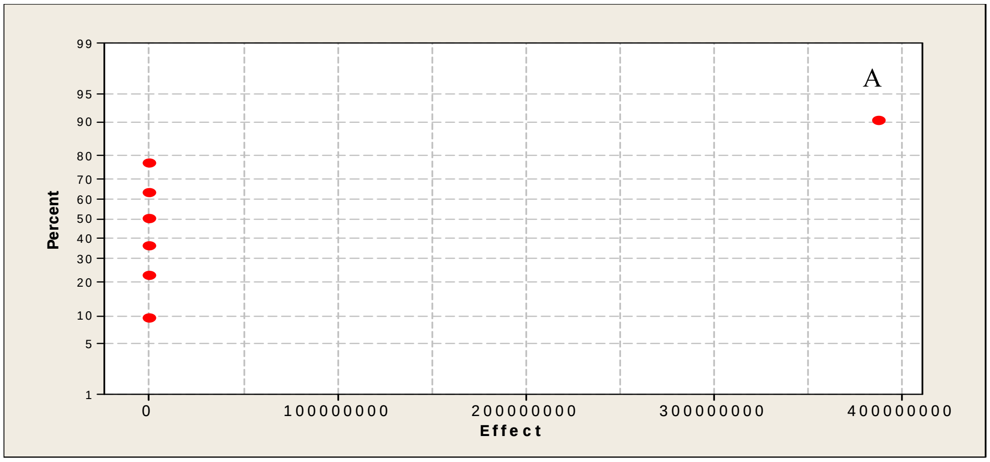


Figure A.19Probability plot of effects of partitioning of Ketoconazole with water

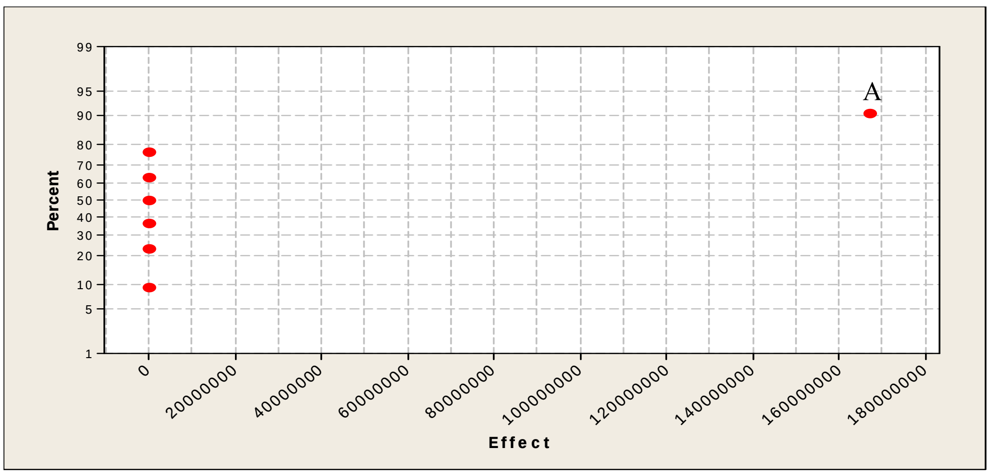


Figure A.20Probability plot of effects of partitioning of Ketoconazole with sediment

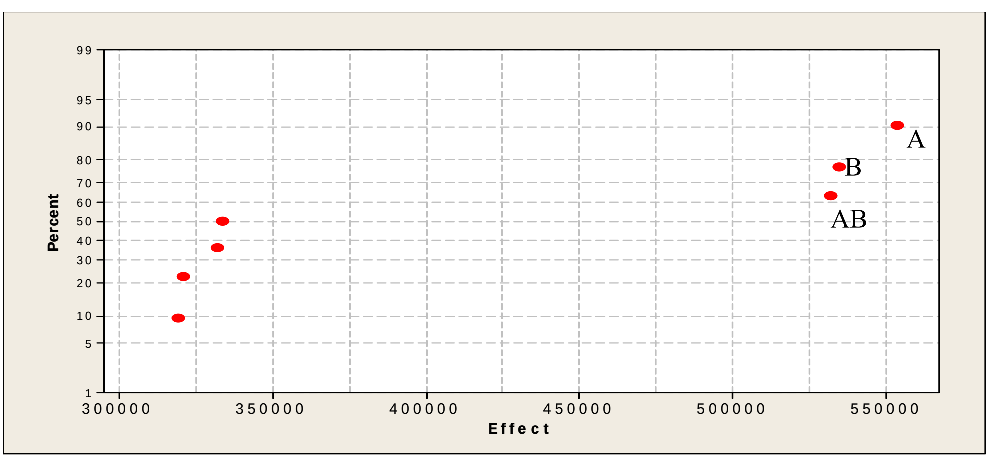


Figure A.21Probability plot of effects of partitioning of Ketoconazole with suspended sediment

Table A.15 Model Predicted Portioning of Carbamazepine with $2^3$ Factorial Design Variables

| Factor Value | | | Moles of Analyte Partitioned Into | | |
|---|---|---|---|---|---|
| **Conc of Carbamazepine(A)** | **Conc of S.S(B)** | **Organic fraction of S.S(C)** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 3.4E+07 | 8.4E+05 | 8.7E+03 |
| + | + | - | 3.4E+07 | 8.4E+05 | 2.2E+03 |
| + | - | + | 3.4E+07 | 8.4E+05 | 1.7E+02 |
| + | - | - | 3.4E+07 | 8.4E+05 | 4.4E+01 |
| - | + | + | 8.3E+05 | 2.0E+04 | 2.1E+02 |
| - | + | - | 8.3E+05 | 2.0E+04 | 5.3E+01 |
| - | - | + | 8.3E+05 | 2.0E+04 | 4.2E+00 |
| - | - | - | 8.3E+05 | 2.0E+04 | 1.1E+00 |

Table A.16 Calculated Effects of Factors and their Interactions on the Associations of Carbamazepine with Different Media

| Factors/Interactions | Effect | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 1.3E+08 | 3.3E+06 | 1.1E+04 |
| B | -1.1E+04 | -2.6E+02 | 1.1E+04 |
| C | -6.7E+03 | -1.6E+02 | 6.8E+03 |
| AB | -1.0E+04 | -2.5E+02 | 1.0E+04 |
| AC | -6.4E+03 | -1.6E+02 | 6.5E+03 |
| BC | -6.4E+03 | -1.6E+02 | 6.6E+03 |
| ABC | -6.1E+03 | -1.5E+02 | 6.3E+03 |

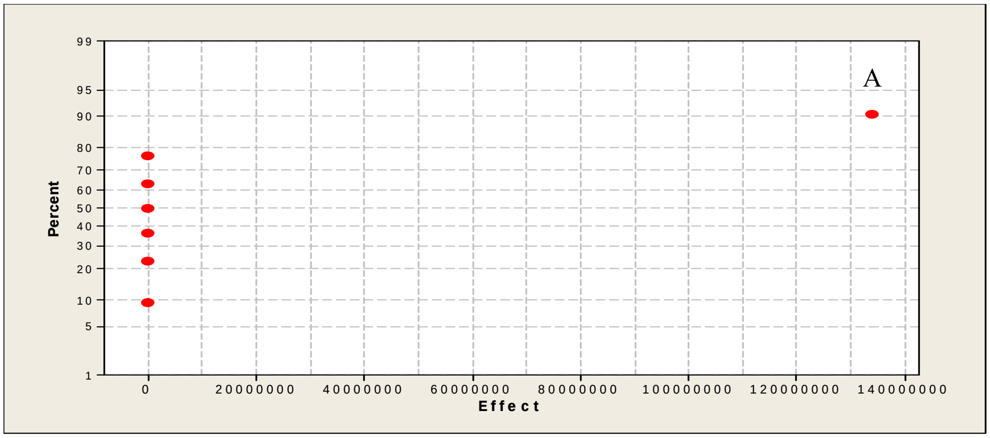


Figure A.22Probability plot of effects of partitioning of Carbamazepine with water

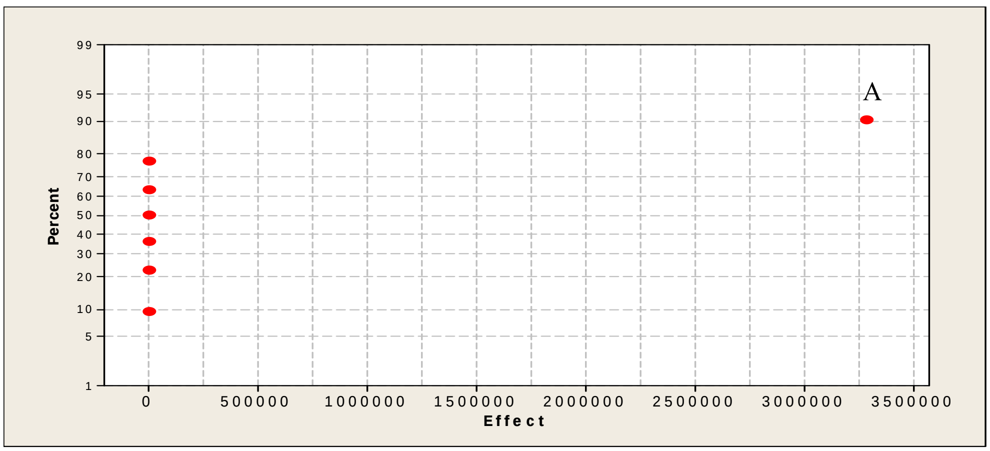


Figure A.23Probability plot of effects of partitioning of Carbamazepine with sediment

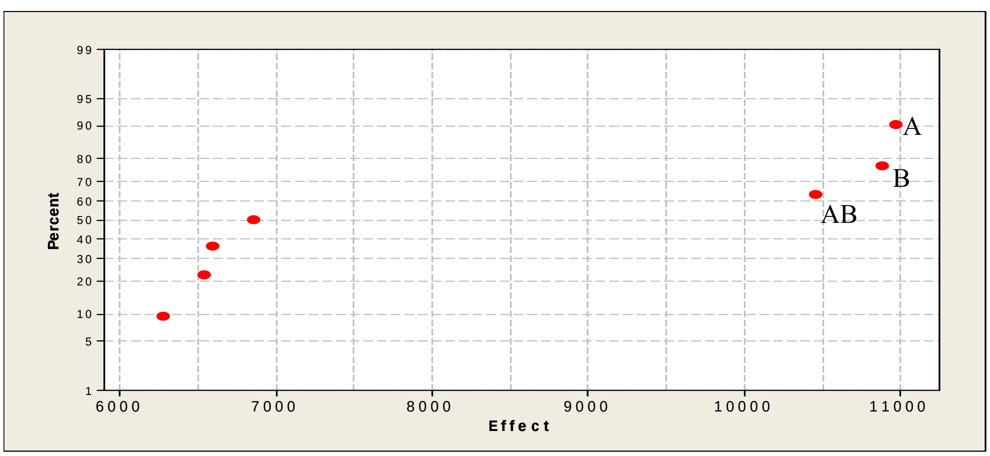


Figure A.24Probability plot of effects of partitioning of Carbamazepine with suspended sediment

Table A.17 Model Predicted Portioning of Caffeine with $2^3$ Factorial Design Variables

| **Factor Value** | | | **Moles of Analyte Partitioned Into** | | |
|---|---|---|---|---|---|
| **Conc of Caffeine (A)** | **Conc of S.S(B)** | **Organic fraction of S.S(C)** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 1.2E+08 | 1.3E+05 | 1.4E+03 |
| + | + | - | 1.2E+08 | 1.3E+05 | 3.4E+02 |
| + | - | + | 1.2E+08 | 1.3E+05 | 2.7E+01 |
| + | - | - | 1.2E+08 | 1.3E+05 | 6.8E+00 |
| - | + | + | 2.1E+06 | 2.2E+03 | 2.3E+01 |
| - | + | - | 2.1E+06 | 2.2E+03 | 5.7E+00 |
| - | - | + | 2.1E+06 | 2.2E+03 | 4.5E-01 |
| - | - | - | 2.1E+06 | 2.2E+03 | 1.1E-01 |

Table A.18 Calculated Effects of Factors and their Interactions on the Associations of Caffeine with Different Media

| **Factors/Interactions** | **Effect** | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 4.9E+08 | 5.1E+05 | 1.7E+03 |
| B | -1.7E+03 | -1.8E+00 | 1.7E+03 |
| C | -1.1E+03 | -1.1E+00 | 1.1E+03 |
| AB | -1.6E+03 | -1.7E+00 | 1.6E+03 |
| AC | -1.0E+03 | -1.1E+00 | 1.0E+03 |
| BC | -1.0E+03 | -1.1E+00 | 1.0E+03 |
| ABC | -9.8E+02 | -1.0E+00 | 9.8E+02 |

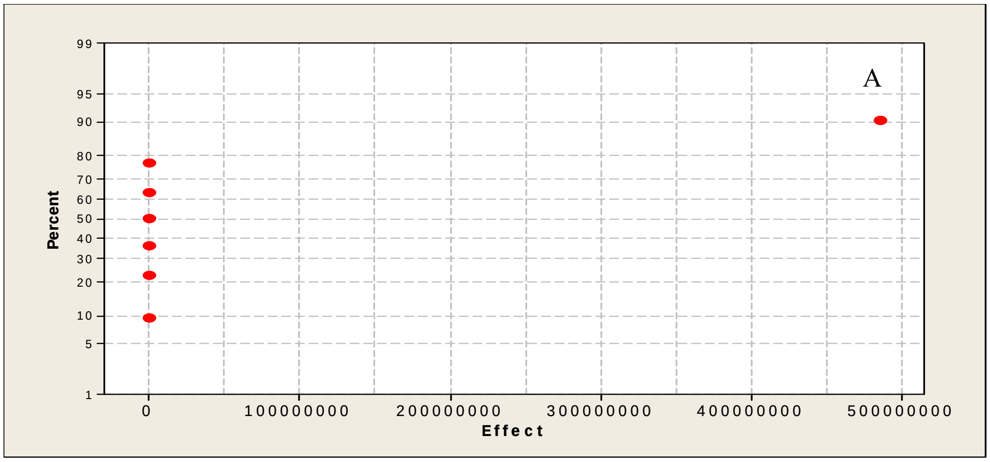


Figure A.25Probability plot of effects of partitioning of Caffeine with water

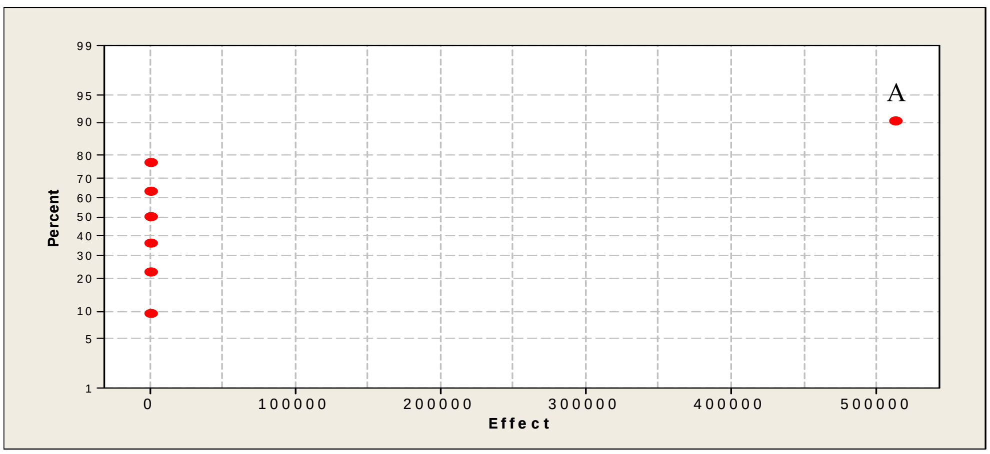


Figure A.26Probability plot of effects of partitioning of Caffeine with sediment

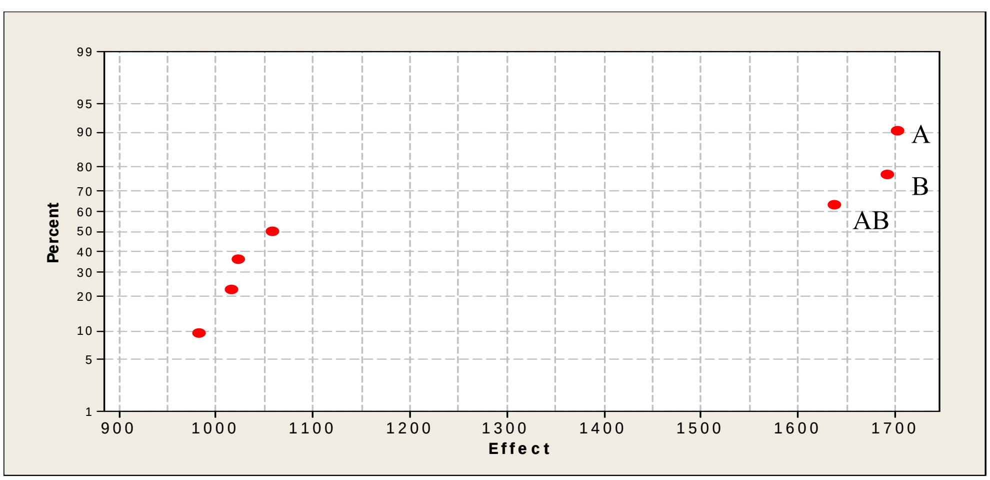


Figure A.27Probability plot of effects of partitioning of Caffeine with suspended sediment

Table A.19 Model Predicted Portioning of Ibuprofen with $2^3$ Factorial Design Variables

| **Factor Value** | | | **Moles of Analyte Partitioned Into** | | |
|---|---|---|---|---|---|
| **Conc of Ibuprofen(A)** | **Conc of S.S(B)** | **Organic fraction of S.S(C)** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 2.5E+08 | 4.1E+07 | 4.2E+05 |
| + | + | - | 2.5E+08 | 4.1E+07 | 1.1E+05 |
| + | - | + | 2.5E+08 | 4.1E+07 | 8.5E+03 |
| + | - | - | 2.5E+08 | 4.1E+07 | 2.1E+03 |
| - | + | + | 1.2E+06 | 2.0E+05 | 2.1E+03 |
| - | + | - | 1.2E+06 | 2.0E+05 | 5.3E+02 |
| - | - | + | 1.2E+06 | 2.0E+05 | 4.2E+01 |
| - | - | - | 1.2E+06 | 2.0E+05 | 1.1E+01 |

Table A.20 Calculated Effects of Factors and their Interactions on the Associations of Ibuprofen with Different Media

| **Factors/Interactions** | **Effect** | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 9.9E+08 | 1.6E+08 | 5.4E+05 |
| B | -4.5E+05 | -7.3E+04 | 5.2E+05 |
| C | -2.8E+05 | -4.5E+04 | 3.3E+05 |
| AB | -4.4E+05 | -7.2E+04 | 5.2E+05 |
| AC | -2.8E+05 | -4.5E+04 | 3.2E+05 |
| BC | -2.7E+05 | -4.4E+04 | 3.1E+05 |
| ABC | -2.7E+05 | -4.3E+04 | 3.1E+05 |

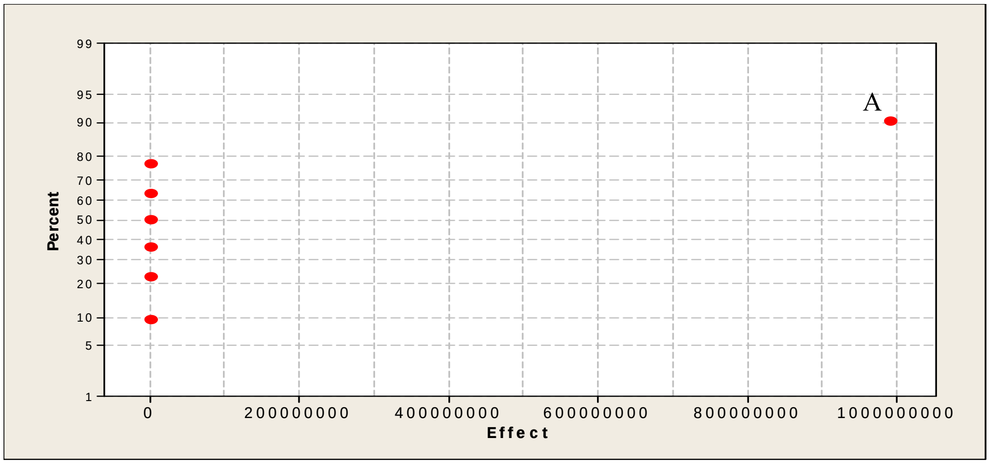


Figure A.28Probability plot of effects of partitioning of Ibuprofen with water

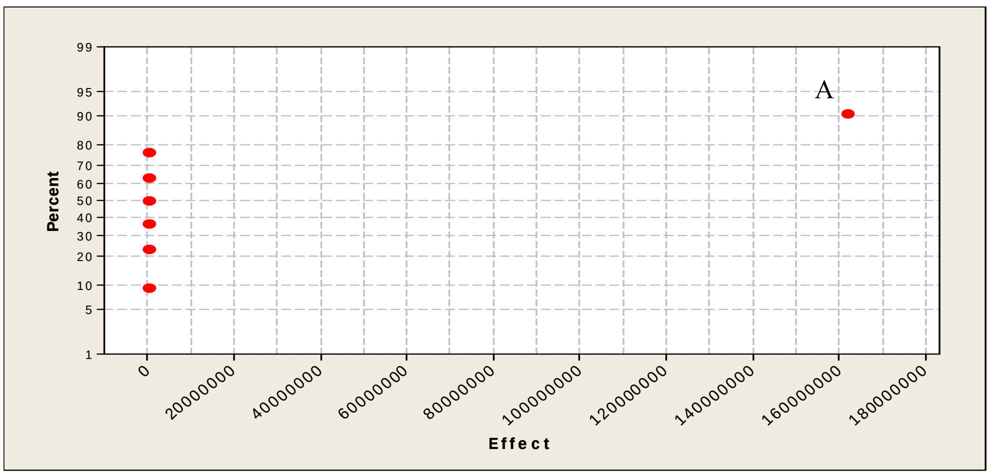


Figure A.29Probability plot of effects of partitioning of Ibuprofen with sediment

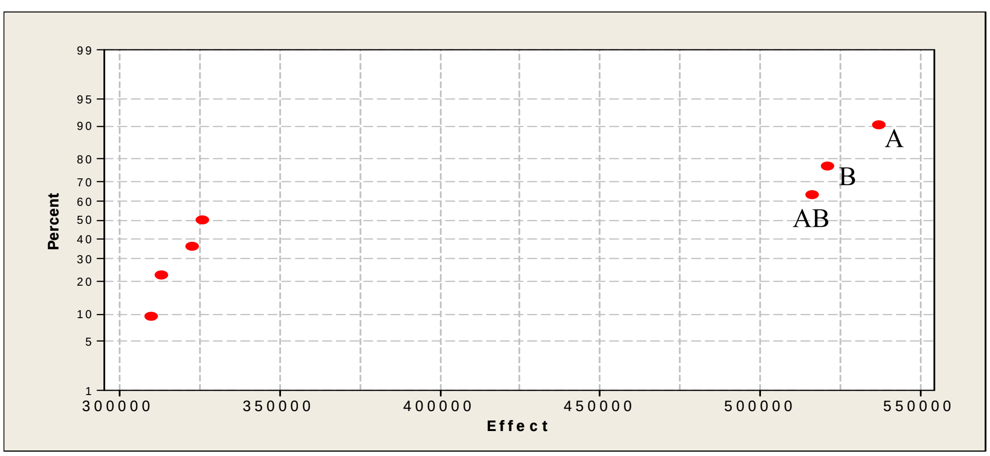


Figure A.30Probability plot of effects of partitioning of Ibuprofen with suspended sediment

Table A.21 Model Predicted Portioning of Diclofenac with $2^3$ Factorial Design Variables

| **Factor Value** | | | **Moles of Analyte Partitioned Into** | | |
|---|---|---|---|---|---|
| **Conc of Diclofenac(A)** | **Conc of S.S(B)** | **Organic fraction of S.S(C)** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 5.8E+07 | 2.3E+06 | 2.4E+04 |
| + | + | - | 5.8E+07 | 2.3E+06 | 6.1E+03 |
| + | - | + | 5.8E+07 | 2.3E+06 | 4.8E+02 |
| + | - | - | 5.8E+07 | 2.3E+06 | 1.2E+02 |
| - | + | + | 2.3E+06 | 9.0E+04 | 9.4E+02 |
| - | + | - | 2.3E+06 | 9.0E+04 | 2.4E+02 |
| - | - | + | 2.3E+06 | 9.0E+04 | 1.9E+01 |
| - | - | - | 2.3E+06 | 9.0E+04 | 4.7E+00 |

Table A.22 Calculated Effects of Factors and their Interactions on the Associations of Diclofenac with Different Media

| **Factors/Interactions** | **Effect** | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 2.2E+08 | 8.9E+06 | 3.0E+04 |
| B | -3.0E+04 | -1.2E+03 | 3.1E+04 |
| C | -1.8E+04 | -7.4E+02 | 1.9E+04 |
| AB | -2.7E+04 | -1.1E+03 | 2.9E+04 |
| AC | -1.7E+04 | -6.8E+02 | 1.8E+04 |
| BC | -1.8E+04 | -7.1E+02 | 1.8E+04 |
| ABC | -1.6E+04 | -6.5E+02 | 1.7E+04 |

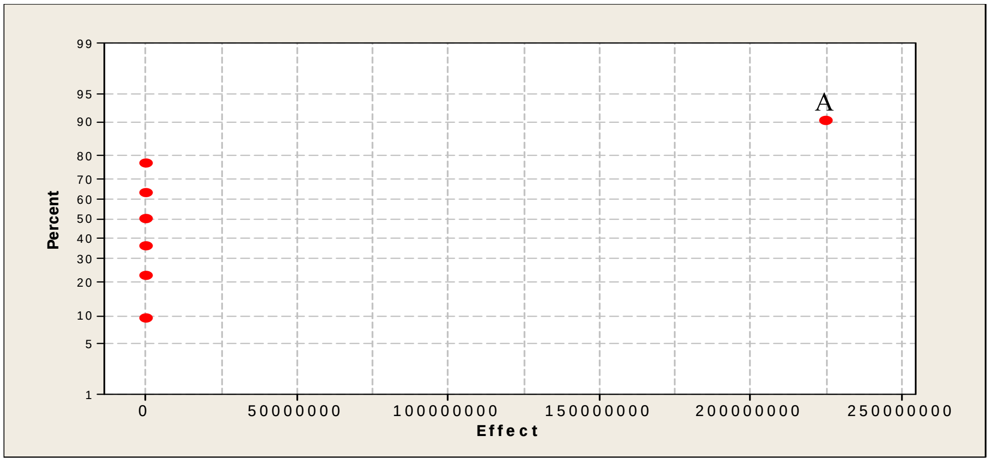


Figure A.31Probability plot of effects of partitioning of Diclofenac with water

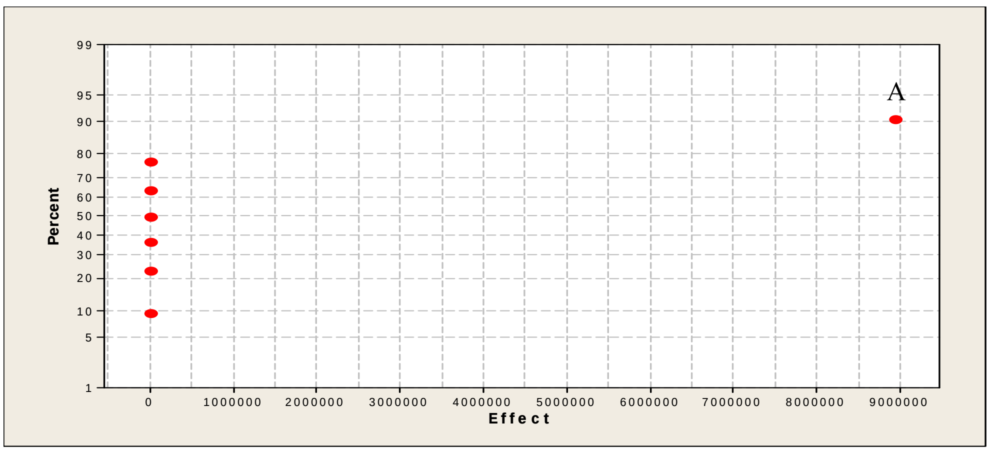


Figure A.32Probability plot of effects of partitioning of Diclofenac with sediment

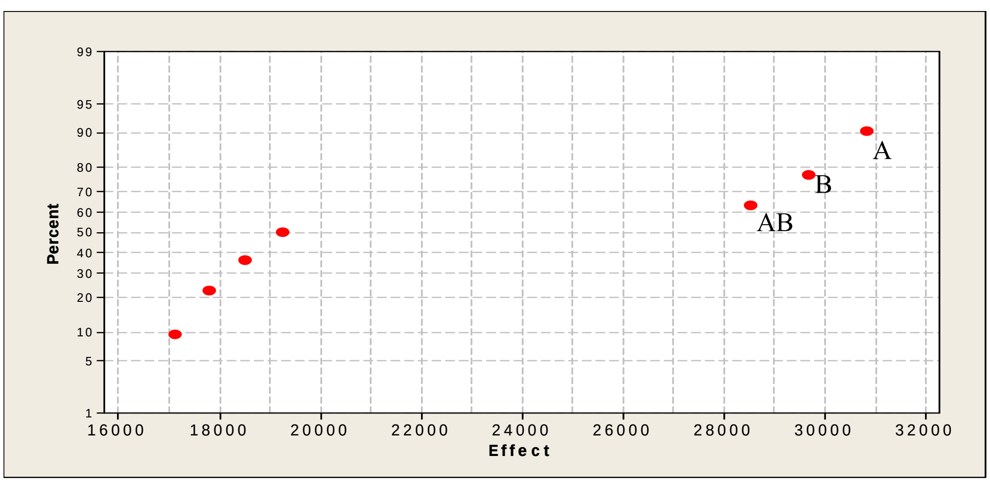


Figure A.33Probability plot of effects of partitioning of Diclofenac with suspended sediment

Table A.23 Model Predicted Portioning of Acetaminophen with $2^3$ Factorial Design Variables

| **Factor Value** | | | **Moles of Analyte Partitioned Into** | | |
|---|---|---|---|---|---|
| **Conc of Acetaminophen(A)** | **Conc of S.S(B)** | **Organic fraction of S.S(C)** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 2.0E+07 | 4.0E+04 | 4.2E+02 |
| + | + | - | 2.0E+07 | 4.0E+04 | 1.0E+02 |
| + | - | + | 2.0E+07 | 4.0E+04 | 8.3E+00 |
| + | - | - | 2.0E+07 | 4.0E+04 | 2.1E+00 |
| - | + | + | 7.9E+06 | 1.6E+04 | 1.7E+02 |
| - | + | - | 7.9E+06 | 1.6E+04 | 4.2E+01 |
| - | - | + | 7.9E+06 | 1.6E+04 | 3.3E+00 |
| - | - | - | 7.9E+06 | 1.6E+04 | 8.3E-01 |

Table A.24 Calculated Effects of Factors and their Interactions on the Associations of Acetaminophen with Different Media

| **Factors/Interactions** | **Effect** | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 4.8E+07 | 9.6E+04 | 3.2E+02 |
| B | -7.1E+02 | -1.4E+00 | 7.1E+02 |
| C | -4.4E+02 | -9.0E-01 | 4.5E+02 |
| AB | -3.1E+02 | -6.2E-01 | 3.1E+02 |
| AC | -1.9E+02 | -3.8E-01 | 1.9E+02 |
| BC | -4.3E+02 | -8.6E-01 | 4.3E+02 |
| ABC | -1.8E+02 | -3.7E-01 | 1.8E+02 |

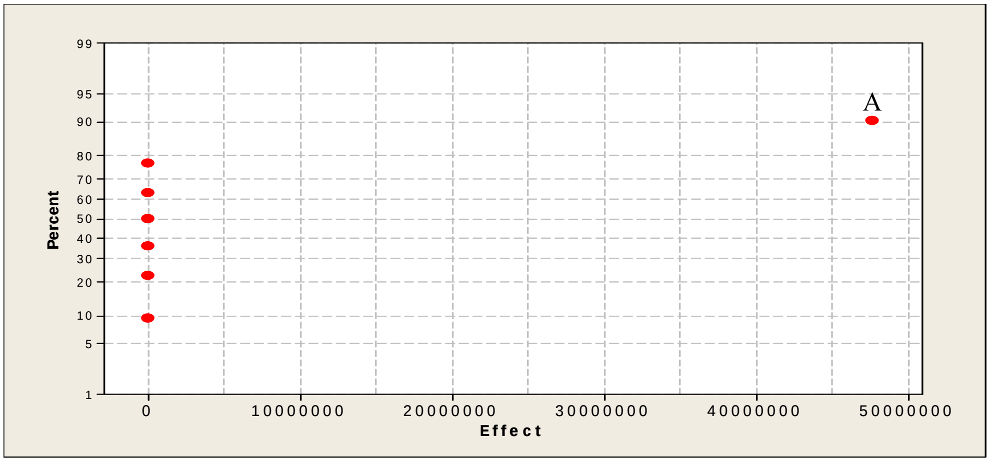


Figure A.34Probability plot of effects of partitioning of Acetaminophen with water

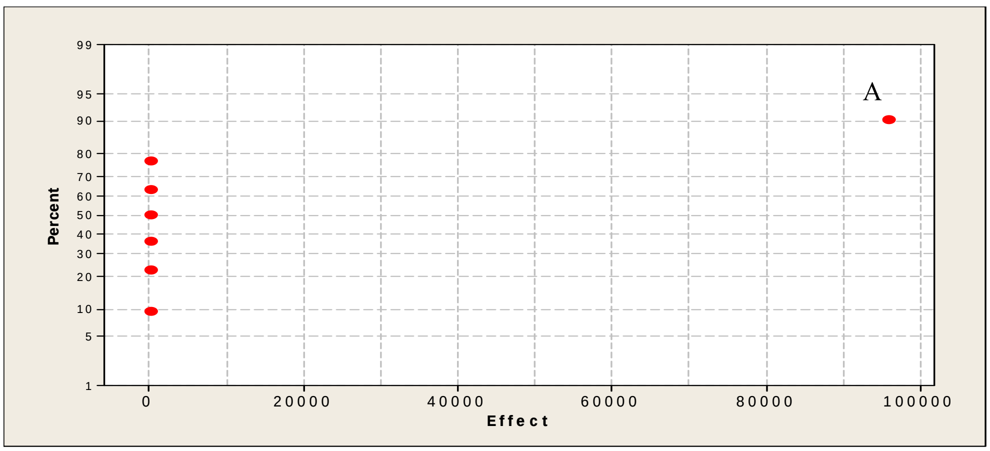


Figure A.35Probability plot of effects of partitioning of Acetaminophen with sediment

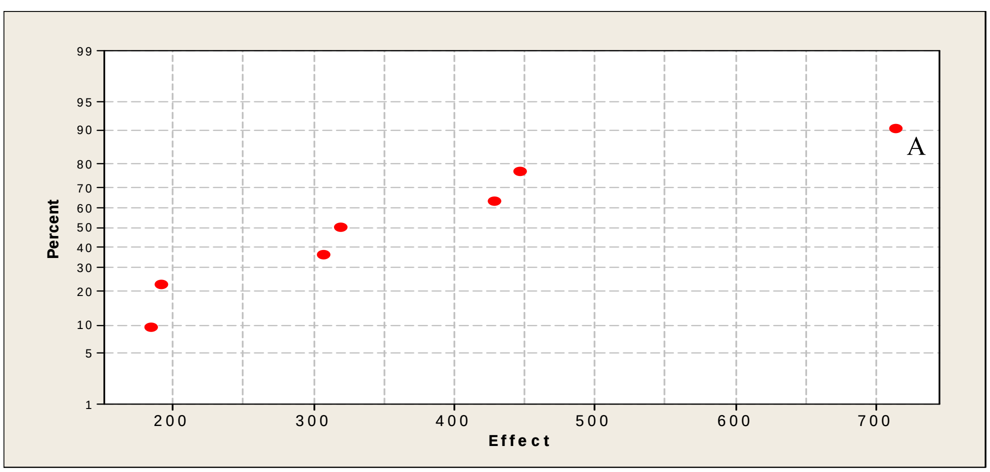


Figure A.36Probability plot of effects of partitioning of Acetaminophen with suspended sediment

Table A.25 Model Predicted Portioning of Triclosan with $2^3$ Factorial Design Variables

| Factor Value | | | Moles of Analyte Partitioned Into | | |
|---|---|---|---|---|---|
| **Conc of Triclosan(A)** | **Conc of S.S(B)** | **Organic fraction of S.S(C)** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 1.8E+08 | 7.8E+07 | 8.1E+05 |
| + | + | - | 1.8E+08 | 7.8E+07 | 2.0E+05 |
| + | - | + | 1.8E+08 | 7.8E+07 | 1.6E+04 |
| + | - | - | 1.8E+08 | 7.8E+07 | 4.1E+03 |
| - | + | + | 7.1E+06 | 3.2E+06 | 3.3E+04 |
| - | + | - | 7.2E+06 | 3.2E+06 | 8.2E+03 |
| - | - | + | 7.2E+06 | 3.2E+06 | 6.6E+02 |
| - | - | - | 7.2E+06 | 3.2E+06 | 1.6E+02 |

Table A.26 Calculated Effects of Factors and their Interactions on the Associations of Triclosan with Different Media

| Factors/Interactions | Effect | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 6.8E+08 | 3.0E+08 | 9.9E+05 |
| B | -7.1E+05 | -3.1E+05 | 1.0E+06 |
| C | -4.4E+05 | -2.0E+05 | 6.4E+05 |
| AB | -6.6E+05 | -2.9E+05 | 9.5E+05 |
| AC | -4.1E+05 | -1.8E+05 | 5.9E+05 |
| BC | -4.3E+05 | -1.9E+05 | 6.2E+05 |
| ABC | -3.9E+05 | -1.7E+05 | 5.7E+05 |

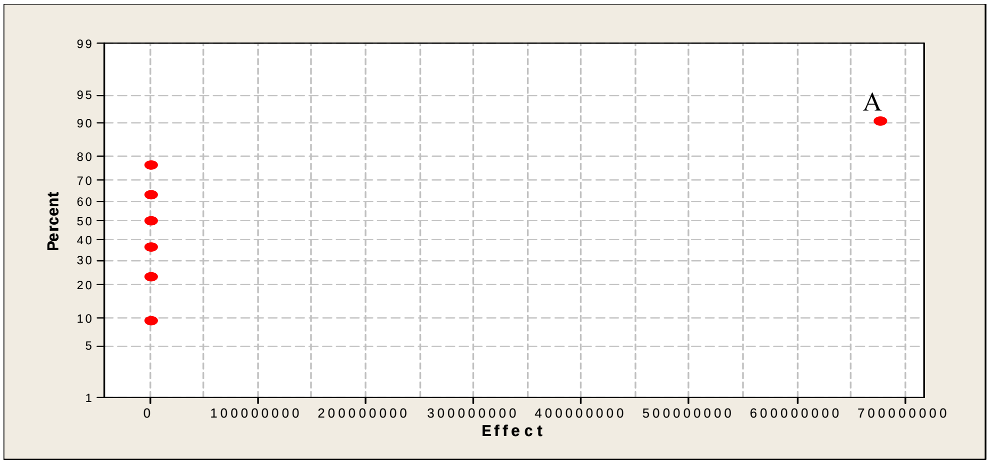


Figure A.37Probability plot of effects of partitioning of Triclosan with water

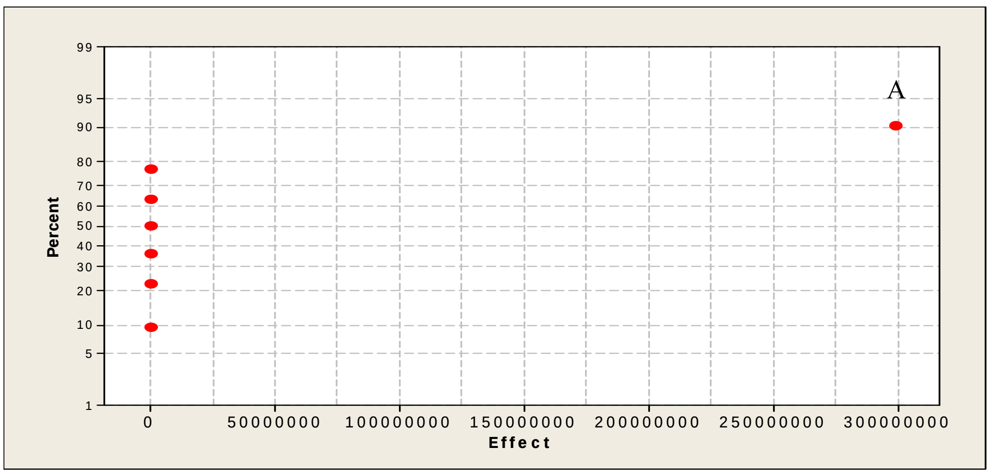


Figure A.38Probability plot of effects of partitioning of Triclosan with sediment

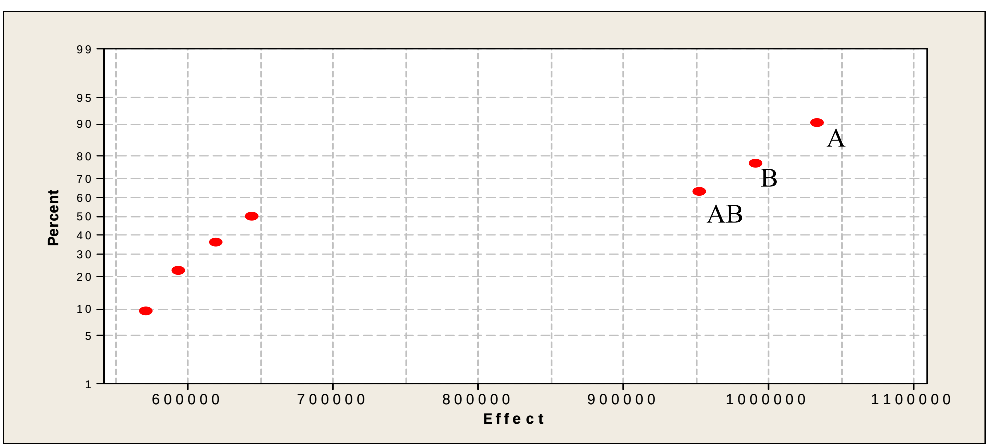


Figure A.39Probability plot of effects of partitioning of Triclosan with suspended sediment

Table A.27 Model Predicted Portioning of Ciprofloxacin with $2^3$ Factorial Design Variables

| **Factor Value** | | | **Moles of Analyte Partitioned Into** | | |
|---|---|---|---|---|---|
| **Conc of Ciprofloxacin(A)** | **Conc of S.S.(B)** | **Organic fraction of S.S(C)** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 3.8E+07 | 1.1E+08 | 1.2E+06 |
| + | + | - | 3.8E+07 | 1.1E+08 | 2.9E+05 |
| + | - | + | 3.8E+07 | 1.1E+08 | 2.3E+04 |
| + | - | - | 3.8E+07 | 1.1E+08 | 5.9E+03 |
| - | + | + | 2.1E+06 | 6.0E+06 | 6.3E+04 |
| - | + | - | 2.1E+06 | 6.1E+06 | 1.6E+04 |
| - | - | + | 2.1E+06 | 6.1E+06 | 1.3E+03 |
| - | - | - | 2.1E+06 | 6.1E+06 | 3.2E+02 |

Table A.28 Calculated Effects of Factors and their Interactions on the Associations of Ciprofloxacin with Different Media

| **Factors/Interactions** | **Effect** | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 1.5E+08 | 4.2E+08 | 1.4E+06 |
| B | -3.8E+05 | -1.1E+06 | 1.5E+06 |
| C | -2.4E+05 | -7.0E+05 | 9.4E+05 |
| AB | -3.4E+05 | -1.0E+06 | 1.3E+06 |
| AC | -2.1E+05 | -6.3E+05 | 8.4E+05 |
| BC | -2.3E+05 | -6.7E+05 | 9.0E+05 |
| ABC | -2.1E+05 | -6.0E+05 | 8.1E+05 |

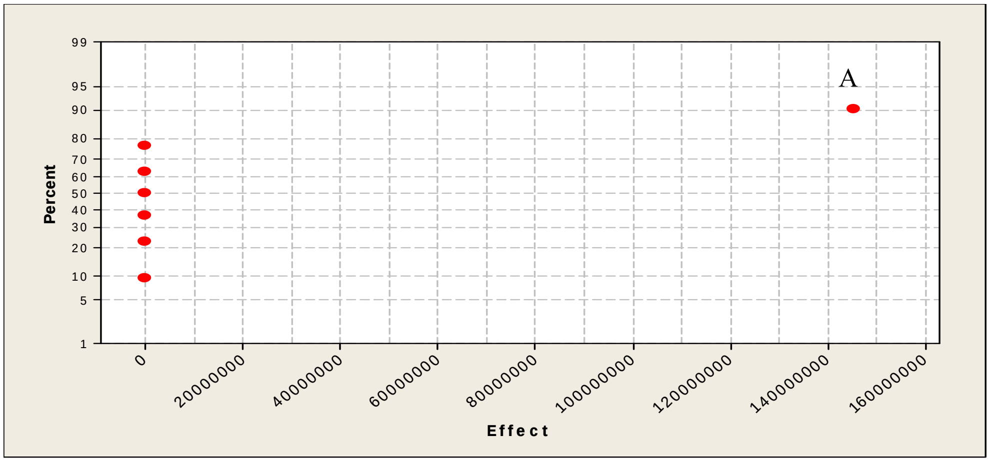


Figure A.40Probability plot of effects of partitioning of Ciprofloxacin with water

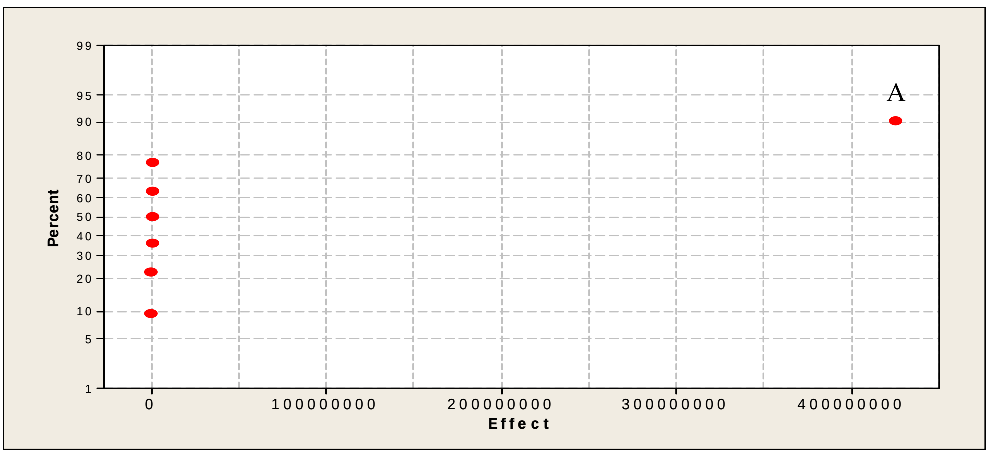


Figure A.41Probability plot of effects of partitioning of Ciprofloxacin with sediment

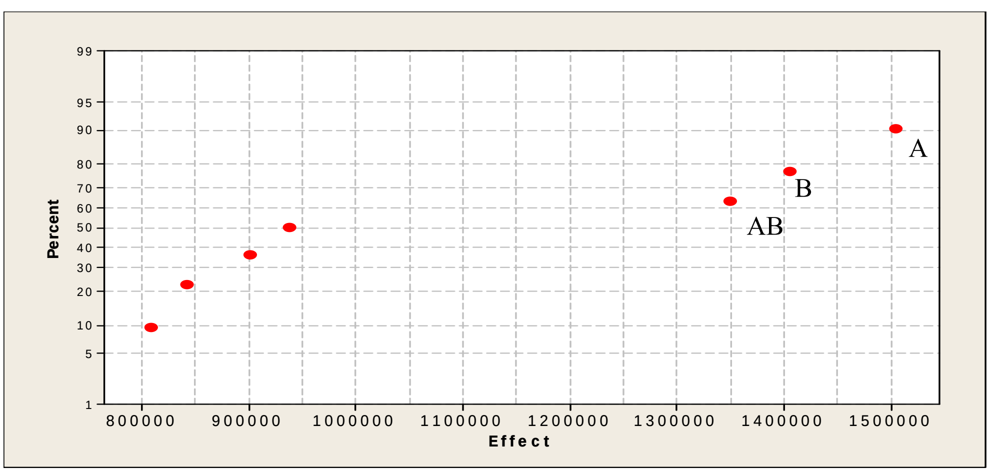


Figure A.42Probability plot of effects of partitioning of Ciprofloxacin with suspended sediment

Table A.29 Model Predicted Portioning of Metoprolol with $2^3$ Factorial Design Variables

| **Factor Value** | | | **Moles of Analyte Partitioned Into** | | |
|---|---|---|---|---|---|
| **Conc of Metoprolol(A)** | **Conc of S.S.(B)** | **Organic fraction of S.S(C)** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 4.5E+07 | 1.3E+05 | 1.4E+03 |
| + | + | - | 4.5E+07 | 1.3E+05 | 3.5E+02 |
| + | - | + | 4.5E+07 | 1.3E+05 | 2.8E+01 |
| + | - | - | 4.5E+07 | 1.3E+05 | 6.9E+00 |
| - | + | + | 7.5E+06 | 2.2E+04 | 2.3E+02 |
| - | + | - | 7.5E+06 | 2.2E+04 | 5.8E+01 |
| - | - | + | 7.5E+06 | 2.2E+04 | 4.6E+00 |
| - | - | - | 7.5E+06 | 2.2E+04 | 1.2E+00 |

Table A.30 Calculated Effects of Factors and their Interactions on the Associations of Metoprolol with Different Media

| **Factors/Interactions** | **Effect** | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 1.5E+08 | 4.4E+05 | 1.5E+03 |
| B | -2.0E+03 | -5.9E+00 | 2.0E+03 |
| C | -1.2E+03 | -3.7E+00 | 1.2E+03 |
| AB | -1.4E+03 | -4.2E+00 | 1.4E+03 |
| AC | -8.8E+02 | -2.6E+00 | 8.8E+02 |
| BC | -1.2E+03 | -3.5E+00 | 1.2E+03 |
| ABC | -8.5E+02 | -2.5E+00 | 8.5E+02 |

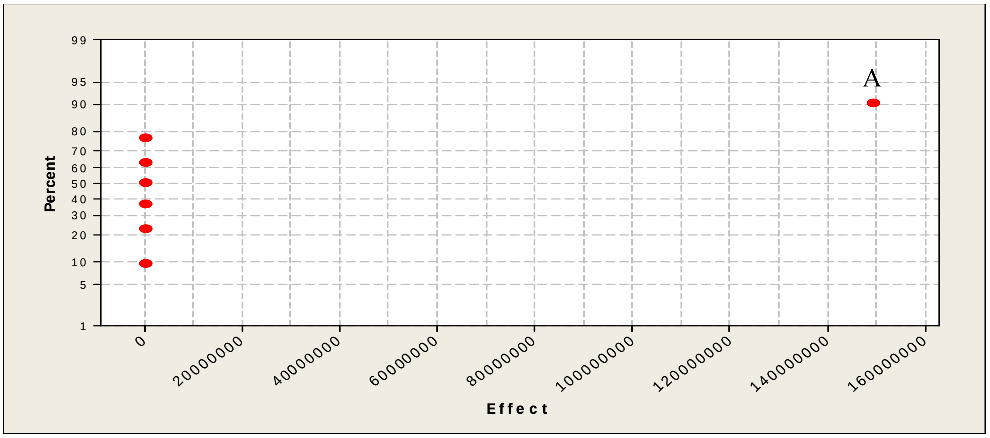


Figure A.43Probability plot of effects of partitioning of Metoprolol with water

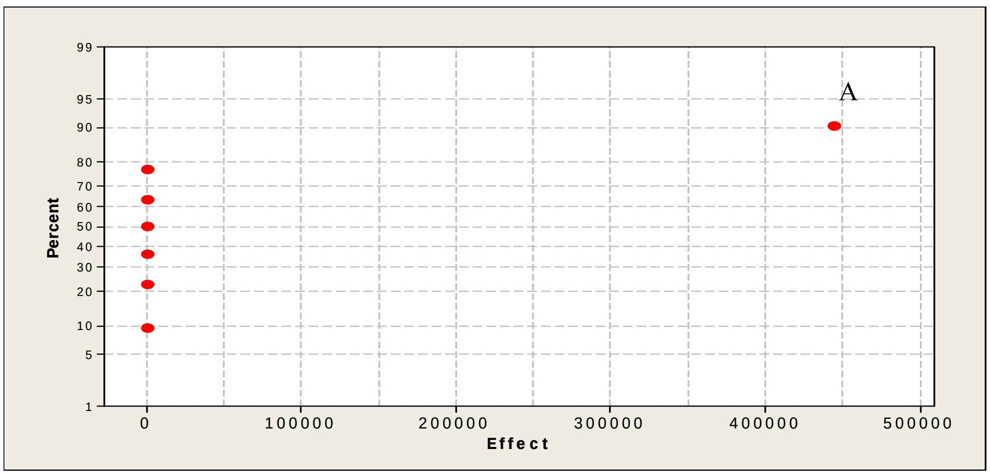


Figure A.44Probability plot of effects of partitioning of Metoprolol with sediment

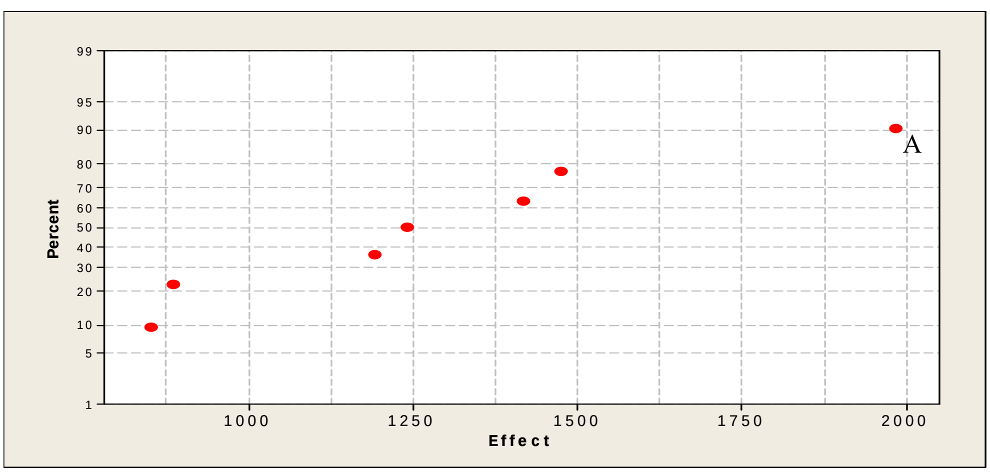


Figure A.45Probability plot of effects of partitioning of Metoprolol with suspended sediment

Table A.31 Model Predicted Portioning of Salicylic acid with $2^3$ Factorial Design Variables

| Factor Value | | | Moles of Analyte Partitioned Into | | |
|---|---|---|---|---|---|
| Conc of Salicylic acid(A) | Conc of S.S(B) | Organic fraction of S.S(C) | Water | Sediment | Suspended Sediment |
| + | + | + | 3.8E+07 | 1.2E+08 | 1.2E+06 |
| + | + | - | 3.9E+07 | 1.2E+08 | 3.1E+05 |
| + | - | + | 3.9E+07 | 1.2E+08 | 2.5E+04 |
| + | - | - | 3.9E+07 | 1.2E+08 | 6.3E+03 |
| - | + | + | 2.3E+06 | 7.1E+06 | 7.4E+04 |
| - | + | - | 2.3E+06 | 7.1E+06 | 1.9E+04 |
| - | - | + | 2.3E+06 | 7.1E+06 | 1.5E+03 |
| - | - | - | 2.3E+06 | 7.1E+06 | 3.7E+02 |

Table A.32 Calculated Effects of Factors and their Interactions on the Associations of Salicylic acid with Different Media

| Factors/Interactions | Effect | | |
|---|---|---|---|
| | Water | Sediment | Suspended Sediment |
| A | 1.4E+08 | 4.5E+08 | 1.5E+06 |
| B | -3.9E+05 | -1.2E+06 | 1.6E+06 |
| C | -2.4E+05 | -7.6E+05 | 1.0E+06 |
| AB | -3.5E+05 | -1.1E+06 | 1.4E+06 |
| AC | -2.2E+05 | -6.8E+05 | 9.0E+05 |
| BC | -2.3E+05 | -7.3E+05 | 9.7E+05 |
| ABC | -2.1E+05 | -6.5E+05 | 8.6E+05 |

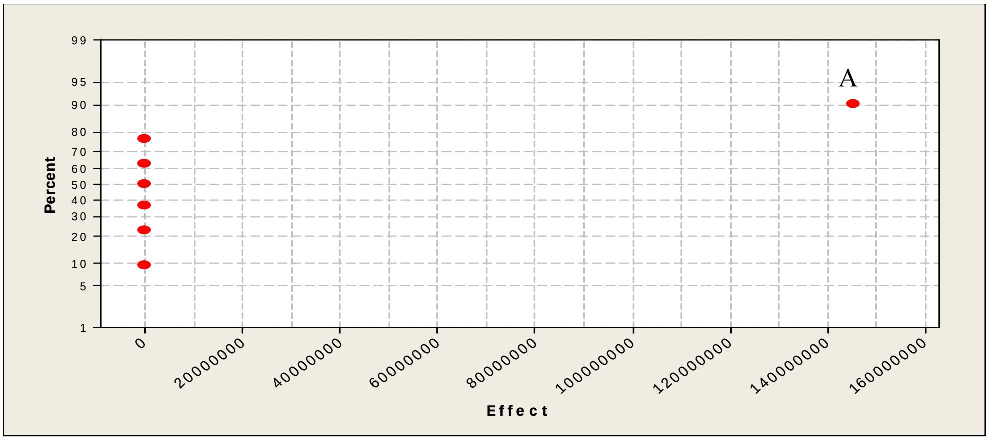


Figure A.46Probability plot of effects of partitioning of Salicylic acid with water

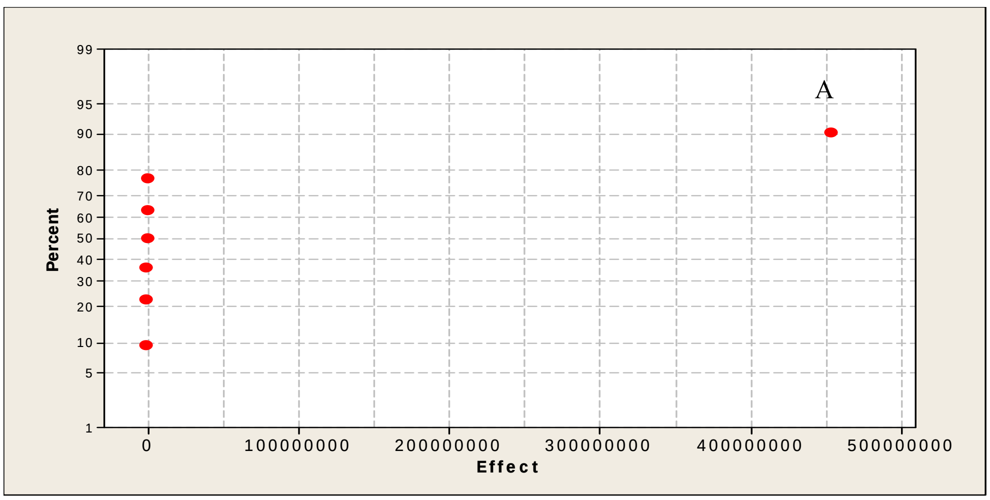


Figure A.47Probability plot of effects of partitioning of Salicylic acid with sediment

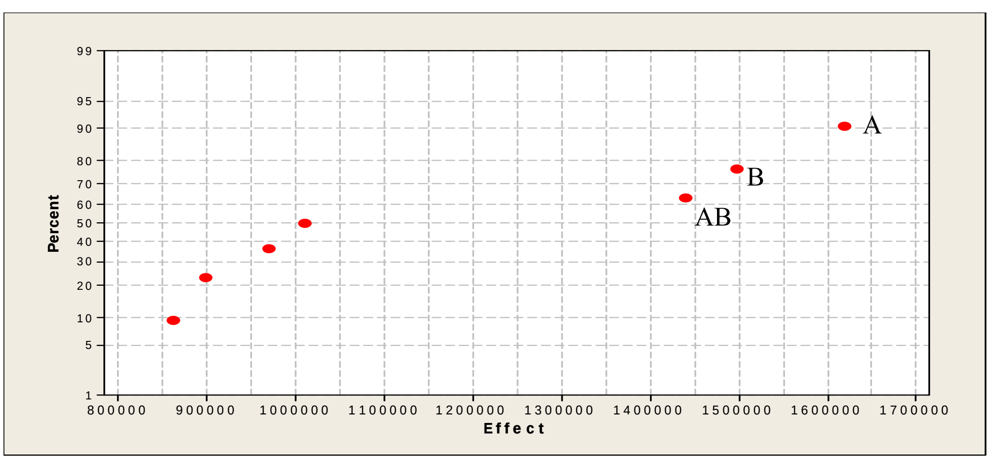


Figure A.48Probability plot of effects of partitioning of Salicylic acid with suspended sediment

Table A.33 Model Predicted Portioning of Dioxin with $2^3$ Factorial Design Variables

| **Factor Value** | | | **Moles of Analyte Partitioned Into** | | |
|---|---|---|---|---|---|
| **Conc of Dioxin(A)** | **Conc of S.S(B)** | **Organic fraction of S.S(C)** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 4.0E+07 | 4.6E+10 | 4.8E+08 |
| + | + | - | 4.0E+07 | 4.6E+10 | 1.2E+08 |
| + | - | + | 4.0E+07 | 4.6E+10 | 9.7E+06 |
| + | - | - | 4.0E+07 | 4.6E+10 | 2.4E+06 |
| - | + | + | 2.7E+02 | 3.1E+05 | 3.2E+03 |
| - | + | - | 2.7E+02 | 3.1E+05 | 8.1E+02 |
| - | - | + | 2.7E+02 | 3.1E+05 | 6.5E+01 |
| - | - | - | 2.7E+02 | 3.1E+05 | 1.6E+01 |

Table A.34 Calculated Effects of Factors and their Interactions on the Associations of Dioxin with Different Media

| **Factors/Interactions** | **Effect** | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 1.6E+08 | 1.9E+11 | 6.1E+08 |
| B | -5.1E+05 | -5.9E+08 | 5.9E+08 |
| C | -3.2E+05 | -3.7E+08 | 3.7E+08 |
| AB | -5.1E+05 | -5.9E+08 | 5.9E+08 |
| AC | -3.2E+05 | -3.7E+08 | 3.7E+08 |
| BC | -3.0E+05 | -3.5E+08 | 3.5E+08 |
| ABC | -3.0E+05 | -3.5E+08 | 3.5E+08 |

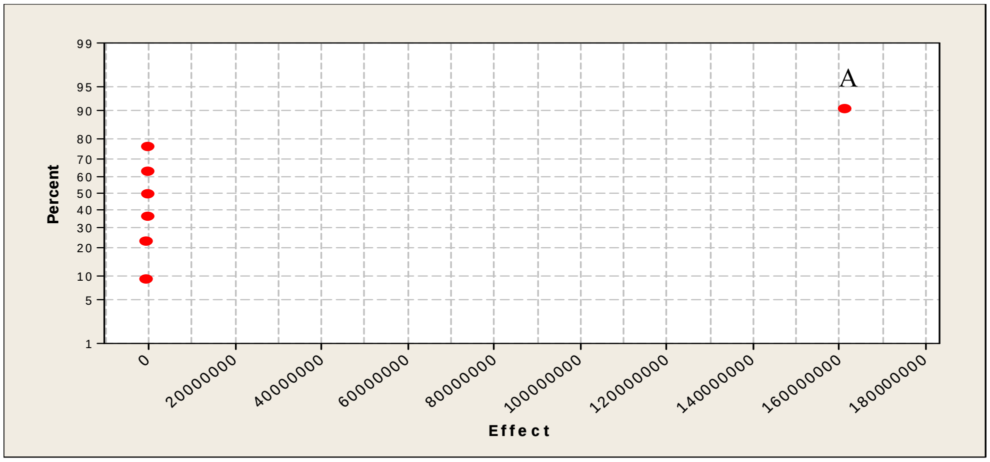


Figure A.49Probability plot of effects of partitioning of Dioxin with water

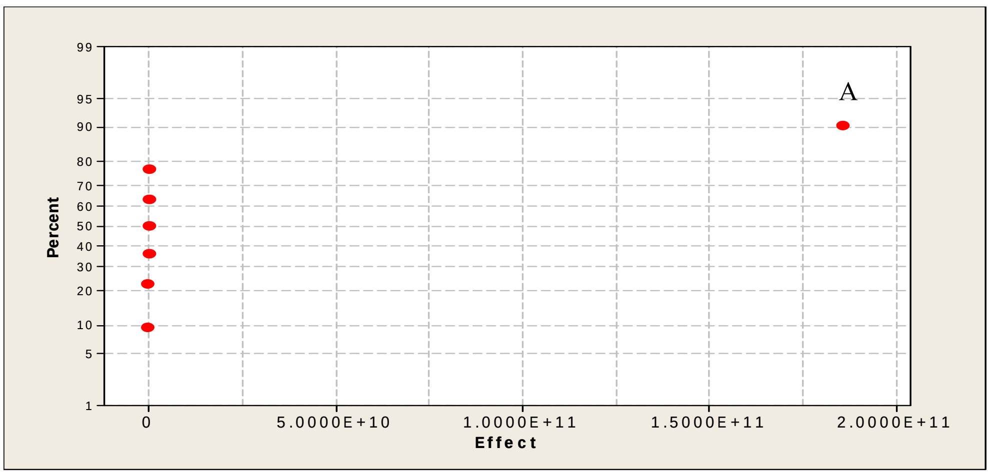


Figure A.50Probability plot of effects of partitioning of Dioxin with sediment

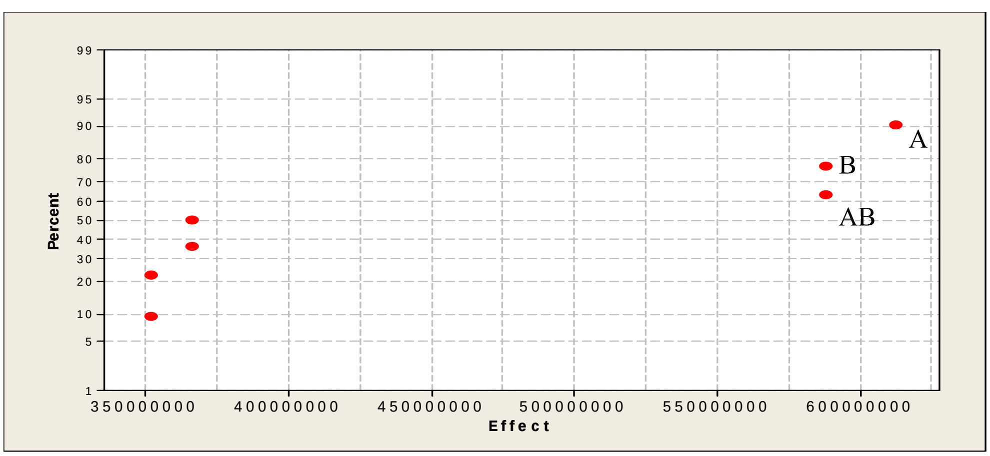


Figure A.51Probability plot of effects of partitioning of Dioxin with suspended sediment

## APPENDIX B

## PROPERTIES AND FATE MODELING OF PESTICIDES

Table B.1 Model Predicted Portioning of Aldrin with $2^3$ Factorial Design Variables

| Factor Value | | | Moles of Analyte Partitioned Into | | |
|---|---|---|---|---|---|
| **Conc of Aldrin(A)** | **Conc of S.S(B)** | **Organic fraction of S.S(C)** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 8.6E+08 | 9.5E+08 | 9.9E+06 |
| + | + | - | 8.7E+08 | 9.5E+08 | 2.5E+06 |
| + | - | + | 8.7E+08 | 9.5E+08 | 2.0E+05 |
| + | - | - | 8.7E+08 | 9.5E+08 | 5.0E+04 |
| - | + | + | 8.6E+06 | 9.5E+06 | 9.9E+04 |
| - | + | - | 8.7E+06 | 9.5E+06 | 2.5E+04 |
| - | - | + | 8.7E+06 | 9.5E+06 | 2.0E+03 |
| - | - | - | 8.7E+06 | 9.5E+06 | 5.0E+02 |

Table B.2 Calculated Effects of Factors and their Interactions on the Associations of Aldrin with Different Media

| Factors/Interactions | Effect | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 3.4E+09 | 3.8E+09 | 1.3E+07 |
| B | -3.9E+06 | -4.3E+06 | 1.2E+07 |
| C | -2.4E+06 | -2.7E+06 | 7.6E+06 |
| AB | -3.8E+06 | -4.2E+06 | 1.2E+07 |
| AC | -2.4E+06 | -2.6E+06 | 7.5E+06 |
| BC | -2.3E+06 | -2.6E+06 | 7.3E+06 |
| ABC | -2.3E+06 | -2.5E+06 | 7.2E+06 |

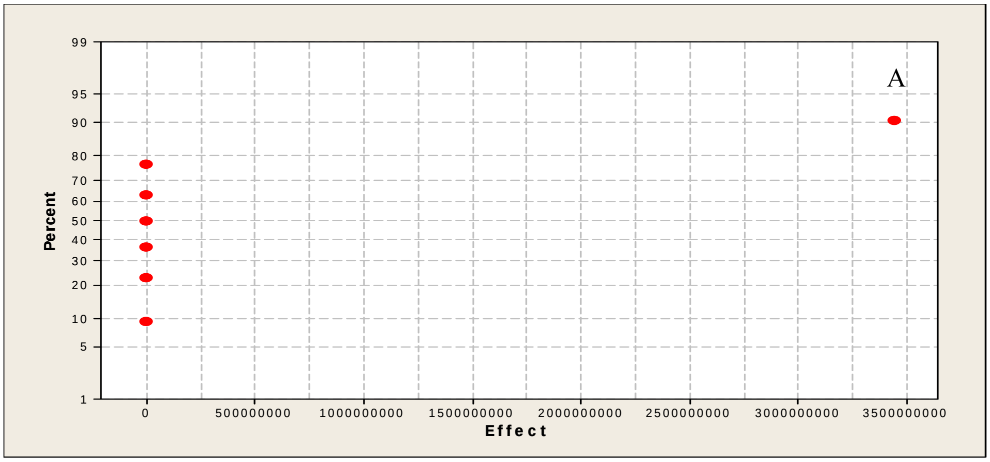


Figure B.1 Probability plot of effects of partitioning of Aldrin with water

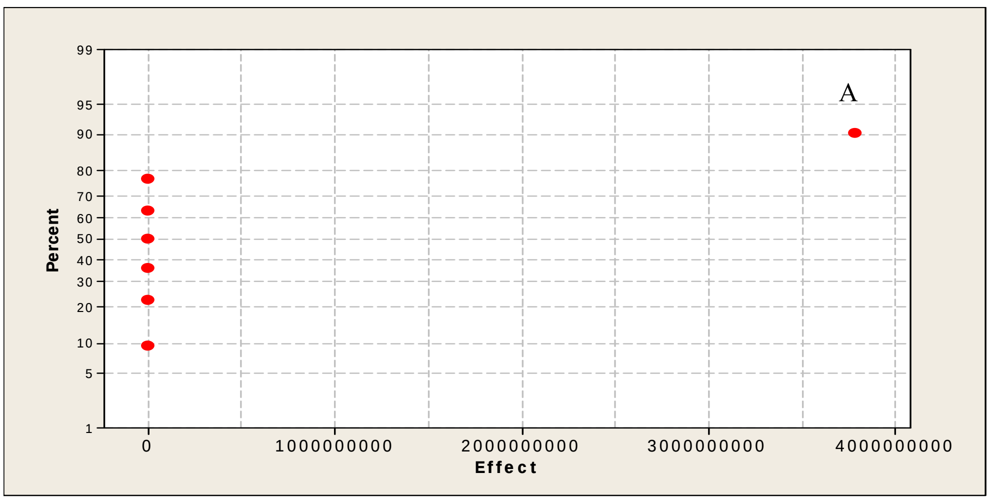


Figure B.2 Probability plot of effects of partitioning of Aldrin with sediment

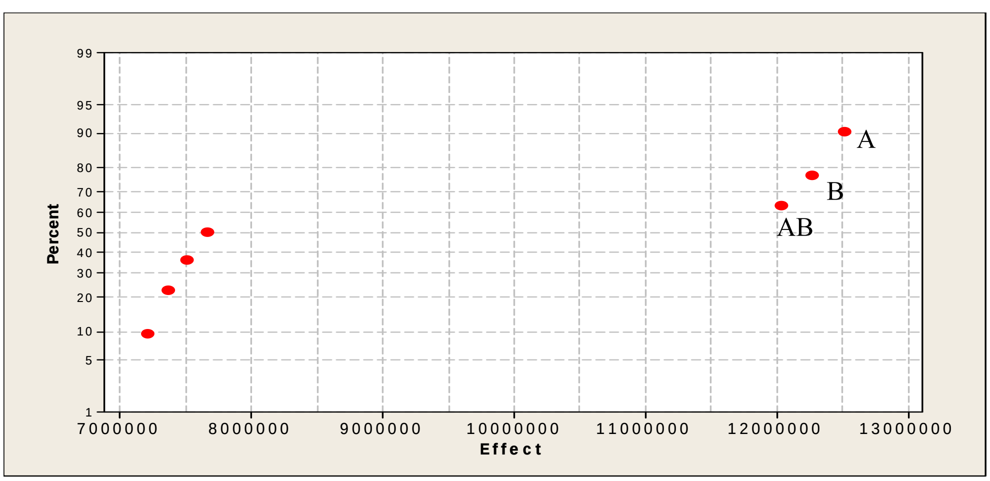


Figure B.3 Probability plot of effects of partitioning of Aldrin with suspended sediment

Table B.3 Model Predicted Portioning of Chloroneb with $2^3$ Factorial Design Variables

| Factor Value | | | Moles of Analyte Partitioned Into | | |
|---|---|---|---|---|---|
| Conc of Chloroneb(A) | Conc of S.S(B) | Organic fraction of S.S(C) | Water | Sediment | Suspended Sediment |
| + | + | + | 1.5E+09 | 9.3E+07 | 9.7E+05 |
| + | + | - | 1.5E+09 | 9.3E+07 | 2.4E+05 |
| + | - | + | 1.5E+09 | 9.3E+07 | 1.9E+04 |
| + | - | - | 1.5E+09 | 9.3E+07 | 4.8E+03 |
| - | + | + | 1.5E+07 | 9.3E+05 | 9.7E+03 |
| - | + | - | 1.5E+07 | 9.3E+05 | 2.4E+03 |
| - | - | + | 1.5E+07 | 9.3E+05 | 1.9E+02 |
| - | - | - | 1.5E+07 | 9.3E+05 | 4.8E+01 |

Table B.4 Calculated Effects of Factors and their Interactions on the Associations of Chloroneb with Different Media

| Factors/Interactions | Effect | | |
|---|---|---|---|
| | Water | Sediment | Suspended Sediment |
| A | 6.1E+09 | 3.7E+08 | 1.2E+06 |
| B | -3.8E+05 | -2.3E+04 | 1.2E+06 |
| C | -2.4E+05 | -1.4E+04 | 7.5E+05 |
| AB | -3.7E+05 | -2.3E+04 | 1.2E+06 |
| AC | -2.3E+05 | -1.4E+04 | 7.3E+05 |
| BC | -2.3E+05 | -1.4E+04 | 7.2E+05 |
| ABC | -2.2E+05 | -1.4E+04 | 7.0E+05 |

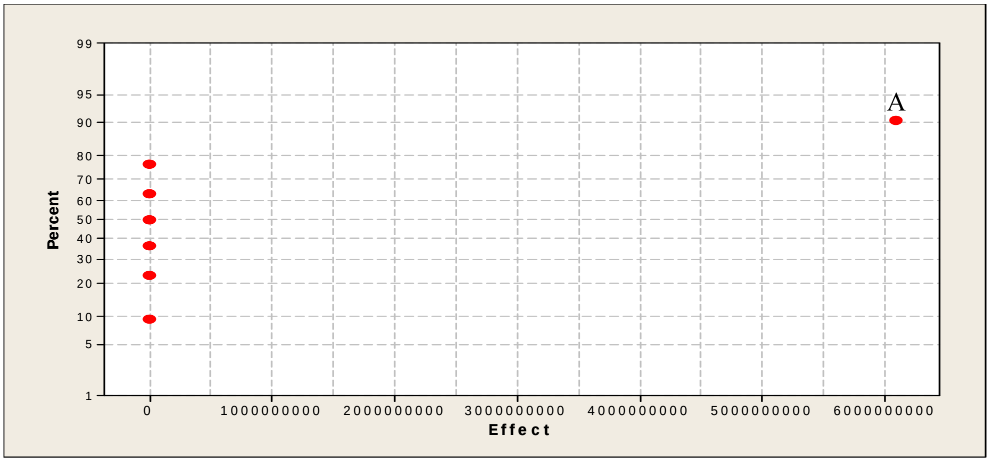


Figure B.4 Probability plot of effects of partitioning of Chloroneb with water

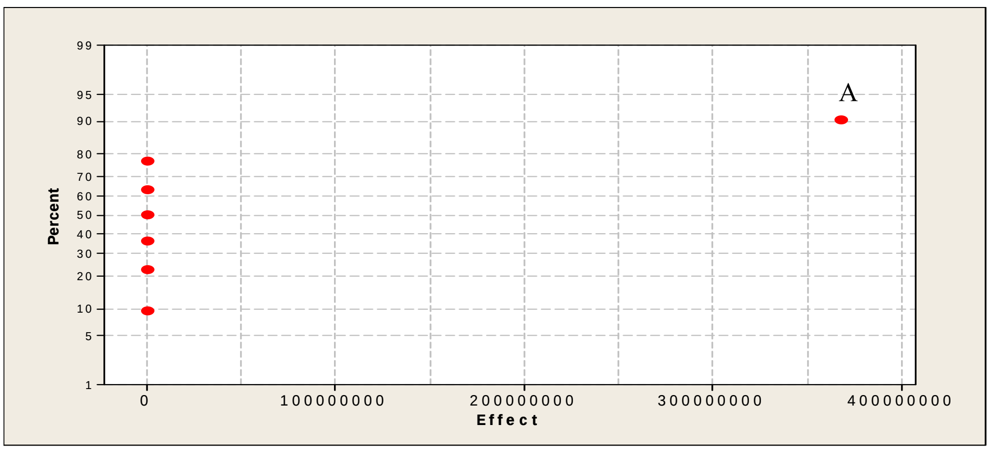


Figure B.5 Probability plot of effects of partitioning of Chloroneb with sediment

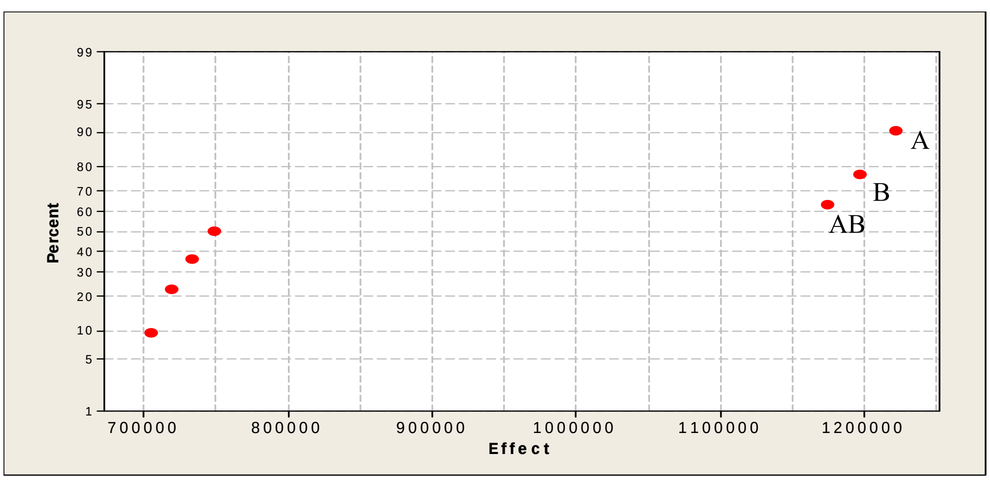


Figure B.6 Probability plot of effects of partitioning of Chloroneb with suspended sediment

Table B.5 Model Predicted Portioning of Chlorothalonil with $2^3$ Factorial Design Variables

| **Factor Value** | | | **Moles of Analyte Partitioned Into** | | |
|---|---|---|---|---|---|
| **Conc of Chlorothalonil(A)** | **Conc of S.S(B)** | **Organic fraction of S.S(C)** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 3.4E+09 | 3.0E+08 | 3.1E+06 |
| + | + | - | 3.4E+09 | 3.0E+08 | 7.8E+05 |
| + | - | + | 3.4E+09 | 3.0E+08 | 6.2E+04 |
| + | - | - | 3.4E+09 | 3.0E+08 | 1.6E+04 |
| - | + | + | 3.4E+07 | 3.0E+06 | 3.1E+04 |
| - | + | - | 3.4E+07 | 3.0E+06 | 7.8E+03 |
| - | - | + | 3.4E+07 | 3.0E+06 | 6.2E+02 |
| - | - | - | 3.4E+07 | 3.0E+06 | 1.6E+02 |

Table B.6 Calculated Effects of Factors and their Interactions on the Associations of Chlorothalonil with Different Media

| **Factors/Interactions** | **Effect** | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 1.4E+10 | 1.2E+09 | 3.9E+06 |
| B | -3.5E+06 | -3.0E+05 | 3.8E+06 |
| C | -2.2E+06 | -1.9E+05 | 2.4E+06 |
| AB | -3.4E+06 | -3.0E+05 | 3.8E+06 |
| AC | -2.1E+06 | -1.9E+05 | 2.3E+06 |
| BC | -2.1E+06 | -1.8E+05 | 2.3E+06 |
| ABC | -2.1E+06 | -1.8E+05 | 2.3E+06 |

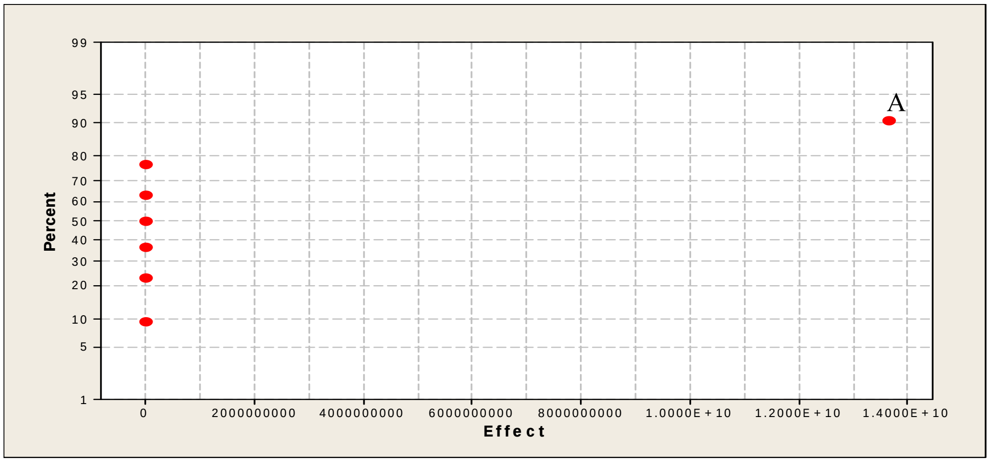


Figure B.7 Probability plot of effects of partitioning of Chlorothalonil with water

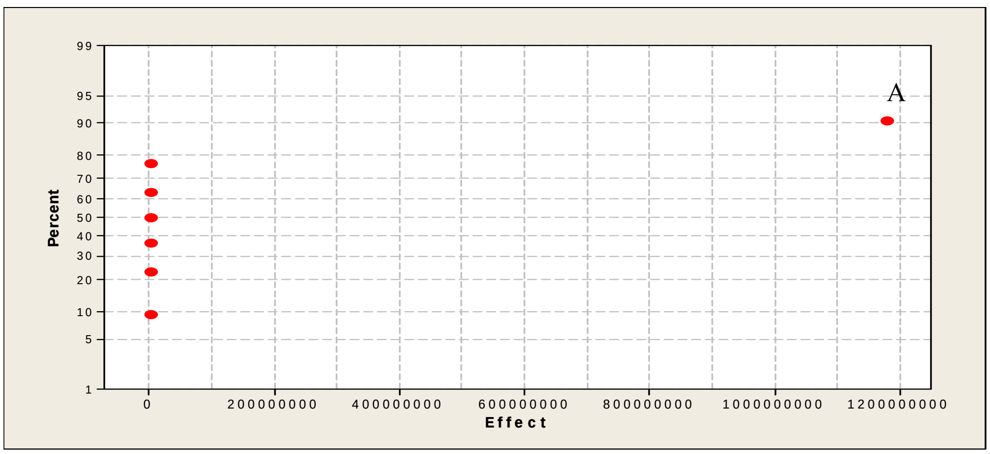


Figure B.8 Probability plot of effects of partitioning of Chlorothalonil with sediment

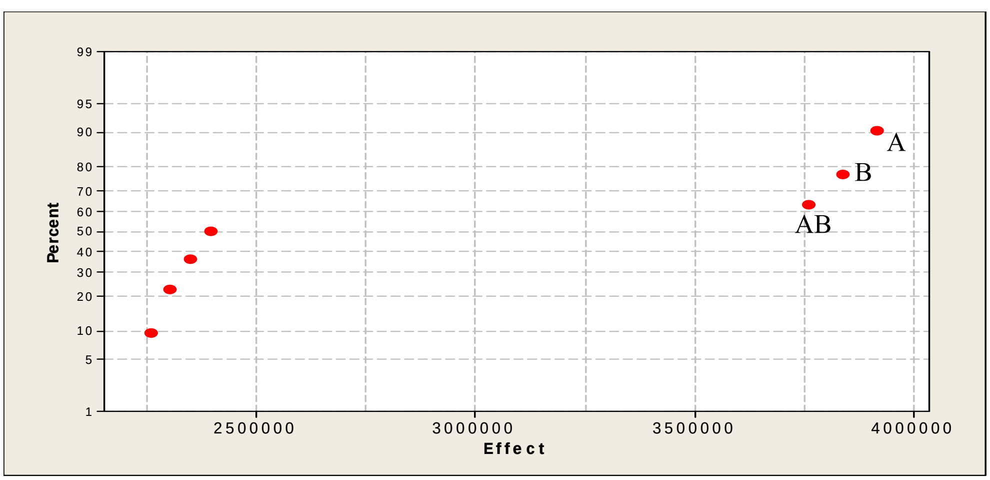


Figure B.9 Probability plot of effects of partitioning of Chlorothalonil with suspended sediment

Table B.7 Model Predicted Portioning of DDD with $2^3$ Factorial Design Variables

| **Factor Value** | | | **Moles of Analyte Partitioned Into** | | |
|---|---|---|---|---|---|
| **Conc of DDD(A)** | **Conc of S.S(B)** | **Organic fraction of S.S(C)** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 8.6E+07 | 3.0E+09 | 3.1E+07 |
| + | + | - | 8.6E+07 | 3.0E+09 | 7.8E+06 |
| + | - | + | 8.7E+07 | 3.0E+09 | 6.3E+05 |
| + | - | - | 8.7E+07 | 3.0E+09 | 1.6E+05 |
| - | + | + | 8.6E+05 | 3.0E+07 | 3.1E+05 |
| - | + | - | 8.6E+05 | 3.0E+07 | 7.8E+04 |
| - | - | + | 8.7E+05 | 3.0E+07 | 6.3E+03 |
| - | - | - | 8.7E+05 | 3.0E+07 | 1.6E+03 |

Table B.8 Calculated Effects of Factors and their Interactions on the Associations of DDD with Different Media

| **Factors/Interactions** | **Effect** | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 3.4E+08 | 1.2E+10 | 3.9E+07 |
| B | -1.1E+06 | -3.7E+07 | 3.8E+07 |
| C | -6.6E+05 | -2.3E+07 | 2.4E+07 |
| AB | -1.0E+06 | -3.6E+07 | 3.8E+07 |
| AC | -6.5E+05 | -2.3E+07 | 2.3E+07 |
| BC | -6.4E+05 | -2.2E+07 | 2.3E+07 |
| ABC | -6.3E+05 | -2.2E+07 | 2.3E+07 |

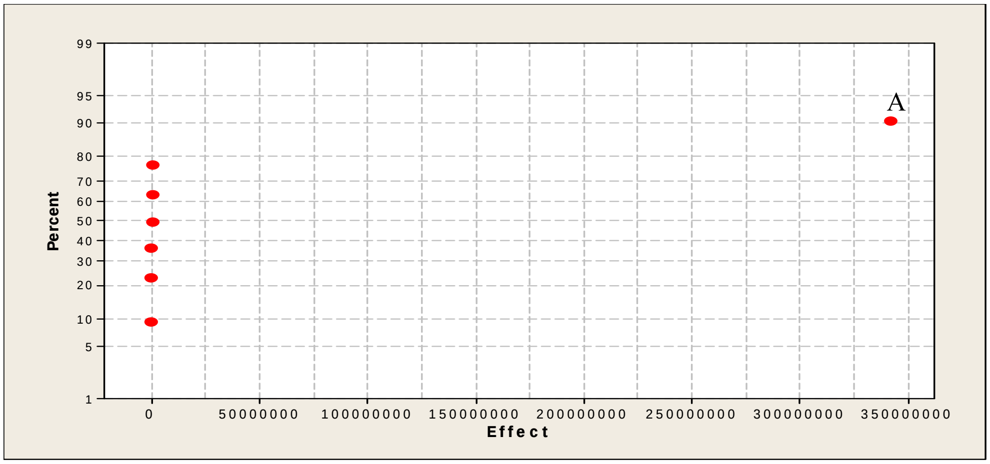


Figure B.10 Probability plot of effects of partitioning of DDD with water

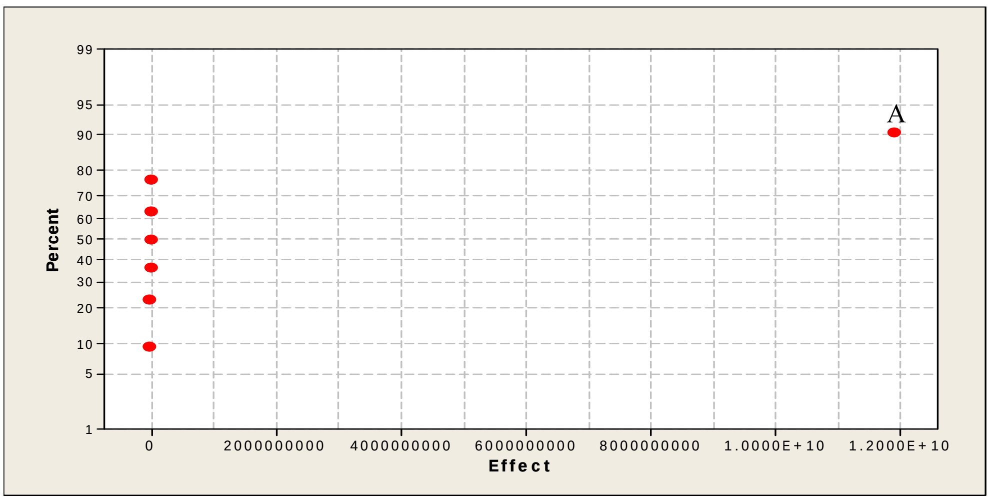


Figure B.11 Probability plot of effects of partitioning of DDD with sediment

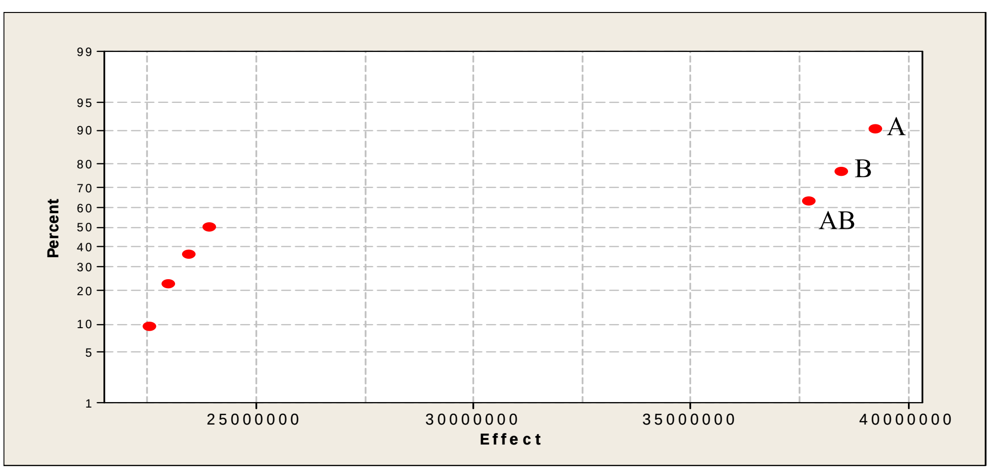


Figure B.12 Probability plot of effects of partitioning of DDD with suspended sediment

Table B.9 Model Predicted Portioning of DDE with $2^3$ Factorial Design Variables

| Factor Value | | | Moles of Analyte Partitioned Into | | |
|---|---|---|---|---|---|
| Conc of DDE(A) | Conc of S.S(B) | Organic fraction of S.S(C) | Water | Sediment | Suspended Sediment |
| + | + | + | 6.6E+08 | 1.6E+09 | 1.7E+07 |
| + | + | - | 6.6E+08 | 1.6E+09 | 4.2E+06 |
| + | - | + | 6.7E+08 | 1.6E+09 | 3.3E+05 |
| + | - | - | 6.7E+08 | 1.6E+09 | 8.3E+04 |
| - | + | + | 6.6E+06 | 1.6E+07 | 1.7E+05 |
| - | + | - | 6.6E+06 | 1.6E+07 | 4.2E+04 |
| - | - | + | 6.7E+06 | 1.6E+07 | 3.3E+03 |
| - | - | - | 6.7E+06 | 1.6E+07 | 8.3E+02 |

Table B.10 Calculated Effects of Factors and their Interactions on the Associations of DDE with Different Media

| Factors/Interactions | Effect | | |
|---|---|---|---|
| | Water | Sediment | Suspended Sediment |
| A | 2.6E+09 | 6.3E+09 | 2.1E+07 |
| B | -4.4E+06 | -1.0E+07 | 2.1E+07 |
| C | -2.7E+06 | -6.5E+06 | 1.3E+07 |
| AB | -4.3E+06 | -1.0E+07 | 2.0E+07 |
| AC | -2.7E+06 | -6.4E+06 | 1.3E+07 |
| BC | -2.6E+06 | -6.3E+06 | 1.2E+07 |
| ABC | -2.6E+06 | -6.2E+06 | 1.2E+07 |

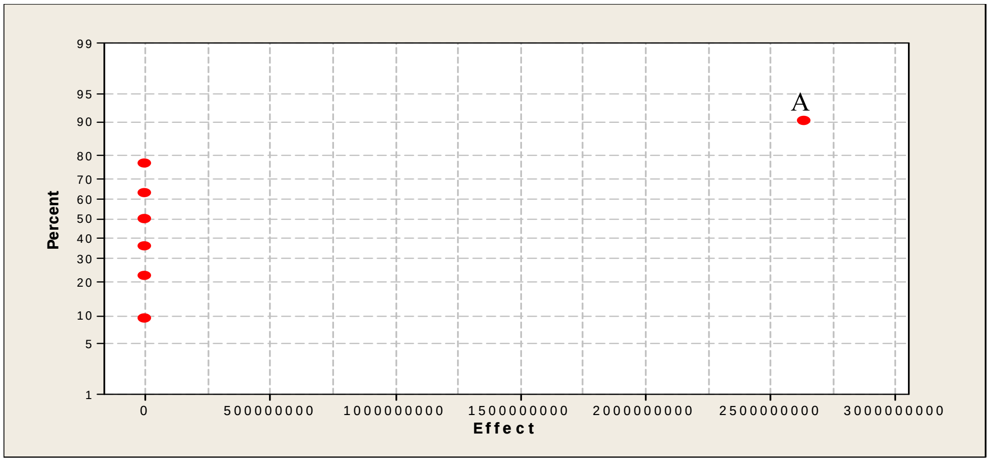


Figure B.13 Probability plot of effects of partitioning of DDE with water

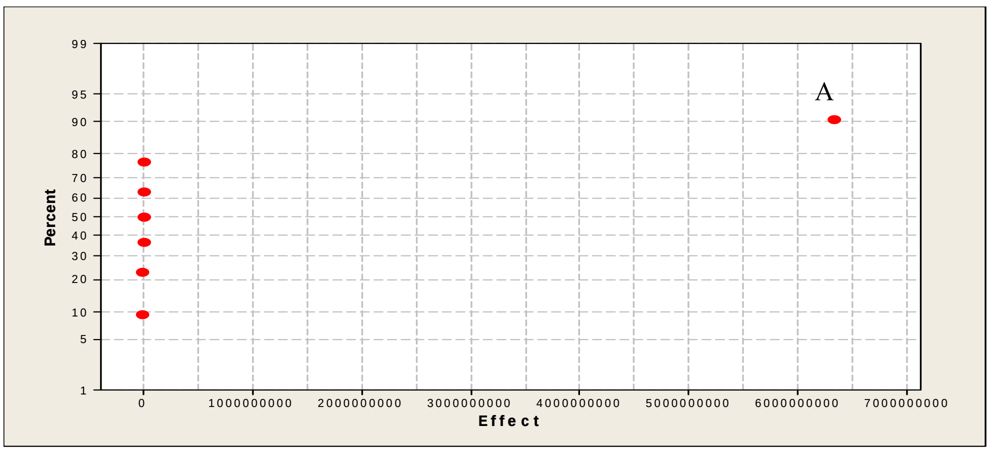


Figure B.14 Probability plot of effects of partitioning of DDE with sediment

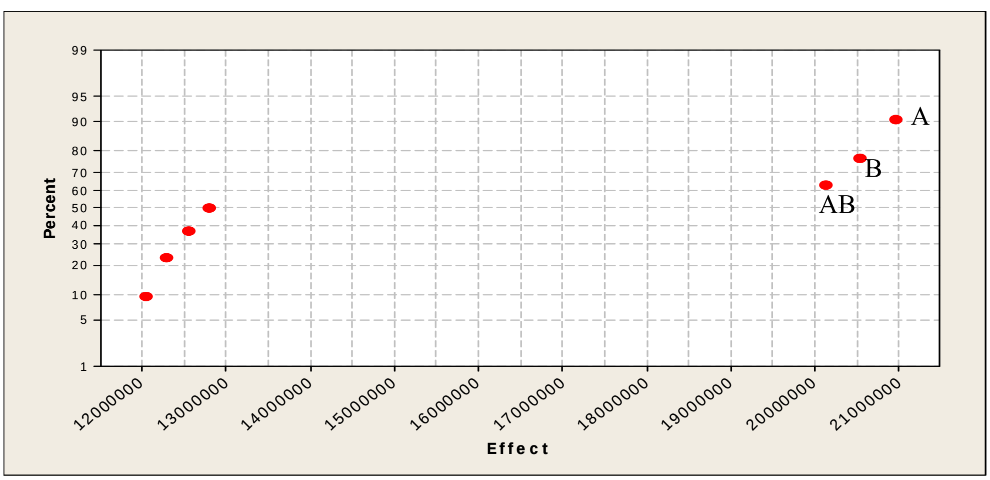


Figure B.15 Probability plot of effects of partitioning of DDE with suspended sediment

Table B.11 Model Predicted Portioning of DDT with $2^3$ Factorial Design Variables

| **Factor Value** | | | **Moles of Analyte Partitioned Into** | | |
|---|---|---|---|---|---|
| **Conc of DDT(A)** | **Conc of S.S(B)** | **Organic fraction of S.S(C)** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 2.1E+08 | 2.5E+09 | 2.6E+07 |
| + | + | - | 2.1E+08 | 2.5E+09 | 6.4E+06 |
| + | - | + | 2.2E+08 | 2.5E+09 | 5.2E+05 |
| + | - | - | 2.2E+08 | 2.5E+09 | 1.3E+05 |
| - | + | + | 2.1E+06 | 2.5E+07 | 2.6E+05 |
| - | + | - | 2.1E+06 | 2.5E+07 | 6.4E+04 |
| - | - | + | 2.2E+06 | 2.5E+07 | 5.2E+03 |
| - | - | - | 2.2E+06 | 2.5E+07 | 1.3E+03 |

Table B.12 Calculated Effects of Factors and their Interactions on the Associations of DDT with Different Media

| **Factors/Interactions** | **Effect** | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 8.5E+08 | 9.8E+09 | 3.2E+07 |
| B | -2.4E+06 | -2.8E+07 | 3.2E+07 |
| C | -1.5E+06 | -1.7E+07 | 2.0E+07 |
| AB | -2.4E+06 | -2.7E+07 | 3.1E+07 |
| AC | -1.5E+06 | -1.7E+07 | 1.9E+07 |
| BC | -1.4E+06 | -1.7E+07 | 1.9E+07 |
| ABC | -1.4E+06 | -1.6E+07 | 1.9E+07 |

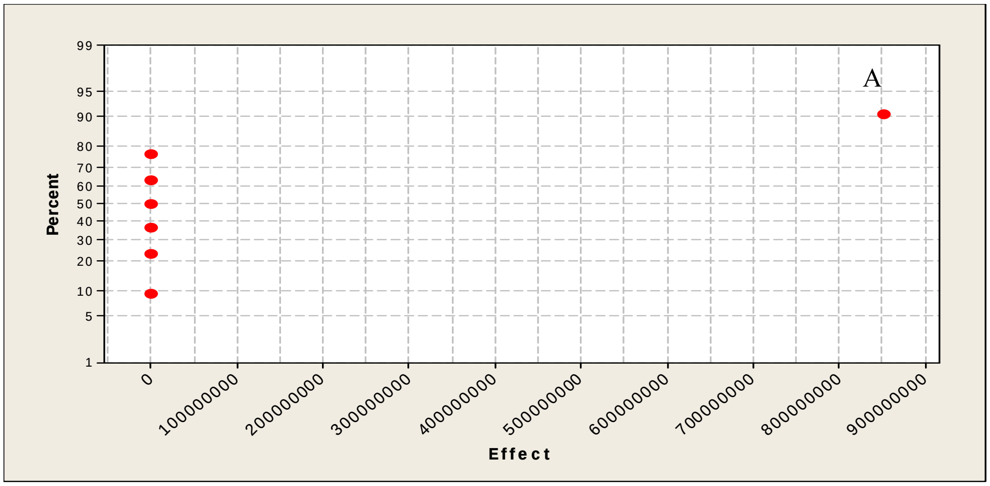


Figure B.16 Probability plot of effects of partitioning of DDT with water

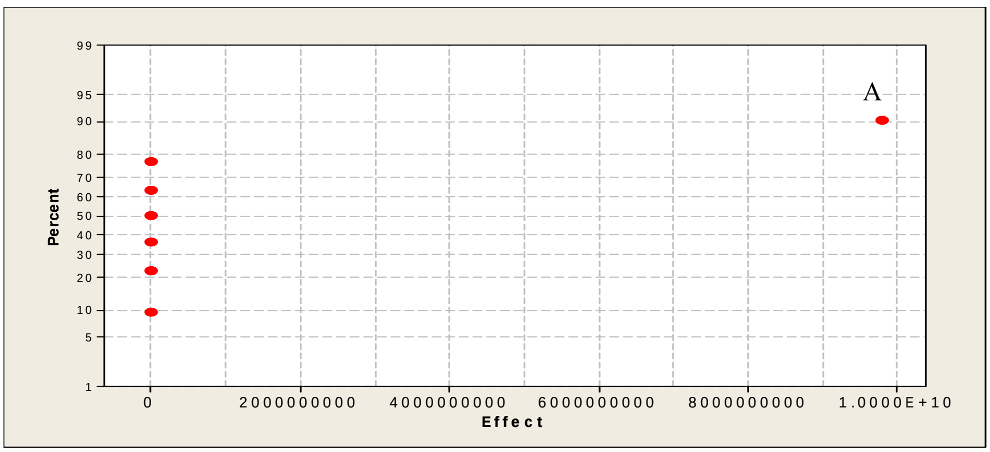


Figure B.17 Probability plot of effects of partitioning of DDT with sediment

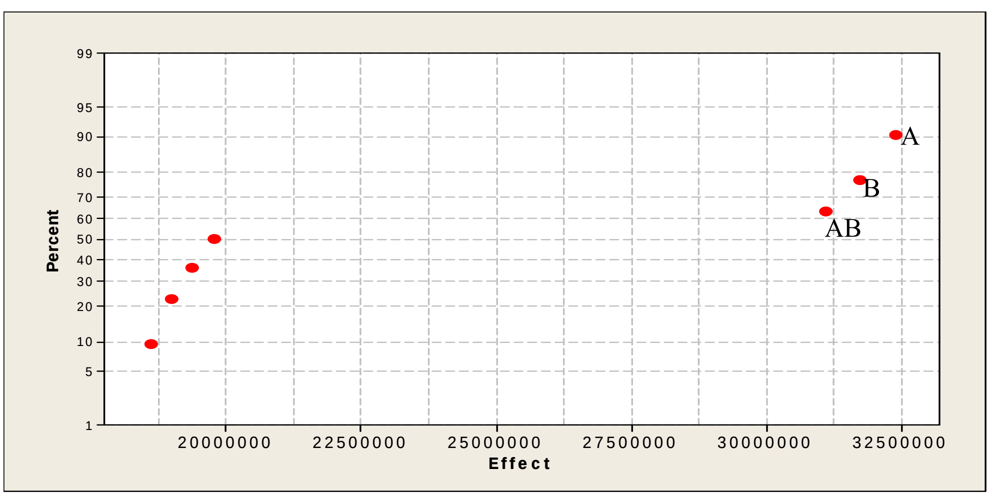


Figure B.18 Probability plot of effects of partitioning of DDT with suspended sediment

Table B.13 Model Predicted Portioning of Dieldrin with $2^3$ Factorial Design Variables

| Factor Value | | | Moles of Analyte Partitioned Into | | |
|---|---|---|---|---|---|
| **Conc of Dieldrin(A)** | **Conc of S.S(B)** | **Organic fraction of S.S(C)** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 1.6E+09 | 6.7E+08 | 7.0E+06 |
| + | + | - | 1.6E+09 | 6.7E+08 | 1.8E+06 |
| + | - | + | 1.6E+09 | 6.7E+08 | 1.4E+05 |
| + | - | - | 1.6E+09 | 6.7E+08 | 3.5E+04 |
| - | + | + | 1.6E+07 | 6.7E+06 | 7.0E+04 |
| - | + | - | 1.6E+07 | 6.7E+06 | 1.8E+04 |
| - | - | + | 1.6E+07 | 6.7E+06 | 1.4E+03 |
| - | - | - | 1.6E+07 | 6.7E+06 | 3.5E+02 |

Table B.14 Calculated Effects of Factors and their Interactions on the Associations of Dieldrin with Different Media

| Factors/Interactions | Effect | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 6.4E+09 | 2.7E+09 | 8.8E+06 |
| B | -5.3E+06 | -2.2E+06 | 8.7E+06 |
| C | -3.3E+06 | -1.4E+06 | 5.4E+06 |
| AB | -5.2E+06 | -2.2E+06 | 8.5E+06 |
| AC | -3.3E+06 | -1.4E+06 | 5.3E+06 |
| BC | -3.2E+06 | -1.3E+06 | 5.2E+06 |
| ABC | -3.1E+06 | -1.3E+06 | 5.1E+06 |

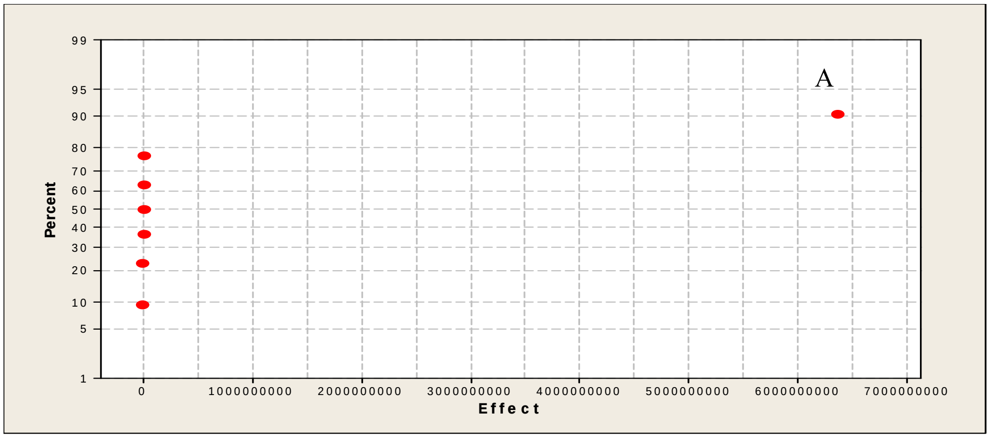


Figure B.19 Probability plot of effects of partitioning of Dieldrin with water

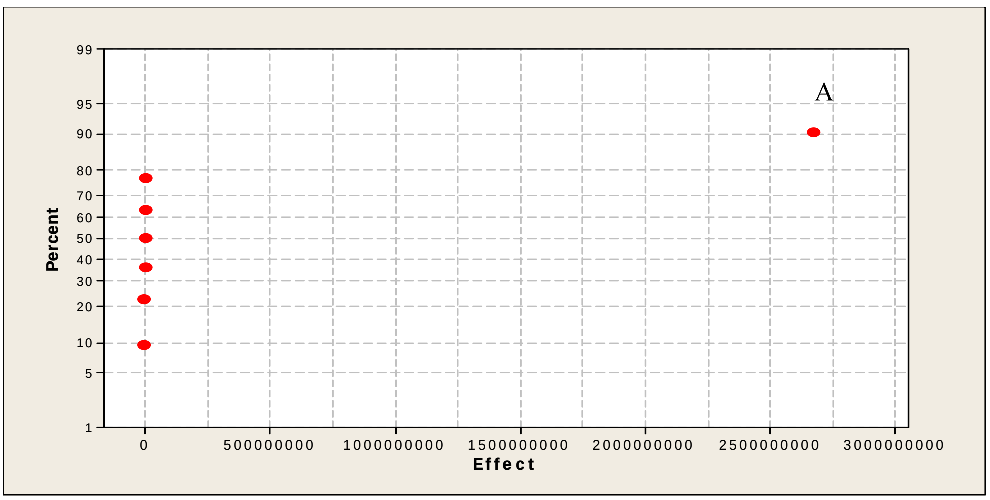


Figure B.20 Probability plot of effects of partitioning of Dieldrin with sediment

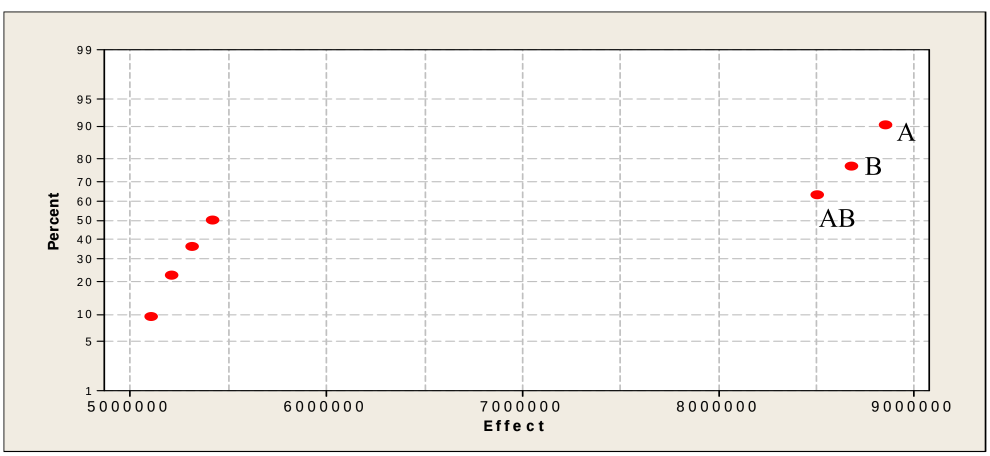


Figure B.21 Probability plot of effects of partitioning of Dieldrin with suspended sediment

Table B.15 Model Predicted Portioning of Endosulfan with $2^3$ Factorial Design Variables

| **Factor Value** | | | **Moles of Analyte Partitioned Into** | | |
|---|---|---|---|---|---|
| **Conc of Endosulfan(A)** | **Conc of S.S(B)** | **Organic fraction of S.S(C)** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 9.9E+08 | 1.4E+08 | 1.4E+06 |
| + | + | - | 9.9E+08 | 1.4E+08 | 3.6E+05 |
| + | - | + | 9.9E+08 | 1.4E+08 | 2.8E+04 |
| + | - | - | 9.9E+08 | 1.4E+08 | 7.1E+03 |
| - | + | + | 9.9E+06 | 1.4E+06 | 1.4E+04 |
| - | + | - | 9.9E+06 | 1.4E+06 | 3.6E+03 |
| - | - | + | 9.9E+06 | 1.4E+06 | 2.8E+02 |
| - | - | - | 9.9E+06 | 1.4E+06 | 7.1E+01 |

Table B.16 Calculated Effects of Factors and their Interactions on the Associations of Endosulfan with Different Media

| **Factors/Interactions** | **Effect** | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 3.9E+09 | 5.4E+08 | 1.8E+06 |
| B | -7.1E+05 | -9.8E+04 | 1.8E+06 |
| C | -4.4E+05 | -6.1E+04 | 1.1E+06 |
| AB | -6.9E+05 | -9.6E+04 | 1.7E+06 |
| AC | -4.3E+05 | -6.0E+04 | 1.1E+06 |
| BC | -4.2E+05 | -5.9E+04 | 1.1E+06 |
| ABC | -4.2E+05 | -5.8E+04 | 1.0E+06 |

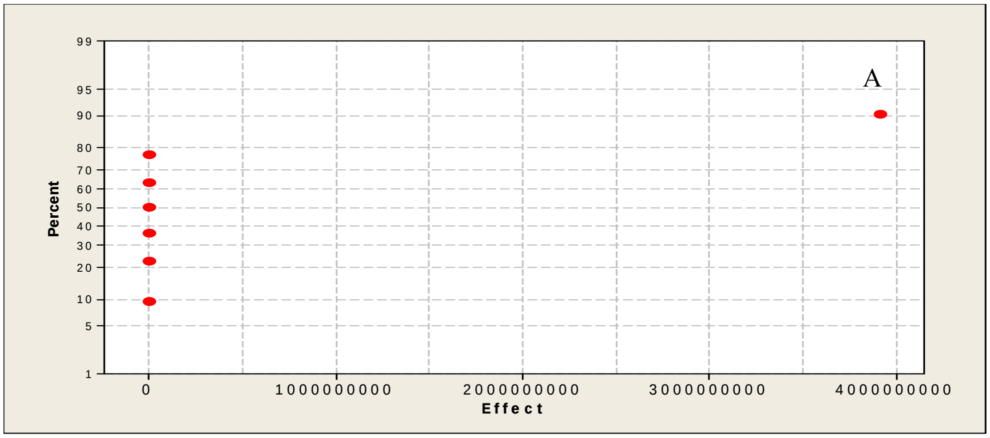


Figure B.22 Probability plot of effects of partitioning of Endosulfan with water

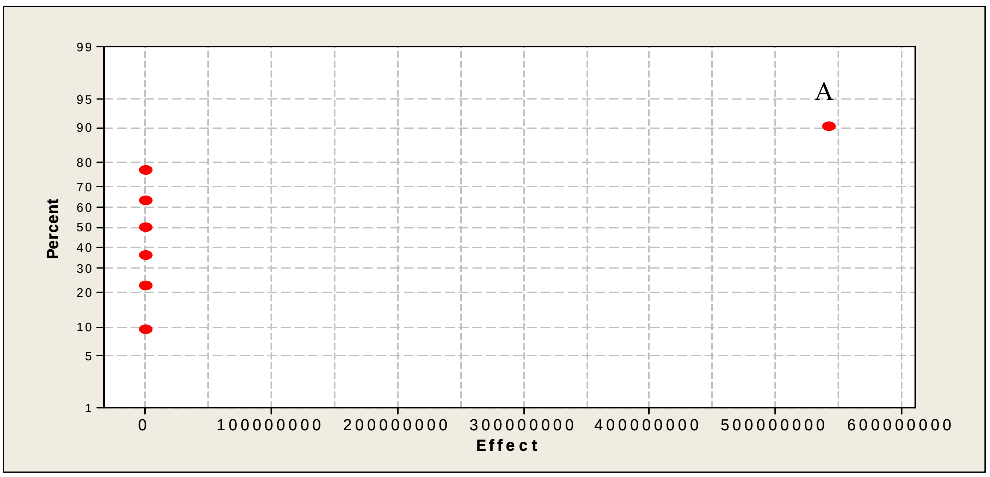


Figure B.23 Probability plot of effects of partitioning of Endosulfan with sediment

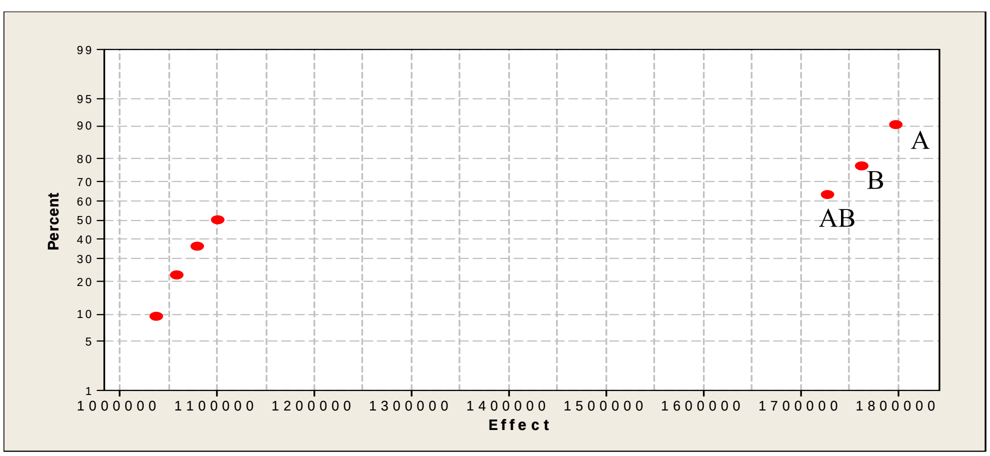


Figure B.24 Probability plot of effects of partitioning of Endosulfan with suspended sediment

Table B.17 Model Predicted Portioning of Endrin with $2^3$ Factorial Design Variables

| Factor Value | | | Moles of Analyte Partitioned Into | | |
|---|---|---|---|---|---|
| Conc of Endrin(A) | Conc of S.S(B) | Organic fraction of S.S(C) | Water | Sediment | Suspended Sediment |
| + | + | + | 1.6E+09 | 7.8E+08 | 8.1E+06 |
| + | + | - | 1.6E+09 | 7.8E+08 | 2.0E+06 |
| + | - | + | 1.6E+09 | 7.8E+08 | 1.6E+05 |
| + | - | - | 1.6E+09 | 7.8E+08 | 4.1E+04 |
| - | + | + | 1.6E+07 | 7.8E+06 | 8.1E+04 |
| - | + | - | 1.6E+07 | 7.8E+06 | 2.0E+04 |
| - | - | + | 1.6E+07 | 7.8E+06 | 1.6E+03 |
| - | - | - | 1.6E+07 | 7.8E+06 | 4.1E+02 |

Table B.18 Calculated Effects of Factors and their Interactions on the Associations of Endrin with Different Media

| Factors/Interactions | Effect | | |
|---|---|---|---|
| | Water | Sediment | Suspended Sediment |
| A | 6.4E+09 | 3.1E+09 | 1.0E+07 |
| B | -6.2E+06 | -3.0E+06 | 1.0E+07 |
| C | -3.9E+06 | -1.9E+06 | 6.2E+06 |
| AB | -6.1E+06 | -2.9E+06 | 9.8E+06 |
| AC | -3.8E+06 | -1.8E+06 | 6.1E+06 |
| BC | -3.7E+06 | -1.8E+06 | 6.0E+06 |
| ABC | -3.6E+06 | -1.7E+06 | 5.9E+06 |

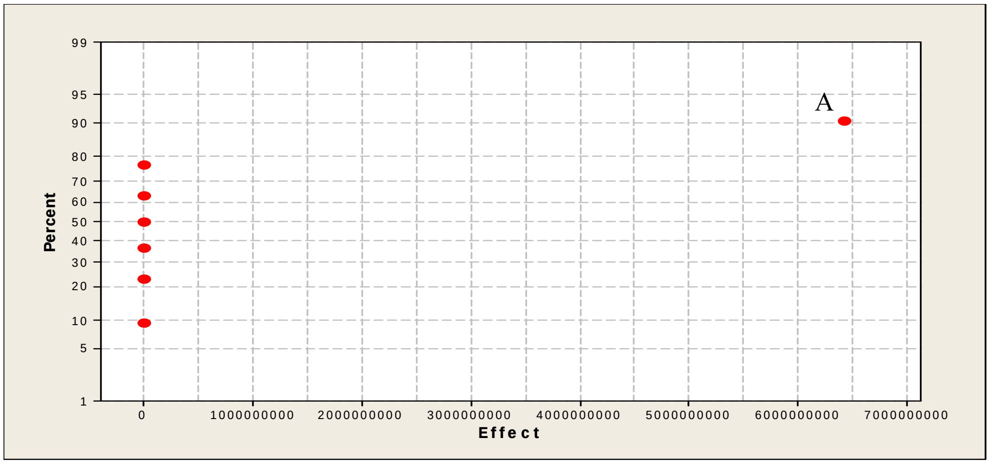


Figure B.25 Probability plot of effects of partitioning of Endrin with water

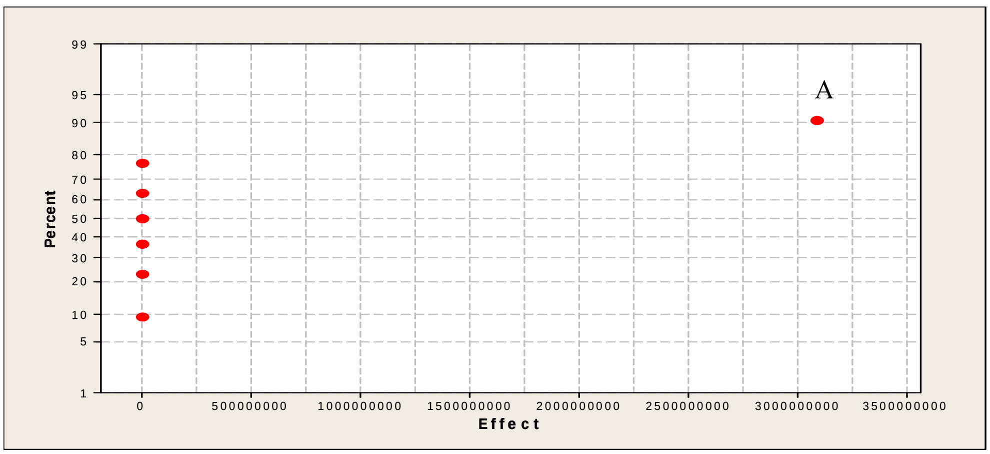


Figure B.26 Probability plot of effects of partitioning of Endrin with sediment

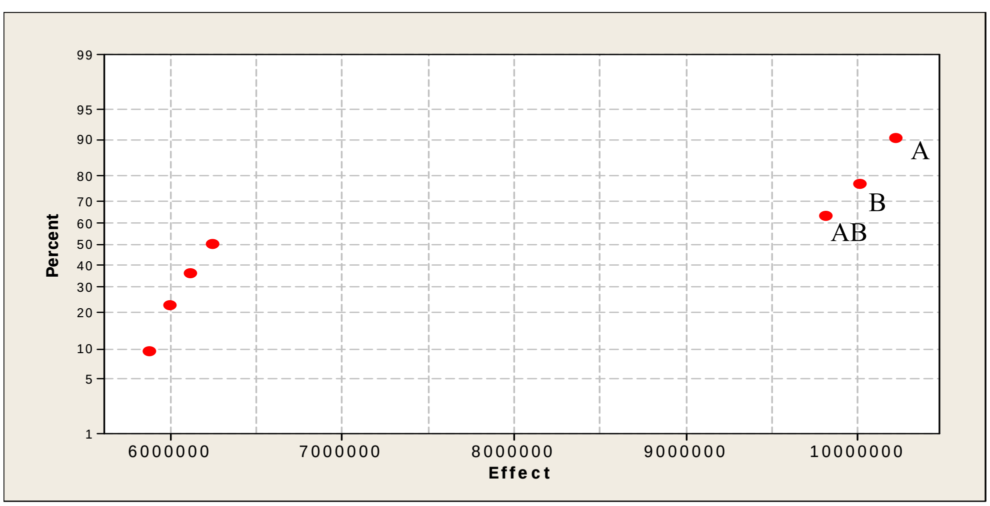


Figure B.27 Probability plot of effects of partitioning of Endrin with suspended sediment

Table B.19 Model Predicted Portioning of Etridiazole with $2^3$ Factorial Design Variables

| **Factor Value** | | | **Moles of Analyte Partitioned Into** | | |
|---|---|---|---|---|---|
| **Conc of Etridiazole(A)** | **Conc of S.S(B)** | **Organic fraction of S.S(C)** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 2.4E+09 | 1.2E+08 | 1.2E+06 |
| + | + | - | 2.4E+09 | 1.2E+08 | 3.0E+05 |
| + | - | + | 2.4E+09 | 1.2E+08 | 2.4E+04 |
| + | - | - | 2.4E+09 | 1.2E+08 | 6.1E+03 |
| - | + | + | 2.4E+07 | 1.2E+06 | 1.2E+04 |
| - | + | - | 2.4E+07 | 1.2E+06 | 3.0E+03 |
| - | - | + | 2.4E+07 | 1.2E+06 | 2.4E+02 |
| - | - | - | 2.4E+07 | 1.2E+06 | 6.1E+01 |

Table B.20 Calculated Effects of Factors and their Interactions on the Associations of Etridiazole with Different Media

| **Factors/Interactions** | **Effect** | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 9.6E+09 | 4.6E+08 | 1.5E+06 |
| B | -9.1E+05 | -4.3E+04 | 1.5E+06 |
| C | -5.7E+05 | -2.7E+04 | 9.4E+05 |
| AB | -8.9E+05 | -4.3E+04 | 1.5E+06 |
| AC | -5.5E+05 | -2.7E+04 | 9.2E+05 |
| BC | -5.4E+05 | -2.6E+04 | 9.0E+05 |
| ABC | -5.3E+05 | -2.6E+04 | 8.8E+05 |

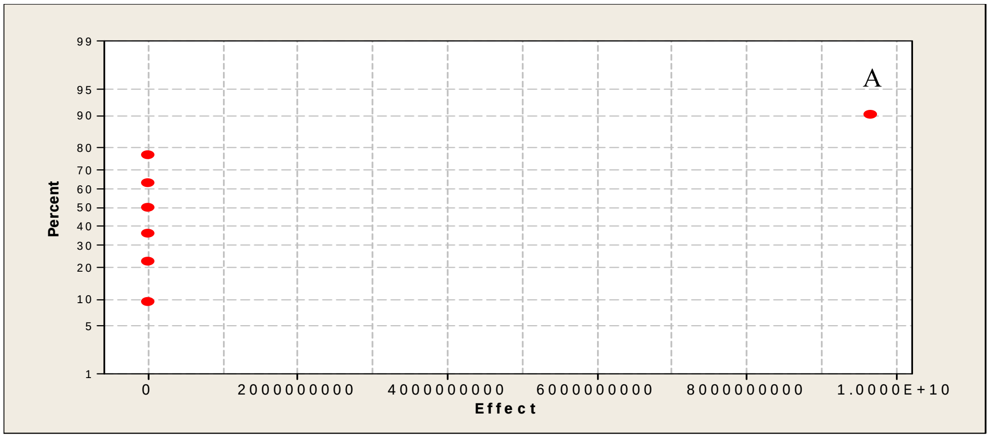


Figure B.28 Probability plot of effects of partitioning of Etridiazole with water

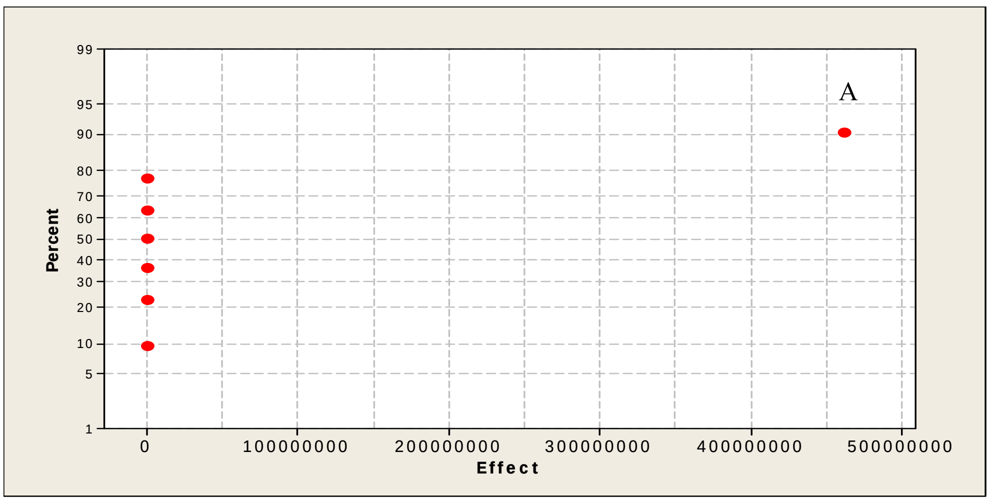


Figure B.29 Probability plot of effects of partitioning of Etridiazole with sediment

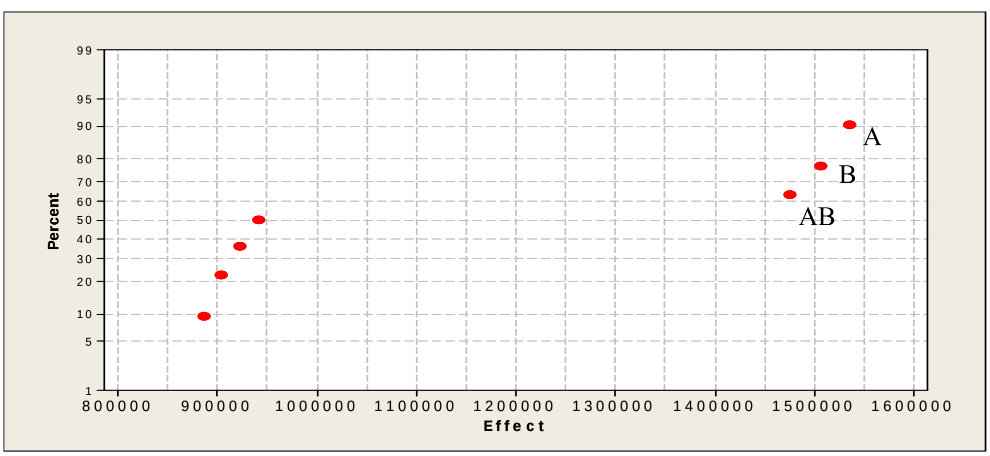


Figure B.30 Probability plot of effects of partitioning of Etridiazole with suspended sediment

Table B.21 Model Predicted Portioning of HCH-α with $2^3$ Factorial Design Variables

| **Factor Value** | | | **Moles of Analyte Partitioned Into** | | |
|---|---|---|---|---|---|
| **Conc of HCH-α(A)** | **Conc of S.S(B)** | **Organic fraction of S.S(C)** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 2.8E+09 | 2.8E+08 | 2.9E+06 |
| + | + | - | 2.8E+09 | 2.8E+08 | 7.3E+05 |
| + | - | + | 2.8E+09 | 2.8E+08 | 5.8E+04 |
| + | - | - | 2.8E+09 | 2.8E+08 | 1.5E+04 |
| - | + | + | 2.8E+07 | 2.8E+06 | 2.9E+04 |
| - | + | - | 2.8E+07 | 2.8E+06 | 7.3E+03 |
| - | - | + | 2.8E+07 | 2.8E+06 | 5.8E+02 |
| - | - | - | 2.8E+07 | 2.8E+06 | 1.5E+02 |

Table B.22 Calculated Effects of Factors and their Interactions on the Associations of HCH-α with Different Media

| **Factors/Interactions** | **Effect** | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 1.1E+10 | 1.1E+09 | 3.7E+06 |
| B | -2.9E+06 | -2.9E+05 | 3.6E+06 |
| C | -1.8E+06 | -1.8E+05 | 2.2E+06 |
| AB | -2.8E+06 | -2.9E+05 | 3.5E+06 |
| AC | -1.8E+06 | -1.8E+05 | 2.2E+06 |
| BC | -1.7E+06 | -1.7E+05 | 2.2E+06 |
| ABC | -1.7E+06 | -1.7E+05 | 2.1E+06 |

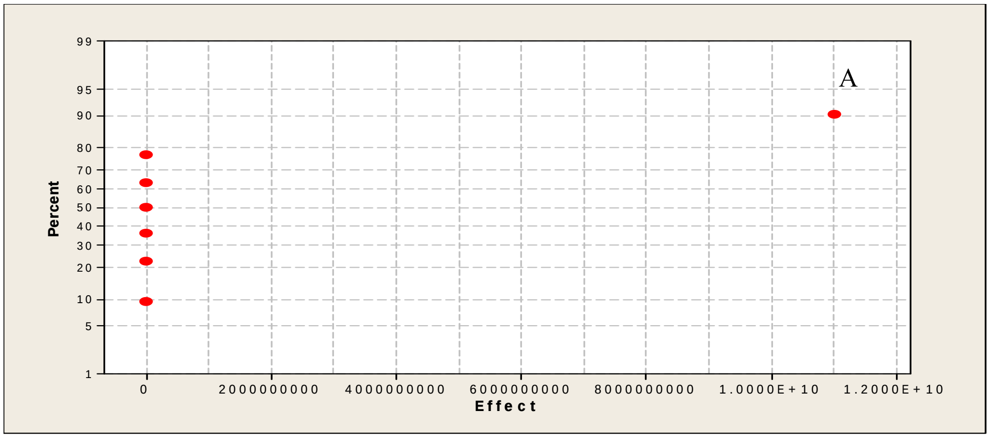


Figure B.31 Probability plot of effects of partitioning of HCH-α with water

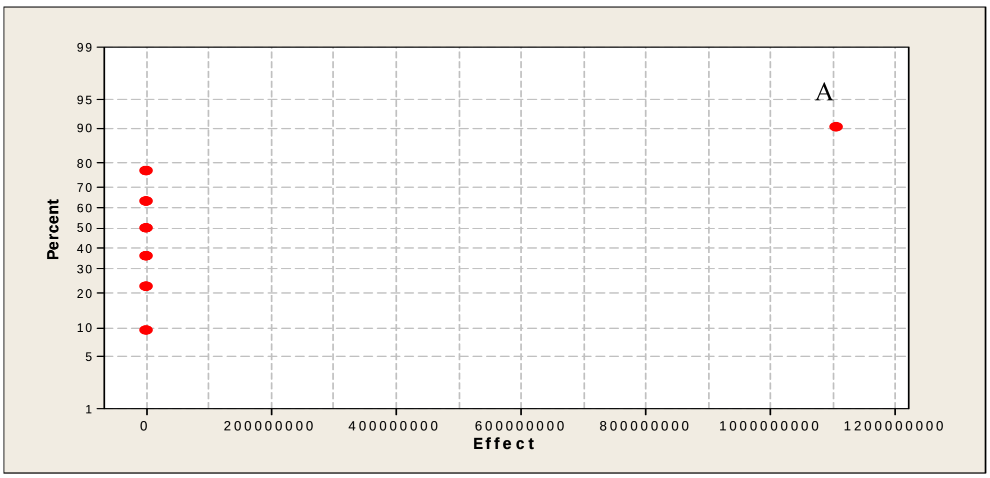


Figure B.32 Probability plot of effects of partitioning of HCH-α with sediment

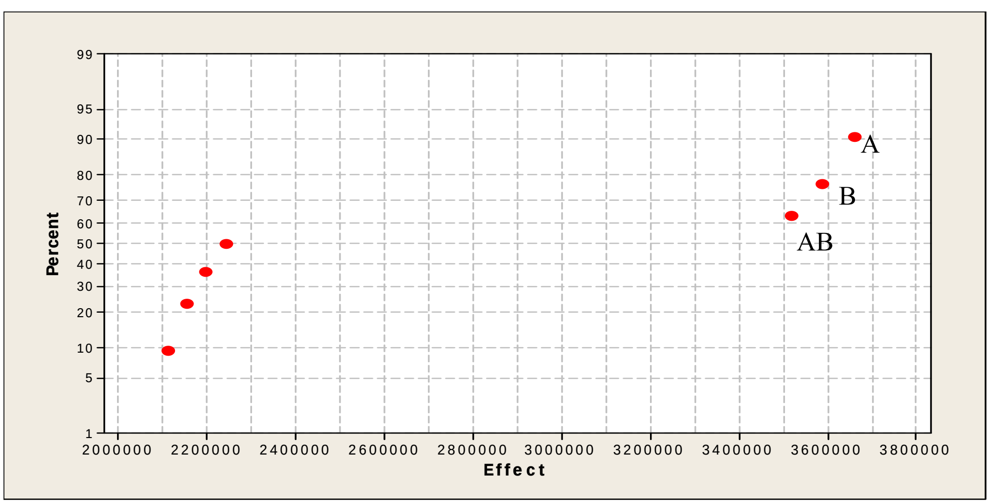


Figure B.33 Probability plot of effects of partitioning of HCH-α with suspended sediment

Table B.23 Model Predicted Portioning of HCH-β with $2^3$ Factorial Design Variables

| Factor Value | | | Moles of Analyte Partitioned Into | | |
|---|---|---|---|---|---|
| Conc of HCH-β(A) | Conc of S.S(B) | Organic fraction of S.S(C) | Water | Sediment | Suspended Sediment |
| + | + | + | 2.3E+09 | 1.1E+09 | 1.1E+07 |
| + | + | - | 2.3E+09 | 1.1E+09 | 2.8E+06 |
| + | - | + | 2.3E+09 | 1.1E+09 | 2.2E+05 |
| + | - | - | 2.3E+09 | 1.1E+09 | 5.6E+04 |
| - | + | + | 2.3E+07 | 1.1E+07 | 1.1E+05 |
| - | + | - | 2.3E+07 | 1.1E+07 | 2.8E+04 |
| - | - | + | 2.3E+07 | 1.1E+07 | 2.2E+03 |
| - | - | - | 2.3E+07 | 1.1E+07 | 5.6E+02 |

Table B.24 Calculated Effects of Factors and their Interactions on the Associations of HCH-β with Different Media

| Factors/Interactions | Effect | | |
|---|---|---|---|
| | Water | Sediment | Suspended Sediment |
| A | 9.3E+09 | 4.2E+09 | 1.4E+07 |
| B | -9.4E+06 | -4.3E+06 | 1.4E+07 |
| C | -5.9E+06 | -2.7E+06 | 8.6E+06 |
| AB | -9.2E+06 | -4.2E+06 | 1.4E+07 |
| AC | -5.8E+06 | -2.6E+06 | 8.4E+06 |
| BC | -5.6E+06 | -2.6E+06 | 8.3E+06 |
| ABC | -5.5E+06 | -2.5E+06 | 8.1E+06 |

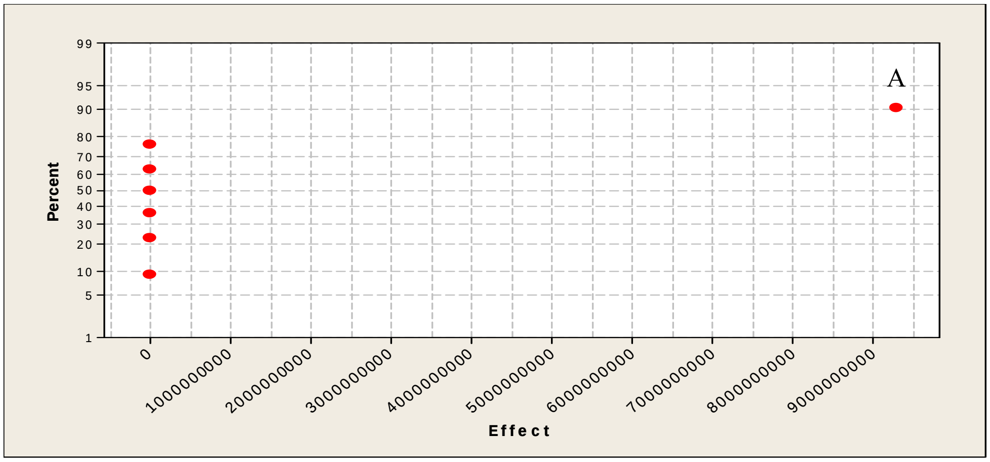


Figure B.34 Probability plot of effects of partitioning of HCH-β with water

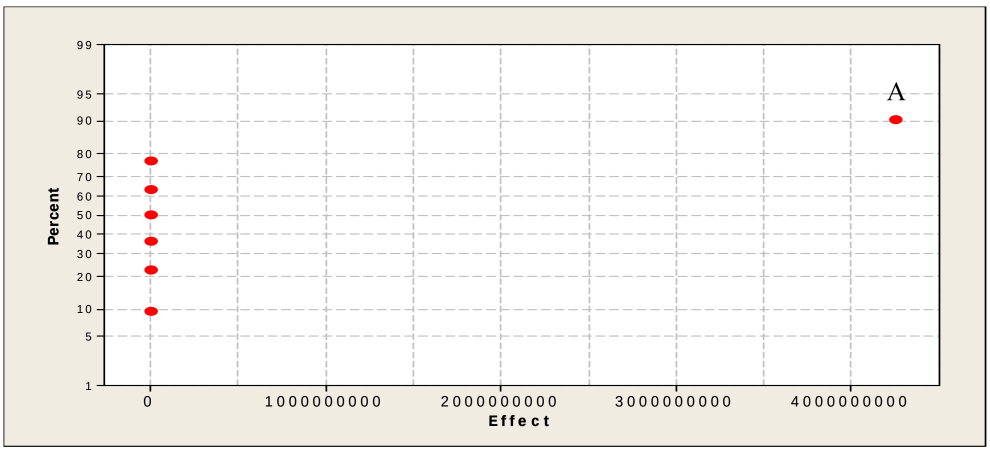


Figure B.35 Probability plot of effects of partitioning of HCH-β with sediment

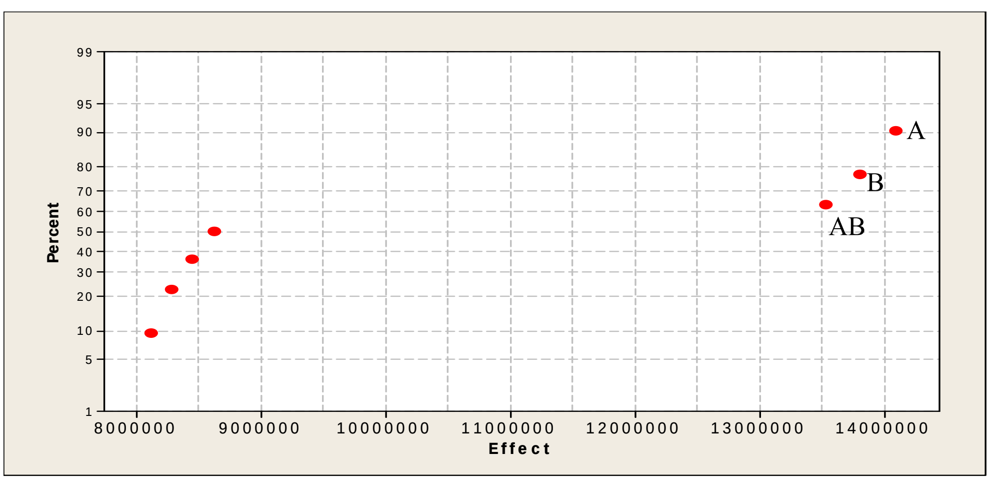


Figure B.36 Probability plot of effects of partitioning of HCH-β with suspended sediment

Table B.25 Model Predicted Portioning of HCH-δ with $2^3$ Factorial Design Variables

| Factor Value | | | Moles of Analyte Partitioned Into | | |
|---|---|---|---|---|---|
| Conc of HCH-δ(A) | Conc of S.S(B) | Organic fraction of S.S(C) | Water | Sediment | Suspended Sediment |
| + | + | + | 3.3E+09 | 1.0E+08 | 1.1E+06 |
| + | + | - | 3.3E+09 | 1.0E+08 | 2.7E+05 |
| + | - | + | 3.3E+09 | 1.0E+08 | 2.2E+04 |
| + | - | - | 3.3E+09 | 1.0E+08 | 5.5E+03 |
| - | + | + | 3.3E+07 | 1.0E+06 | 1.1E+04 |
| - | + | - | 3.3E+07 | 1.0E+06 | 2.7E+03 |
| - | - | + | 3.3E+07 | 1.0E+06 | 2.2E+02 |
| - | - | - | 3.3E+07 | 1.0E+06 | 5.5E+01 |

Table B.26 Calculated Effects of Factors and their Interactions on the Associations of HCH-δ with Different Media

| Factors/Interactions | Effect | | |
|---|---|---|---|
| | Water | Sediment | Suspended Sediment |
| A | 1.3E+10 | 4.1E+08 | 1.4E+06 |
| B | -1.3E+06 | -4.1E+04 | 1.4E+06 |
| C | -8.1E+05 | -2.6E+04 | 8.4E+05 |
| AB | -1.3E+06 | -4.0E+04 | 1.3E+06 |
| AC | -7.9E+05 | -2.5E+04 | 8.3E+05 |
| BC | -7.8E+05 | -2.5E+04 | 8.1E+05 |
| ABC | -7.6E+05 | -2.4E+04 | 7.9E+05 |

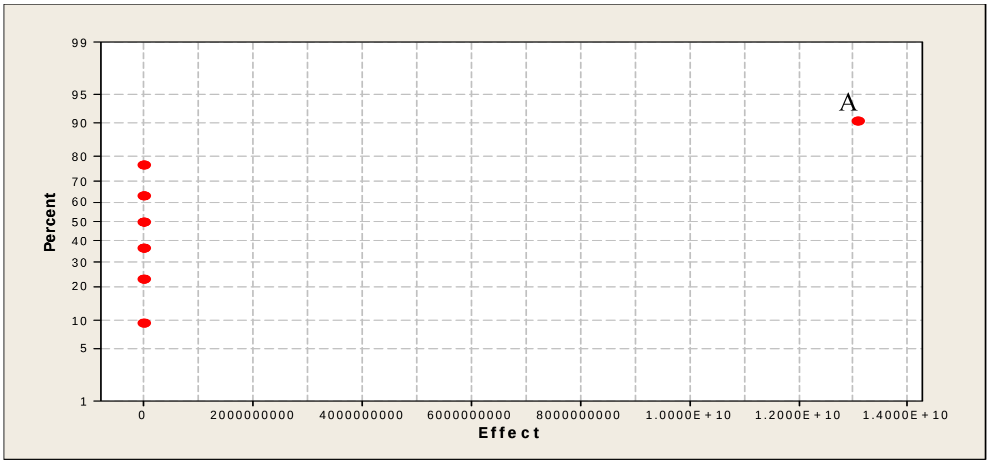


Figure B.37 Probability plot of effects of partitioning of HCH-δ with water

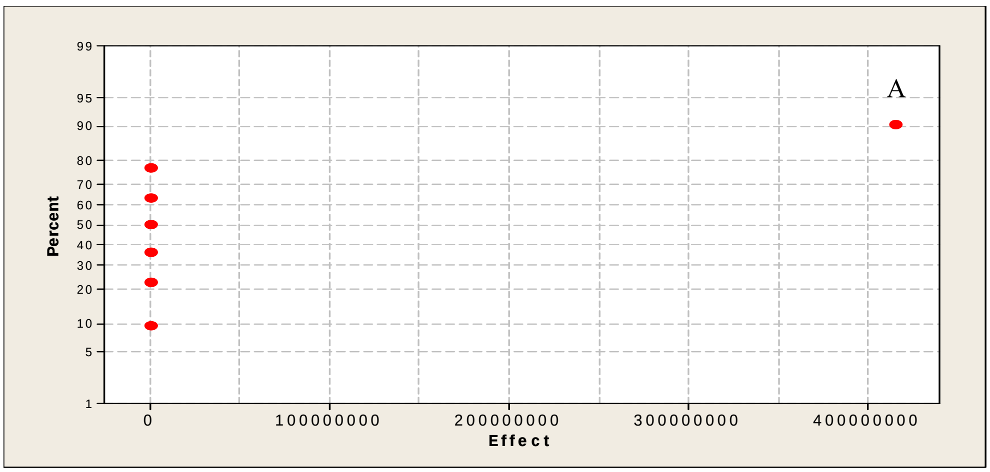


Figure B.38 Probability plot of effects of partitioning of HCH-δ with sediment

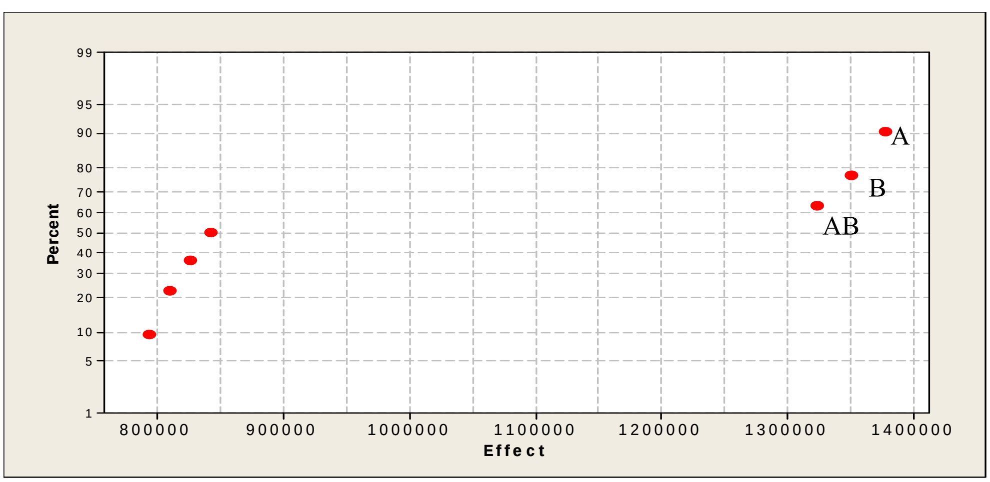


Figure B.39 Probability plot of effects of partitioning of HCH-δ with suspended sediment

Table B.27 Model Predicted Portioning of HCH-γ with $2^3$ Factorial Design Variables

| Factor Value | | | Moles of Analyte Partitioned Into | | |
|---|---|---|---|---|---|
| **Conc of HCH-γ(A)** | **Conc of S.S(B)** | **Organic fraction of S.S(C)** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 3.0E+09 | 1.5E+08 | 1.6E+06 |
| + | + | - | 3.0E+09 | 1.5E+08 | 4.0E+05 |
| + | - | + | 3.0E+09 | 1.5E+08 | 3.2E+04 |
| + | - | - | 3.0E+09 | 1.5E+08 | 8.0E+03 |
| - | + | + | 3.0E+07 | 1.5E+06 | 1.6E+04 |
| - | + | - | 3.0E+07 | 1.5E+06 | 4.0E+03 |
| - | - | + | 3.0E+07 | 1.5E+06 | 3.2E+02 |
| - | - | - | 3.0E+07 | 1.5E+06 | 8.0E+01 |

Table B.28 Calculated Effects of Factors and their Interactions on the Associations of HCH-γ with Different Media

| Factors/Interactions | Effect | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 1.2E+10 | 6.1E+08 | 2.0E+06 |
| B | -1.7E+06 | -8.8E+04 | 2.0E+06 |
| C | -1.1E+06 | -5.5E+04 | 1.2E+06 |
| AB | -1.7E+06 | -8.6E+04 | 1.9E+06 |
| AC | -1.0E+06 | -5.4E+04 | 1.2E+06 |
| BC | -1.0E+06 | -5.2E+04 | 1.2E+06 |
| ABC | -1.0E+06 | -5.1E+04 | 1.2E+06 |

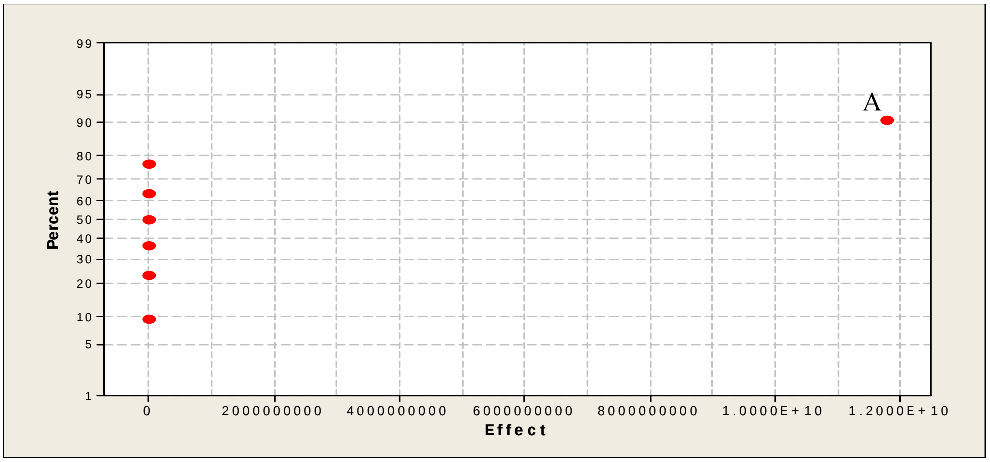


Figure B.40 Probability plot of effects of partitioning of HCH-γ with water

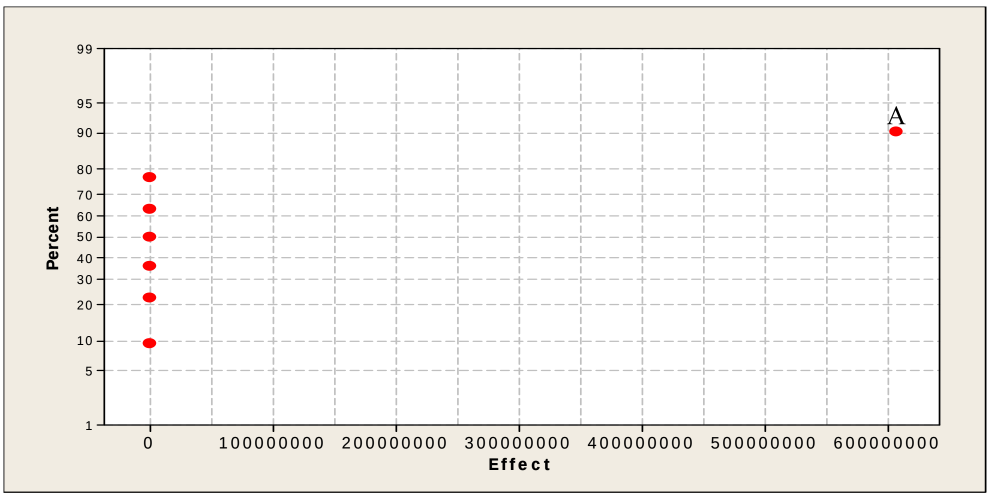


Figure B.41 Probability plot of effects of partitioning of HCH-γ with sediment

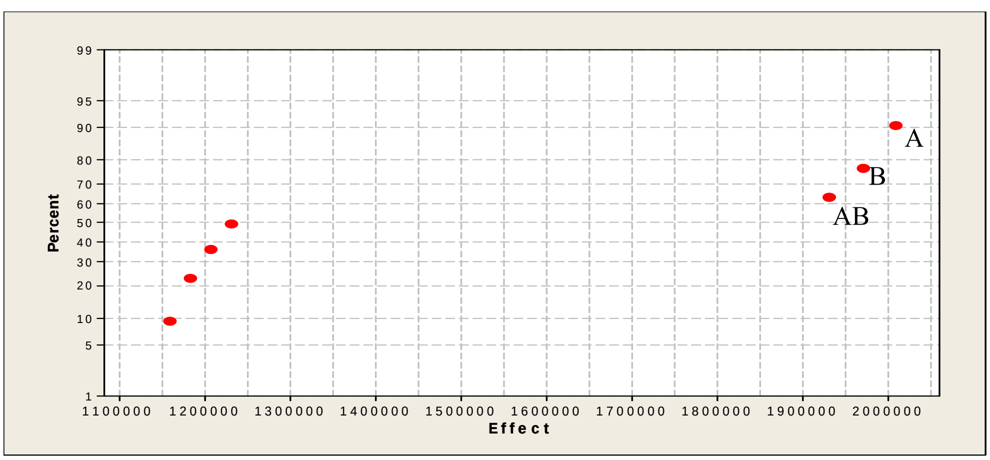


Figure B.42 Probability plot of effects of partitioning of HCH-γ with suspended sediment

Table B.29 Model Predicted Portioning of Heptachlor with $2^3$ Factorial Design Variables

| **Factor Value** | | | **Moles of Analyte Partitioned Into** | | |
|---|---|---|---|---|---|
| **Conc of Heptachlor(A)** | **Conc of S.S(B)** | **Organic fraction of S.S(C)** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 3.3E+08 | 3.8E+08 | 3.9E+06 |
| + | + | - | 3.3E+08 | 3.8E+08 | 9.8E+05 |
| + | - | + | 3.3E+08 | 3.8E+08 | 7.9E+04 |
| + | - | - | 3.3E+08 | 3.8E+08 | 2.0E+04 |
| - | + | + | 3.3E+06 | 3.8E+06 | 3.9E+04 |
| - | + | - | 3.3E+06 | 3.8E+06 | 9.8E+03 |
| - | - | + | 3.3E+06 | 3.8E+06 | 7.9E+02 |
| - | - | - | 3.3E+06 | 3.8E+06 | 2.0E+02 |

Table B.30 Calculated Effects of Factors and their Interactions on the Associations of Heptachlor with Different Media

| **Factors/Interactions** | **Effect** | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 1.3E+09 | 1.5E+09 | 5.0E+06 |
| B | -5.9E+05 | -6.9E+05 | 4.9E+06 |
| C | -3.7E+05 | -4.3E+05 | 3.0E+06 |
| AB | -5.8E+05 | -6.7E+05 | 4.8E+06 |
| AC | -3.6E+05 | -4.2E+05 | 3.0E+06 |
| BC | -3.6E+05 | -4.1E+05 | 2.9E+06 |
| ABC | -3.5E+05 | -4.0E+05 | 2.9E+06 |

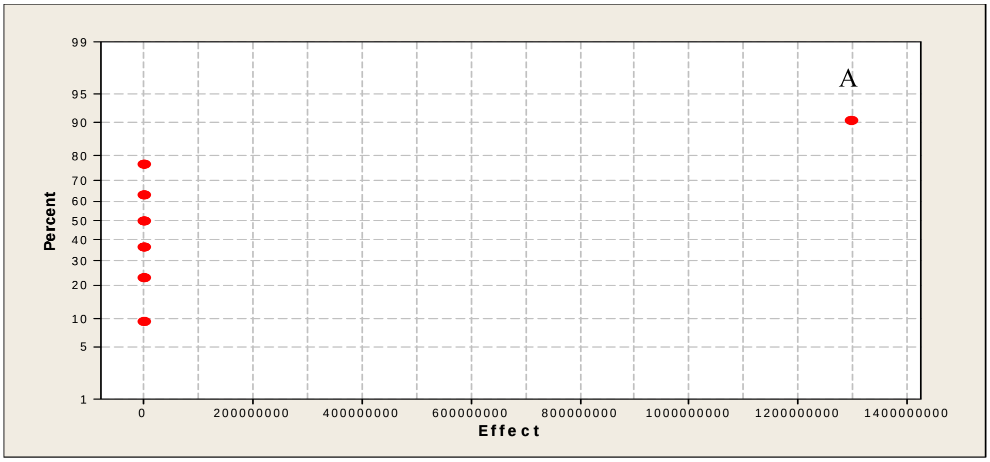


Figure B.43 Probability plot of effects of partitioning of Heptachlor with water

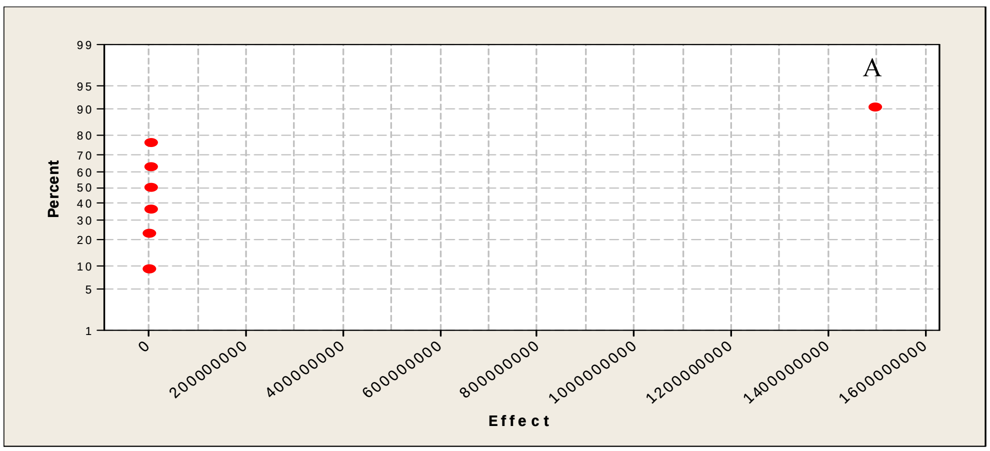


Figure B.44 Probability plot of effects of partitioning of Heptachlor with sediment

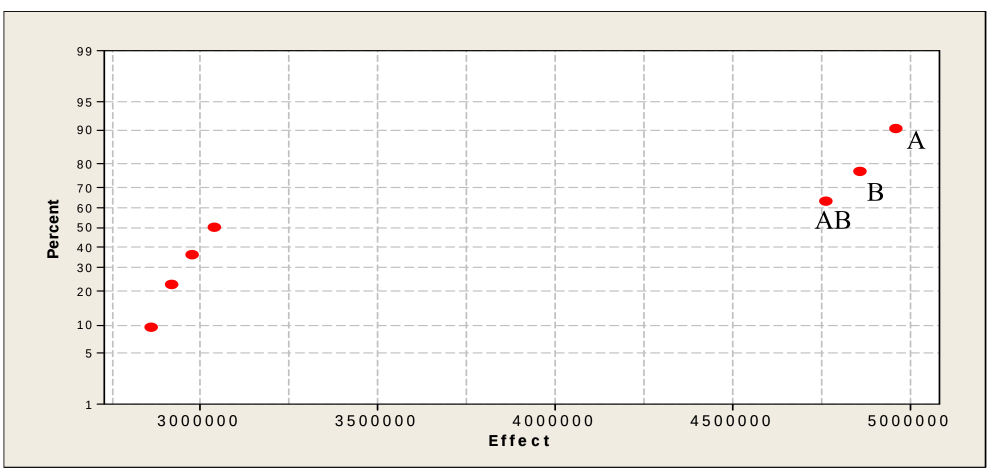


Figure B.45 Probability plot of effects of partitioning of Heptachlor with suspended sediment

Table B.31 Model Predicted Portioning of Heptachlor epoxide with $2^3$ Factorial Design Variables

| **Factor Value** | | | **Moles of Analyte Partitioned Into** | | |
|---|---|---|---|---|---|
| **Conc of Heptachlor epoxide(A)** | **Conc of S.S(B)** | **Organic fraction of S.S(C)** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 1.3E+09 | 4.7E+08 | 4.9E+06 |
| + | + | - | 1.3E+09 | 4.7E+08 | 1.2E+06 |
| + | - | + | 1.3E+09 | 4.7E+08 | 9.8E+04 |
| + | - | - | 1.3E+09 | 4.7E+08 | 2.5E+04 |
| - | + | + | 1.3E+07 | 4.7E+06 | 4.9E+04 |
| - | + | - | 1.3E+07 | 4.7E+06 | 1.2E+04 |
| - | - | + | 1.3E+07 | 4.7E+06 | 9.8E+02 |
| - | - | - | 1.3E+07 | 4.7E+06 | 2.5E+02 |

Table B.32 Calculated Effects of Factors and their Interactions on the Associations of Heptachlor epoxide with Different Media

| **Factors/Interactions** | **Effect** | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 5.0E+09 | 1.9E+09 | 6.2E+06 |
| B | -3.0E+06 | -1.1E+06 | 6.1E+06 |
| C | -1.9E+06 | -6.9E+05 | 3.8E+06 |
| AB | -2.9E+06 | -1.1E+06 | 5.9E+06 |
| AC | -1.8E+06 | -6.8E+05 | 3.7E+06 |
| BC | -1.8E+06 | -6.7E+05 | 3.6E+06 |
| ABC | -1.7E+06 | -6.5E+05 | 3.6E+06 |

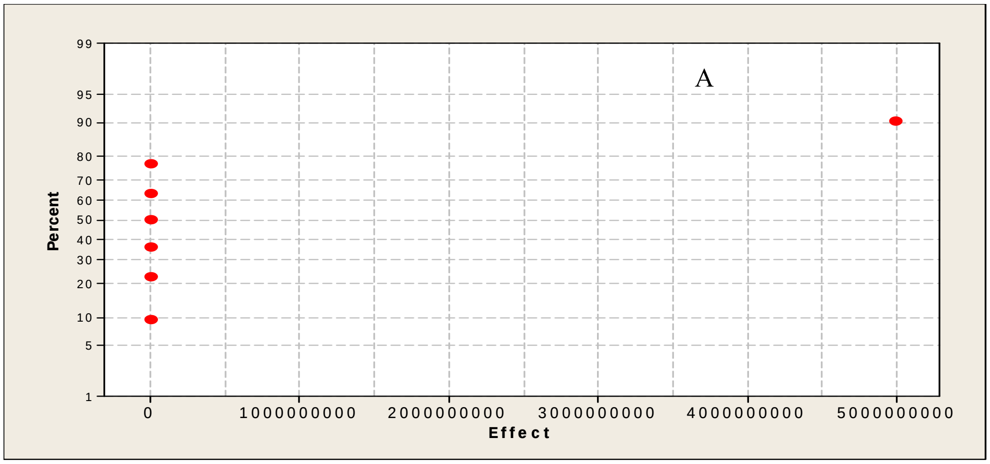


Figure B.46 Probability plot of effects of partitioning of Heptachlor epoxide with water

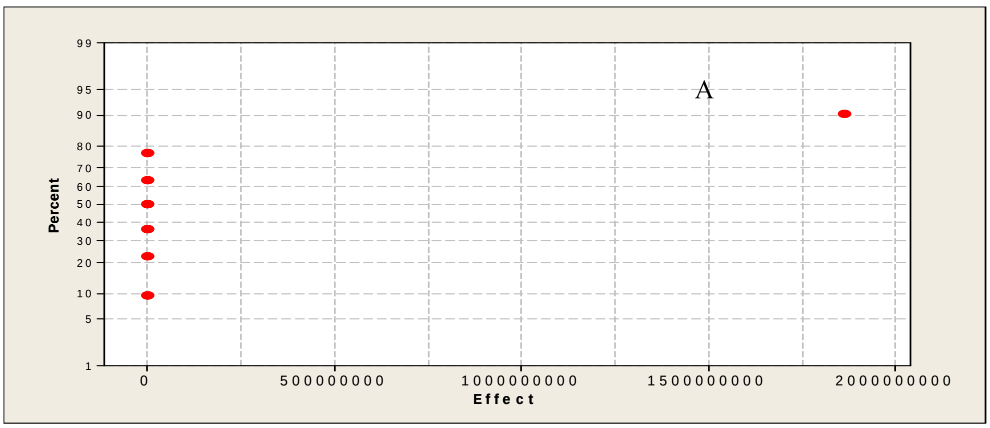


Figure B.47 Probability plot of effects of partitioning of Heptachlor epoxide with sediment

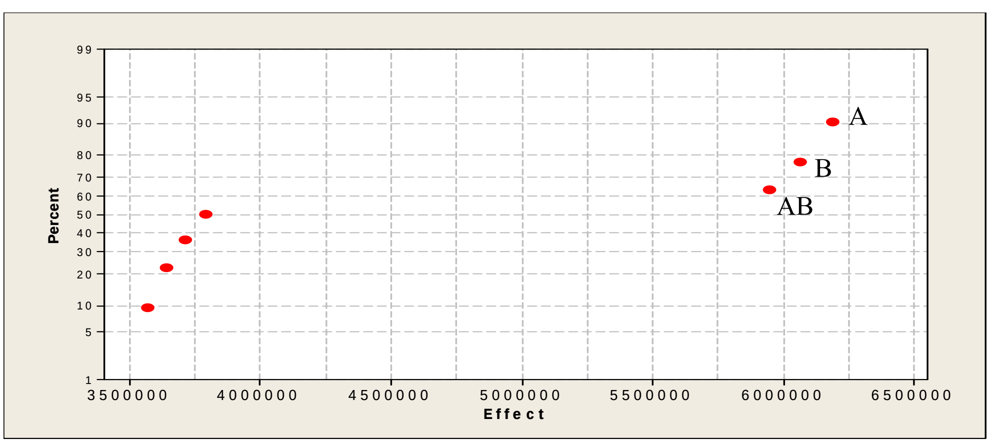


Figure B.48 Probability plot of effects of partitioning of Heptachlor epoxide with suspended sediment

Table B.33 Model Predicted Portioning of Methoxychlor with $2^3$ Factorial Design Variables

| **Factor Value** | | | **Moles of Analyte Partitioned Into** | | |
|---|---|---|---|---|---|
| **Conc of Methoxychlor(A)** | **Conc of S.S(B)** | **Organic fraction of S.S(C)** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 5.9E+08 | 2.3E+09 | 2.4E+07 |
| + | + | - | 6.0E+08 | 2.3E+09 | 6.0E+06 |
| + | - | + | 6.0E+08 | 2.3E+09 | 4.8E+05 |
| + | - | - | 6.0E+08 | 2.3E+09 | 1.2E+05 |
| - | + | + | 5.9E+06 | 2.3E+07 | 2.4E+05 |
| - | + | - | 6.0E+06 | 2.3E+07 | 6.0E+04 |
| - | - | + | 6.0E+06 | 2.3E+07 | 4.8E+03 |
| - | - | - | 6.0E+06 | 2.3E+07 | 1.2E+03 |

Table B.34 Calculated Effects of Factors and their Interactions on the Associations of Methoxychlor with Different Media

| **Factors/Interactions** | **Effect** | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 2.4E+09 | 9.0E+09 | 3.0E+07 |
| B | -6.0E+06 | -2.3E+07 | 2.9E+07 |
| C | -3.8E+06 | -1.4E+07 | 1.8E+07 |
| AB | -5.9E+06 | -2.3E+07 | 2.9E+07 |
| AC | -3.7E+06 | -1.4E+07 | 1.8E+07 |
| BC | -3.6E+06 | -1.4E+07 | 1.8E+07 |
| ABC | -3.5E+06 | -1.4E+07 | 1.7E+07 |

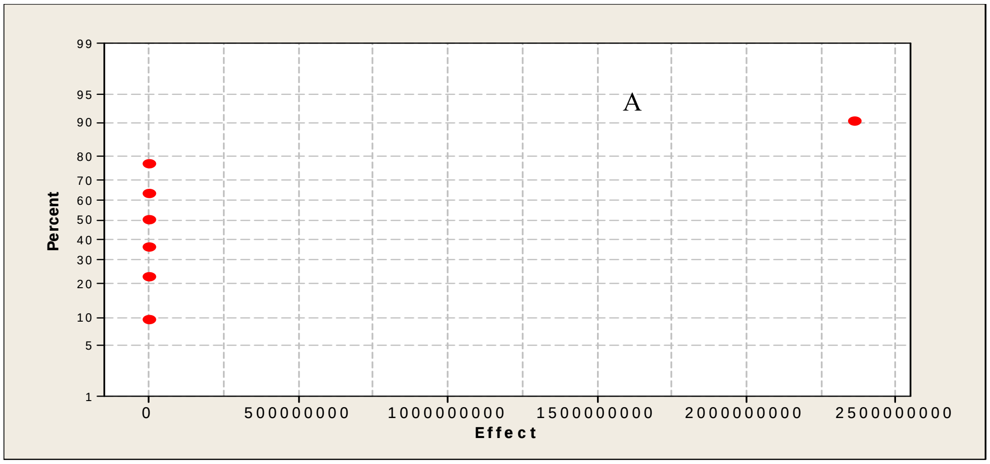


Figure B.49 Probability plot of effects of partitioning of Methoxychlor with water

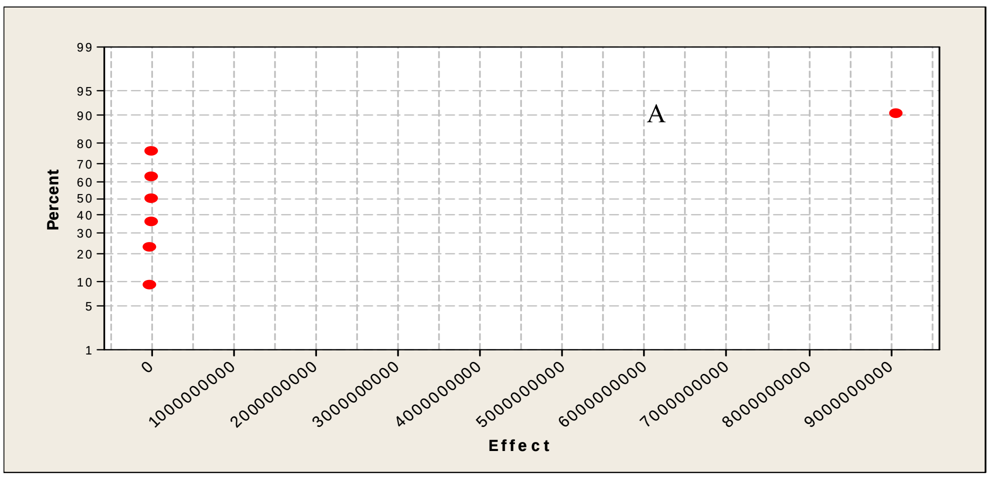


Figure B.50 Probability plot of effects of partitioning of Methoxychlor with sediment

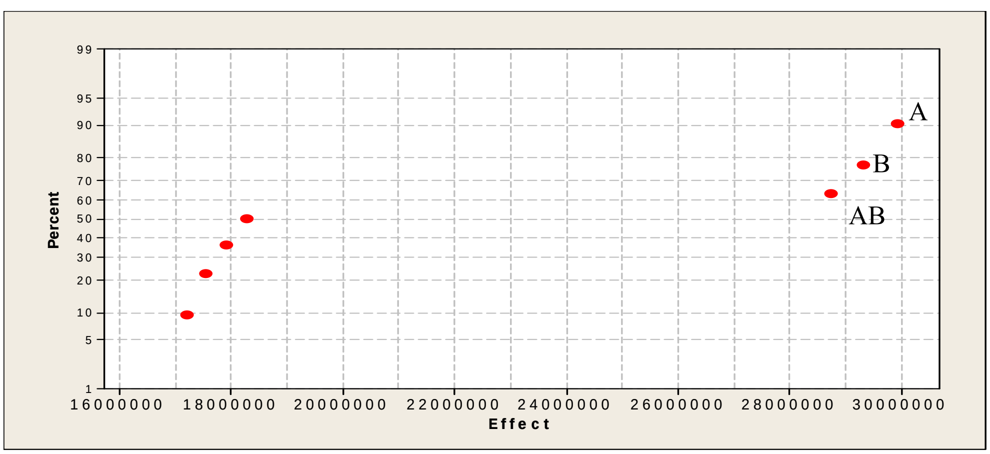


Figure B.51 Probability plot of effects of partitioning of Methoxychlor with suspended sediment

Table B.35 Model Predicted Portioning of Permethrin with $2^3$ Factorial Design Variables

| Factor Value | | | Moles of Analyte Partitioned Into | | |
|---|---|---|---|---|---|
| **Conc of Permethrin(A)** | **Conc of S.S(B)** | **Organic fraction of S.S(C)** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 1.1E+09 | 1.2E+09 | 1.2E+07 |
| + | + | - | 1.1E+09 | 1.2E+09 | 3.1E+06 |
| + | - | + | 1.1E+09 | 1.2E+09 | 2.5E+05 |
| + | - | - | 1.1E+09 | 1.2E+09 | 6.2E+04 |
| - | + | + | 1.1E+07 | 1.2E+07 | 1.2E+05 |
| - | + | - | 1.1E+07 | 1.2E+07 | 3.1E+04 |
| - | - | + | 1.1E+07 | 1.2E+07 | 2.5E+03 |
| - | - | - | 1.1E+07 | 1.2E+07 | 6.2E+02 |

Table B.36 Calculated Effects of Factors and their Interactions on the Associations of Permethrin with Different Media

| Factors/Interactions | Effect | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 4.3E+09 | 4.7E+09 | 1.6E+07 |
| B | -4.9E+06 | -5.3E+06 | 1.5E+07 |
| C | -3.0E+06 | -3.3E+06 | 9.6E+06 |
| AB | -4.8E+06 | -5.2E+06 | 1.5E+07 |
| AC | -3.0E+06 | -3.3E+06 | 9.4E+06 |
| BC | -2.9E+06 | -3.2E+06 | 9.2E+06 |
| ABC | -2.9E+06 | -3.1E+06 | 9.0E+06 |

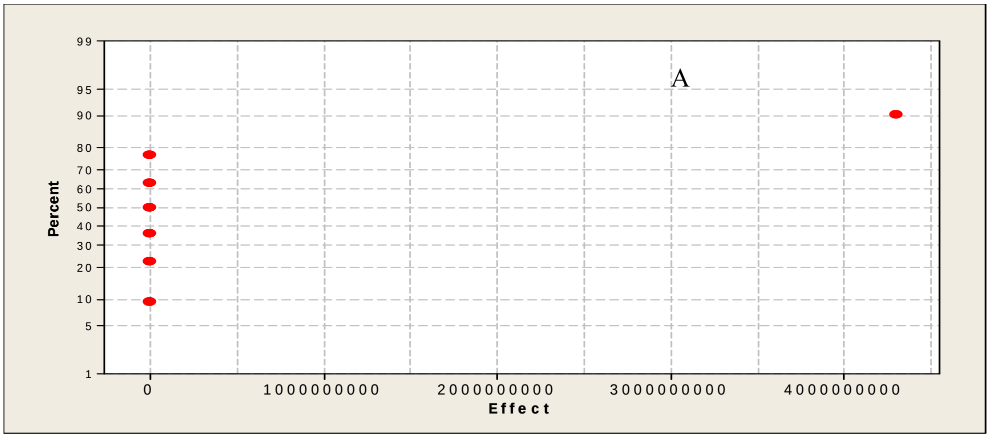


Figure B.52 Probability plot of effects of partitioning of Permethrin with water

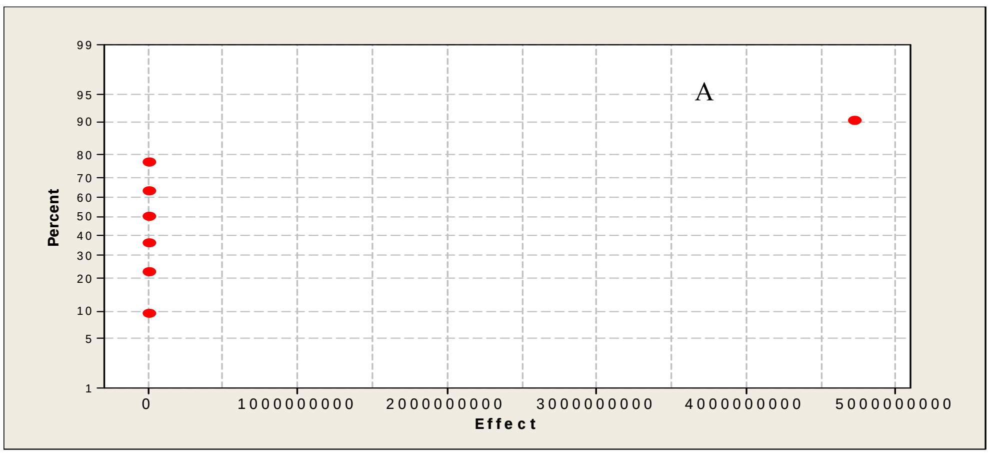


Figure B.53 Probability plot of effects of partitioning of Permethrin with sediment

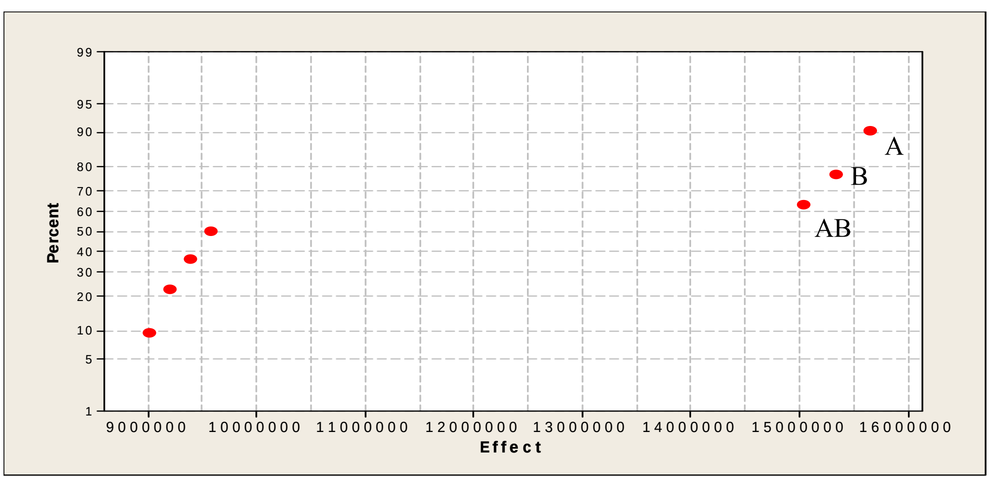


Figure B.54 Probability plot of effects of partitioning of Permethrin with suspended sediment

Table B.37 Model Predicted Portioning of Propachlor with $2^3$ Factorial Design Variables

| Factor Value | | | Moles of Analyte Partitioned Into | | |
|---|---|---|---|---|---|
| Conc of Propachlor(A) | Conc of S.S(B) | Organic fraction of S.S(C) | Water | Sediment | Suspended Sediment |
| + | + | + | 1.8E+09 | 1.1E+08 | 1.2E+06 |
| + | + | - | 1.8E+09 | 1.1E+08 | 2.9E+05 |
| + | - | + | 1.8E+09 | 1.1E+08 | 2.3E+04 |
| + | - | - | 1.8E+09 | 1.1E+08 | 5.8E+03 |
| - | + | + | 1.8E+07 | 1.1E+06 | 1.2E+04 |
| - | + | - | 1.8E+07 | 1.1E+06 | 2.9E+03 |
| - | - | + | 1.8E+07 | 1.1E+06 | 2.3E+02 |
| - | - | - | 1.8E+07 | 1.1E+06 | 5.8E+01 |

Table B.38 Calculated Effects of Factors and their Interactions on the Associations of Propachlor with Different Media

| Factors/Interactions | Effect | | |
|---|---|---|---|
| | Water | Sediment | Suspended Sediment |
| A | 7.3E+09 | 4.4E+08 | 1.5E+06 |
| B | -4.6E+05 | -2.8E+04 | 1.4E+06 |
| C | -2.9E+05 | -1.7E+04 | 9.0E+05 |
| AB | -4.5E+05 | -2.7E+04 | 1.4E+06 |
| AC | -2.8E+05 | -1.7E+04 | 8.8E+05 |
| BC | -2.7E+05 | -1.7E+04 | 8.6E+05 |
| ABC | -2.7E+05 | -1.6E+04 | 8.4E+05 |

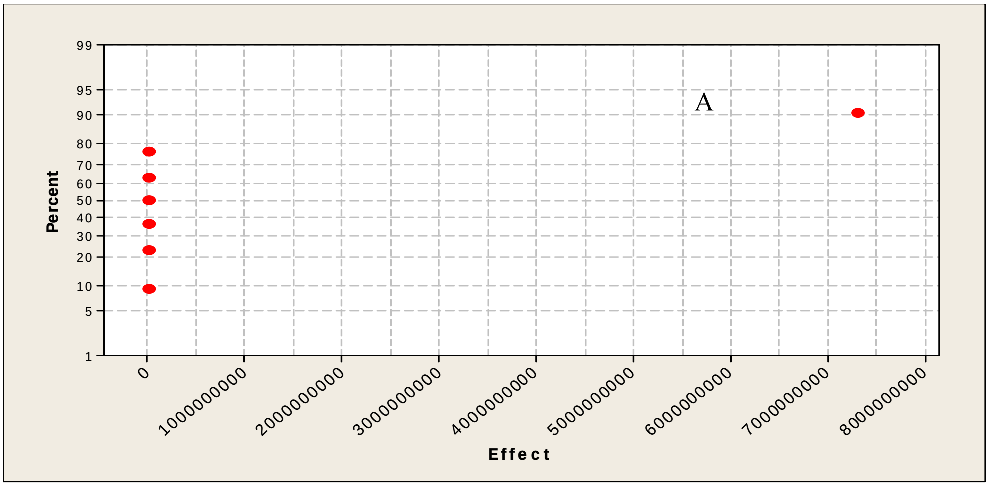


Figure B.55 Probability plot of effects of partitioning of Propachlor with water

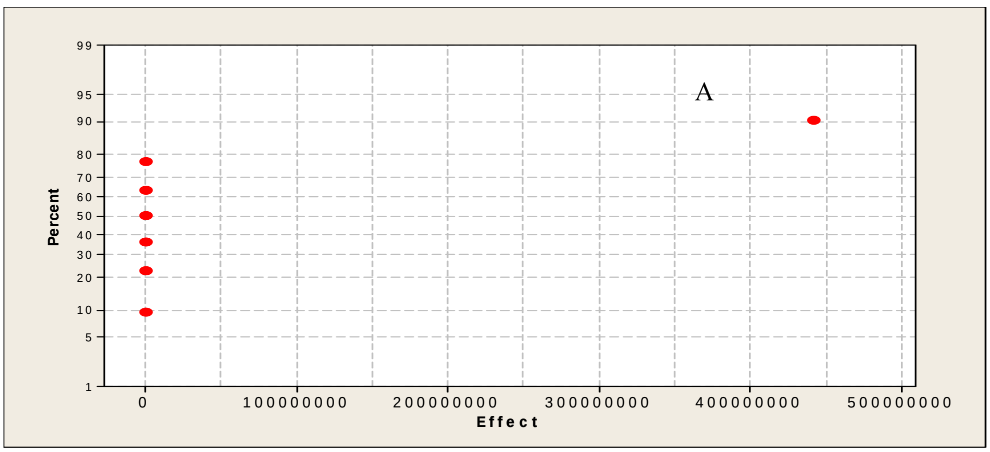


Figure B.56 Probability plot of effects of partitioning of Propachlor with sediment

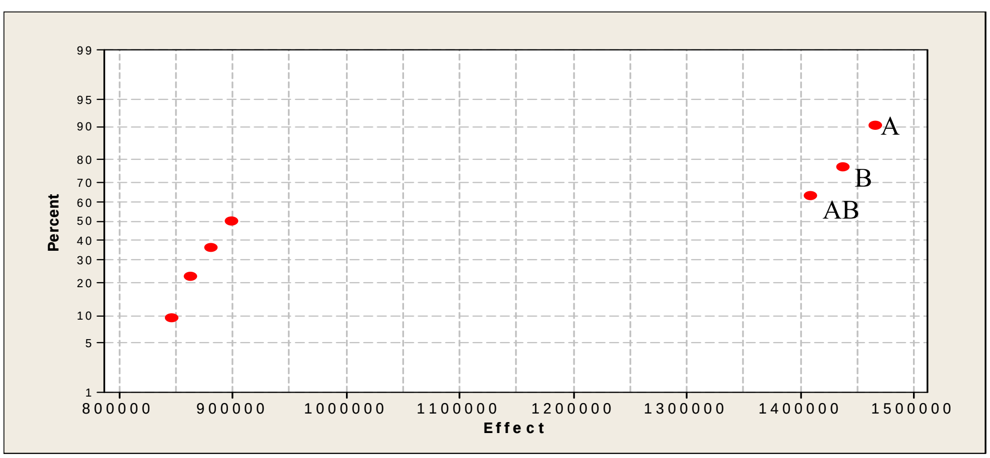


Figure B.57 Probability plot of effects of partitioning of Propachlor with suspended sediment

Table B.39 Model Predicted Portioning of Trifluralin with $2^3$ Factorial Design Variables

| Factor Value | | | Moles of Analyte Partitioned Into | | |
|---|---|---|---|---|---|
| Conc of Trifluralin(A) | Conc of S.S(B) | Organic fraction of S.S(C) | Water | Sediment | Suspended Sediment |
| + | + | + | 3.1E+09 | 2.7E+08 | 2.8E+06 |
| + | + | - | 3.1E+09 | 2.7E+08 | 7.0E+05 |
| + | - | + | 3.1E+09 | 2.7E+08 | 5.6E+04 |
| + | - | - | 3.1E+09 | 2.7E+08 | 1.4E+04 |
| - | + | + | 3.1E+07 | 2.7E+06 | 2.8E+04 |
| - | + | - | 3.1E+07 | 2.7E+06 | 7.0E+03 |
| - | - | + | 3.1E+07 | 2.7E+06 | 5.6E+02 |
| - | - | - | 3.1E+07 | 2.7E+06 | 1.4E+02 |

Table B.40 Calculated Effects of Factors and their Interactions on the Associations of Trifluralin with Different Media

| Factors/Interactions | Effect | | |
|---|---|---|---|
| | Water | Sediment | Suspended Sediment |
| A | 1.2E+10 | 1.1E+09 | 3.5E+06 |
| B | -3.2E+06 | -2.7E+05 | 3.5E+06 |
| C | -2.0E+06 | -1.7E+05 | 2.2E+06 |
| AB | -3.1E+06 | -2.7E+05 | 3.4E+06 |
| AC | -1.9E+06 | -1.7E+05 | 2.1E+06 |
| BC | -1.9E+06 | -1.6E+05 | 2.1E+06 |
| ABC | -1.9E+06 | -1.6E+05 | 2.0E+06 |

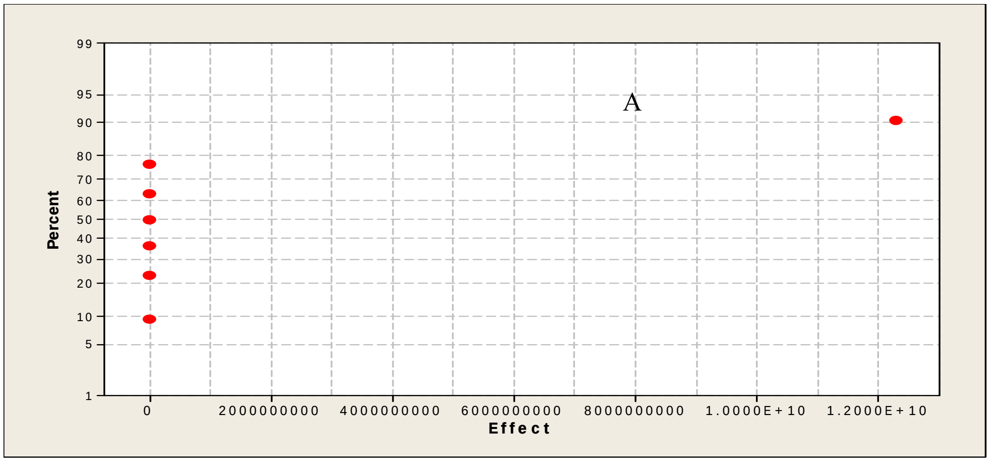


Figure B.58 Probability plot of effects of partitioning of Trifluralin with water

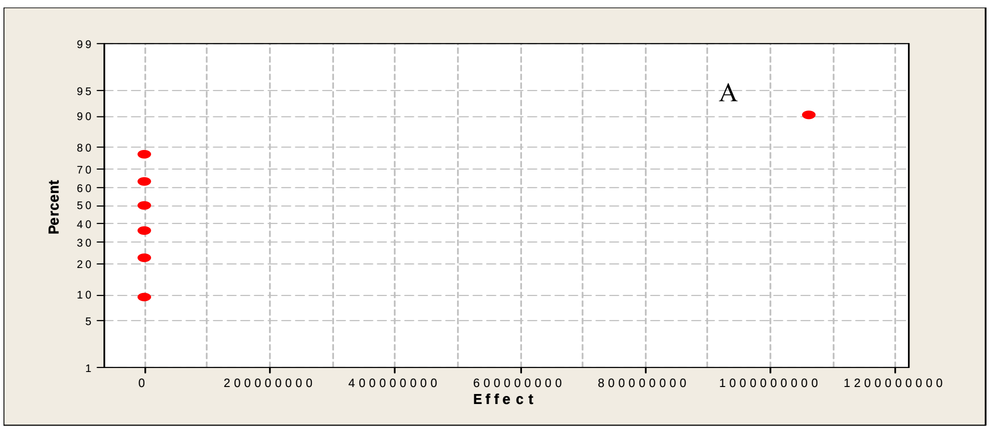


Figure B.59 Probability plot of effects of partitioning of Trifluralin with sediment

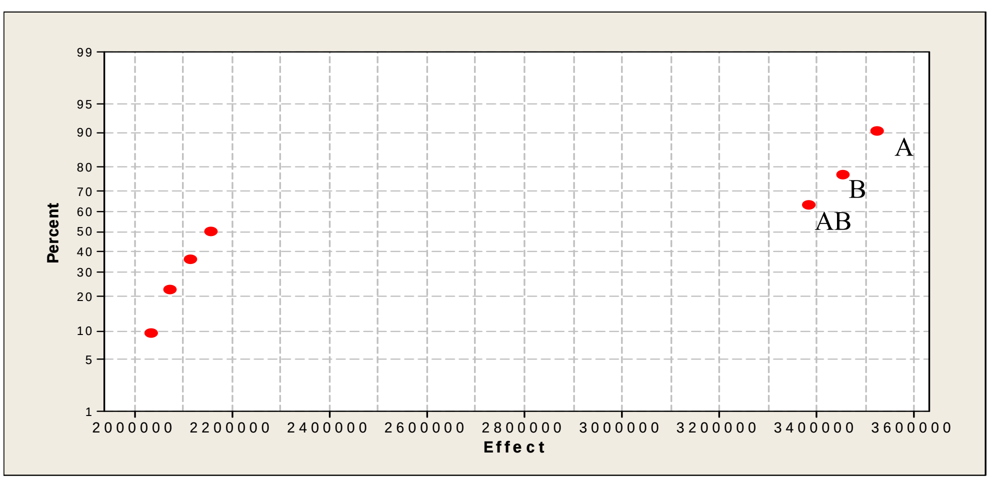


Figure B.60 Probability plot of effects of partitioning of Trifluralin with suspended sediment

Table B.41 Model Predicted Portioning of Aroclor 1016 with $2^3$ Factorial Design Variables

| Factor Value | | | Moles of Analyte Partitioned Into | | |
|---|---|---|---|---|---|
| Conc of Aroclor 1016(A) | Conc of S.S(B) | Organic fraction of S.S(C) | Water | Sediment | Suspended Sediment |
| + | + | + | 1.3E+09 | 5.4E+08 | 5.6E+06 |
| + | + | - | 1.3E+09 | 5.4E+08 | 1.4E+06 |
| + | - | + | 1.3E+09 | 5.4E+08 | 1.1E+05 |
| + | - | - | 1.3E+09 | 5.4E+08 | 2.8E+04 |
| - | + | + | 1.3E+07 | 5.4E+06 | 5.6E+04 |
| - | + | - | 1.3E+07 | 5.4E+06 | 1.4E+04 |
| - | - | + | 1.3E+07 | 5.4E+06 | 1.1E+03 |
| - | - | - | 1.3E+07 | 5.4E+06 | 2.8E+02 |

Table B.42 Calculated Effects of Factors and their Interactions on the Associations of Aroclor 1016 with Different Media

| Factors/Interactions | Effect | | |
|---|---|---|---|
| | Water | Sediment | Suspended Sediment |
| A | 5.1E+09 | 2.1E+09 | 7.1E+06 |
| B | -4.3E+06 | -1.8E+06 | 6.9E+06 |
| C | -2.7E+06 | -1.1E+06 | 4.3E+06 |
| AB | -4.2E+06 | -1.7E+06 | 6.8E+06 |
| AC | -2.6E+06 | -1.1E+06 | 4.2E+06 |
| BC | -2.5E+06 | -1.1E+06 | 4.2E+06 |
| ABC | -2.5E+06 | -1.0E+06 | 4.1E+06 |

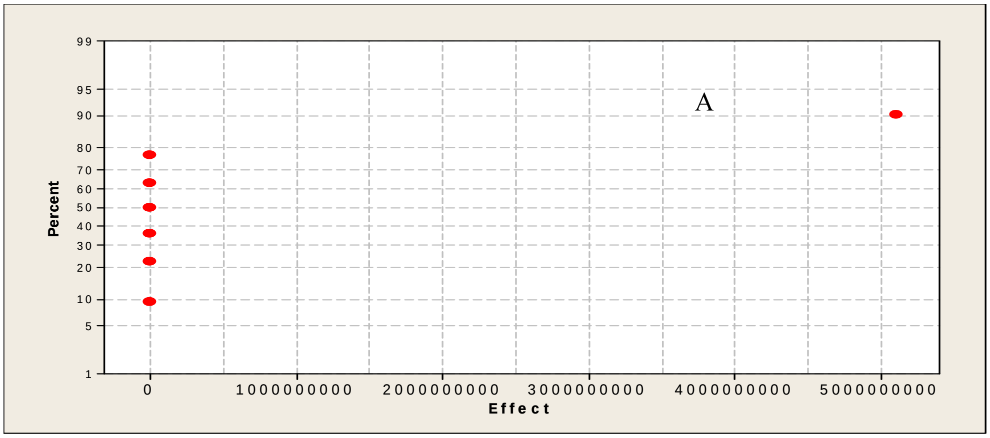


Figure B.61 Probability plot of effects of partitioning of Aroclor 1016 with water

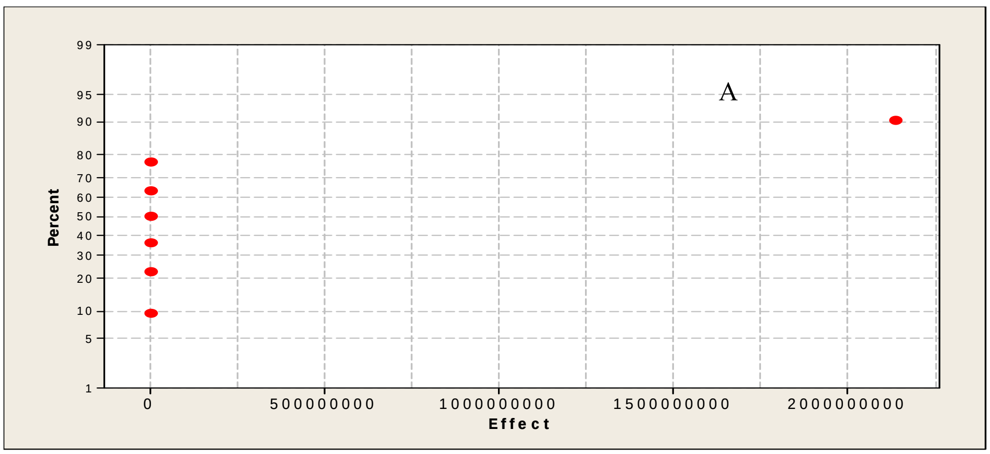


Figure B.62 Probability plot of effects of partitioning of Aroclor 1016 with sediment

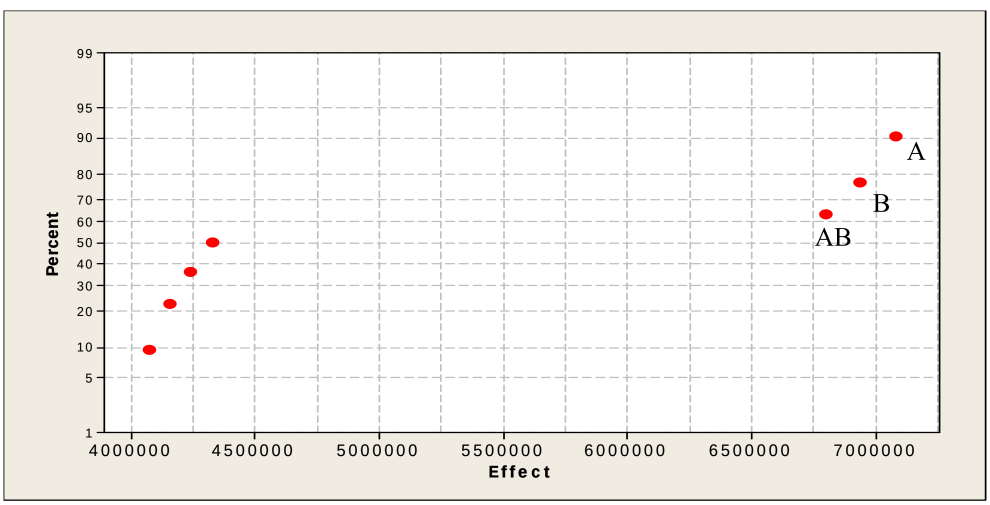


Figure B.63 Probability plot of effects of partitioning of Aroclor 1016 with suspended sediment

Table B.43 Model Predicted Portioning of Aroclor 1221 with $2^3$ Factorial Design Variables

| **Factor Value** | | | **Moles of Analyte Partitioned Into** | | |
|---|---|---|---|---|---|
| **Conc of Aroclor 1221(A)** | **Conc of S.S(B)** | **Organic fraction of S.S(C)** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 1.4E+09 | 6.1E+08 | 6.3E+06 |
| + | + | - | 1.4E+09 | 6.1E+08 | 1.6E+06 |
| + | - | + | 1.4E+09 | 6.1E+08 | 1.3E+05 |
| + | - | - | 1.4E+09 | 6.1E+08 | 3.2E+04 |
| - | + | + | 1.4E+07 | 6.1E+06 | 6.3E+04 |
| - | + | - | 1.4E+07 | 6.1E+06 | 1.6E+04 |
| - | - | + | 1.4E+07 | 6.1E+06 | 1.3E+03 |
| - | - | - | 1.4E+07 | 6.1E+06 | 3.2E+02 |

Table B.44 Calculated Effects of Factors and their Interactions on the Associations of Aroclor 1221 with Different Media

| **Factors/Interactions** | **Effect** | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 5.7E+09 | 2.4E+09 | 8.0E+06 |
| B | -4.8E+06 | -2.0E+06 | 7.8E+06 |
| C | -3.0E+06 | -1.3E+06 | 4.9E+06 |
| AB | -4.7E+06 | -2.0E+06 | 7.6E+06 |
| AC | -2.9E+06 | -1.2E+06 | 4.8E+06 |
| BC | -2.9E+06 | -1.2E+06 | 4.7E+06 |
| ABC | -2.8E+06 | -1.2E+06 | 4.6E+06 |

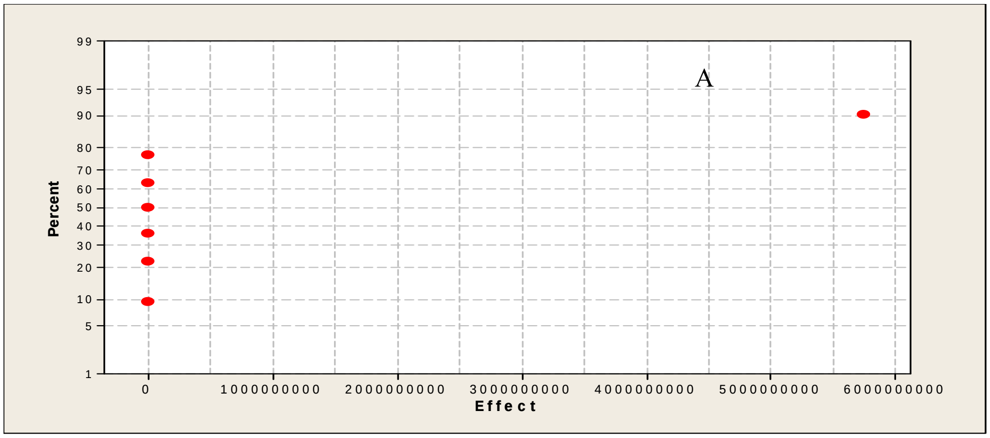


Figure B.64 Probability plot of effects of partitioning of Aroclor 1221 with water

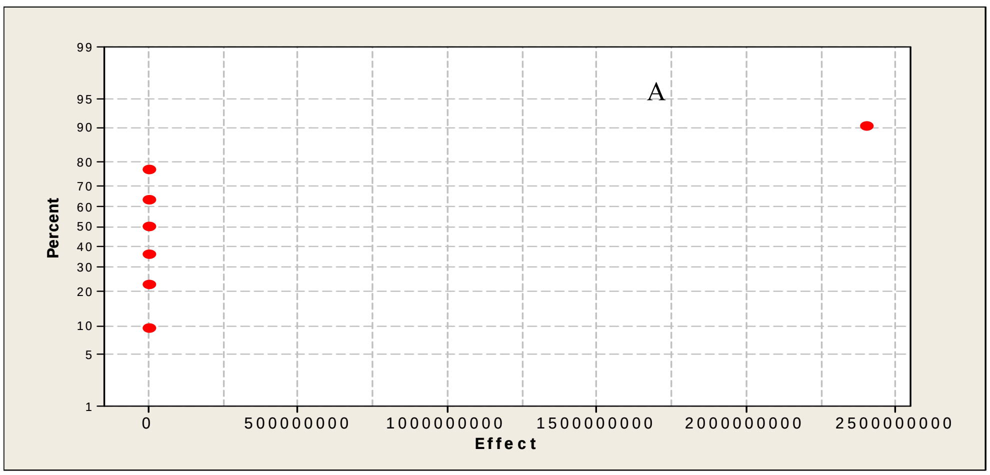


Figure B.65 Probability plot of effects of partitioning of Aroclor 1221 with sediment

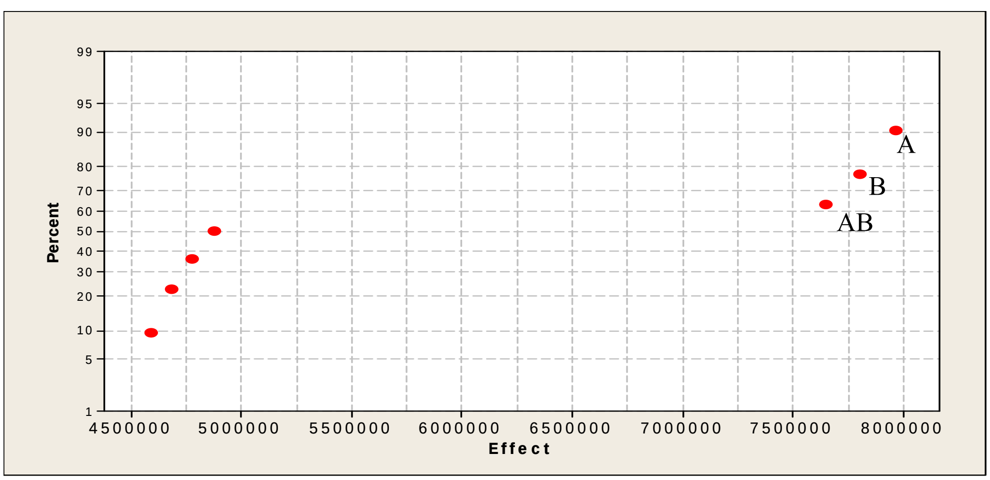


Figure B.66 Probability plot of effects of partitioning of Aroclor 1221 with suspended sediment

Table B.45 Model Predicted Portioning of Aroclor 1232 with $2^3$ Factorial Design Variables

| Factor Value | | | Moles of Analyte Partitioned Into | | |
|---|---|---|---|---|---|
| **Conc of Aroclor 1232(A)** | **Conc of S.S(B)** | **Organic fraction of S.S(C)** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 1.9E+09 | 8.1E+08 | 8.4E+06 |
| + | + | - | 1.9E+09 | 8.1E+08 | 2.1E+06 |
| + | - | + | 1.9E+09 | 8.1E+08 | 1.7E+05 |
| + | - | - | 1.9E+09 | 8.1E+08 | 4.2E+04 |
| - | + | + | 1.9E+07 | 8.1E+06 | 8.4E+04 |
| - | + | - | 1.9E+07 | 8.1E+06 | 2.1E+04 |
| - | - | + | 1.9E+07 | 8.1E+06 | 1.7E+03 |
| - | - | - | 1.9E+07 | 8.1E+06 | 4.2E+02 |

Table B.46 Calculated Effects of Factors and their Interactions on the Associations of Aroclor 1232 with Different Media

| Factors/Interactions | Effect | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 7.6E+09 | 3.2E+09 | 1.1E+07 |
| B | -6.4E+06 | -2.7E+06 | 1.0E+07 |
| C | -4.0E+06 | -1.7E+06 | 6.5E+06 |
| AB | -6.3E+06 | -2.6E+06 | 1.0E+07 |
| AC | -3.9E+06 | -1.6E+06 | 6.4E+06 |
| BC | -3.8E+06 | -1.6E+06 | 6.2E+06 |
| ABC | -3.7E+06 | -1.6E+06 | 6.1E+06 |

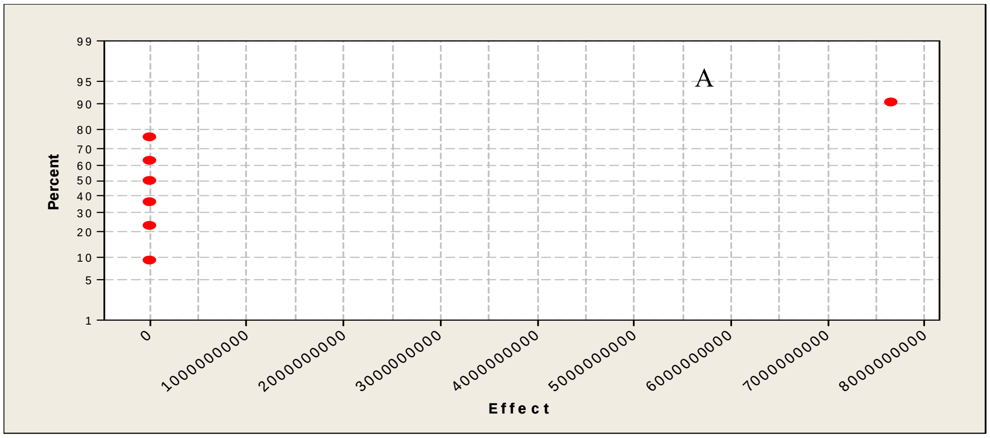


Figure B.67 Probability plot of effects of partitioning of Aroclor 1232 with water

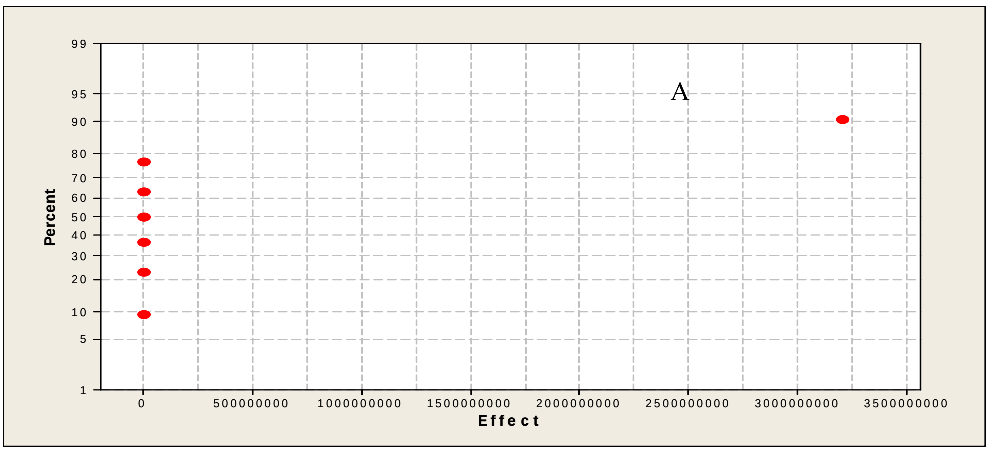


Figure B.68 Probability plot of effects of partitioning of Aroclor 1232 with sediment

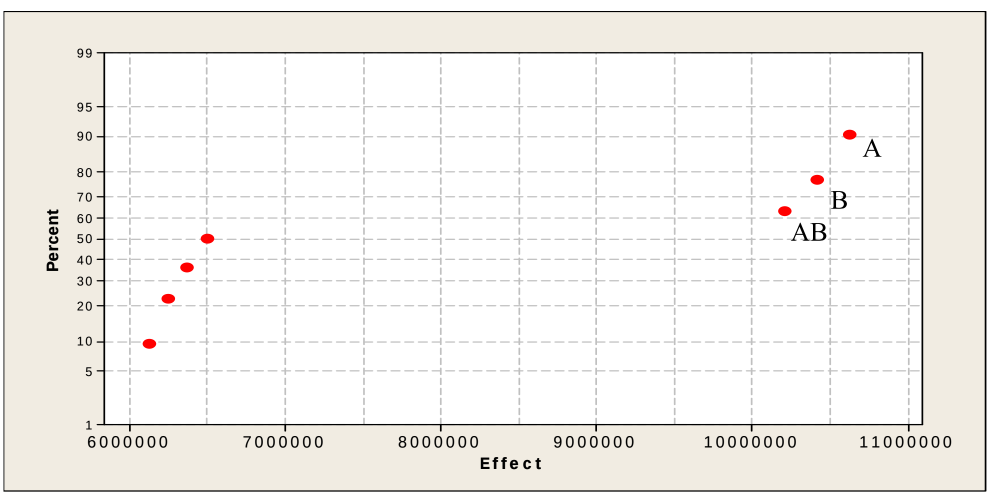


Figure B.69 Probability plot of effects of partitioning of Aroclor 1232 with suspended sediment

Table B.47 Model Predicted Portioning of Aroclor 1242 with $2^3$ Factorial Design Variables

| Factor Value | | | Moles of Analyte Partitioned Into | | |
|---|---|---|---|---|---|
| Conc of Aroclor 1242(A) | Conc of S.S(B) | Organic fraction of S.S(C) | Water | Sediment | Suspended Sediment |
| + | + | + | 1.2E+09 | 5.0E+08 | 5.3E+06 |
| + | + | - | 1.2E+09 | 5.1E+08 | 1.3E+06 |
| + | - | + | 1.2E+09 | 5.1E+08 | 1.1E+05 |
| + | - | - | 1.2E+09 | 5.1E+08 | 2.6E+04 |
| - | + | + | 1.2E+07 | 5.0E+06 | 5.3E+04 |
| - | + | - | 1.2E+07 | 5.1E+06 | 1.3E+04 |
| - | - | + | 1.2E+07 | 5.1E+06 | 1.1E+03 |
| - | - | - | 1.2E+07 | 5.1E+06 | 2.6E+02 |

Table B.48 Calculated Effects of Factors and their Interactions on the Associations of Aroclor 1242 with Different Media

| Factors/Interactions | Effect | | |
|---|---|---|---|
| | Water | Sediment | Suspended Sediment |
| A | 4.8E+09 | 2.0E+09 | 6.6E+06 |
| B | -4.0E+06 | -1.7E+06 | 6.5E+06 |
| C | -2.5E+06 | -1.0E+06 | 4.1E+06 |
| AB | -3.9E+06 | -1.6E+06 | 6.4E+06 |
| AC | -2.4E+06 | -1.0E+06 | 4.0E+06 |
| BC | -2.4E+06 | -1.0E+06 | 3.9E+06 |
| ABC | -2.3E+06 | -9.8E+05 | 3.8E+06 |

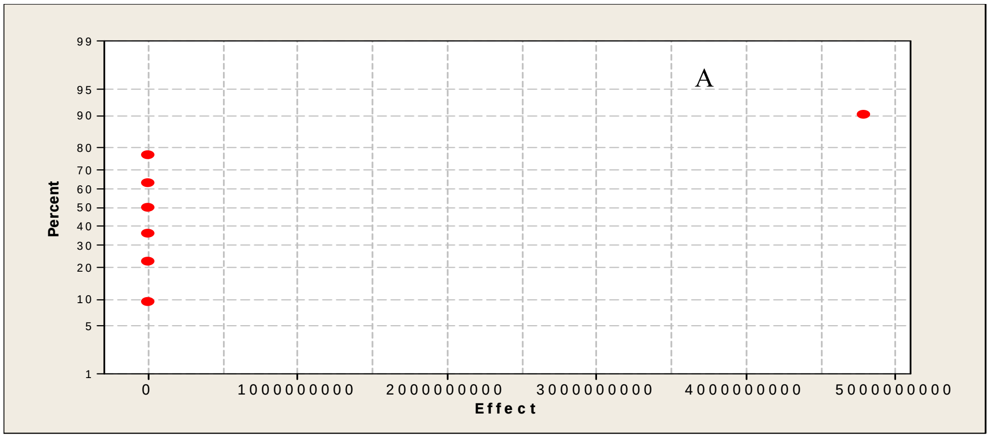


Figure B.70 Probability plot of effects of partitioning of Aroclor 1242 with water

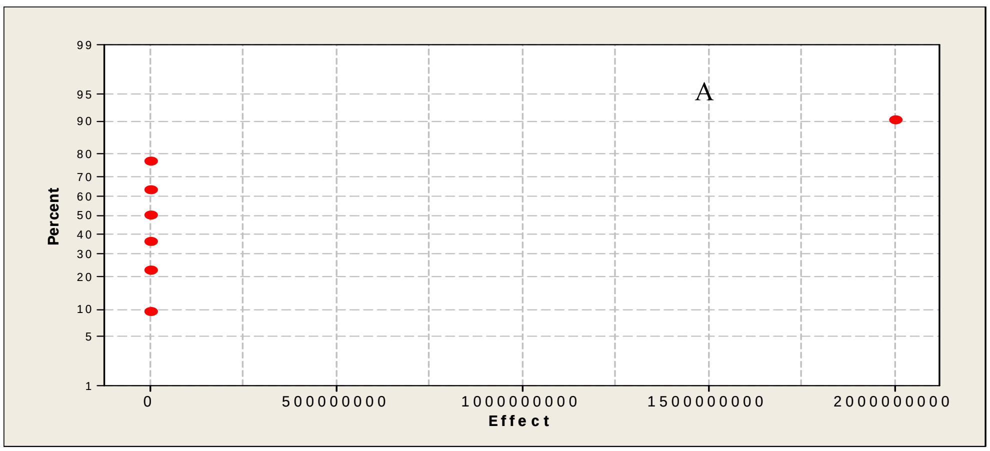


Figure B.71 Probability plot of effects of partitioning of Aroclor 1242 with sediment

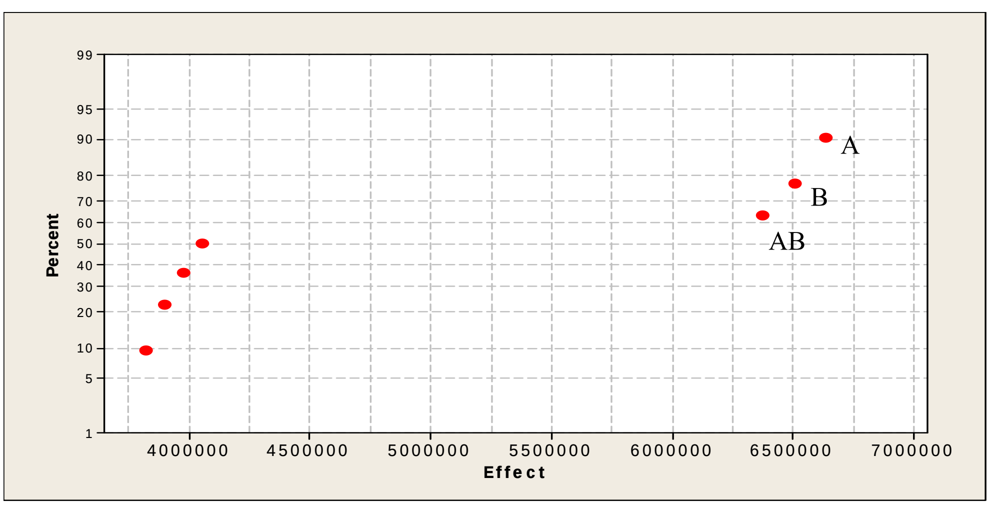


Figure B.72 Probability plot of effects of partitioning of Aroclor 1242 with suspended sediment

Table B.49 Model Predicted Portioning of Aroclor 1248 with $2^3$ Factorial Design Variables

| **Factor Value** | | | **Moles of Analyte Partitioned Into** | | |
|---|---|---|---|---|---|
| **Conc of Aroclor 1248(A)** | **Conc of S.S(B)** | **Organic fraction of S.S(C)** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 1.4E+09 | 5.9E+08 | 6.2E+06 |
| + | + | - | 1.4E+09 | 5.9E+08 | 1.5E+06 |
| + | - | + | 1.4E+09 | 5.9E+08 | 1.2E+05 |
| + | - | - | 1.4E+09 | 5.9E+08 | 3.1E+04 |
| - | + | + | 1.4E+07 | 5.9E+06 | 6.2E+04 |
| - | + | - | 1.4E+07 | 5.9E+06 | 1.5E+04 |
| - | - | + | 1.4E+07 | 5.9E+06 | 1.2E+03 |
| - | - | - | 1.4E+07 | 5.9E+06 | 3.1E+02 |

Table B.50 Calculated Effects of Factors and their Interactions on the Associations of Aroclor 1248 with Different Media

| **Factors/Interactions** | **Effect** | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 5.6E+09 | 2.3E+09 | 7.8E+06 |
| B | -4.7E+06 | -2.0E+06 | 7.6E+06 |
| C | -2.9E+06 | -1.2E+06 | 4.8E+06 |
| AB | -4.6E+06 | -1.9E+06 | 7.5E+06 |
| AC | -2.9E+06 | -1.2E+06 | 4.7E+06 |
| BC | -2.8E+06 | -1.2E+06 | 4.6E+06 |
| ABC | -2.7E+06 | -1.2E+06 | 4.5E+06 |

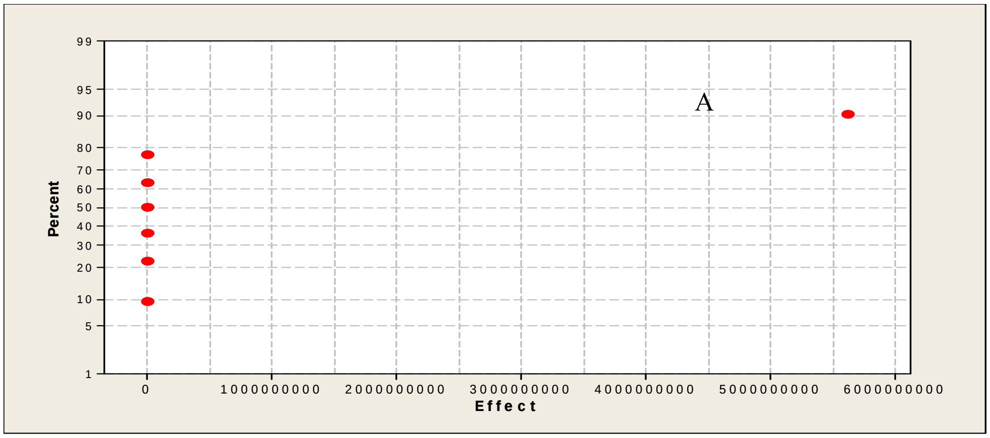


Figure B.73 Probability plot of effects of partitioning of Aroclor 1248 with water

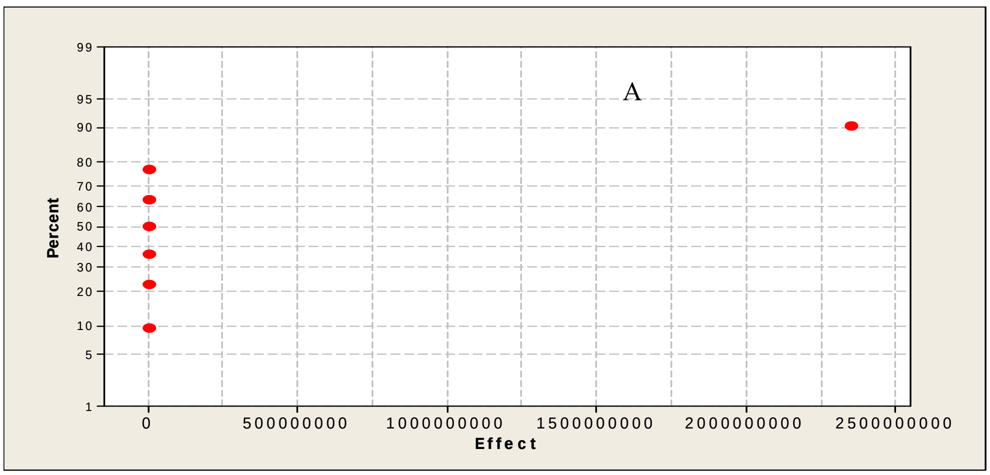


Figure B.74 Probability plot of effects of partitioning of Aroclor 1248 with sediment

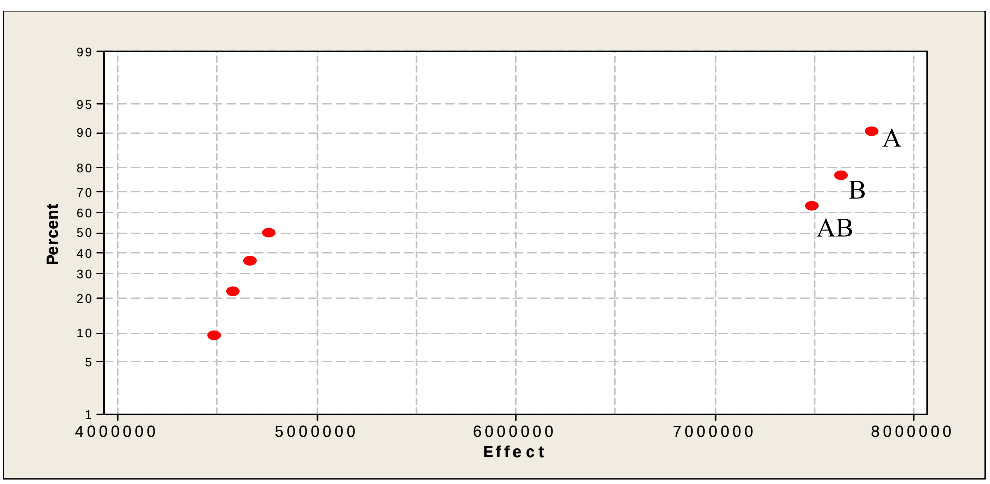


Figure B.75 Probability plot of effects of partitioning of Aroclor 1248 with suspended sediment

Table B.51 Model Predicted Portioning of Aroclor 1254 with $2^3$ Factorial Design Variables

| Factor Value | | | Moles of Analyte Partitioned Into | | |
|---|---|---|---|---|---|
| Conc of Aroclor 1254(A) | Conc of S.S(B) | Organic fraction of S.S(C) | Water | Sediment | Suspended Sediment |
| + | + | + | 2.4E+09 | 1.0E+09 | 1.1E+07 |
| + | + | - | 2.4E+09 | 1.0E+09 | 2.6E+06 |
| + | - | + | 2.4E+09 | 1.0E+09 | 2.1E+05 |
| + | - | - | 2.4E+09 | 1.0E+09 | 5.3E+04 |
| - | + | + | 2.4E+07 | 1.0E+07 | 1.1E+05 |
| - | + | - | 2.4E+07 | 1.0E+07 | 2.6E+04 |
| - | - | + | 2.4E+07 | 1.0E+07 | 2.1E+03 |
| - | - | - | 2.4E+07 | 1.0E+07 | 5.3E+02 |

Table B.52 Calculated Effects of Factors and their Interactions on the Associations of Aroclor 1254 with Different Media

| Factors/Interactions | Effect | | |
|---|---|---|---|
| | Water | Sediment | Suspended Sediment |
| A | 9.6E+09 | 4.0E+09 | 1.3E+07 |
| B | -8.0E+06 | -3.3E+06 | 1.3E+07 |
| C | -5.0E+06 | -2.1E+06 | 8.1E+06 |
| AB | -7.8E+06 | -3.3E+06 | 1.3E+07 |
| AC | -4.9E+06 | -2.0E+06 | 8.0E+06 |
| BC | -4.8E+06 | -2.0E+06 | 7.8E+06 |
| ABC | -4.7E+06 | -2.0E+06 | 7.6E+06 |

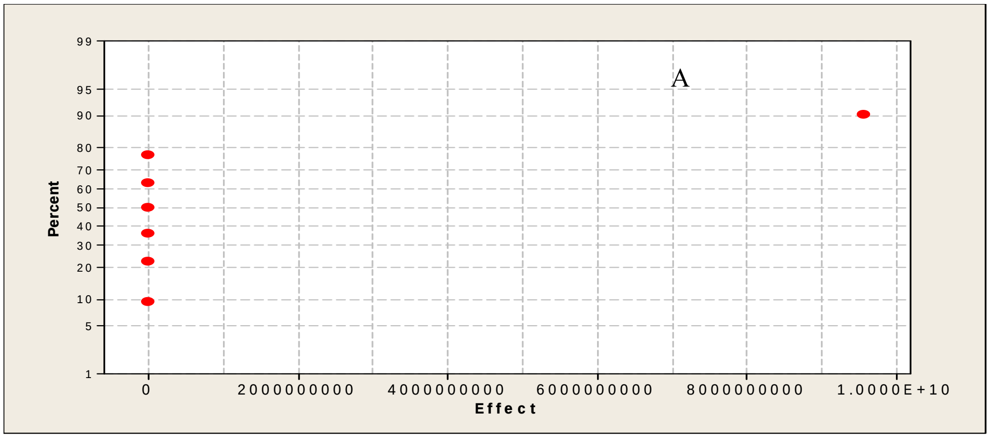


Figure B.76 Probability plot of effects of partitioning of Aroclor 1254 with water

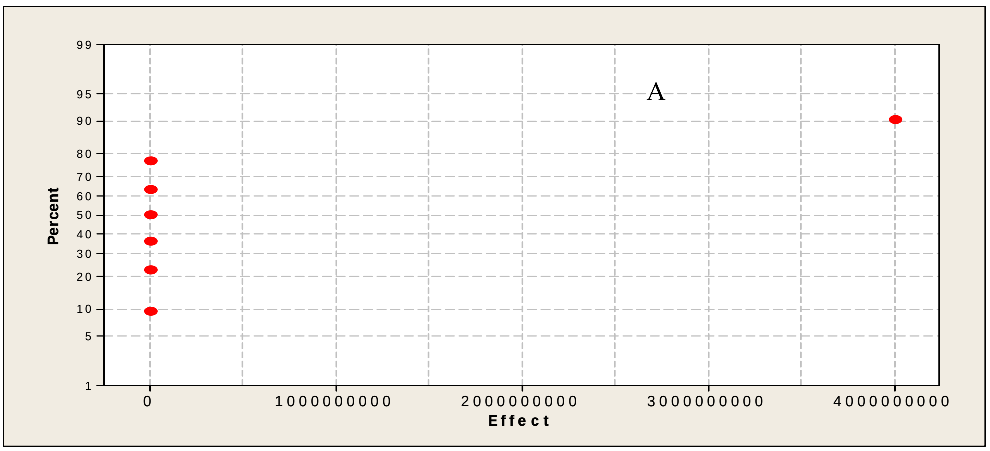


Figure B.77 Probability plot of effects of partitioning of Aroclor 1254 with sediment

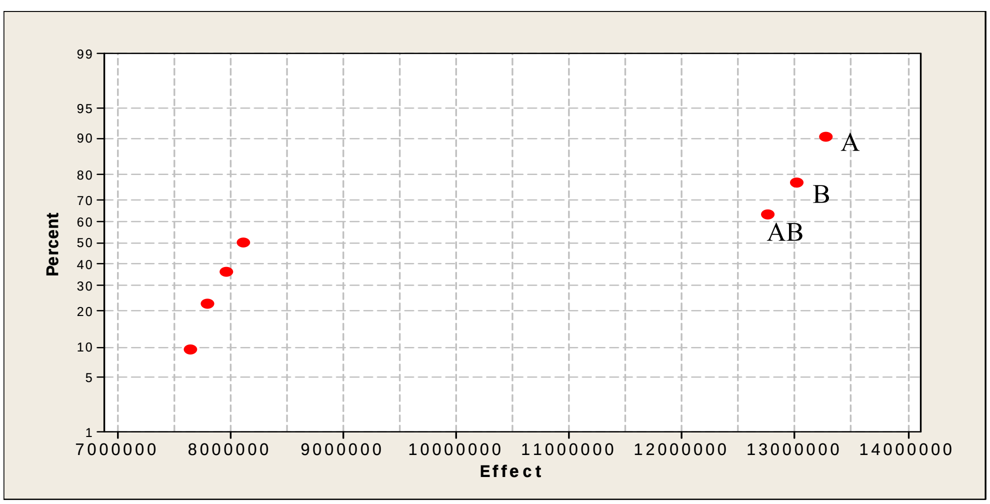


Figure B.78 Probability plot of effects of partitioning of Aroclor 1254 with suspended sediment

Table B.53 Model Predicted Portioning of Aroclor 1260 with $2^3$ Factorial Design Variables

| Factor Value | | | Moles of Analyte Partitioned Into | | |
|---|---|---|---|---|---|
| Conc of Aroclor 1260(A) | Conc of S.S(B) | Organic fraction of S.S(C) | Water | Sediment | Suspended Sediment |
| + | + | + | 2.1E+09 | 8.7E+08 | 9.1E+06 |
| + | + | - | 2.1E+09 | 8.8E+08 | 2.3E+06 |
| + | - | + | 2.1E+09 | 8.8E+08 | 1.8E+05 |
| + | - | - | 2.1E+09 | 8.8E+08 | 4.6E+04 |
| - | + | + | 2.1E+07 | 8.7E+06 | 9.1E+04 |
| - | + | - | 2.1E+07 | 8.8E+06 | 2.3E+04 |
| - | - | + | 2.1E+07 | 8.8E+06 | 1.8E+03 |
| - | - | - | 2.1E+07 | 8.8E+06 | 4.6E+02 |

Table B.54 Calculated Effects of Factors and their Interactions on the Associations of Aroclor 1260 with Different Media

| Factors/Interactions | Effect | | |
|---|---|---|---|
| | Water | Sediment | Suspended Sediment |
| A | 8.3E+09 | 3.5E+09 | 1.2E+07 |
| B | -6.9E+06 | -2.9E+06 | 1.1E+07 |
| C | -4.3E+06 | -1.8E+06 | 7.0E+06 |
| AB | -6.8E+06 | -2.8E+06 | 1.1E+07 |
| AC | -4.2E+06 | -1.8E+06 | 6.9E+06 |
| BC | -4.1E+06 | -1.7E+06 | 6.8E+06 |
| ABC | -4.1E+06 | -1.7E+06 | 6.6E+06 |

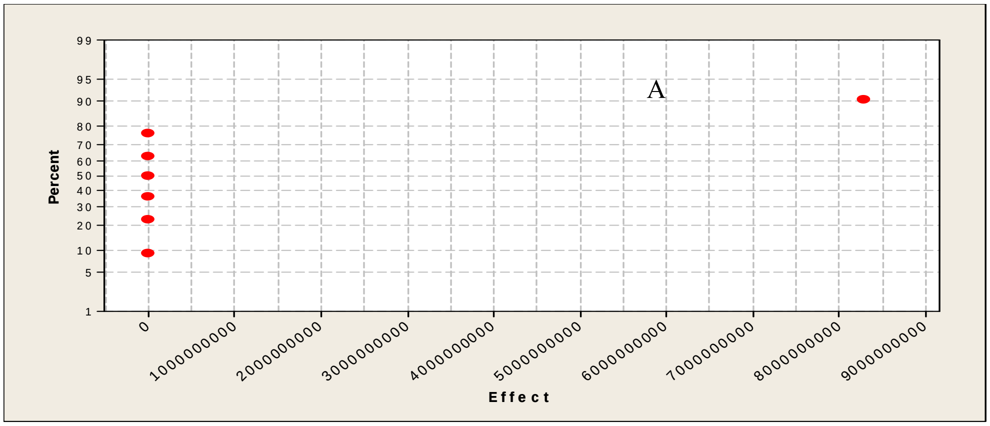


Figure B.79 Probability plot of effects of partitioning of Aroclor 1260 with water

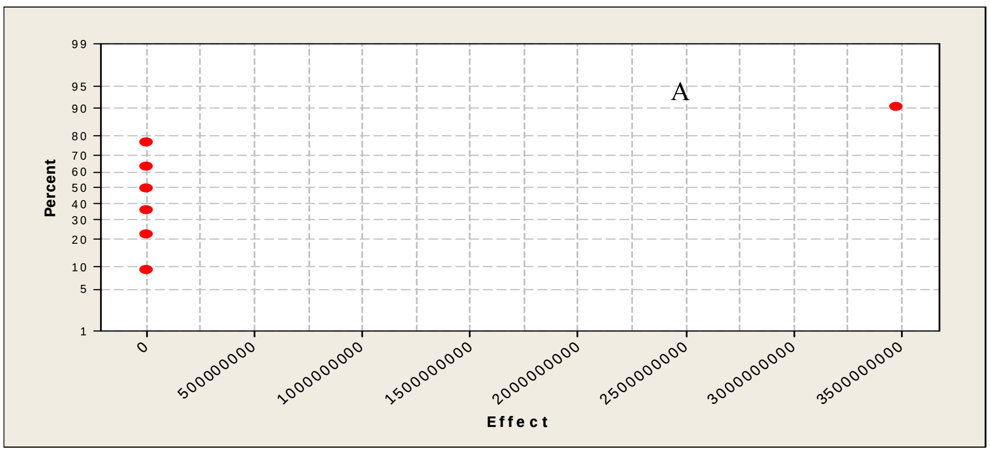


Figure B.80 Probability plot of effects of partitioning of Aroclor 1260 with sediment

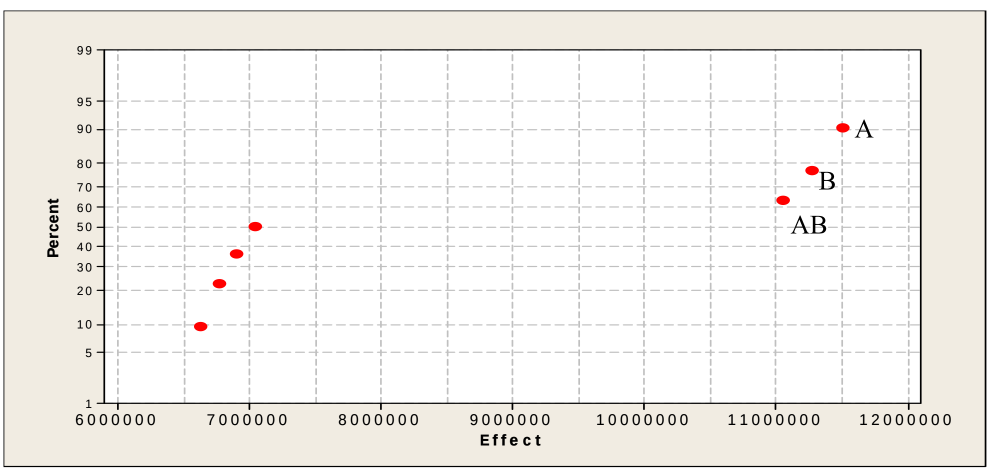


Figure B.81 Probability plot of effects of partitioning of Aroclor 1260 with suspended sediment

Table B.55 Model Predicted Portioning of Toxaphene with $2^3$ Factorial Design Variables

| **Factor Value** | | | **Moles of Analyte Partitioned Into** | | |
|---|---|---|---|---|---|
| **Conc of Toxaphene(A)** | **Conc of S.S(B)** | **Organic fraction of S.S(C)** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 4.0E+09 | 1.3E+08 | 1.3E+06 |
| + | + | - | 4.0E+09 | 1.3E+08 | 3.3E+05 |
| + | - | + | 4.0E+09 | 1.3E+08 | 2.6E+04 |
| + | - | - | 4.0E+09 | 1.3E+08 | 6.5E+03 |
| - | + | + | 4.0E+07 | 1.3E+06 | 1.3E+04 |
| - | + | - | 4.0E+07 | 1.3E+06 | 3.3E+03 |
| - | - | + | 4.0E+07 | 1.3E+06 | 2.6E+02 |
| - | - | - | 4.0E+07 | 1.3E+06 | 6.5E+01 |

Table B.56 Calculated Effects of Factors and their Interactions on the Associations of Toxaphene with Different Media

| **Factors/Interactions** | **Effect** | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 1.6E+10 | 5.0E+08 | 1.7E+06 |
| B | -1.6E+06 | -4.9E+04 | 1.6E+06 |
| C | -9.7E+05 | -3.1E+04 | 1.0E+06 |
| AB | -1.5E+06 | -4.8E+04 | 1.6E+06 |
| AC | -9.5E+05 | -3.0E+04 | 9.9E+05 |
| BC | -9.3E+05 | -3.0E+04 | 9.7E+05 |
| ABC | -9.2E+05 | -2.9E+04 | 9.5E+05 |

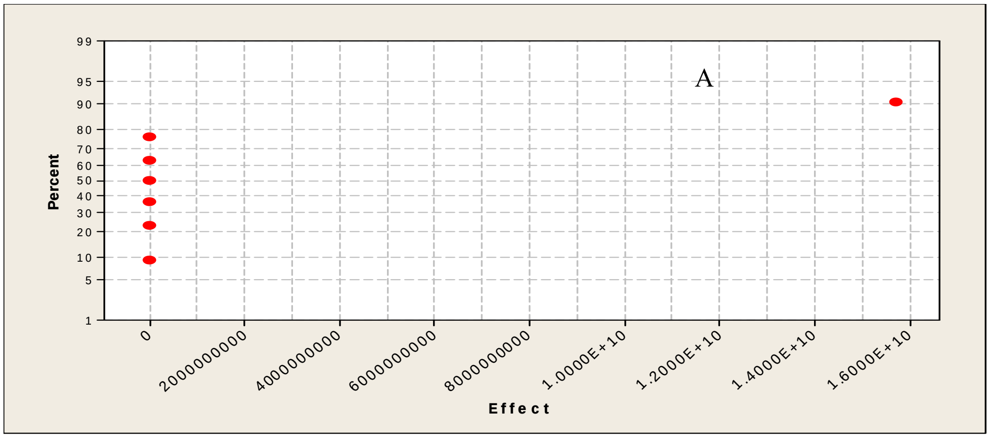


Figure B.82 Probability plot of effects of partitioning of Toxaphene with water

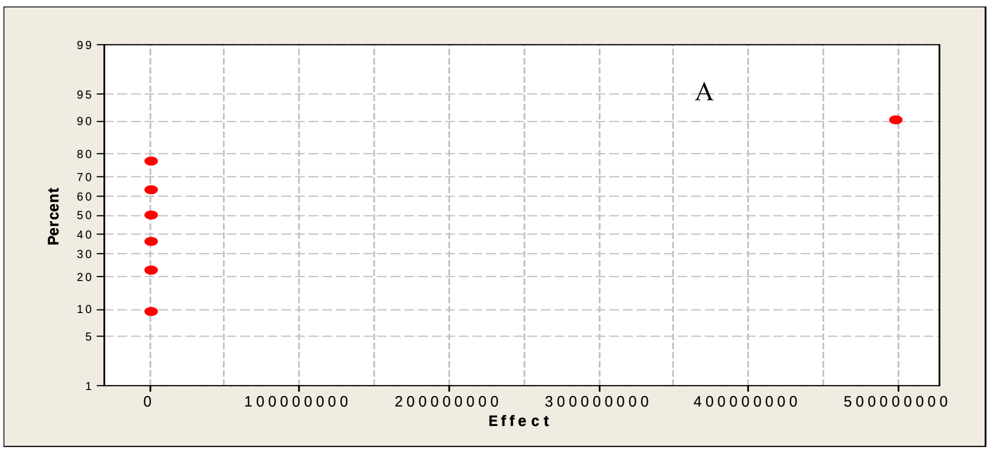


Figure B.83 Probability plot of effects of partitioning of Toxaphene with sediment

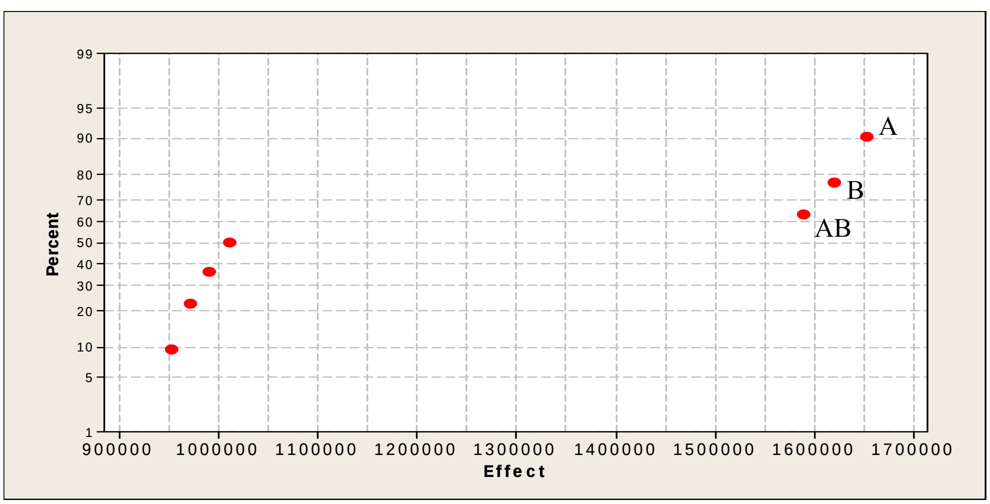


Figure B.84 Probability plot of effects of partitioning of Toxaphene with suspended sediment

Table B.57 Model Predicted Portioning of Chlordane with $2^3$ Factorial Design Variables

| **Factor Value** | | | **Moles of Analyte Partitioned Into** | | |
|---|---|---|---|---|---|
| **Conc of Chlordane(A)** | **Conc of S.S(B)** | **Organic fraction of S.S(C)** | **Water** | **Sediment** | **Suspended Sediment** |
| + | + | + | 4.7E+08 | 1.8E+09 | 1.9E+07 |
| + | + | - | 4.8E+08 | 1.8E+09 | 4.8E+06 |
| + | - | + | 4.8E+08 | 1.8E+09 | 3.8E+05 |
| + | - | - | 4.8E+08 | 1.8E+09 | 9.5E+04 |
| - | + | + | 4.7E+06 | 1.8E+07 | 1.9E+05 |
| - | + | - | 4.8E+06 | 1.8E+07 | 4.8E+04 |
| - | - | + | 4.8E+06 | 1.8E+07 | 3.8E+03 |
| - | - | - | 4.8E+06 | 1.8E+07 | 9.5E+02 |

Table B.58 Calculated Effects of Factors and their Interactions on the Associations of Chlordane with Different Media

| **Factors/Interactions** | **Effect** | | |
|---|---|---|---|
| | **Water** | **Sediment** | **Suspended Sediment** |
| A | 1.9E+09 | 7.2E+09 | 2.4E+07 |
| B | -4.8E+06 | -1.9E+07 | 2.3E+07 |
| C | -3.0E+06 | -1.2E+07 | 1.5E+07 |
| AB | -4.7E+06 | -1.8E+07 | 2.3E+07 |
| AC | -3.0E+06 | -1.1E+07 | 1.4E+07 |
| BC | -2.9E+06 | -1.1E+07 | 1.4E+07 |
| ABC | -2.8E+06 | -1.1E+07 | 1.4E+07 |

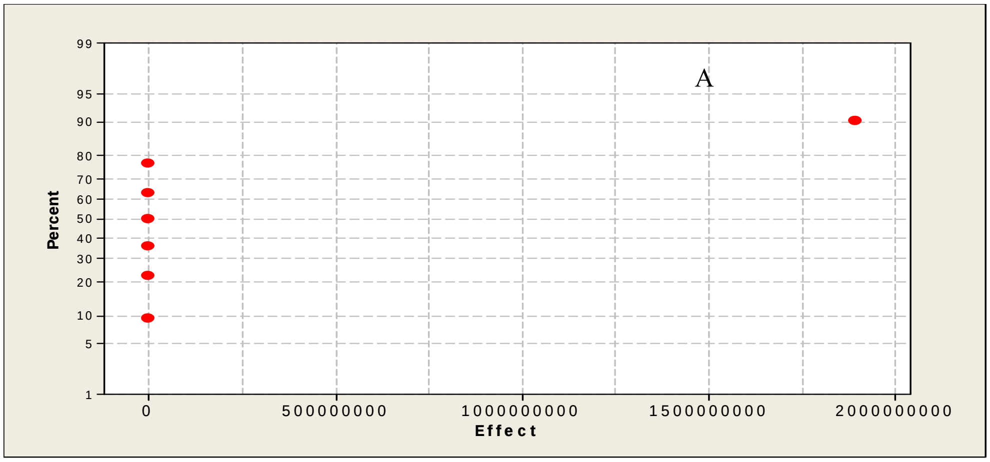


Figure B.85 Probability plot of effects of partitioning of Chlordane with water

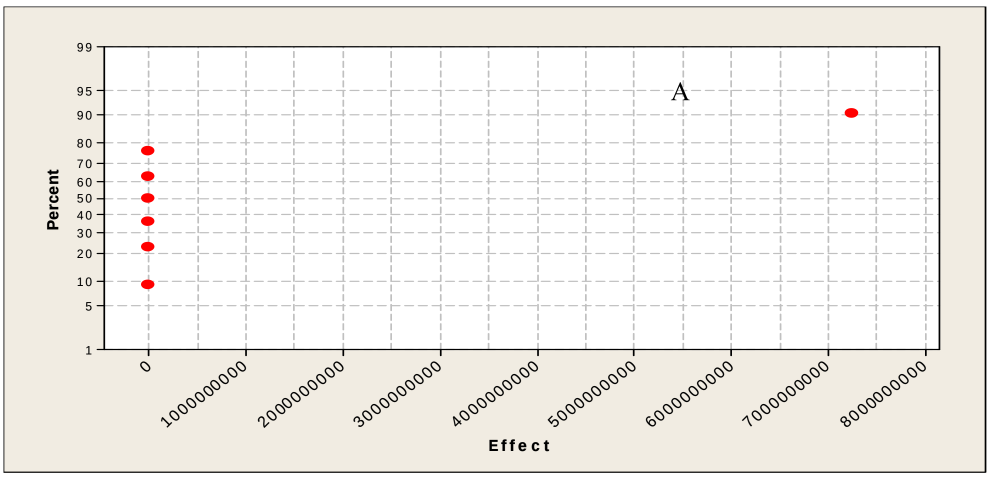


Figure B.86 Probability plot of effects of partitioning of Chlordane with sediment

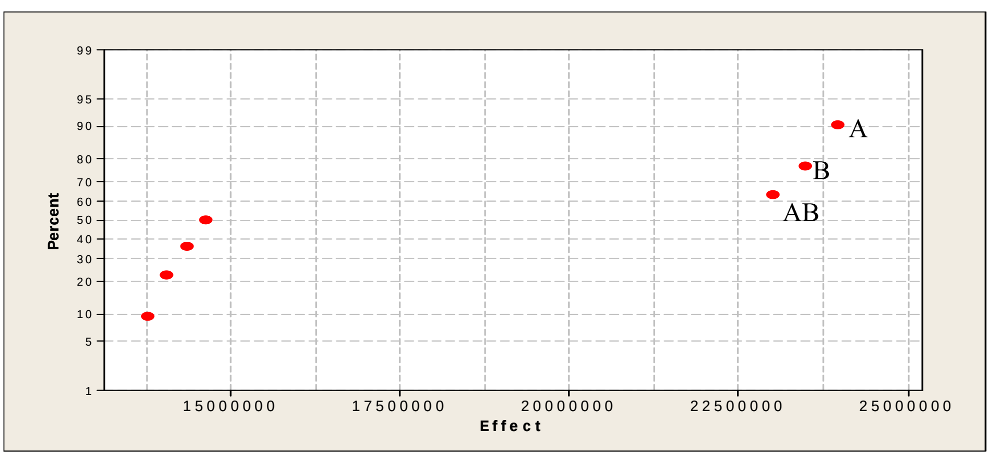


Figure B.87 Probability plot of effects of partitioning of Chlordane with suspended sediment

## APPENDIX C

## VADOSE ZONE MODELING OF PPCPs

Table C.1 Properties of PPCPs included in the study

| Compound | Solubility (mg/L) | Molecularwt. (g/mole) |
|---|---|---|
| Nystatin | 360 | 926.09 |
| Dexamethasone | 89 | 392.46 |
| Methoprene | 1.4 | 310.48 |
| Prednisone | 312 | 358.43 |
| Metronidazole | 11000 | 171.15 |
| Clindamycin | 30.61 | 424.99 |
| ketoconazole | 0.29 | 531.44 |
| Carbamazepine | 18 | 236.27 |
| Caffeine | 21600 | 194.19 |
| Ibuprofen | 21 | 206.28 |
| Diclofenac | 2.37 | 296.15 |
| Acetaminophen | 14000 | 151.16 |
| Triclosan | 10 | 289.55 |
| Ciprofloxacin | 30000 | 331.35 |
| Metoprolol | 1000 | 267.36 |
| Salicylic acid | 2240 | 138.12 |

Table C.2 SESOIL input values for Nystatin

| Run | Conc | Rainfall | Vadose Zone Thickness | Intrinsic permeability | Organic Content | pH | Soil Type | Soil Description | CEC | Kd |
|---|---|---|---|---|---|---|---|---|---|---|
| | μg/L | cm | cm | $cm^2$ | % | | | | meq/100g | |
| 1 | 0.74 | 153.6 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 2 | 0.74 | 6.708 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 3 | 0.74 | 153.6 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 4 | 0.74 | 6.708 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 5 | 0.74 | 153.6 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 6 | 0.74 | 6.708 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 7 | 0.74 | 153.6 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 8 | 0.74 | 6.708 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 9 | 0.74 | 153.6 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 10 | 0.74 | 6.708 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 11 | 0.74 | 153.6 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 12 | 0.74 | 6.708 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 13 | 0.74 | 153.6 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 14 | 0.74 | 6.708 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 15 | 0.74 | 153.6 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 16 | 0.74 | 6.708 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 17 | 0.74 | 153.6 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 18 | 0.74 | 6.708 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 19 | 0.74 | 153.6 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 20 | 0.74 | 6.708 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 21 | 0.74 | 153.6 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 22 | 0.74 | 6.708 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 23 | 0.74 | 153.6 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 24 | 0.74 | 6.708 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 25 | 0.74 | 153.6 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 26 | 0.74 | 6.708 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 27 | 0.74 | 153.6 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 28 | 0.74 | 6.708 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 29 | 0.74 | 153.6 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 30 | 0.74 | 6.708 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 31 | 0.74 | 153.6 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 32 | 0.74 | 6.708 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 33 | 0.002 | 153.6 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 34 | 0.002 | 6.708 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 35 | 0.002 | 153.6 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 36 | 0.002 | 6.708 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 37 | 0.002 | 153.6 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |

Continuation of above table

| Run | Conc | Rainfall | Vadose Zone Thickness | Intrinsic permeability | Organic Content | pH | Soil Type | Soil Description | CEC | Kd |
|---|---|---|---|---|---|---|---|---|---|---|
| | µg/L | cm | cm | $cm^2$ | % | | | | meq/100g | |
| 38 | 0.002 | 6.708 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 39 | 0.002 | 153.6 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 40 | 0.002 | 6.708 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 41 | 0.002 | 153.6 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 42 | 0.002 | 6.708 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 43 | 0.002 | 153.6 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 44 | 0.002 | 6.708 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 45 | 0.002 | 153.6 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 46 | 0.002 | 6.708 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 47 | 0.002 | 153.6 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 48 | 0.002 | 6.708 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 49 | 0.002 | 153.6 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 50 | 0.002 | 6.708 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 51 | 0.002 | 153.6 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 52 | 0.002 | 6.708 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 53 | 0.002 | 153.6 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 54 | 0.002 | 6.708 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 55 | 0.002 | 153.6 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 56 | 0.002 | 6.708 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 57 | 0.002 | 153.6 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 58 | 0.002 | 6.708 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 59 | 0.002 | 153.6 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 60 | 0.002 | 6.708 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 61 | 0.002 | 153.6 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 62 | 0.002 | 6.708 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 63 | 0.002 | 153.6 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 64 | 0.002 | 6.708 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |

Table C.3 SESOIL input values for Dexamethasone

| Run | Conc | Rainfall | Vadose Zone Thickness | Intrinsic permeability | Organic Content | pH | Soil Type | Soil Description | CEC | Kd |
|---|---|---|---|---|---|---|---|---|---|---|
| | µg/L | cm | cm | $cm^2$ | % | | | | meq/100g | |
| 1 | 0.74 | 153.6 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 2 | 0.74 | 6.708 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 3 | 0.74 | 153.6 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 4 | 0.74 | 6.708 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 5 | 0.74 | 153.6 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 6 | 0.74 | 6.708 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 7 | 0.74 | 153.6 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 8 | 0.74 | 6.708 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 9 | 0.74 | 153.6 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 10 | 0.74 | 6.708 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 11 | 0.74 | 153.6 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 12 | 0.74 | 6.708 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 13 | 0.74 | 153.6 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 14 | 0.74 | 6.708 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 15 | 0.74 | 153.6 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 16 | 0.74 | 6.708 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 17 | 0.74 | 153.6 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 18 | 0.74 | 6.708 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 19 | 0.74 | 153.6 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 20 | 0.74 | 6.708 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 21 | 0.74 | 153.6 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 22 | 0.74 | 6.708 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 23 | 0.74 | 153.6 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 24 | 0.74 | 6.708 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 25 | 0.74 | 153.6 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 26 | 0.74 | 6.708 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 27 | 0.74 | 153.6 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 28 | 0.74 | 6.708 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 29 | 0.74 | 153.6 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 30 | 0.74 | 6.708 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 31 | 0.74 | 153.6 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 32 | 0.74 | 6.708 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 33 | 0.002 | 153.6 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 34 | 0.002 | 6.708 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 35 | 0.002 | 153.6 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 36 | 0.002 | 6.708 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 37 | 0.002 | 153.6 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |

Continuation of above table

| Run | Conc | Rainfall | Vadose Zone Thickness | Intrinsic permeability | Organic Content | pH | Soil Type | Soil Description | CEC | Kd |
|---|---|---|---|---|---|---|---|---|---|---|
| | μg/L | cm | cm | $cm^2$ | % | | | | meq/100g | |
| 38 | 0.002 | 6.708 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 39 | 0.002 | 153.6 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 40 | 0.002 | 6.708 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 41 | 0.002 | 153.6 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 42 | 0.002 | 6.708 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 43 | 0.002 | 153.6 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 44 | 0.002 | 6.708 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 45 | 0.002 | 153.6 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 46 | 0.002 | 6.708 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 47 | 0.002 | 153.6 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 48 | 0.002 | 6.708 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 49 | 0.002 | 153.6 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 50 | 0.002 | 6.708 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 51 | 0.002 | 153.6 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 52 | 0.002 | 6.708 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 53 | 0.002 | 153.6 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 54 | 0.002 | 6.708 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 55 | 0.002 | 153.6 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 56 | 0.002 | 6.708 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 57 | 0.002 | 153.6 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 58 | 0.002 | 6.708 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 59 | 0.002 | 153.6 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 60 | 0.002 | 6.708 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 61 | 0.002 | 153.6 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 62 | 0.002 | 6.708 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 63 | 0.002 | 153.6 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 64 | 0.002 | 6.708 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |

Table C.4 SESOIL input values for Methoprene

| Run | Conc | Rainfall | Vadose Zone Thickness | Intrinsic permeability | Organic Content | pH | Soil Type | Soil Description | CEC | Kd |
|---|---|---|---|---|---|---|---|---|---|---|
| | µg/L | cm | cm | $cm^2$ | % | | | | meq/100g | |
| 1 | 0.74 | 153.6 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 2 | 0.74 | 6.708 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 3 | 0.74 | 153.6 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 4 | 0.74 | 6.708 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 5 | 0.74 | 153.6 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 6 | 0.74 | 6.708 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 7 | 0.74 | 153.6 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 8 | 0.74 | 6.708 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 9 | 0.74 | 153.6 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 10 | 0.74 | 6.708 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 11 | 0.74 | 153.6 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 12 | 0.74 | 6.708 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 13 | 0.74 | 153.6 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 14 | 0.74 | 6.708 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 15 | 0.74 | 153.6 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 16 | 0.74 | 6.708 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 17 | 0.74 | 153.6 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 18 | 0.74 | 6.708 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 19 | 0.74 | 153.6 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 20 | 0.74 | 6.708 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 21 | 0.74 | 153.6 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 22 | 0.74 | 6.708 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 23 | 0.74 | 153.6 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 24 | 0.74 | 6.708 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 25 | 0.74 | 153.6 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 26 | 0.74 | 6.708 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 27 | 0.74 | 153.6 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 28 | 0.74 | 6.708 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 29 | 0.74 | 153.6 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 30 | 0.74 | 6.708 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 31 | 0.74 | 153.6 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 32 | 0.74 | 6.708 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 33 | 0.002 | 153.6 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 34 | 0.002 | 6.708 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 35 | 0.002 | 153.6 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 36 | 0.002 | 6.708 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 37 | 0.002 | 153.6 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |

Continuation of above table

| Run | Conc | Rainfall | Vadose Zone Thickness | Intrinsic permeability | Organic Content | pH | Soil Type | Soil Description | CEC | Kd |
|---|---|---|---|---|---|---|---|---|---|---|
| | µg/L | cm | cm | $cm^2$ | % | | | | meq/100g | |
| 38 | 0.002 | 6.708 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 39 | 0.002 | 153.6 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 40 | 0.002 | 6.708 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 41 | 0.002 | 153.6 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 42 | 0.002 | 6.708 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 43 | 0.002 | 153.6 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 44 | 0.002 | 6.708 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 45 | 0.002 | 153.6 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 46 | 0.002 | 6.708 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 47 | 0.002 | 153.6 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 48 | 0.002 | 6.708 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 49 | 0.002 | 153.6 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 50 | 0.002 | 6.708 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 51 | 0.002 | 153.6 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 52 | 0.002 | 6.708 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 53 | 0.002 | 153.6 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 54 | 0.002 | 6.708 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 55 | 0.002 | 153.6 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 56 | 0.002 | 6.708 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 57 | 0.002 | 153.6 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 58 | 0.002 | 6.708 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 59 | 0.002 | 153.6 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 60 | 0.002 | 6.708 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 61 | 0.002 | 153.6 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 62 | 0.002 | 6.708 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 63 | 0.002 | 153.6 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 64 | 0.002 | 6.708 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |

Table C.5 SESOIL input values for Prednisone

| Run | Conc | Rainfall | Vadose Zone Thickness | Intrinsic permeability | Organic Content | pH | Soil Type | Soil Description | CEC | Kd |
|---|---|---|---|---|---|---|---|---|---|---|
| | µg/L | cm | cm | $cm^2$ | % | | | | meq/100g | |
| 1 | 0.74 | 153.6 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 2 | 0.74 | 6.708 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 3 | 0.74 | 153.6 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 4 | 0.74 | 6.708 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 5 | 0.74 | 153.6 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 6 | 0.74 | 6.708 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 7 | 0.74 | 153.6 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 8 | 0.74 | 6.708 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 9 | 0.74 | 153.6 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 10 | 0.74 | 6.708 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 11 | 0.74 | 153.6 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 12 | 0.74 | 6.708 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 13 | 0.74 | 153.6 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 14 | 0.74 | 6.708 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 15 | 0.74 | 153.6 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 16 | 0.74 | 6.708 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 17 | 0.74 | 153.6 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 18 | 0.74 | 6.708 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 19 | 0.74 | 153.6 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 20 | 0.74 | 6.708 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 21 | 0.74 | 153.6 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 22 | 0.74 | 6.708 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 23 | 0.74 | 153.6 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 24 | 0.74 | 6.708 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 25 | 0.74 | 153.6 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 26 | 0.74 | 6.708 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 27 | 0.74 | 153.6 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 28 | 0.74 | 6.708 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 29 | 0.74 | 153.6 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 30 | 0.74 | 6.708 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 31 | 0.74 | 153.6 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 32 | 0.74 | 6.708 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 33 | 0.002 | 153.6 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 34 | 0.002 | 6.708 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 35 | 0.002 | 153.6 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 36 | 0.002 | 6.708 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 37 | 0.002 | 153.6 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |

Continuation of above table

| Run | Conc | Rainfall | Vadose Zone Thickness | Intrinsic permeability | Organic Content | pH | Soil Type | Soil Description | CEC | Kd |
|---|---|---|---|---|---|---|---|---|---|---|
| | µg/L | cm | cm | $cm^2$ | % | | | | meq/100g | |
| 38 | 0.002 | 6.708 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 39 | 0.002 | 153.6 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 40 | 0.002 | 6.708 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 41 | 0.002 | 153.6 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 42 | 0.002 | 6.708 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 43 | 0.002 | 153.6 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 44 | 0.002 | 6.708 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 45 | 0.002 | 153.6 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 46 | 0.002 | 6.708 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 47 | 0.002 | 153.6 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 48 | 0.002 | 6.708 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 49 | 0.002 | 153.6 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 50 | 0.002 | 6.708 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 51 | 0.002 | 153.6 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 52 | 0.002 | 6.708 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 53 | 0.002 | 153.6 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 54 | 0.002 | 6.708 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 55 | 0.002 | 153.6 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 56 | 0.002 | 6.708 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 57 | 0.002 | 153.6 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 58 | 0.002 | 6.708 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 59 | 0.002 | 153.6 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 60 | 0.002 | 6.708 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 61 | 0.002 | 153.6 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 62 | 0.002 | 6.708 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 63 | 0.002 | 153.6 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 64 | 0.002 | 6.708 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |

Table C.6 SESOIL input values for Metronidazole

| Run | Conc | Rainfall | Vadose Zone Thickness | Intrinsic permeability | Organic Content | pH | Soil Type | Soil Description | CEC | Kd |
|---|---|---|---|---|---|---|---|---|---|---|
| | μg/L | cm | cm | $cm^2$ | % | | | | meq/100g | |
| 1 | 0.74 | 153.6 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 2 | 0.74 | 6.708 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 3 | 0.74 | 153.6 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 4 | 0.74 | 6.708 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 5 | 0.74 | 153.6 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 6 | 0.74 | 6.708 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 7 | 0.74 | 153.6 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 8 | 0.74 | 6.708 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 9 | 0.74 | 153.6 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 10 | 0.74 | 6.708 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 11 | 0.74 | 153.6 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 12 | 0.74 | 6.708 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 13 | 0.74 | 153.6 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 14 | 0.74 | 6.708 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 15 | 0.74 | 153.6 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 16 | 0.74 | 6.708 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 17 | 0.74 | 153.6 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 18 | 0.74 | 6.708 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 19 | 0.74 | 153.6 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 20 | 0.74 | 6.708 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 21 | 0.74 | 153.6 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 22 | 0.74 | 6.708 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 23 | 0.74 | 153.6 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 24 | 0.74 | 6.708 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 25 | 0.74 | 153.6 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 26 | 0.74 | 6.708 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 27 | 0.74 | 153.6 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 28 | 0.74 | 6.708 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 29 | 0.74 | 153.6 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 30 | 0.74 | 6.708 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 31 | 0.74 | 153.6 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 32 | 0.74 | 6.708 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 33 | 0.002 | 153.6 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 34 | 0.002 | 6.708 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 35 | 0.002 | 153.6 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 36 | 0.002 | 6.708 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 37 | 0.002 | 153.6 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |

Continuation of above table

| Run | Conc | Rainfall | Vadose Zone Thickness | Intrinsic permeability | Organic Content | pH | Soil Type | Soil Description | CEC | Kd |
|---|---|---|---|---|---|---|---|---|---|---|
| | µg/L | cm | cm | $cm^2$ | % | | | | meq/100g | |
| 38 | 0.002 | 6.708 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 39 | 0.002 | 153.6 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 40 | 0.002 | 6.708 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 41 | 0.002 | 153.6 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 42 | 0.002 | 6.708 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 43 | 0.002 | 153.6 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 44 | 0.002 | 6.708 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 45 | 0.002 | 153.6 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 46 | 0.002 | 6.708 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 47 | 0.002 | 153.6 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 48 | 0.002 | 6.708 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 49 | 0.002 | 153.6 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 50 | 0.002 | 6.708 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 51 | 0.002 | 153.6 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 52 | 0.002 | 6.708 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 53 | 0.002 | 153.6 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 54 | 0.002 | 6.708 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 55 | 0.002 | 153.6 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 56 | 0.002 | 6.708 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 57 | 0.002 | 153.6 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 58 | 0.002 | 6.708 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 59 | 0.002 | 153.6 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 60 | 0.002 | 6.708 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 61 | 0.002 | 153.6 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 62 | 0.002 | 6.708 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 63 | 0.002 | 153.6 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 64 | 0.002 | 6.708 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |

Table C.7 SESOIL input values for Clindamycin

| Run | Conc | Rainfall | Vadose Zone Thickness | Intrinsic permeability | Organic Content | pH | Soil Type | Soil Description | CEC | Kd |
|---|---|---|---|---|---|---|---|---|---|---|
| | μg/L | cm | cm | $cm^2$ | % | | | | meq/100g | |
| 1 | 0.74 | 153.6 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 2 | 0.74 | 6.708 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 3 | 0.74 | 153.6 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 4 | 0.74 | 6.708 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 5 | 0.74 | 153.6 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 6 | 0.74 | 6.708 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 7 | 0.74 | 153.6 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 8 | 0.74 | 6.708 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 9 | 0.74 | 153.6 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 10 | 0.74 | 6.708 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 11 | 0.74 | 153.6 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 12 | 0.74 | 6.708 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 13 | 0.74 | 153.6 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 14 | 0.74 | 6.708 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 15 | 0.74 | 153.6 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 16 | 0.74 | 6.708 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 17 | 0.74 | 153.6 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 18 | 0.74 | 6.708 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 19 | 0.74 | 153.6 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 20 | 0.74 | 6.708 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 21 | 0.74 | 153.6 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 22 | 0.74 | 6.708 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 23 | 0.74 | 153.6 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 24 | 0.74 | 6.708 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 25 | 0.74 | 153.6 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 26 | 0.74 | 6.708 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 27 | 0.74 | 153.6 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 28 | 0.74 | 6.708 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 29 | 0.74 | 153.6 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 30 | 0.74 | 6.708 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 31 | 0.74 | 153.6 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 32 | 0.74 | 6.708 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 33 | 0.002 | 153.6 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 34 | 0.002 | 6.708 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 35 | 0.002 | 153.6 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 36 | 0.002 | 6.708 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 37 | 0.002 | 153.6 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |

Continuation of above table

| Run | Conc | Rainfall | Vadose Zone Thickness | Intrinsic permeability | Organic Content | pH | Soil Type | Soil Description | CEC | Kd |
|---|---|---|---|---|---|---|---|---|---|---|
| | µg/L | cm | cm | $cm^2$ | % | | | | meq/100g | |
| 38 | 0.002 | 6.708 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 39 | 0.002 | 153.6 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 40 | 0.002 | 6.708 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 41 | 0.002 | 153.6 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 42 | 0.002 | 6.708 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 43 | 0.002 | 153.6 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 44 | 0.002 | 6.708 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 45 | 0.002 | 153.6 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 46 | 0.002 | 6.708 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 47 | 0.002 | 153.6 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 48 | 0.002 | 6.708 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 49 | 0.002 | 153.6 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 50 | 0.002 | 6.708 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 51 | 0.002 | 153.6 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 52 | 0.002 | 6.708 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 53 | 0.002 | 153.6 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 54 | 0.002 | 6.708 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 55 | 0.002 | 153.6 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 56 | 0.002 | 6.708 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 57 | 0.002 | 153.6 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 58 | 0.002 | 6.708 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 59 | 0.002 | 153.6 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 60 | 0.002 | 6.708 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 61 | 0.002 | 153.6 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 62 | 0.002 | 6.708 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 63 | 0.002 | 153.6 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 64 | 0.002 | 6.708 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |

Table C.8 SESOIL input values for Ketoconazole

| Run | Conc | Rainfall | Vadose Zone Thickness | Intrinsic permeability | Organic Content | pH | Soil Type | Soil Description | CEC | Kd |
|---|---|---|---|---|---|---|---|---|---|---|
| | µg/L | cm | cm | $cm^2$ | % | | | | meq/100g | |
| 1 | 0.74 | 153.6 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 2 | 0.74 | 6.708 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 3 | 0.74 | 153.6 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 4 | 0.74 | 6.708 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 5 | 0.74 | 153.6 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 6 | 0.74 | 6.708 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 7 | 0.74 | 153.6 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 8 | 0.74 | 6.708 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 9 | 0.74 | 153.6 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 10 | 0.74 | 6.708 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 11 | 0.74 | 153.6 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 12 | 0.74 | 6.708 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 13 | 0.74 | 153.6 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 14 | 0.74 | 6.708 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 15 | 0.74 | 153.6 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 16 | 0.74 | 6.708 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 17 | 0.74 | 153.6 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 18 | 0.74 | 6.708 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 19 | 0.74 | 153.6 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 20 | 0.74 | 6.708 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 21 | 0.74 | 153.6 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 22 | 0.74 | 6.708 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 23 | 0.74 | 153.6 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 24 | 0.74 | 6.708 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 25 | 0.74 | 153.6 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 26 | 0.74 | 6.708 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 27 | 0.74 | 153.6 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 28 | 0.74 | 6.708 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 29 | 0.74 | 153.6 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 30 | 0.74 | 6.708 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 31 | 0.74 | 153.6 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 32 | 0.74 | 6.708 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 33 | 0.002 | 153.6 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 34 | 0.002 | 6.708 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 35 | 0.002 | 153.6 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 36 | 0.002 | 6.708 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 37 | 0.002 | 153.6 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |

Continuation of above table

| Run | Conc | Rainfall | Vadose Zone Thickness | Intrinsic permeability | Organic Content | pH | Soil Type | Soil Description | CEC | Kd |
|---|---|---|---|---|---|---|---|---|---|---|
| | μg/L | cm | cm | $cm^2$ | % | | | | meq/100g | |
| 38 | 0.002 | 6.708 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 39 | 0.002 | 153.6 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 40 | 0.002 | 6.708 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 41 | 0.002 | 153.6 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 42 | 0.002 | 6.708 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 43 | 0.002 | 153.6 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 44 | 0.002 | 6.708 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 45 | 0.002 | 153.6 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 46 | 0.002 | 6.708 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 47 | 0.002 | 153.6 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 48 | 0.002 | 6.708 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 49 | 0.002 | 153.6 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 50 | 0.002 | 6.708 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 51 | 0.002 | 153.6 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 52 | 0.002 | 6.708 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 53 | 0.002 | 153.6 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 54 | 0.002 | 6.708 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 55 | 0.002 | 153.6 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 56 | 0.002 | 6.708 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 57 | 0.002 | 153.6 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 58 | 0.002 | 6.708 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 59 | 0.002 | 153.6 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 60 | 0.002 | 6.708 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 61 | 0.002 | 153.6 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 62 | 0.002 | 6.708 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 63 | 0.002 | 153.6 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 64 | 0.002 | 6.708 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |

Table C.9 SESOIL input values for Carbamazepine

| Run | Conc | Rainfall | Vadose Zone Thickness | Intrinsic permeability | Organic Content | pH | Soil Type | Soil Description | CEC | Kd |
|---|---|---|---|---|---|---|---|---|---|---|
| | μg/L | cm | cm | $cm^2$ | % | | | | meq/100g | |
| 1 | 0.083 | 153.6 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 2 | 0.083 | 6.708 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 3 | 0.083 | 153.6 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 4 | 0.083 | 6.708 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 5 | 0.083 | 153.6 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 6 | 0.083 | 6.708 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 7 | 0.083 | 153.6 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 8 | 0.083 | 6.708 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 9 | 0.083 | 153.6 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 10 | 0.083 | 6.708 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 11 | 0.083 | 153.6 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 12 | 0.083 | 6.708 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 13 | 0.083 | 153.6 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 14 | 0.083 | 6.708 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 15 | 0.083 | 153.6 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 16 | 0.083 | 6.708 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 17 | 0.083 | 153.6 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 18 | 0.083 | 6.708 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 19 | 0.083 | 153.6 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 20 | 0.083 | 6.708 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 21 | 0.083 | 153.6 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 22 | 0.083 | 6.708 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 23 | 0.083 | 153.6 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 24 | 0.083 | 6.708 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 25 | 0.083 | 153.6 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 26 | 0.083 | 6.708 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 27 | 0.083 | 153.6 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 28 | 0.083 | 6.708 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 29 | 0.083 | 153.6 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 30 | 0.083 | 6.708 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 31 | 0.083 | 153.6 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 32 | 0.083 | 6.708 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 33 | 0.002 | 153.6 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 34 | 0.002 | 6.708 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 35 | 0.002 | 153.6 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 36 | 0.002 | 6.708 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 37 | 0.002 | 153.6 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |

Continuation of above table

| Run | Conc | Rainfall | Vadose Zone Thickness | Intrinsic permeability | Organic Content | pH | Soil Type | Soil Description | CEC | Kd |
|---|---|---|---|---|---|---|---|---|---|---|
| | µg/L | cm | cm | $cm^2$ | % | | | | meq/100g | |
| 38 | 0.002 | 6.708 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 39 | 0.002 | 153.6 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 40 | 0.002 | 6.708 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 41 | 0.002 | 153.6 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 42 | 0.002 | 6.708 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 43 | 0.002 | 153.6 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 44 | 0.002 | 6.708 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 45 | 0.002 | 153.6 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 46 | 0.002 | 6.708 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 47 | 0.002 | 153.6 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 48 | 0.002 | 6.708 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 49 | 0.002 | 153.6 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 50 | 0.002 | 6.708 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 51 | 0.002 | 153.6 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 52 | 0.002 | 6.708 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 53 | 0.002 | 153.6 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 54 | 0.002 | 6.708 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 55 | 0.002 | 153.6 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 56 | 0.002 | 6.708 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 57 | 0.002 | 153.6 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 58 | 0.002 | 6.708 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 59 | 0.002 | 153.6 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 60 | 0.002 | 6.708 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 61 | 0.002 | 153.6 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 62 | 0.002 | 6.708 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 63 | 0.002 | 153.6 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 64 | 0.002 | 6.708 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |

Table C.10 SESOIL input values for Caffeine

| Run | Conc | Rainfall | Vadose Zone Thickness | Intrinsic permeability | Organic Content | pH | Soil Type | Soil Description | CEC | Kd |
|---|---|---|---|---|---|---|---|---|---|---|
| | μg/L | cm | cm | $cm^2$ | % | | | | meq/100g | |
| 1 | 0.24 | 153.6 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 2 | 0.24 | 6.708 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 3 | 0.24 | 153.6 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 4 | 0.24 | 6.708 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 5 | 0.24 | 153.6 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 6 | 0.24 | 6.708 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 7 | 0.24 | 153.6 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 8 | 0.24 | 6.708 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 9 | 0.24 | 153.6 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 10 | 0.24 | 6.708 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 11 | 0.24 | 153.6 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 12 | 0.24 | 6.708 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 13 | 0.24 | 153.6 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 14 | 0.24 | 6.708 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 15 | 0.24 | 153.6 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 16 | 0.24 | 6.708 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 17 | 0.24 | 153.6 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 18 | 0.24 | 6.708 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 19 | 0.24 | 153.6 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 20 | 0.24 | 6.708 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 21 | 0.24 | 153.6 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 22 | 0.24 | 6.708 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 23 | 0.24 | 153.6 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 24 | 0.24 | 6.708 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 25 | 0.24 | 153.6 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 26 | 0.24 | 6.708 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 27 | 0.24 | 153.6 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 28 | 0.24 | 6.708 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 29 | 0.24 | 153.6 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 30 | 0.24 | 6.708 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 31 | 0.24 | 153.6 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 32 | 0.24 | 6.708 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 33 | 0.004 | 153.6 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 34 | 0.004 | 6.708 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 35 | 0.004 | 153.6 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 36 | 0.004 | 6.708 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 37 | 0.004 | 153.6 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |

Continuation of above table

| Run | Conc | Rainfall | Vadose Zone Thickness | Intrinsic permeability | Organic Content | pH | Soil Type | Soil Description | CEC | Kd |
|---|---|---|---|---|---|---|---|---|---|---|
| | μg/L | cm | cm | $cm^2$ | % | | | | meq/100g | |
| 38 | 0.004 | 6.708 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 39 | 0.004 | 153.6 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 40 | 0.004 | 6.708 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 41 | 0.004 | 153.6 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 42 | 0.004 | 6.708 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 43 | 0.004 | 153.6 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 44 | 0.004 | 6.708 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 45 | 0.004 | 153.6 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 46 | 0.004 | 6.708 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 47 | 0.004 | 153.6 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 48 | 0.004 | 6.708 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 49 | 0.004 | 153.6 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 50 | 0.004 | 6.708 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 51 | 0.004 | 153.6 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 52 | 0.004 | 6.708 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 53 | 0.004 | 153.6 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 54 | 0.004 | 6.708 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 55 | 0.004 | 153.6 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 56 | 0.004 | 6.708 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 57 | 0.004 | 153.6 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 58 | 0.004 | 6.708 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 59 | 0.004 | 153.6 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 60 | 0.004 | 6.708 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 61 | 0.004 | 153.6 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 62 | 0.004 | 6.708 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 63 | 0.004 | 153.6 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 64 | 0.004 | 6.708 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |

Table C.11 SESOIL input values for Ibuprofen

| Run | Conc | Rainfall | Vadose Zone Thickness | Intrinsic permeability | Organic Content | pH | Soil Type | Soil Description | CEC | Kd |
|---|---|---|---|---|---|---|---|---|---|---|
| | µg/L | cm | cm | $cm^2$ | % | | | | meq/100g | |
| 1 | 0.6 | 153.6 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 2 | 0.6 | 6.708 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 3 | 0.6 | 153.6 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 4 | 0.6 | 6.708 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 5 | 0.6 | 153.6 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 6 | 0.6 | 6.708 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 7 | 0.6 | 153.6 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 8 | 0.6 | 6.708 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 9 | 0.6 | 153.6 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 10 | 0.6 | 6.708 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 11 | 0.6 | 153.6 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 12 | 0.6 | 6.708 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 13 | 0.6 | 153.6 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 14 | 0.6 | 6.708 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 15 | 0.6 | 153.6 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 16 | 0.6 | 6.708 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 17 | 0.6 | 153.6 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 18 | 0.6 | 6.708 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 19 | 0.6 | 153.6 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 20 | 0.6 | 6.708 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 21 | 0.6 | 153.6 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 22 | 0.6 | 6.708 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 23 | 0.6 | 153.6 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 24 | 0.6 | 6.708 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 25 | 0.6 | 153.6 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 26 | 0.6 | 6.708 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 27 | 0.6 | 153.6 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 28 | 0.6 | 6.708 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 29 | 0.6 | 153.6 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 30 | 0.6 | 6.708 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 31 | 0.6 | 153.6 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 32 | 0.6 | 6.708 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 33 | 0.003 | 153.6 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 34 | 0.003 | 6.708 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 35 | 0.003 | 153.6 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 36 | 0.003 | 6.708 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 37 | 0.003 | 153.6 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |

Continuation of above table

| Run | Conc | Rainfall | Vadose Zone Thickness | Intrinsic permeability | Organic Content | pH | Soil Type | Soil Description | CEC | Kd |
|---|---|---|---|---|---|---|---|---|---|---|
| | μg/L | cm | cm | $cm^2$ | % | | | | meq/100g | |
| 38 | 0.003 | 6.708 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 39 | 0.003 | 153.6 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 40 | 0.003 | 6.708 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 41 | 0.003 | 153.6 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 42 | 0.003 | 6.708 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 43 | 0.003 | 153.6 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 44 | 0.003 | 6.708 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 45 | 0.003 | 153.6 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 46 | 0.003 | 6.708 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 47 | 0.003 | 153.6 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 48 | 0.003 | 6.708 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 49 | 0.003 | 153.6 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 50 | 0.003 | 6.708 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 51 | 0.003 | 153.6 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 52 | 0.003 | 6.708 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 53 | 0.003 | 153.6 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 54 | 0.003 | 6.708 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 55 | 0.003 | 153.6 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 56 | 0.003 | 6.708 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 57 | 0.003 | 153.6 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 58 | 0.003 | 6.708 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 59 | 0.003 | 153.6 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 60 | 0.003 | 6.708 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 61 | 0.003 | 153.6 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 62 | 0.003 | 6.708 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 63 | 0.003 | 153.6 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 64 | 0.003 | 6.708 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |

Table C.12 SESOIL input values for Diclofenac

| Run | Conc | Rainfall | Vadose Zone Thickness | Intrinsic permeability | Organic Content | pH | Soil Type | Soil Description | CEC | Kd |
|---|---|---|---|---|---|---|---|---|---|---|
| | μg/L | cm | cm | $cm^2$ | % | | | | meq/100g | |
| 1 | 0.18 | 153.6 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 2 | 0.18 | 6.708 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 3 | 0.18 | 153.6 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 4 | 0.18 | 6.708 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 5 | 0.18 | 153.6 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 6 | 0.18 | 6.708 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 7 | 0.18 | 153.6 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 8 | 0.18 | 6.708 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 9 | 0.18 | 153.6 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 10 | 0.18 | 6.708 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 11 | 0.18 | 153.6 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 12 | 0.18 | 6.708 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 13 | 0.18 | 153.6 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 14 | 0.18 | 6.708 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 15 | 0.18 | 153.6 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 16 | 0.18 | 6.708 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 17 | 0.18 | 153.6 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 18 | 0.18 | 6.708 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 19 | 0.18 | 153.6 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 20 | 0.18 | 6.708 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 21 | 0.18 | 153.6 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 22 | 0.18 | 6.708 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 23 | 0.18 | 153.6 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 24 | 0.18 | 6.708 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 25 | 0.18 | 153.6 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 26 | 0.18 | 6.708 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 27 | 0.18 | 153.6 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 28 | 0.18 | 6.708 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 29 | 0.18 | 153.6 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 30 | 0.18 | 6.708 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 31 | 0.18 | 153.6 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 32 | 0.18 | 6.708 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 33 | 0.007 | 153.6 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 34 | 0.007 | 6.708 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 35 | 0.007 | 153.6 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 36 | 0.007 | 6.708 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 37 | 0.007 | 153.6 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |

Continuation of above table

| Run | Conc | Rainfall | Vadose Zone Thickness | Intrinsic permeability | Organic Content | pH | Soil Type | Soil Description | CEC | Kd |
|---|---|---|---|---|---|---|---|---|---|---|
| | µg/L | cm | cm | $cm^2$ | % | | | | meq/100g | |
| 38 | 0.007 | 6.708 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 39 | 0.007 | 153.6 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 40 | 0.007 | 6.708 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 41 | 0.007 | 153.6 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 42 | 0.007 | 6.708 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 43 | 0.007 | 153.6 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 44 | 0.007 | 6.708 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 45 | 0.007 | 153.6 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 46 | 0.007 | 6.708 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 47 | 0.007 | 153.6 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 48 | 0.007 | 6.708 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 49 | 0.007 | 153.6 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 50 | 0.007 | 6.708 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 51 | 0.007 | 153.6 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 52 | 0.007 | 6.708 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 53 | 0.007 | 153.6 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 54 | 0.007 | 6.708 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 55 | 0.007 | 153.6 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 56 | 0.007 | 6.708 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 57 | 0.007 | 153.6 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 58 | 0.007 | 6.708 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 59 | 0.007 | 153.6 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 60 | 0.007 | 6.708 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 61 | 0.007 | 153.6 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 62 | 0.007 | 6.708 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 63 | 0.007 | 153.6 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 64 | 0.007 | 6.708 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |

Table C.13 SESOIL input values for Acetaminophen

| Run | Conc | Rainfall | Vadose Zone Thickness | Intrinsic permeability | Organic Content | pH | Soil Type | Soil Description | CEC | Kd |
|---|---|---|---|---|---|---|---|---|---|---|
| | μg/L | cm | cm | $cm^2$ | % | | | | meq/100g | |
| 1 | 0.03 | 153.6 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 2 | 0.03 | 6.708 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 3 | 0.03 | 153.6 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 4 | 0.03 | 6.708 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 5 | 0.03 | 153.6 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 6 | 0.03 | 6.708 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 7 | 0.03 | 153.6 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 8 | 0.03 | 6.708 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 9 | 0.03 | 153.6 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 10 | 0.03 | 6.708 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 11 | 0.03 | 153.6 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 12 | 0.03 | 6.708 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 13 | 0.03 | 153.6 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 14 | 0.03 | 6.708 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 15 | 0.03 | 153.6 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 16 | 0.03 | 6.708 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 17 | 0.03 | 153.6 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 18 | 0.03 | 6.708 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 19 | 0.03 | 153.6 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 20 | 0.03 | 6.708 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 21 | 0.03 | 153.6 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 22 | 0.03 | 6.708 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 23 | 0.03 | 153.6 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 24 | 0.03 | 6.708 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 25 | 0.03 | 153.6 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 26 | 0.03 | 6.708 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 27 | 0.03 | 153.6 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 28 | 0.03 | 6.708 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 29 | 0.03 | 153.6 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 30 | 0.03 | 6.708 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 31 | 0.03 | 153.6 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 32 | 0.03 | 6.708 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 33 | 0.012 | 153.6 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 34 | 0.012 | 6.708 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 35 | 0.012 | 153.6 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 36 | 0.012 | 6.708 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 37 | 0.012 | 153.6 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |

Continuation of above table

| Run | Conc | Rainfall | Vadose Zone Thickness | Intrinsic permeability | Organic Content | pH | Soil Type | Soil Description | CEC | Kd |
|---|---|---|---|---|---|---|---|---|---|---|
| | μg/L | cm | cm | $cm^2$ | % | | | | meq/100g | |
| 38 | 0.012 | 6.708 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 39 | 0.012 | 153.6 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 40 | 0.012 | 6.708 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 41 | 0.012 | 153.6 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 42 | 0.012 | 6.708 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 43 | 0.012 | 153.6 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 44 | 0.012 | 6.708 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 45 | 0.012 | 153.6 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 46 | 0.012 | 6.708 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 47 | 0.012 | 153.6 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 48 | 0.012 | 6.708 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 49 | 0.012 | 153.6 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 50 | 0.012 | 6.708 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 51 | 0.012 | 153.6 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 52 | 0.012 | 6.708 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 53 | 0.012 | 153.6 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 54 | 0.012 | 6.708 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 55 | 0.012 | 153.6 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 56 | 0.012 | 6.708 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 57 | 0.012 | 153.6 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 58 | 0.012 | 6.708 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 59 | 0.012 | 153.6 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 60 | 0.012 | 6.708 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 61 | 0.012 | 153.6 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 62 | 0.012 | 6.708 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 63 | 0.012 | 153.6 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 64 | 0.012 | 6.708 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |

Table C.14 SESOIL input values for Triclosan

| Run | Conc | Rainfall | Vadose Zone Thickness | Intrinsic permeability | Organic Content | pH | Soil Type | Soil Description | CEC | Kd |
|---|---|---|---|---|---|---|---|---|---|---|
| | μg/L | cm | cm | $cm^2$ | % | | | | meq/100g | |
| 1 | 0.74 | 153.6 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 2 | 0.74 | 6.708 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 3 | 0.74 | 153.6 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 4 | 0.74 | 6.708 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 5 | 0.74 | 153.6 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 6 | 0.74 | 6.708 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 7 | 0.74 | 153.6 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 8 | 0.74 | 6.708 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 9 | 0.74 | 153.6 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 10 | 0.74 | 6.708 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 11 | 0.74 | 153.6 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 12 | 0.74 | 6.708 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 13 | 0.74 | 153.6 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 14 | 0.74 | 6.708 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 15 | 0.74 | 153.6 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 16 | 0.74 | 6.708 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 17 | 0.74 | 153.6 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 18 | 0.74 | 6.708 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 19 | 0.74 | 153.6 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 20 | 0.74 | 6.708 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 21 | 0.74 | 153.6 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 22 | 0.74 | 6.708 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 23 | 0.74 | 153.6 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 24 | 0.74 | 6.708 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 25 | 0.74 | 153.6 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 26 | 0.74 | 6.708 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 27 | 0.74 | 153.6 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 28 | 0.74 | 6.708 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 29 | 0.74 | 153.6 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 30 | 0.74 | 6.708 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 31 | 0.74 | 153.6 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 32 | 0.74 | 6.708 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 33 | 0.003 | 153.6 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 34 | 0.003 | 6.708 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 35 | 0.003 | 153.6 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 36 | 0.003 | 6.708 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 37 | 0.003 | 153.6 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |

Continuation of above table

| Run | Conc | Rainfall | Vadose Zone Thickness | Intrinsic permeability | Organic Content | pH | Soil Type | Soil Description | CEC | Kd |
|---|---|---|---|---|---|---|---|---|---|---|
| | µg/L | cm | cm | $cm^2$ | % | | | | meq/100g | |
| 38 | 0.003 | 6.708 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 39 | 0.003 | 153.6 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 40 | 0.003 | 6.708 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 41 | 0.003 | 153.6 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 42 | 0.003 | 6.708 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 43 | 0.003 | 153.6 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 44 | 0.003 | 6.708 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 45 | 0.003 | 153.6 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 46 | 0.003 | 6.708 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 47 | 0.003 | 153.6 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 48 | 0.003 | 6.708 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 49 | 0.003 | 153.6 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 50 | 0.003 | 6.708 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 51 | 0.003 | 153.6 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 52 | 0.003 | 6.708 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 53 | 0.003 | 153.6 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 54 | 0.003 | 6.708 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 55 | 0.003 | 153.6 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 56 | 0.003 | 6.708 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 57 | 0.003 | 153.6 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 58 | 0.003 | 6.708 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 59 | 0.003 | 153.6 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 60 | 0.003 | 6.708 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 61 | 0.003 | 153.6 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 62 | 0.003 | 6.708 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 63 | 0.003 | 153.6 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 64 | 0.003 | 6.708 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |

Table C.15 SESOIL input values for Ciprofloxacin

| Run | Conc | Rainfall | Vadose Zone Thickness | Intrinsic permeability | Organic Content | pH | Soil Type | Soil Description | CEC | Kd |
|---|---|---|---|---|---|---|---|---|---|---|
| | µg/L | cm | cm | $cm^2$ | % | | | | meq/100g | |
| 1 | 0.5 | 153.6 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 2 | 0.5 | 6.708 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 3 | 0.5 | 153.6 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 4 | 0.5 | 6.708 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 5 | 0.5 | 153.6 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 6 | 0.5 | 6.708 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 7 | 0.5 | 153.6 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 8 | 0.5 | 6.708 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 9 | 0.5 | 153.6 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 10 | 0.5 | 6.708 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 11 | 0.5 | 153.6 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 12 | 0.5 | 6.708 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 13 | 0.5 | 153.6 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 14 | 0.5 | 6.708 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 15 | 0.5 | 153.6 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 16 | 0.5 | 6.708 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 17 | 0.5 | 153.6 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 18 | 0.5 | 6.708 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 19 | 0.5 | 153.6 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 20 | 0.5 | 6.708 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 21 | 0.5 | 153.6 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 22 | 0.5 | 6.708 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 23 | 0.5 | 153.6 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 24 | 0.5 | 6.708 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 25 | 0.5 | 153.6 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 26 | 0.5 | 6.708 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 27 | 0.5 | 153.6 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 28 | 0.5 | 6.708 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 29 | 0.5 | 153.6 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 30 | 0.5 | 6.708 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 31 | 0.5 | 153.6 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 32 | 0.5 | 6.708 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 33 | 0.027 | 153.6 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 34 | 0.027 | 6.708 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 35 | 0.027 | 153.6 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 36 | 0.027 | 6.708 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 37 | 0.027 | 153.6 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |

Continuation of above table

| Run | Conc | Rainfall | Vadose Zone Thickness | Intrinsic permeability | Organic Content | pH | Soil Type | Soil Description | CEC | Kd |
|---|---|---|---|---|---|---|---|---|---|---|
| | μg/L | cm | cm | $cm^2$ | % | | | | meq/100g | |
| 38 | 0.027 | 6.708 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 39 | 0.027 | 153.6 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 40 | 0.027 | 6.708 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 41 | 0.027 | 153.6 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 42 | 0.027 | 6.708 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 43 | 0.027 | 153.6 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 44 | 0.027 | 6.708 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 45 | 0.027 | 153.6 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 46 | 0.027 | 6.708 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 47 | 0.027 | 153.6 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 48 | 0.027 | 6.708 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 49 | 0.027 | 153.6 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 50 | 0.027 | 6.708 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 51 | 0.027 | 153.6 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 52 | 0.027 | 6.708 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 53 | 0.027 | 153.6 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 54 | 0.027 | 6.708 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 55 | 0.027 | 153.6 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 56 | 0.027 | 6.708 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 57 | 0.027 | 153.6 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 58 | 0.027 | 6.708 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 59 | 0.027 | 153.6 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 60 | 0.027 | 6.708 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 61 | 0.027 | 153.6 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 62 | 0.027 | 6.708 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 63 | 0.027 | 153.6 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 64 | 0.027 | 6.708 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |

Table C.16 SESOIL input values for Metoprolol

| Run | Conc | Rainfall | Vadose Zone Thickness | Intrinsic permeability | Organic Content | pH | Soil Type | Soil Description | CEC | Kd |
|---|---|---|---|---|---|---|---|---|---|---|
| | µg/L | cm | cm | $cm^2$ | % | | | | meq/100g | |
| 1 | 0.12 | 153.6 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 2 | 0.12 | 6.708 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 3 | 0.12 | 153.6 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 4 | 0.12 | 6.708 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 5 | 0.12 | 153.6 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 6 | 0.12 | 6.708 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 7 | 0.12 | 153.6 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 8 | 0.12 | 6.708 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 9 | 0.12 | 153.6 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 10 | 0.12 | 6.708 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 11 | 0.12 | 153.6 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 12 | 0.12 | 6.708 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 13 | 0.12 | 153.6 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 14 | 0.12 | 6.708 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 15 | 0.12 | 153.6 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 16 | 0.12 | 6.708 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 17 | 0.12 | 153.6 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 18 | 0.12 | 6.708 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 19 | 0.12 | 153.6 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 20 | 0.12 | 6.708 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 21 | 0.12 | 153.6 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 22 | 0.12 | 6.708 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 23 | 0.12 | 153.6 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 24 | 0.12 | 6.708 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 25 | 0.12 | 153.6 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 26 | 0.12 | 6.708 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 27 | 0.12 | 153.6 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 28 | 0.12 | 6.708 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 29 | 0.12 | 153.6 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 30 | 0.12 | 6.708 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 31 | 0.12 | 153.6 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 32 | 0.12 | 6.708 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 33 | 0.02 | 153.6 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 34 | 0.02 | 6.708 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 35 | 0.02 | 153.6 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 36 | 0.02 | 6.708 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 37 | 0.02 | 153.6 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |

Continuation of above table

| Run | Conc | Rainfall | Vadose Zone Thickness | Intrinsic permeability | Organic Content | pH | Soil Type | Soil Description | CEC | Kd |
|---|---|---|---|---|---|---|---|---|---|---|
| | μg/L | cm | cm | $cm^2$ | % | | | | meq/100g | |
| 38 | 0.02 | 6.708 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 39 | 0.02 | 153.6 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 40 | 0.02 | 6.708 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 41 | 0.02 | 153.6 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 42 | 0.02 | 6.708 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 43 | 0.02 | 153.6 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 44 | 0.02 | 6.708 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 45 | 0.02 | 153.6 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 46 | 0.02 | 6.708 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 47 | 0.02 | 153.6 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 48 | 0.02 | 6.708 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 49 | 0.02 | 153.6 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 50 | 0.02 | 6.708 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 51 | 0.02 | 153.6 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 52 | 0.02 | 6.708 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 53 | 0.02 | 153.6 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 54 | 0.02 | 6.708 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 55 | 0.02 | 153.6 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 56 | 0.02 | 6.708 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 57 | 0.02 | 153.6 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 58 | 0.02 | 6.708 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 59 | 0.02 | 153.6 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 60 | 0.02 | 6.708 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 61 | 0.02 | 153.6 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 62 | 0.02 | 6.708 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 63 | 0.02 | 153.6 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 64 | 0.02 | 6.708 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |

Table C.17 SESOIL input values for Salicylic acid

| Run | Conc | Rainfall | Vadose Zone Thickness | Intrinsic permeability | Organic Content | pH | Soil Type | Soil Description | CEC | Kd |
|---|---|---|---|---|---|---|---|---|---|---|
| | μg/L | cm | cm | $cm^2$ | % | | | | meq/100g | |
| 1 | 0.22 | 153.6 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 2 | 0.22 | 6.708 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 3 | 0.22 | 153.6 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 4 | 0.22 | 6.708 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 5 | 0.22 | 153.6 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 6 | 0.22 | 6.708 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 7 | 0.22 | 153.6 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 8 | 0.22 | 6.708 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 9 | 0.22 | 153.6 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 10 | 0.22 | 6.708 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 11 | 0.22 | 153.6 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 12 | 0.22 | 6.708 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 13 | 0.22 | 153.6 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 14 | 0.22 | 6.708 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 15 | 0.22 | 153.6 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 16 | 0.22 | 6.708 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 17 | 0.22 | 153.6 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 18 | 0.22 | 6.708 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 19 | 0.22 | 153.6 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 20 | 0.22 | 6.708 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 21 | 0.22 | 153.6 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 22 | 0.22 | 6.708 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 23 | 0.22 | 153.6 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 24 | 0.22 | 6.708 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 25 | 0.22 | 153.6 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 26 | 0.22 | 6.708 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 27 | 0.22 | 153.6 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 28 | 0.22 | 6.708 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 29 | 0.22 | 153.6 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 30 | 0.22 | 6.708 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 31 | 0.22 | 153.6 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 32 | 0.22 | 6.708 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 33 | 0.013 | 153.6 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 34 | 0.013 | 6.708 | 1200 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 35 | 0.013 | 153.6 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 36 | 0.013 | 6.708 | 300 | 1E-07 | 3 | 7.2 | Julesburg | sand lm | 10 | 80 |
| 37 | 0.013 | 153.6 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |

Continuation of above table

| Run | Conc | Rainfall | Vadose Zone Thickness | Intrinsic permeability | Organic Content | pH | Soil Type | Soil Description | CEC | Kd |
|---|---|---|---|---|---|---|---|---|---|---|
| | µg/L | cm | cm | $cm^2$ | % | | | | meq/100g | |
| 38 | 0.013 | 6.708 | 1200 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 39 | 0.013 | 153.6 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 40 | 0.013 | 6.708 | 300 | 1E-10 | 3 | 8 | Lewisville | silty cly | 23 | 1500 |
| 41 | 0.013 | 153.6 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 42 | 0.013 | 6.708 | 1200 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 43 | 0.013 | 153.6 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 44 | 0.013 | 6.708 | 300 | 1E-07 | 0.5 | 7.5 | Pompano | fn sand | 5 | 30 |
| 45 | 0.013 | 153.6 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 46 | 0.013 | 6.708 | 1200 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 47 | 0.013 | 153.6 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 48 | 0.013 | 6.708 | 300 | 1E-10 | 0.5 | 7.5 | Climara | clay | 38 | 2000 |
| 49 | 0.013 | 153.6 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 50 | 0.013 | 6.708 | 1200 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 51 | 0.013 | 153.6 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 52 | 0.013 | 6.708 | 300 | 1E-07 | 3 | 5 | Hazelton | ch loam | 4 | 150 |
| 53 | 0.013 | 153.6 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 54 | 0.013 | 6.708 | 1200 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 55 | 0.013 | 153.6 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 56 | 0.013 | 6.708 | 300 | 1E-10 | 3 | 5 | Charles | slt lm | 9 | 500 |
| 57 | 0.013 | 153.6 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 58 | 0.013 | 6.708 | 1200 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 59 | 0.013 | 153.6 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 60 | 0.013 | 6.708 | 300 | 1E-07 | 0.5 | 4.3 | Lakewood | sand | 3 | 20 |
| 61 | 0.013 | 153.6 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 62 | 0.013 | 6.708 | 1200 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 63 | 0.013 | 153.6 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |
| 64 | 0.013 | 6.708 | 300 | 1E-10 | 0.5 | 5 | Waynesboro | cly lm | 10 | 800 |

Table C.18 SESOIL out put values for Nystatin (10 yrs of simulation)

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH | Conc at groundwater (μg/L) | Adsorbed Conc (μg/g) | Maximum pollutant depth (m) |
|---|---|---|---|---|---|---|---|---|---|
| 1 | + | + | + | + | + | + | 2.03E-04 | 6.38E-07 | 2.64 |
| 2 | + | - | + | + | + | + | 1.09E-03 | 3.41E-06 | 2.64 |
| 3 | + | + | - | + | + | + | 3.31E-03 | 1.04E-05 | 26.40 |
| 4 | + | - | - | + | + | + | 8.84E-03 | 2.77E-05 | 2.63 |
| 5 | + | + | + | - | + | + | 2.75E-03 | 8.63E-06 | 2.77 |
| 6 | + | - | + | - | + | + | 3.19E-03 | 1.00E-05 | 0.66 |
| 7 | + | + | - | - | + | + | 3.15E-03 | 9.89E-06 | 2.64 |
| 8 | + | - | - | - | + | + | 4.81E-03 | 1.51E-05 | 0.66 |
| 9 | + | + | + | + | - | + | 3.06E-03 | 9.60E-06 | 26.71 |
| 10 | + | - | + | + | - | + | 9.51E-05 | 2.98E-07 | 2.66 |
| 11 | + | + | - | + | - | + | 5.73E-03 | 1.80E-05 | 26.59 |
| 12 | + | - | - | + | - | + | 8.47E-03 | 2.66E-05 | 2.62 |
| 13 | + | + | + | - | - | + | 3.02E-04 | 9.46E-07 | 2.70 |
| 14 | + | - | + | - | - | + | 3.65E-03 | 1.14E-05 | 6.81 |
| 15 | + | + | - | - | - | + | 9.54E-03 | 2.99E-05 | 2.64 |
| 16 | + | - | - | - | - | + | 1.23E-03 | 3.85E-06 | 6.81 |
| 17 | + | + | + | + | + | - | 3.22E-03 | 1.01E-05 | 26.67 |
| 18 | + | - | + | + | + | - | 1.08E-03 | 3.40E-06 | 2.60 |
| 19 | + | + | - | + | + | - | 6.13E-03 | 1.92E-05 | 26.62 |
| 20 | + | - | - | + | + | - | 8.84E-03 | 2.77E-05 | 2.64 |
| 21 | + | + | + | - | + | - | 8.61E-04 | 2.70E-06 | 2.60 |
| 22 | + | - | + | - | + | - | 3.26E-03 | 1.02E-05 | 0.66 |
| 23 | + | + | - | - | + | - | 7.72E-04 | 2.42E-06 | 2.64 |
| 24 | + | - | - | - | + | - | 6.79E-03 | 2.13E-05 | 0.66 |
| 25 | + | + | + | + | - | - | 3.06E-03 | 9.60E-06 | 26.61 |
| 26 | + | - | + | + | - | - | 9.51E-05 | 2.98E-07 | 2.67 |
| 27 | + | + | - | + | - | - | 5.73E-03 | 1.80E-05 | 26.62 |
| 28 | + | - | - | + | - | - | 8.47E-03 | 2.66E-05 | 2.64 |
| 29 | + | + | + | - | - | - | 1.03E-03 | 3.24E-06 | 2.64 |
| 30 | + | - | + | - | - | - | 2.93E-05 | 9.21E-08 | 0.66 |
| 31 | + | + | - | - | - | - | 5.75E-03 | 1.81E-05 | 2.64 |
| 32 | + | - | - | - | - | - | 6.86E-03 | 2.15E-05 | 6.81 |
| 33 | - | + | + | + | + | + | 4.40E-07 | 7.12E-08 | 26.61 |
| 34 | - | - | + | + | + | + | 2.35E-06 | 3.80E-07 | 2.65 |
| 35 | - | + | - | + | + | + | 7.15E-06 | 1.16E-06 | 26.69 |
| 36 | - | - | - | + | + | + | 1.91E-05 | 3.10E-06 | 2.65 |
| 37 | - | + | + | - | + | + | 5.95E-06 | 9.63E-07 | 2.64 |
| 38 | - | - | + | - | + | + | 6.90E-06 | 1.12E-06 | 0.66 |
| 39 | - | + | - | - | + | + | 6.81E-06 | 1.10E-06 | 2.64 |
| 40 | - | - | - | - | + | + | 1.04E-05 | 1.68E-06 | 0.66 |
| 41 | - | + | + | + | - | + | 6.23E-06 | 1.01E-06 | 26.62 |

Continuation of above table

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH | Conc at groundwater (µg/L) | Adsorbed Conc (µg/g) | Maximum pollutant depth (m) |
|---|---|---|---|---|---|---|---|---|---|
| 42 | - | - | + | + | - | + | 2.06E-07 | 3.33E-08 | 2.66 |
| 43 | - | + | - | + | - | + | 1.24E-05 | 2.00E-06 | 26.61 |
| 44 | - | - | - | + | - | + | 1.83E-05 | 2.96E-06 | 2.66 |
| 45 | - | + | + | - | - | + | 6.52E-07 | 1.06E-07 | 2.64 |
| 46 | - | - | + | - | - | + | 7.89E-06 | 1.28E-06 | 6.80 |
| 47 | - | + | - | - | - | + | 2.06E-05 | 3.34E-06 | 2.64 |
| 48 | - | - | - | - | - | + | 2.65E-06 | 4.29E-07 | 6.81 |
| 49 | - | + | + | + | + | - | 6.95E-06 | 1.13E-06 | 26.61 |
| 50 | - | - | + | + | + | - | 2.35E-06 | 3.80E-07 | 2.64 |
| 51 | - | + | - | + | + | - | 1.33E-05 | 2.15E-06 | 26.21 |
| 52 | - | - | - | + | + | - | 1.91E-05 | 3.10E-06 | 2.64 |
| 53 | - | + | + | - | + | - | 1.86E-06 | 3.01E-07 | 2.64 |
| 54 | - | - | + | - | + | - | 7.04E-06 | 1.14E-06 | 0.66 |
| 55 | - | + | - | - | + | - | 1.67E-06 | 2.70E-07 | 2.64 |
| 56 | - | - | - | - | + | - | 1.47E-05 | 2.38E-06 | 0.66 |
| 57 | - | + | + | + | - | - | 6.62E-06 | 1.07E-06 | 26.60 |
| 58 | - | - | + | + | - | - | 2.06E-07 | 3.33E-08 | 2.66 |
| 59 | - | + | - | + | - | - | 1.24E-05 | 2.00E-06 | 26.61 |
| 60 | - | - | - | + | - | - | 1.83E-05 | 2.96E-06 | 2.61 |
| 61 | - | + | + | - | - | - | 2.23E-06 | 3.62E-07 | 2.64 |
| 62 | - | - | + | - | - | - | 6.34E-08 | 1.03E-08 | 6.80 |
| 63 | - | + | - | - | - | - | 1.24E-05 | 2.01E-06 | 2.64 |
| 64 | - | - | - | - | - | - | 1.48E-05 | 2.40E-06 | 6.81 |

Table C.19 SESOIL out put values for Dexamethasone (10 yrs of simulation)

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH | Conc at groundwater (µg/L) | Adsorbed Conc (µg/g) | Maximum pollutant depth (m) |
|---|---|---|---|---|---|---|---|---|---|
| 1 | + | + | + | + | + | + | 1.56E-04 | 9.25E-07 | 2.95 |
| 2 | + | - | + | + | + | + | 8.36E-04 | 4.94E-06 | 2.94 |
| 3 | + | + | - | + | + | + | 2.55E-03 | 1.51E-05 | 29.40 |
| 4 | + | - | - | + | + | + | 6.80E-03 | 4.02E-05 | 2.94 |
| 5 | + | + | + | - | + | + | 2.12E-03 | 1.25E-05 | 2.97 |
| 6 | + | - | + | - | + | + | 2.45E-03 | 1.45E-05 | 0.74 |
| 7 | + | + | - | - | + | + | 2.42E-03 | 1.43E-05 | 2.94 |
| 8 | + | - | - | - | + | + | 3.70E-03 | 2.19E-05 | 0.74 |
| 9 | + | + | + | + | - | + | 2.35E-03 | 1.39E-05 | 29.63 |
| 10 | + | - | + | + | - | + | 7.31E-05 | 4.33E-07 | 2.96 |
| 11 | + | + | - | + | - | + | 4.41E-03 | 2.61E-05 | 29.64 |
| 12 | + | - | - | + | - | + | 6.51E-03 | 3.85E-05 | 2.94 |
| 13 | + | + | + | - | - | + | 2.32E-04 | 1.37E-06 | 2.94 |
| 14 | + | - | + | - | - | + | 2.81E-03 | 1.66E-05 | 7.58 |
| 15 | + | + | - | - | - | + | 7.34E-03 | 4.34E-05 | 2.95 |
| 16 | + | - | - | - | - | + | 9.43E-04 | 5.58E-06 | 7.58 |
| 17 | + | + | + | + | + | - | 2.47E-03 | 1.46E-05 | 29.65 |
| 18 | + | - | + | + | + | - | 8.33E-04 | 4.92E-06 | 2.94 |
| 19 | + | + | - | + | + | - | 4.72E-03 | 2.79E-05 | 29.41 |
| 20 | + | - | - | + | + | - | 6.80E-03 | 4.02E-05 | 2.94 |
| 21 | + | + | + | - | + | - | 6.62E-04 | 3.91E-06 | 2.94 |
| 22 | + | - | + | - | + | - | 2.51E-03 | 1.48E-05 | 0.73 |
| 23 | + | + | - | - | + | - | 5.94E-04 | 3.51E-06 | 2.94 |
| 24 | + | - | - | - | + | - | 5.22E-03 | 3.09E-05 | 0.74 |
| 25 | + | + | + | + | - | - | 2.35E-03 | 1.39E-05 | 29.63 |
| 26 | + | - | + | + | - | - | 7.31E-05 | 4.33E-07 | 2.97 |
| 27 | + | + | - | + | - | - | 4.41E-03 | 2.61E-05 | 29.63 |
| 28 | + | - | - | + | - | - | 6.51E-03 | 3.85E-05 | 2.94 |
| 29 | + | + | + | - | - | - | 7.95E-04 | 4.70E-06 | 2.94 |
| 30 | + | - | + | - | - | - | 2.26E-05 | 1.33E-07 | 0.74 |
| 31 | + | + | - | - | - | - | 4.43E-03 | 2.62E-05 | 2.94 |
| 32 | + | - | - | - | - | - | 5.28E-03 | 3.12E-05 | 7.58 |
| 33 | - | + | + | + | + | + | 3.89E-07 | 8.05E-08 | 29.63 |
| 34 | - | - | + | + | + | + | 2.08E-06 | 4.30E-07 | 2.94 |
| 35 | - | + | - | + | + | + | 6.33E-06 | 1.31E-06 | 29.50 |
| 36 | - | - | - | + | + | + | 1.69E-05 | 3.50E-06 | 2.94 |
| 37 | - | + | + | - | + | + | 5.26E-06 | 1.09E-06 | 2.94 |
| 38 | - | - | + | - | + | + | 6.10E-06 | 1.26E-06 | 0.73 |
| 39 | - | + | - | - | + | + | 6.03E-06 | 1.25E-06 | 2.94 |
| 40 | - | - | - | - | + | + | 9.21E-06 | 1.90E-06 | 0.73 |
| 41 | - | + | + | + | - | + | 5.52E-06 | 1.14E-06 | 29.64 |
| 42 | - | - | + | + | - | + | 1.82E-07 | 3.76E-08 | 2.96 |

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH | Conc at groundwater (μg/L) | Adsorbed Conc (μg/g) | Maximum pollutant depth (m) |
|---|---|---|---|---|---|---|---|---|---|
| 43 | - | + | - | + | - | + | 1.10E-05 | 2.27E-06 | 29.63 |
| 44 | - | - | - | + | - | + | 1.62E-05 | 3.35E-06 | 2.94 |
| 45 | - | + | + | - | - | + | 5.77E-07 | 1.19E-07 | 2.94 |
| 46 | - | - | + | - | - | + | 6.98E-06 | 1.44E-06 | 7.58 |
| 47 | - | + | - | - | - | + | 1.83E-05 | 3.78E-06 | 2.94 |
| 48 | - | - | - | - | - | + | 2.35E-06 | 4.85E-07 | 7.58 |
| 49 | - | + | + | + | + | - | 6.15E-06 | 1.27E-06 | 29.66 |
| 50 | - | - | + | + | + | - | 2.08E-06 | 4.30E-07 | 2.94 |
| 51 | - | + | - | + | + | - | 1.17E-05 | 2.43E-06 | 29.40 |
| 52 | - | - | - | + | + | - | 1.69E-05 | 3.50E-06 | 2.94 |
| 53 | - | + | + | - | + | - | 1.65E-06 | 3.40E-07 | 2.94 |
| 54 | - | - | + | - | + | - | 6.23E-06 | 1.29E-06 | 0.74 |
| 55 | - | + | - | - | + | - | 1.48E-06 | 3.05E-07 | 2.94 |
| 56 | - | - | - | - | + | - | 1.30E-05 | 2.68E-06 | 0.74 |
| 57 | - | + | + | + | - | - | 5.86E-06 | 1.21E-06 | 29.63 |
| 58 | - | - | + | + | - | - | 1.82E-07 | 3.76E-08 | 2.96 |
| 59 | - | + | - | + | - | - | 1.10E-05 | 2.27E-06 | 29.64 |
| 60 | - | - | - | + | - | - | 1.62E-05 | 3.35E-06 | 2.94 |
| 61 | - | + | + | - | - | - | 1.98E-06 | 4.09E-07 | 2.94 |
| 62 | - | - | + | - | - | - | 5.61E-08 | 1.16E-08 | 7.58 |
| 63 | - | + | - | - | - | - | 1.10E-05 | 2.28E-06 | 2.94 |
| 64 | - | - | - | - | - | - | 1.31E-05 | 2.71E-06 | 7.58 |

Table C.20 SESOIL out put values for Methoprene (10 yrs of simulation)

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH | Conc at groundwater (µg/L) | Adsorbed Conc (µg/g) | Maximum pollutant depth (m) |
|---|---|---|---|---|---|---|---|---|---|
| 1 | + | + | + | + | + | + | 4.07E-05 | 5.10E-06 | 0.78 |
| 2 | + | - | + | + | + | + | 2.17E-04 | 2.73E-05 | 0.78 |
| 3 | + | + | - | + | + | + | 6.62E-04 | 8.31E-05 | 7.80 |
| 4 | + | - | - | + | + | + | 1.77E-03 | 2.22E-04 | 0.78 |
| 5 | + | + | + | - | + | + | 5.50E-04 | 6.91E-05 | 0.79 |
| 6 | + | - | + | - | + | + | 6.38E-04 | 8.00E-05 | 0.20 |
| 7 | + | + | - | - | + | + | 6.30E-04 | 7.91E-05 | 0.78 |
| 8 | + | - | - | - | + | + | 9.61E-04 | 1.21E-04 | 0.20 |
| 9 | + | + | + | + | - | + | 6.12E-04 | 7.68E-05 | 7.86 |
| 10 | + | - | + | + | - | + | 1.90E-05 | 2.39E-06 | 0.79 |
| 11 | + | + | - | + | - | + | 1.15E-03 | 1.44E-04 | 7.86 |
| 12 | + | - | - | + | - | + | 1.69E-03 | 2.12E-04 | 0.78 |
| 13 | + | + | + | - | - | + | 6.03E-05 | 7.57E-06 | 0.78 |
| 14 | + | - | + | - | - | + | 7.29E-04 | 9.15E-05 | 2.02 |
| 15 | + | + | - | - | - | + | 1.91E-03 | 2.40E-04 | 0.78 |
| 16 | + | - | - | - | - | + | 2.45E-04 | 3.08E-05 | 2.01 |
| 17 | + | + | + | + | + | - | 6.43E-04 | 8.07E-05 | 7.86 |
| 18 | + | - | + | + | + | - | 2.16E-04 | 2.72E-05 | 0.78 |
| 19 | + | + | - | + | + | - | 1.23E-03 | 1.54E-04 | 7.80 |
| 20 | + | - | - | + | + | - | 1.77E-03 | 2.22E-04 | 0.78 |
| 21 | + | + | + | - | + | - | 1.72E-04 | 2.16E-05 | 0.78 |
| 22 | + | - | + | - | + | - | 6.52E-04 | 8.18E-05 | 0.20 |
| 23 | + | + | - | - | + | - | 1.54E-04 | 1.94E-05 | 0.78 |
| 24 | + | - | - | - | + | - | 1.36E-03 | 1.70E-04 | 0.20 |
| 25 | + | + | + | + | - | - | 6.12E-04 | 7.68E-05 | 7.86 |
| 26 | + | - | + | + | - | - | 1.90E-05 | 2.39E-06 | 0.79 |
| 27 | + | + | - | + | - | - | 1.15E-03 | 1.44E-04 | 7.86 |
| 28 | + | - | - | + | - | - | 1.69E-03 | 2.12E-04 | 0.78 |
| 29 | + | + | + | - | - | - | 2.07E-04 | 2.59E-05 | 0.78 |
| 30 | + | - | + | - | - | - | 5.87E-06 | 7.37E-07 | 0.20 |
| 31 | + | + | - | - | - | - | 1.15E-03 | 1.44E-04 | 0.78 |
| 32 | + | - | - | - | - | - | 1.37E-03 | 1.72E-04 | 2.01 |
| 33 | - | + | + | + | + | + | 7.33E-08 | 7.12E-07 | 7.86 |
| 34 | - | - | + | + | + | + | 3.92E-07 | 3.80E-06 | 0.78 |
| 35 | - | + | - | + | + | + | 1.19E-06 | 1.16E-05 | 7.80 |
| 36 | - | - | - | + | + | + | 3.19E-06 | 3.10E-05 | 0.78 |
| 37 | - | + | + | - | + | + | 9.91E-07 | 9.63E-06 | 0.78 |
| 38 | - | - | + | - | + | + | 1.15E-06 | 1.12E-05 | 0.20 |
| 39 | - | + | - | - | + | + | 1.14E-06 | 1.10E-05 | 0.78 |

Continuation of above table

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH | Conc at groundwater (µg/L) | Adsorbed Conc (µg/g) | Maximum pollutant depth (m) |
|---|---|---|---|---|---|---|---|---|---|
| 40 | - | - | - | - | + | + | 1.73E-06 | 1.68E-05 | 0.20 |
| 41 | - | + | + | + | - | + | 1.04E-06 | 1.01E-05 | 7.86 |
| 42 | - | - | + | + | - | + | 3.43E-08 | 3.33E-07 | 0.79 |
| 43 | - | + | - | + | - | + | 2.06E-06 | 2.00E-05 | 7.86 |
| 44 | - | - | - | + | - | + | 3.05E-06 | 2.96E-05 | 0.78 |
| 45 | - | + | + | - | - | + | 1.09E-07 | 1.06E-06 | 0.78 |
| 46 | - | - | + | - | - | + | 1.31E-06 | 1.28E-05 | 2.01 |
| 47 | - | + | - | - | - | + | 3.44E-06 | 3.34E-05 | 0.78 |
| 48 | - | - | - | - | - | + | 4.42E-07 | 4.29E-06 | 2.01 |
| 49 | - | + | + | + | + | - | 1.16E-06 | 1.13E-05 | 7.86 |
| 50 | - | - | + | + | + | - | 3.92E-07 | 3.80E-06 | 0.78 |
| 51 | - | + | - | + | + | - | 2.21E-06 | 2.15E-05 | 7.80 |
| 52 | - | - | - | + | + | - | 3.19E-06 | 3.10E-05 | 0.78 |
| 53 | - | + | + | - | + | - | 3.10E-07 | 3.01E-06 | 0.78 |
| 54 | - | - | + | - | + | - | 1.17E-06 | 1.14E-05 | 0.20 |
| 55 | - | + | - | - | + | - | 2.78E-07 | 2.70E-06 | 0.78 |
| 56 | - | - | - | - | + | - | 2.45E-06 | 2.38E-05 | 0.20 |
| 57 | - | + | + | + | - | - | 1.10E-06 | 1.07E-05 | 7.86 |
| 58 | - | - | + | + | - | - | 3.43E-08 | 3.33E-07 | 0.79 |
| 59 | - | + | - | + | - | - | 2.06E-06 | 2.00E-05 | 7.86 |
| 60 | - | - | - | + | - | - | 3.05E-06 | 2.96E-05 | 0.78 |
| 61 | - | + | + | - | - | - | 3.72E-07 | 3.62E-06 | 0.78 |
| 62 | - | - | + | - | - | - | 1.06E-08 | 1.03E-07 | 2.01 |
| 63 | - | + | - | - | - | - | 2.07E-06 | 2.01E-05 | 0.78 |
| 64 | - | - | - | - | - | - | 2.47E-06 | 2.40E-05 | 2.01 |

Table C.21 SESOIL out put values for Prednisone (10 yrs of simulation)

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH | Conc at groundwater (µg/L) | Adsorbed Conc (µg/g) | Maximum pollutant depth (m) |
|---|---|---|---|---|---|---|---|---|---|
| 1 | + | + | + | + | + | + | 2.44E-04 | 7.33E-07 | 5.11 |
| 2 | + | - | + | + | + | + | 1.30E-03 | 3.92E-06 | 5.11 |
| 3 | + | + | - | + | + | + | 3.97E-03 | 1.19E-05 | 51.01 |
| 4 | + | - | - | + | + | + | 1.06E-02 | 3.19E-05 | 5.10 |
| 5 | + | + | + | - | + | + | 3.30E-03 | 9.92E-06 | 5.14 |
| 6 | + | - | + | - | + | + | 3.83E-03 | 1.15E-05 | 1.28 |
| 7 | + | + | - | - | + | + | 3.78E-03 | 1.14E-05 | 5.10 |
| 8 | + | - | - | - | + | + | 5.77E-03 | 1.73E-05 | 1.28 |
| 9 | + | + | + | + | - | + | 3.67E-03 | 1.10E-05 | 51.40 |
| 10 | + | - | + | + | - | + | 1.14E-04 | 3.43E-07 | 5.14 |
| 11 | + | + | - | + | - | + | 6.87E-03 | 2.07E-05 | 51.40 |
| 12 | + | - | - | + | - | + | 1.02E-02 | 3.05E-05 | 5.10 |
| 13 | + | + | + | - | - | + | 3.62E-04 | 1.09E-06 | 5.10 |
| 14 | + | - | + | - | - | + | 4.38E-03 | 1.32E-05 | 13.15 |
| 15 | + | + | - | - | - | + | 1.15E-02 | 3.44E-05 | 5.10 |
| 16 | + | - | - | - | - | + | 1.47E-03 | 4.42E-06 | 13.15 |
| 17 | + | + | + | + | + | - | 3.86E-03 | 1.16E-05 | 51.40 |
| 18 | + | - | + | + | + | - | 1.30E-03 | 3.90E-06 | 5.10 |
| 19 | + | + | - | + | + | - | 7.36E-03 | 2.21E-05 | 51.01 |
| 20 | + | - | - | + | + | - | 1.06E-02 | 3.19E-05 | 5.10 |
| 21 | + | + | + | - | + | - | 1.03E-03 | 3.10E-06 | 5.10 |
| 22 | + | - | + | - | + | - | 3.91E-03 | 1.17E-05 | 1.28 |
| 23 | + | + | - | - | + | - | 9.26E-04 | 2.78E-06 | 5.10 |
| 24 | + | - | - | - | + | - | 8.15E-03 | 2.45E-05 | 1.28 |
| 25 | + | + | + | + | - | - | 3.67E-03 | 1.10E-05 | 51.40 |
| 26 | + | - | + | + | - | - | 1.14E-04 | 3.43E-07 | 5.14 |
| 27 | + | + | - | + | - | - | 6.87E-03 | 2.07E-05 | 51.40 |
| 28 | + | - | - | + | - | - | 1.02E-02 | 3.05E-05 | 5.10 |
| 29 | + | + | + | - | - | - | 1.24E-03 | 3.72E-06 | 5.10 |
| 30 | + | - | + | - | - | - | 3.52E-05 | 1.06E-07 | 1.28 |
| 31 | + | + | - | - | - | - | 6.90E-03 | 2.07E-05 | 5.10 |
| 32 | + | - | - | - | - | - | 8.24E-03 | 2.48E-05 | 13.15 |
| 33 | - | + | + | + | + | + | 7.04E-07 | 7.42E-08 | 51.40 |
| 34 | - | - | + | + | + | + | 3.76E-06 | 3.96E-07 | 5.11 |
| 35 | - | + | - | + | + | + | 1.14E-05 | 1.21E-06 | 51.01 |
| 36 | - | - | - | + | + | + | 3.06E-05 | 3.22E-06 | 5.10 |
| 37 | - | + | + | - | + | + | 9.52E-06 | 1.00E-06 | 5.10 |
| 38 | - | - | + | - | + | + | 1.10E-05 | 1.16E-06 | 1.28 |
| 39 | - | + | - | - | + | + | 1.09E-05 | 1.15E-06 | 5.10 |

Continuation of above table

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH | Conc at groundwater (μg/L) | Adsorbed Conc (μg/g) | Maximum pollutant depth (m) |
|---|---|---|---|---|---|---|---|---|---|
| 40 | - | - | - | - | + | + | 1.66E-05 | 1.75E-06 | 1.28 |
| 41 | - | + | + | + | - | + | 9.97E-06 | 1.05E-06 | 51.40 |
| 42 | - | - | + | + | - | + | 3.29E-07 | 3.47E-08 | 5.14 |
| 43 | - | + | - | + | - | + | 1.98E-05 | 2.09E-06 | 51.40 |
| 44 | - | - | - | + | - | + | 2.93E-05 | 3.09E-06 | 5.10 |
| 45 | - | + | + | - | - | + | 1.04E-06 | 1.10E-07 | 5.10 |
| 46 | - | - | + | - | - | + | 1.26E-05 | 1.33E-06 | 13.15 |
| 47 | - | + | - | - | - | + | 3.30E-05 | 3.48E-06 | 5.10 |
| 48 | - | - | - | - | - | + | 4.24E-06 | 4.47E-07 | 13.15 |
| 49 | - | + | + | + | + | - | 1.11E-05 | 1.17E-06 | 51.40 |
| 50 | - | - | + | + | + | - | 3.76E-06 | 3.96E-07 | 5.10 |
| 51 | - | + | - | + | + | - | 2.12E-05 | 2.24E-06 | 51.01 |
| 52 | - | - | - | + | + | - | 3.06E-05 | 3.22E-06 | 5.10 |
| 53 | - | + | + | - | + | - | 2.98E-06 | 3.14E-07 | 5.10 |
| 54 | - | - | + | - | + | - | 1.13E-05 | 1.19E-06 | 1.28 |
| 55 | - | + | - | - | + | - | 2.67E-06 | 2.81E-07 | 5.10 |
| 56 | - | - | - | - | + | - | 2.35E-05 | 2.47E-06 | 1.28 |
| 57 | - | + | + | + | - | - | 1.06E-05 | 1.12E-06 | 51.40 |
| 58 | - | - | + | + | - | - | 3.29E-07 | 3.47E-08 | 5.14 |
| 59 | - | + | - | + | - | - | 1.98E-05 | 2.09E-06 | 51.40 |
| 60 | - | - | - | + | - | - | 2.93E-05 | 3.09E-06 | 5.10 |
| 61 | - | + | + | - | - | - | 3.57E-06 | 3.77E-07 | 5.10 |
| 62 | - | - | + | - | - | - | 1.01E-07 | 1.07E-08 | 13.15 |
| 63 | - | + | - | - | - | - | 1.99E-05 | 2.10E-06 | 5.10 |
| 64 | - | - | - | - | - | - | 2.37E-05 | 2.50E-06 | 13.15 |

Table C.22 SESOIL out put values for Metronidazole (10 yrs of simulation)

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH | Conc at groundwater (µg/L) | Adsorbed Conc (µg/g) | Maximum pollutant depth (m) |
|---|---|---|---|---|---|---|---|---|---|
| 1 | + | + | + | + | + | + | 8.13E-04 | 6.19E-08 | 5.59 |
| 2 | + | - | + | + | + | + | 4.35E-03 | 3.31E-07 | 5.59 |
| 3 | + | + | - | + | + | + | 1.32E-02 | 1.01E-06 | 55.81 |
| 4 | + | - | - | + | + | + | 3.54E-02 | 2.69E-06 | 5.58 |
| 5 | + | + | + | - | + | + | 1.10E-02 | 8.38E-07 | 5.62 |
| 6 | + | - | + | - | + | + | 1.28E-02 | 9.71E-07 | 1.40 |
| 7 | + | + | - | - | + | + | 1.26E-02 | 9.60E-07 | 5.58 |
| 8 | + | - | - | - | + | + | 1.92E-02 | 1.46E-06 | 1.40 |
| 9 | + | + | + | + | - | + | 1.22E-02 | 9.32E-07 | 56.24 |
| 10 | + | - | + | + | - | + | 3.80E-04 | 2.90E-08 | 5.62 |
| 11 | + | + | - | + | - | + | 2.29E-02 | 1.74E-06 | 56.24 |
| 12 | + | - | - | + | - | + | 3.39E-02 | 2.58E-06 | 5.58 |
| 13 | + | + | + | - | - | + | 1.21E-03 | 9.19E-08 | 5.58 |
| 14 | + | - | + | - | - | + | 1.46E-02 | 1.11E-06 | 14.39 |
| 15 | + | + | - | - | - | + | 3.82E-02 | 2.91E-06 | 5.58 |
| 16 | + | - | - | - | - | + | 4.90E-03 | 3.73E-07 | 14.39 |
| 17 | + | + | + | + | + | - | 1.29E-02 | 9.79E-07 | 56.24 |
| 18 | + | - | + | + | + | - | 4.33E-03 | 3.30E-07 | 5.58 |
| 19 | + | + | - | + | + | - | 2.45E-02 | 1.87E-06 | 55.81 |
| 20 | + | - | - | + | + | - | 3.54E-02 | 2.69E-06 | 5.58 |
| 21 | + | + | + | - | + | - | 3.44E-03 | 2.62E-07 | 5.58 |
| 22 | + | - | + | - | + | - | 1.30E-02 | 9.92E-07 | 1.40 |
| 23 | + | + | - | - | + | - | 3.09E-03 | 2.35E-07 | 5.58 |
| 24 | + | - | - | - | + | - | 2.72E-02 | 2.07E-06 | 1.40 |
| 25 | + | + | + | + | - | - | 1.22E-02 | 9.32E-07 | 56.24 |
| 26 | + | - | + | + | - | - | 3.80E-04 | 2.90E-08 | 5.62 |
| 27 | + | + | - | + | - | - | 2.29E-02 | 1.74E-06 | 56.24 |
| 28 | + | - | - | + | - | - | 3.39E-02 | 2.58E-06 | 5.58 |
| 29 | + | + | + | - | - | - | 4.13E-03 | 3.15E-07 | 5.58 |
| 30 | + | - | + | - | - | - | 1.17E-04 | 8.94E-09 | 1.40 |
| 31 | + | + | - | - | - | - | 2.30E-02 | 1.75E-06 | 5.58 |
| 32 | + | - | - | - | - | - | 2.75E-02 | 2.09E-06 | 14.39 |
| 33 | - | + | + | + | + | + | 2.64E-06 | 6.14E-09 | 56.24 |
| 34 | - | - | + | + | + | + | 1.41E-05 | 3.28E-08 | 5.59 |
| 35 | - | + | - | + | + | + | 4.29E-05 | 9.98E-08 | 55.81 |
| 36 | - | - | - | + | + | + | 1.15E-04 | 2.67E-07 | 5.58 |
| 37 | - | + | + | - | + | + | 3.57E-05 | 8.30E-08 | 5.58 |
| 38 | - | - | + | - | + | + | 4.14E-05 | 9.62E-08 | 1.40 |
| 39 | - | + | - | - | + | + | 4.09E-05 | 9.51E-08 | 5.58 |

Continuation of above table

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH | Conc at groundwater (µg/L) | Adsorbed Conc (µg/g) | Maximum pollutant depth (m) |
|---|---|---|---|---|---|---|---|---|---|
| 40 | - | - | - | - | + | + | 6.24E-05 | 1.45E-07 | 1.40 |
| 41 | - | + | + | + | - | + | 3.74E-05 | 8.70E-08 | 56.24 |
| 42 | - | - | + | + | - | + | 1.23E-06 | 2.87E-09 | 5.62 |
| 43 | - | + | - | + | - | + | 7.43E-05 | 1.73E-07 | 56.24 |
| 44 | - | - | - | + | - | + | 1.10E-04 | 2.55E-07 | 5.58 |
| 45 | - | + | + | - | - | + | 3.91E-06 | 9.10E-09 | 5.58 |
| 46 | - | - | + | - | - | + | 4.73E-05 | 1.10E-07 | 14.39 |
| 47 | - | + | - | - | - | + | 1.24E-04 | 2.88E-07 | 5.58 |
| 48 | - | - | - | - | - | + | 1.59E-05 | 3.70E-08 | 14.39 |
| 49 | - | + | + | + | + | - | 4.17E-05 | 9.70E-08 | 56.24 |
| 50 | - | - | + | + | + | - | 1.41E-05 | 3.28E-08 | 5.58 |
| 51 | - | + | - | + | + | - | 7.96E-05 | 1.85E-07 | 55.81 |
| 52 | - | - | - | + | + | - | 1.15E-04 | 2.67E-07 | 5.58 |
| 53 | - | + | + | - | + | - | 1.12E-05 | 2.60E-08 | 5.58 |
| 54 | - | - | + | - | + | - | 4.23E-05 | 9.83E-08 | 1.40 |
| 55 | - | + | - | - | + | - | 1.00E-05 | 2.33E-08 | 5.58 |
| 56 | - | - | - | - | + | - | 8.80E-05 | 2.05E-07 | 1.40 |
| 57 | - | + | + | + | - | - | 3.97E-05 | 9.24E-08 | 56.24 |
| 58 | - | - | + | + | - | - | 1.23E-06 | 2.87E-09 | 5.62 |
| 59 | - | + | - | + | - | - | 7.43E-05 | 1.73E-07 | 56.24 |
| 60 | - | - | - | + | - | - | 1.10E-04 | 2.55E-07 | 5.58 |
| 61 | - | + | + | - | - | - | 1.34E-05 | 3.12E-08 | 5.58 |
| 62 | - | - | + | - | - | - | 3.81E-07 | 8.85E-10 | 14.39 |
| 63 | - | + | - | - | - | - | 7.47E-05 | 1.74E-07 | 5.58 |
| 64 | - | - | - | - | - | - | 8.90E-05 | 2.07E-07 | 14.39 |

Table C.23 SESOIL out put values for Clindamycin (10 yrs of simulation)

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH | Conc at groundwater (µg/L) | Adsorbed Conc (µg/g) | Maximum pollutant depth (m) |
|---|---|---|---|---|---|---|---|---|---|
| 1 | + | + | + | + | + | + | 1.27E-04 | 1.40E-06 | 3.18 |
| 2 | + | - | + | + | + | + | 6.79E-04 | 7.50E-06 | 3.18 |
| 3 | + | + | - | + | + | + | 2.07E-03 | 2.28E-05 | 31.81 |
| 4 | + | - | - | + | + | + | 5.53E-03 | 6.10E-05 | 3.18 |
| 5 | + | + | + | - | + | + | 1.72E-03 | 1.90E-05 | 3.20 |
| 6 | + | - | + | - | + | + | 1.99E-03 | 2.20E-05 | 0.80 |
| 7 | + | + | - | - | + | + | 1.97E-03 | 2.18E-05 | 3.18 |
| 8 | + | - | - | - | + | + | 3.00E-03 | 3.32E-05 | 0.80 |
| 9 | + | + | + | + | - | + | 1.91E-03 | 2.11E-05 | 32.05 |
| 10 | + | - | + | + | - | + | 5.94E-05 | 6.56E-07 | 3.20 |
| 11 | + | + | - | + | - | + | 3.58E-03 | 3.95E-05 | 32.05 |
| 12 | + | - | - | + | - | + | 5.29E-03 | 5.84E-05 | 3.18 |
| 13 | + | + | + | - | - | + | 1.89E-04 | 2.08E-06 | 3.18 |
| 14 | + | - | + | - | - | + | 2.28E-03 | 2.52E-05 | 8.20 |
| 15 | + | + | - | - | - | + | 5.97E-03 | 6.59E-05 | 3.18 |
| 16 | + | - | - | - | - | + | 7.66E-04 | 8.46E-06 | 8.20 |
| 17 | + | + | + | + | + | - | 2.01E-03 | 2.22E-05 | 32.05 |
| 18 | + | - | + | + | + | - | 6.76E-04 | 7.47E-06 | 3.18 |
| 19 | + | + | - | + | + | - | 3.83E-03 | 4.23E-05 | 31.81 |
| 20 | + | - | - | + | + | - | 5.53E-03 | 6.10E-05 | 3.18 |
| 21 | + | + | + | - | + | - | 5.38E-04 | 5.94E-06 | 3.18 |
| 22 | + | - | + | - | + | - | 2.04E-03 | 2.25E-05 | 0.80 |
| 23 | + | + | - | - | + | - | 4.82E-04 | 5.33E-06 | 3.18 |
| 24 | + | - | - | - | + | - | 4.24E-03 | 4.68E-05 | 0.80 |
| 25 | + | + | + | + | - | - | 1.91E-03 | 2.11E-05 | 32.05 |
| 26 | + | - | + | + | - | - | 5.94E-05 | 6.56E-07 | 3.20 |
| 27 | + | + | - | + | - | - | 3.58E-03 | 3.95E-05 | 32.05 |
| 28 | + | - | - | + | - | - | 5.29E-03 | 5.84E-05 | 3.18 |
| 29 | + | + | + | - | - | - | 6.46E-04 | 7.13E-06 | 3.18 |
| 30 | + | - | + | - | - | - | 1.83E-05 | 2.03E-07 | 0.80 |
| 31 | + | + | - | - | - | - | 3.60E-03 | 3.97E-05 | 3.18 |
| 32 | + | - | - | - | - | - | 4.29E-03 | 4.74E-05 | 8.20 |
| 33 | - | + | + | + | + | + | 3.38E-07 | 1.26E-07 | 32.05 |
| 34 | - | - | + | + | + | + | 1.81E-06 | 6.73E-07 | 3.18 |
| 35 | - | + | - | + | + | + | 5.50E-06 | 2.05E-06 | 31.81 |
| 36 | - | - | - | + | + | + | 1.47E-05 | 5.48E-06 | 3.18 |
| 37 | - | + | + | - | + | + | 4.58E-06 | 1.70E-06 | 3.18 |
| 38 | - | - | + | - | + | + | 5.30E-06 | 1.98E-06 | 0.80 |
| 39 | - | + | - | - | + | + | 5.24E-06 | 1.95E-06 | 3.18 |

Continuation of above table

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH | Conc at groundwater (μg/L) | Adsorbed Conc (μg/g) | Maximum pollutant depth (m) |
|---|---|---|---|---|---|---|---|---|---|
| 40 | - | - | - | - | + | + | 8.00E-06 | 2.98E-06 | 0.80 |
| 41 | - | + | + | + | - | + | 4.79E-06 | 1.79E-06 | 32.05 |
| 42 | - | - | + | + | - | + | 1.58E-07 | 5.89E-08 | 3.20 |
| 43 | - | + | - | + | - | + | 9.52E-06 | 3.55E-06 | 32.05 |
| 44 | - | - | - | + | - | + | 1.41E-05 | 5.24E-06 | 3.18 |
| 45 | - | + | + | - | - | + | 5.01E-07 | 1.87E-07 | 3.18 |
| 46 | - | - | + | - | - | + | 6.07E-06 | 2.26E-06 | 8.20 |
| 47 | - | + | - | - | - | + | 1.59E-05 | 5.91E-06 | 3.18 |
| 48 | - | - | - | - | - | + | 2.04E-06 | 7.60E-07 | 8.20 |
| 49 | - | + | + | + | + | - | 5.35E-06 | 1.99E-06 | 32.05 |
| 50 | - | - | + | + | + | - | 1.81E-06 | 6.73E-07 | 3.18 |
| 51 | - | + | - | + | + | - | 1.02E-05 | 3.80E-06 | 31.81 |
| 52 | - | - | - | + | + | - | 1.47E-05 | 5.48E-06 | 3.18 |
| 53 | - | + | + | - | + | - | 1.43E-06 | 5.33E-07 | 3.18 |
| 54 | - | - | + | - | + | - | 5.42E-06 | 2.02E-06 | 0.80 |
| 55 | - | + | - | - | + | - | 1.28E-06 | 4.78E-07 | 3.18 |
| 56 | - | - | - | - | + | - | 1.13E-05 | 4.20E-06 | 0.80 |
| 57 | - | + | + | + | - | - | 5.09E-06 | 1.90E-06 | 32.05 |
| 58 | - | - | + | + | - | - | 1.58E-07 | 5.89E-08 | 3.20 |
| 59 | - | + | - | + | - | - | 9.52E-06 | 3.55E-06 | 32.05 |
| 60 | - | - | - | + | - | - | 1.41E-05 | 5.24E-06 | 3.18 |
| 61 | - | + | + | - | - | - | 1.72E-06 | 6.40E-07 | 3.18 |
| 62 | - | - | + | - | - | - | 4.88E-08 | 1.82E-08 | 8.20 |
| 63 | - | + | - | - | - | - | 9.57E-06 | 3.57E-06 | 3.18 |
| 64 | - | - | - | - | - | - | 1.14E-05 | 4.25E-06 | 8.20 |

Table C.24 SESOIL out put values for Ketoconazole (10 yrs of simulation)

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH | Conc at groundwater (µg/L) | Adsorbed Conc (µg/g) | Maximum pollutant depth (m) |
|---|---|---|---|---|---|---|---|---|---|
| 1 | + | + | + | + | + | + | 9.68E-05 | 3.83E-06 | 3.78 |
| 2 | + | - | + | + | + | + | 5.18E-04 | 2.05E-05 | 3.78 |
| 3 | + | + | - | + | + | + | 1.58E-03 | 6.23E-05 | 37.81 |
| 4 | + | - | - | + | + | + | 4.21E-03 | 1.66E-04 | 3.78 |
| 5 | + | + | + | - | + | + | 1.31E-03 | 5.18E-05 | 3.81 |
| 6 | + | - | + | - | + | + | 1.52E-03 | 6.00E-05 | 0.95 |
| 7 | + | + | - | - | + | + | 1.50E-03 | 5.93E-05 | 3.78 |
| 8 | + | - | - | - | + | + | 2.29E-03 | 9.05E-05 | 0.95 |
| 9 | + | + | + | + | - | + | 1.46E-03 | 5.76E-05 | 38.10 |
| 10 | + | - | + | + | - | + | 4.53E-05 | 1.79E-06 | 3.81 |
| 11 | + | + | - | + | - | + | 2.73E-03 | 1.08E-04 | 38.10 |
| 12 | + | - | - | + | - | + | 4.03E-03 | 1.59E-04 | 3.78 |
| 13 | + | + | + | - | - | + | 1.44E-04 | 5.68E-06 | 3.78 |
| 14 | + | - | + | - | - | + | 1.74E-03 | 6.87E-05 | 9.75 |
| 15 | + | + | - | - | - | + | 4.55E-03 | 1.80E-04 | 3.78 |
| 16 | + | - | - | - | - | + | 5.84E-04 | 2.31E-05 | 9.75 |
| 17 | + | + | + | + | + | - | 1.53E-03 | 6.05E-05 | 38.10 |
| 18 | + | - | + | + | + | - | 5.15E-04 | 2.04E-05 | 3.78 |
| 19 | + | + | - | + | + | - | 2.92E-03 | 1.15E-04 | 37.81 |
| 20 | + | - | - | + | + | - | 4.21E-03 | 1.66E-04 | 3.78 |
| 21 | + | + | + | - | + | - | 4.10E-04 | 1.62E-05 | 3.78 |
| 22 | + | - | + | - | + | - | 1.55E-03 | 6.13E-05 | 0.95 |
| 23 | + | + | - | - | + | - | 3.67E-04 | 1.45E-05 | 3.78 |
| 24 | + | - | - | - | + | - | 3.23E-03 | 1.28E-04 | 0.95 |
| 25 | + | + | + | + | - | - | 1.46E-03 | 5.76E-05 | 38.10 |
| 26 | + | - | + | + | - | - | 4.53E-05 | 1.79E-06 | 3.81 |
| 27 | + | + | - | + | - | - | 2.73E-03 | 1.08E-04 | 38.10 |
| 28 | + | - | - | + | - | - | 4.03E-03 | 1.59E-04 | 3.78 |
| 29 | + | + | + | - | - | - | 4.92E-04 | 1.94E-05 | 3.78 |
| 30 | + | - | + | - | - | - | 1.40E-05 | 5.52E-07 | 0.95 |
| 31 | + | + | - | - | - | - | 2.74E-03 | 1.08E-04 | 3.78 |
| 32 | + | - | - | - | - | - | 3.27E-03 | 1.29E-04 | 9.75 |
| 33 | - | + | + | + | + | + | 1.37E-07 | 5.62E-07 | 38.10 |
| 34 | - | - | + | + | + | + | 7.34E-07 | 3.01E-06 | 3.78 |
| 35 | - | + | - | + | + | + | 2.24E-06 | 9.15E-06 | 37.81 |
| 36 | - | - | - | + | + | + | 5.97E-06 | 2.45E-05 | 3.78 |
| 37 | - | + | + | - | + | + | 1.86E-06 | 7.61E-06 | 3.78 |
| 38 | - | - | + | - | + | + | 2.15E-06 | 8.82E-06 | 0.95 |
| 39 | - | + | - | - | + | + | 2.13E-06 | 8.72E-06 | 3.78 |

Continuation of above table

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH | Conc at groundwater (µg/L) | Adsorbed Conc (µg/g) | Maximum pollutant depth (m) |
|---|---|---|---|---|---|---|---|---|---|
| 40 | - | - | - | - | + | + | 3.25E-06 | 1.33E-05 | 0.95 |
| 41 | - | + | + | + | - | + | 1.95E-06 | 7.97E-06 | 38.10 |
| 42 | - | - | + | + | - | + | 6.42E-08 | 2.63E-07 | 3.81 |
| 43 | - | + | - | + | - | + | 3.87E-06 | 1.58E-05 | 38.10 |
| 44 | - | - | - | + | - | + | 5.72E-06 | 2.34E-05 | 3.78 |
| 45 | - | + | + | - | - | + | 2.04E-07 | 8.34E-07 | 3.78 |
| 46 | - | - | + | - | - | + | 2.46E-06 | 1.01E-05 | 9.75 |
| 47 | - | + | - | - | - | + | 6.45E-06 | 2.64E-05 | 3.78 |
| 48 | - | - | - | - | - | + | 8.28E-07 | 3.39E-06 | 9.75 |
| 49 | - | + | + | + | + | - | 2.17E-06 | 8.89E-06 | 38.10 |
| 50 | - | - | + | + | + | - | 7.34E-07 | 3.01E-06 | 3.78 |
| 51 | - | + | - | + | + | - | 4.15E-06 | 1.70E-05 | 37.81 |
| 52 | - | - | - | + | + | - | 5.97E-06 | 2.45E-05 | 3.78 |
| 53 | - | + | + | - | + | - | 5.81E-07 | 2.38E-06 | 3.78 |
| 54 | - | - | + | - | + | - | 2.20E-06 | 9.01E-06 | 0.95 |
| 55 | - | + | - | - | + | - | 5.22E-07 | 2.13E-06 | 3.78 |
| 56 | - | - | - | - | + | - | 4.58E-06 | 1.88E-05 | 0.95 |
| 57 | - | + | + | + | - | - | 2.07E-06 | 8.47E-06 | 38.10 |
| 58 | - | - | + | + | - | - | 6.42E-08 | 2.63E-07 | 3.81 |
| 59 | - | + | - | + | - | - | 3.87E-06 | 1.58E-05 | 38.10 |
| 60 | - | - | - | + | - | - | 5.72E-06 | 2.34E-05 | 3.78 |
| 61 | - | + | + | - | - | - | 6.98E-07 | 2.86E-06 | 3.78 |
| 62 | - | - | + | - | - | - | 1.98E-08 | 8.11E-08 | 9.75 |
| 63 | - | + | - | - | - | - | 3.89E-06 | 1.59E-05 | 3.78 |
| 64 | - | - | - | - | - | - | 4.64E-06 | 1.90E-05 | 9.75 |

Table C.25 SESOIL out put values for Carbamazepine (10 yrs of simulation)

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH | Conc at groundwater (µg/L) | Adsorbed Conc (µg/g) | Maximum pollutant depth (m) |
|---|---|---|---|---|---|---|---|---|---|
| 1 | + | + | + | + | + | + | 1.79E-05 | 8.06E-07 | 3.54 |
| 2 | + | - | + | + | + | + | 9.56E-05 | 4.31E-06 | 3.54 |
| 3 | + | + | - | + | + | + | 2.91E-04 | 1.31E-05 | 35.41 |
| 4 | + | - | - | + | + | + | 7.78E-04 | 3.50E-05 | 3.54 |
| 5 | + | + | + | - | + | + | 2.42E-04 | 1.09E-05 | 3.57 |
| 6 | + | - | + | - | + | + | 2.81E-04 | 1.26E-05 | 0.89 |
| 7 | + | + | - | - | + | + | 2.77E-04 | 1.25E-05 | 3.54 |
| 8 | + | - | - | - | + | + | 4.23E-04 | 1.90E-05 | 0.89 |
| 9 | + | + | + | + | - | + | 2.69E-04 | 1.21E-05 | 35.68 |
| 10 | + | - | + | + | - | + | 8.36E-06 | 3.77E-07 | 3.57 |
| 11 | + | + | - | + | - | + | 5.04E-04 | 2.27E-05 | 35.68 |
| 12 | + | - | - | + | - | + | 7.45E-04 | 3.35E-05 | 3.54 |
| 13 | + | + | + | - | - | + | 2.65E-05 | 1.20E-06 | 3.54 |
| 14 | + | - | + | - | - | + | 3.21E-04 | 1.45E-05 | 9.13 |
| 15 | + | + | - | - | - | + | 8.40E-04 | 3.78E-05 | 3.54 |
| 16 | + | - | - | - | - | + | 1.08E-04 | 4.86E-06 | 9.13 |
| 17 | + | + | + | + | + | - | 2.83E-04 | 1.27E-05 | 35.68 |
| 18 | + | - | + | + | + | - | 9.52E-05 | 4.29E-06 | 3.54 |
| 19 | + | + | - | + | + | - | 5.40E-04 | 2.43E-05 | 35.41 |
| 20 | + | - | - | + | + | - | 7.78E-04 | 3.50E-05 | 3.54 |
| 21 | + | + | + | - | + | - | 7.57E-05 | 3.41E-06 | 3.54 |
| 22 | + | - | + | - | + | - | 2.87E-04 | 1.29E-05 | 0.89 |
| 23 | + | + | - | - | + | - | 6.79E-05 | 3.06E-06 | 3.54 |
| 24 | + | - | - | - | + | - | 5.97E-04 | 2.69E-05 | 0.89 |
| 25 | + | + | + | + | - | - | 2.69E-04 | 1.21E-05 | 35.68 |
| 26 | + | - | + | + | - | - | 8.36E-06 | 3.77E-07 | 3.57 |
| 27 | + | + | - | + | - | - | 5.04E-04 | 2.27E-05 | 35.68 |
| 28 | + | - | - | + | - | - | 7.45E-04 | 3.35E-05 | 3.54 |
| 29 | + | + | + | - | - | - | 9.09E-05 | 4.09E-06 | 3.54 |
| 30 | + | - | + | - | - | - | 2.58E-06 | 1.16E-07 | 0.89 |
| 31 | + | + | - | - | - | - | 5.06E-04 | 2.28E-05 | 3.54 |
| 32 | + | - | - | - | - | - | 6.04E-04 | 2.72E-05 | 9.13 |
| 33 | - | + | + | + | + | + | 3.58E-07 | 7.04E-07 | 35.68 |
| 34 | - | - | + | + | + | + | 1.91E-06 | 3.76E-06 | 3.54 |
| 35 | - | + | - | + | + | + | 5.81E-06 | 1.14E-05 | 35.41 |
| 36 | - | - | - | + | + | + | 1.55E-05 | 3.06E-05 | 3.54 |
| 37 | - | + | + | - | + | + | 4.84E-06 | 9.52E-06 | 3.54 |
| 38 | - | - | + | - | + | + | 5.61E-06 | 1.10E-05 | 0.89 |
| 39 | - | + | - | - | + | + | 5.54E-06 | 1.09E-05 | 3.54 |

Continuation of above table

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH | Conc at groundwater (μg/L) | Adsorbed Conc (μg/g) | Maximum pollutant depth (m) |
|---|---|---|---|---|---|---|---|---|---|
| 40 | - | - | - | - | + | + | 8.46E-06 | 1.66E-05 | 0.89 |
| 41 | - | + | + | + | - | + | 5.07E-06 | 9.97E-06 | 35.68 |
| 42 | - | - | + | + | - | + | 1.67E-07 | 3.29E-07 | 3.57 |
| 43 | - | + | - | + | - | + | 1.01E-05 | 1.98E-05 | 35.68 |
| 44 | - | - | - | + | - | + | 1.49E-05 | 2.93E-05 | 3.54 |
| 45 | - | + | + | - | - | + | 5.30E-07 | 1.04E-06 | 3.54 |
| 46 | - | - | + | - | - | + | 6.41E-06 | 1.26E-05 | 9.13 |
| 47 | - | + | - | - | - | + | 1.68E-05 | 3.30E-05 | 3.54 |
| 48 | - | - | - | - | - | + | 2.16E-06 | 4.24E-06 | 9.13 |
| 49 | - | + | + | + | + | - | 5.65E-06 | 1.11E-05 | 35.68 |
| 50 | - | - | + | + | + | - | 1.91E-06 | 3.76E-06 | 3.54 |
| 51 | - | + | - | + | + | - | 1.08E-05 | 2.12E-05 | 35.41 |
| 52 | - | - | - | + | + | - | 1.55E-05 | 3.06E-05 | 3.54 |
| 53 | - | + | + | - | + | - | 1.51E-06 | 2.98E-06 | 3.54 |
| 54 | - | - | + | - | + | - | 5.73E-06 | 1.13E-05 | 0.89 |
| 55 | - | + | - | - | + | - | 1.36E-06 | 2.67E-06 | 3.54 |
| 56 | - | - | - | - | + | - | 1.19E-05 | 2.35E-05 | 0.89 |
| 57 | - | + | + | + | - | - | 5.38E-06 | 1.06E-05 | 35.68 |
| 58 | - | - | + | + | - | - | 1.67E-07 | 3.29E-07 | 3.57 |
| 59 | - | + | - | + | - | - | 1.01E-05 | 1.98E-05 | 35.68 |
| 60 | - | - | - | + | - | - | 1.49E-05 | 2.93E-05 | 3.54 |
| 61 | - | + | + | - | - | - | 1.82E-06 | 3.57E-06 | 3.54 |
| 62 | - | - | + | - | - | - | 5.16E-08 | 1.01E-07 | 9.13 |
| 63 | - | + | - | - | - | - | 1.01E-05 | 1.99E-05 | 3.54 |
| 64 | - | - | - | - | - | - | 1.21E-05 | 2.37E-05 | 9.13 |

Table C.26 SESOIL out put values for Caffeine (10 yrs of simulation)

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH | Conc at groundwater (μg/L) | Adsorbed Conc (μg/g) | Maximum pollutant depth (m) |
|---|---|---|---|---|---|---|---|---|---|
| 1 | + | + | + | + | + | + | 7.54E-04 | 2.59E-07 | 6.25 |
| 2 | + | - | + | + | + | + | 4.03E-03 | 1.38E-06 | 6.25 |
| 3 | + | + | - | + | + | + | 1.23E-02 | 4.21E-06 | 62.41 |
| 4 | + | - | - | + | + | + | 3.28E-02 | 1.12E-05 | 6.24 |
| 5 | + | + | + | - | + | + | 1.02E-02 | 3.50E-06 | 6.29 |
| 6 | + | - | + | - | + | + | 1.18E-02 | 4.06E-06 | 1.56 |
| 7 | + | + | - | - | + | + | 1.17E-02 | 4.01E-06 | 6.24 |
| 8 | + | - | - | - | + | + | 1.78E-02 | 6.11E-06 | 1.57 |
| 9 | + | + | + | + | - | + | 1.13E-02 | 3.89E-06 | 62.89 |
| 10 | + | - | + | + | - | + | 3.52E-04 | 1.21E-07 | 6.29 |
| 11 | + | + | - | + | - | + | 2.12E-02 | 7.28E-06 | 62.89 |
| 12 | + | - | - | + | - | + | 3.14E-02 | 1.08E-05 | 6.24 |
| 13 | + | + | + | - | - | + | 1.12E-03 | 3.84E-07 | 6.24 |
| 14 | + | - | + | - | - | + | 1.35E-02 | 4.64E-06 | 16.09 |
| 15 | + | + | - | - | - | + | 3.54E-02 | 1.21E-05 | 6.24 |
| 16 | + | - | - | - | - | + | 4.54E-03 | 1.56E-06 | 16.09 |
| 17 | + | + | + | + | + | - | 1.19E-02 | 4.09E-06 | 62.89 |
| 18 | + | - | + | + | + | - | 4.01E-03 | 1.38E-06 | 6.24 |
| 19 | + | + | - | + | + | - | 2.27E-02 | 7.80E-06 | 62.41 |
| 20 | + | - | - | + | + | - | 3.28E-02 | 1.12E-05 | 6.24 |
| 21 | + | + | + | - | + | - | 3.19E-03 | 1.09E-06 | 6.24 |
| 22 | + | - | + | - | + | - | 1.21E-02 | 4.14E-06 | 1.56 |
| 23 | + | + | - | - | + | - | 2.86E-03 | 9.82E-07 | 6.24 |
| 24 | + | - | - | - | + | - | 2.52E-02 | 8.63E-06 | 1.57 |
| 25 | + | + | + | + | - | - | 1.13E-02 | 3.89E-06 | 62.89 |
| 26 | + | - | + | + | - | - | 3.52E-04 | 1.21E-07 | 6.29 |
| 27 | + | + | - | + | - | - | 2.12E-02 | 7.28E-06 | 62.89 |
| 28 | + | - | - | + | - | - | 3.14E-02 | 1.08E-05 | 6.24 |
| 29 | + | + | + | - | - | - | 3.83E-03 | 1.31E-06 | 6.24 |
| 30 | + | - | + | - | - | - | 1.09E-04 | 3.73E-08 | 1.56 |
| 31 | + | + | - | - | - | - | 2.13E-02 | 7.32E-06 | 6.24 |
| 32 | + | - | - | - | - | - | 2.54E-02 | 8.73E-06 | 16.09 |
| 33 | - | + | + | + | + | + | 1.07E-05 | 2.30E-09 | 62.79 |
| 34 | - | - | + | + | + | + | 5.73E-05 | 1.23E-08 | 6.25 |
| 35 | - | + | - | + | + | + | 1.74E-04 | 3.75E-08 | 62.41 |
| 36 | - | - | - | + | + | + | 4.66E-04 | 1.00E-07 | 6.24 |
| 37 | - | + | + | - | + | + | 1.45E-04 | 3.12E-08 | 6.24 |
| 38 | - | - | + | - | + | + | 1.68E-04 | 3.61E-08 | 1.56 |
| 39 | - | + | - | - | + | + | 1.66E-04 | 3.57E-08 | 6.24 |
| 40 | - | - | - | - | + | + | 2.54E-04 | 5.45E-08 | 1.57 |
| 41 | - | + | + | + | - | + | 1.52E-04 | 3.27E-08 | 62.89 |
| 42 | - | - | + | + | - | + | 5.01E-06 | 1.08E-09 | 6.29 |
| 43 | - | + | - | + | - | + | 3.02E-04 | 6.49E-08 | 62.89 |

Continuation of above table

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH | Conc at groundwater (µg/L) | Adsorbed Conc (µg/g) | Maximum pollutant depth (m) |
|---|---|---|---|---|---|---|---|---|---|
| 44 | - | - | - | + | - | + | 4.46E-04 | 9.59E-08 | 6.24 |
| 45 | - | + | + | - | - | + | 1.59E-05 | 3.41E-09 | 6.24 |
| 46 | - | - | + | - | - | + | 1.92E-04 | 4.13E-08 | 16.09 |
| 47 | - | + | - | - | - | + | 5.03E-04 | 1.08E-07 | 6.24 |
| 48 | - | - | - | - | - | + | 6.47E-05 | 1.39E-08 | 16.09 |
| 49 | - | + | + | + | + | - | 1.70E-04 | 3.64E-08 | 62.63 |
| 50 | - | - | + | + | + | - | 5.73E-05 | 1.23E-08 | 6.24 |
| 51 | - | + | - | + | + | - | 3.24E-04 | 6.95E-08 | 62.41 |
| 52 | - | - | - | + | + | - | 4.66E-04 | 1.00E-07 | 6.24 |
| 53 | - | + | + | - | + | - | 4.54E-05 | 9.75E-09 | 6.24 |
| 54 | - | - | + | - | + | - | 1.72E-04 | 3.69E-08 | 1.56 |
| 55 | - | + | - | - | + | - | 4.07E-05 | 8.74E-09 | 6.24 |
| 56 | - | - | - | - | + | - | 3.58E-04 | 7.69E-08 | 1.57 |
| 57 | - | + | + | + | - | - | 1.61E-04 | 3.47E-08 | 62.89 |
| 58 | - | - | + | + | - | - | 5.01E-06 | 1.08E-09 | 6.29 |
| 59 | - | + | - | + | - | - | 3.02E-04 | 6.49E-08 | 62.89 |
| 60 | - | - | - | + | - | - | 4.46E-04 | 9.59E-08 | 6.24 |
| 61 | - | + | + | - | - | - | 5.45E-05 | 1.17E-08 | 6.24 |
| 62 | - | - | + | - | - | - | 1.55E-06 | 3.32E-10 | 16.09 |
| 63 | - | + | - | - | - | - | 3.03E-04 | 6.52E-08 | 6.24 |
| 64 | - | - | - | - | - | - | 3.62E-04 | 7.77E-08 | 16.09 |

Table C.27 SESOIL out put values for Ibuprofen (10 yrs of simulation)

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH | Conc at groundwater (µg/L) | Adsorbed Conc (µg/g) | Maximum pollutant depth (m) |
|---|---|---|---|---|---|---|---|---|---|
| 1 | + | + | + | + | + | + | 1.63E-03 | 6.47E-06 | 1.32 |
| 2 | + | - | + | + | + | + | 8.70E-03 | 3.46E-05 | 1.32 |
| 3 | + | + | - | + | + | + | 2.65E-02 | 1.05E-04 | 13.20 |
| 4 | + | - | - | + | + | + | 7.08E-02 | 2.81E-04 | 1.32 |
| 5 | + | + | + | - | + | + | 2.20E-02 | 8.75E-05 | 1.33 |
| 6 | + | - | + | - | + | + | 2.55E-02 | 1.01E-04 | 0.33 |
| 7 | + | + | - | - | + | + | 2.52E-02 | 1.00E-04 | 1.32 |
| 8 | + | - | - | - | + | + | 3.85E-02 | 1.53E-04 | 0.33 |
| 9 | + | + | + | + | - | + | 2.45E-02 | 9.73E-05 | 13.30 |
| 10 | + | - | + | + | - | + | 7.61E-04 | 3.02E-06 | 1.33 |
| 11 | + | + | - | + | - | + | 4.59E-02 | 1.82E-04 | 13.30 |
| 12 | + | - | - | + | - | + | 6.78E-02 | 2.69E-04 | 1.32 |
| 13 | + | + | + | - | - | + | 2.42E-03 | 9.59E-06 | 1.32 |
| 14 | + | - | + | - | - | + | 2.92E-02 | 1.16E-04 | 3.40 |
| 15 | + | + | - | - | - | + | 7.64E-02 | 3.03E-04 | 1.32 |
| 16 | + | - | - | - | - | + | 9.82E-03 | 3.90E-05 | 3.40 |
| 17 | + | + | + | + | + | - | 2.58E-02 | 1.02E-04 | 13.21 |
| 18 | + | - | + | + | + | - | 8.67E-03 | 3.44E-05 | 1.32 |
| 19 | + | + | - | + | + | - | 4.91E-02 | 1.95E-04 | 13.20 |
| 20 | + | - | - | + | + | - | 7.08E-02 | 2.81E-04 | 1.32 |
| 21 | + | + | + | - | + | - | 6.89E-03 | 2.74E-05 | 1.32 |
| 22 | + | - | + | - | + | - | 2.61E-02 | 1.04E-04 | 0.33 |
| 23 | + | + | - | - | + | - | 6.18E-03 | 2.45E-05 | 1.32 |
| 24 | + | - | - | - | + | - | 5.44E-02 | 2.16E-04 | 0.33 |
| 25 | + | + | + | + | - | - | 2.45E-02 | 9.73E-05 | 13.30 |
| 26 | + | - | + | + | - | - | 7.61E-04 | 3.02E-06 | 1.33 |
| 27 | + | + | - | + | - | - | 4.59E-02 | 1.82E-04 | 13.30 |
| 28 | + | - | - | + | - | - | 6.78E-02 | 2.69E-04 | 1.32 |
| 29 | + | + | + | - | - | - | 8.27E-03 | 3.28E-05 | 1.32 |
| 30 | + | - | + | - | - | - | 2.35E-04 | 9.33E-07 | 0.33 |
| 31 | + | + | - | - | - | - | 4.61E-02 | 1.83E-04 | 1.32 |
| 32 | + | - | - | - | - | - | 5.50E-02 | 2.18E-04 | 3.40 |
| 33 | - | + | + | + | + | + | 7.17E-06 | 1.20E-06 | 13.30 |
| 34 | - | - | + | + | + | + | 3.83E-05 | 6.40E-06 | 1.32 |
| 35 | - | + | - | + | + | + | 1.17E-04 | 1.95E-05 | 13.20 |
| 36 | - | - | - | + | + | + | 3.12E-04 | 5.21E-05 | 1.32 |
| 37 | - | + | + | - | + | + | 9.70E-05 | 1.62E-05 | 1.32 |
| 38 | - | - | + | - | + | + | 1.12E-04 | 1.88E-05 | 0.33 |
| 39 | - | + | - | - | + | + | 1.11E-04 | 1.86E-05 | 1.32 |
| 40 | - | - | - | - | + | + | 1.70E-04 | 2.84E-05 | 0.33 |
| 41 | - | + | + | + | - | + | 1.02E-04 | 1.70E-05 | 13.30 |
| 42 | - | - | + | + | - | + | 3.35E-06 | 5.60E-07 | 1.33 |
| 43 | - | + | - | + | - | + | 2.02E-04 | 3.37E-05 | 13.30 |

Continuation of above table

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH | Conc at groundwater (µg/L) | Adsorbed Conc (µg/g) | Maximum pollutant depth (m) |
|---|---|---|---|---|---|---|---|---|---|
| 44 | - | - | - | + | - | + | 2.98E-04 | 4.99E-05 | 1.32 |
| 45 | - | + | + | - | - | + | 1.06E-05 | 1.78E-06 | 1.32 |
| 46 | - | - | + | - | - | + | 1.29E-04 | 2.15E-05 | 3.40 |
| 47 | - | + | - | - | - | + | 3.36E-04 | 5.62E-05 | 1.32 |
| 48 | - | - | - | - | - | + | 4.32E-05 | 7.22E-06 | 3.40 |
| 49 | - | + | + | + | + | - | 1.13E-04 | 1.89E-05 | 13.19 |
| 50 | - | - | + | + | + | - | 3.83E-05 | 6.40E-06 | 1.32 |
| 51 | - | + | - | + | + | - | 2.16E-04 | 3.62E-05 | 13.20 |
| 52 | - | - | - | + | + | - | 3.12E-04 | 5.21E-05 | 1.32 |
| 53 | - | + | + | - | + | - | 3.03E-05 | 5.07E-06 | 1.32 |
| 54 | - | - | + | - | + | - | 1.15E-04 | 1.92E-05 | 0.33 |
| 55 | - | + | - | - | + | - | 2.72E-05 | 4.55E-06 | 1.32 |
| 56 | - | - | - | - | + | - | 2.39E-04 | 4.00E-05 | 0.33 |
| 57 | - | + | + | + | - | - | 1.08E-04 | 1.80E-05 | 13.30 |
| 58 | - | - | + | + | - | - | 3.35E-06 | 5.60E-07 | 1.33 |
| 59 | - | + | - | + | - | - | 2.02E-04 | 3.37E-05 | 13.30 |
| 60 | - | - | - | + | - | - | 2.98E-04 | 4.99E-05 | 1.32 |
| 61 | - | + | + | - | - | - | 3.64E-05 | 6.09E-06 | 1.32 |
| 62 | - | - | + | - | - | - | 1.03E-06 | 1.73E-07 | 3.40 |
| 63 | - | + | - | - | - | - | 2.03E-04 | 3.39E-05 | 1.32 |
| 64 | - | - | - | - | - | - | 2.42E-04 | 4.04E-05 | 3.40 |

Table C.28 SESOIL out put values for Diclofenac (10 yrs of simulation)

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH | Conc at groundwater (μg/L) | Adsorbed Conc (μg/g) | Maximum pollutant depth (m) |
|---|---|---|---|---|---|---|---|---|---|
| 1 | + | + | + | + | + | + | 6.49E-04 | 2.56E-06 | 2.40 |
| 2 | + | - | + | + | + | + | 3.47E-03 | 1.37E-05 | 2.40 |
| 3 | + | + | - | + | + | + | 1.06E-02 | 4.17E-05 | 24.00 |
| 4 | + | - | - | + | + | + | 2.82E-02 | 1.11E-04 | 2.40 |
| 5 | + | + | + | - | + | + | 8.78E-03 | 3.47E-05 | 2.42 |
| 6 | + | - | + | - | + | + | 1.02E-02 | 4.02E-05 | 0.60 |
| 7 | + | + | - | - | + | + | 1.01E-02 | 3.97E-05 | 2.40 |
| 8 | + | - | - | - | + | + | 1.53E-02 | 6.06E-05 | 0.60 |
| 9 | + | + | + | + | - | + | 9.76E-03 | 3.86E-05 | 24.19 |
| 10 | + | - | + | + | - | + | 3.03E-04 | 1.20E-06 | 2.42 |
| 11 | + | + | - | + | - | + | 1.83E-02 | 7.22E-05 | 24.19 |
| 12 | + | - | - | + | - | + | 2.70E-02 | 1.07E-04 | 2.40 |
| 13 | + | + | + | - | - | + | 9.62E-04 | 3.80E-06 | 2.40 |
| 14 | + | - | + | - | - | + | 1.16E-02 | 4.60E-05 | 6.19 |
| 15 | + | + | - | - | - | + | 3.04E-02 | 1.20E-04 | 2.40 |
| 16 | + | - | - | - | - | + | 3.91E-03 | 1.54E-05 | 6.19 |
| 17 | + | + | + | + | + | - | 1.03E-02 | 4.05E-05 | 24.14 |
| 18 | + | - | + | + | + | - | 3.45E-03 | 1.36E-05 | 2.40 |
| 19 | + | + | - | + | + | - | 1.96E-02 | 7.73E-05 | 24.00 |
| 20 | + | - | - | + | + | - | 2.82E-02 | 1.11E-04 | 2.40 |
| 21 | + | + | + | - | + | - | 2.75E-03 | 1.08E-05 | 2.40 |
| 22 | + | - | + | - | + | - | 1.04E-02 | 4.11E-05 | 0.60 |
| 23 | + | + | - | - | + | - | 2.46E-03 | 9.72E-06 | 2.40 |
| 24 | + | - | - | - | + | - | 2.17E-02 | 8.55E-05 | 0.60 |
| 25 | + | + | + | + | - | - | 9.76E-03 | 3.86E-05 | 24.19 |
| 26 | + | - | + | + | - | - | 3.03E-04 | 1.20E-06 | 2.42 |
| 27 | + | + | - | + | - | - | 1.83E-02 | 7.22E-05 | 24.19 |
| 28 | + | - | - | + | - | - | 2.70E-02 | 1.07E-04 | 2.40 |
| 29 | + | + | + | - | - | - | 3.30E-03 | 1.30E-05 | 2.40 |
| 30 | + | - | + | - | - | - | 9.36E-05 | 3.70E-07 | 0.60 |
| 31 | + | + | - | - | - | - | 1.84E-02 | 7.25E-05 | 2.40 |
| 32 | + | - | - | - | - | - | 2.19E-02 | 8.65E-05 | 6.19 |
| 33 | - | + | + | + | + | + | 2.14E-05 | 3.64E-06 | 24.08 |
| 34 | - | - | + | + | + | + | 1.14E-04 | 1.95E-05 | 2.40 |
| 35 | - | + | - | + | + | + | 3.48E-04 | 5.92E-05 | 24.00 |
| 36 | - | - | - | + | + | + | 9.29E-04 | 1.58E-04 | 2.40 |
| 37 | - | + | + | - | + | + | 2.89E-04 | 4.93E-05 | 2.40 |
| 38 | - | - | + | - | + | + | 3.35E-04 | 5.71E-05 | 0.60 |
| 39 | - | + | - | - | + | + | 3.31E-04 | 5.64E-05 | 2.40 |
| 40 | - | - | - | - | + | + | 5.06E-04 | 8.62E-05 | 0.60 |
| 41 | - | + | + | + | - | + | 3.03E-04 | 5.16E-05 | 24.19 |
| 42 | - | - | + | + | - | + | 9.99E-06 | 1.70E-06 | 2.42 |
| 43 | - | + | - | + | - | + | 6.02E-04 | 1.03E-04 | 24.19 |

Continuation of above table

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH | Conc at groundwater (µg/L) | Adsorbed Conc (µg/g) | Maximum pollutant depth (m) |
|---|---|---|---|---|---|---|---|---|---|
| 44 | - | - | - | + | - | + | 8.90E-04 | 1.52E-04 | 2.40 |
| 45 | - | + | + | - | - | + | 3.17E-05 | 5.40E-06 | 2.40 |
| 46 | - | - | + | - | - | + | 3.83E-04 | 6.53E-05 | 6.19 |
| 47 | - | + | - | - | - | + | 1.00E-03 | 1.71E-04 | 2.40 |
| 48 | - | - | - | - | - | + | 1.29E-04 | 2.20E-05 | 6.19 |
| 49 | - | + | + | + | + | - | 3.38E-04 | 5.76E-05 | 24.03 |
| 50 | - | - | + | + | + | - | 1.14E-04 | 1.95E-05 | 2.40 |
| 51 | - | + | - | + | + | - | 6.45E-04 | 1.10E-04 | 24.00 |
| 52 | - | - | - | + | + | - | 9.29E-04 | 1.58E-04 | 2.40 |
| 53 | - | + | + | - | + | - | 9.04E-05 | 1.54E-05 | 2.40 |
| 54 | - | - | + | - | + | - | 3.42E-04 | 5.83E-05 | 0.60 |
| 55 | - | + | - | - | + | - | 8.11E-05 | 1.38E-05 | 2.40 |
| 56 | - | - | - | - | + | - | 7.13E-04 | 1.22E-04 | 0.60 |
| 57 | - | + | + | + | - | - | 3.22E-04 | 5.48E-05 | 24.19 |
| 58 | - | - | + | + | - | - | 9.99E-06 | 1.70E-06 | 2.42 |
| 59 | - | + | - | + | - | - | 6.02E-04 | 1.03E-04 | 24.19 |
| 60 | - | - | - | + | - | - | 8.90E-04 | 1.52E-04 | 2.40 |
| 61 | - | + | + | - | - | - | 1.09E-04 | 1.85E-05 | 2.40 |
| 62 | - | - | + | - | - | - | 3.08E-06 | 5.25E-07 | 6.19 |
| 63 | - | + | - | - | - | - | 6.05E-04 | 1.03E-04 | 2.40 |
| 64 | - | - | - | - | - | - | 7.21E-04 | 1.23E-04 | 6.19 |

Table C.29 SESOIL out put values for Acetaminophen (10 yrs of simulation)

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH | Conc at groundwater (µg/L) | Adsorbed Conc (µg/g) | Maximum pollutant depth (m) |
|---|---|---|---|---|---|---|---|---|---|
| 1 | + | + | + | + | + | + | 9.42E-05 | 5.12E-07 | 6.49 |
| 2 | + | - | + | + | + | + | 5.04E-04 | 2.74E-06 | 6.49 |
| 3 | + | + | - | + | + | + | 1.53E-03 | 8.33E-06 | 64.81 |
| 4 | + | - | - | + | + | + | 4.10E-03 | 2.23E-05 | 6.48 |
| 5 | + | + | + | - | + | + | 1.27E-03 | 6.92E-06 | 6.53 |
| 6 | + | - | + | - | + | + | 1.48E-03 | 8.03E-06 | 1.62 |
| 7 | + | + | - | - | + | + | 1.46E-03 | 7.93E-06 | 6.48 |
| 8 | + | - | - | - | + | + | 2.23E-03 | 1.21E-05 | 1.63 |
| 9 | + | + | + | + | - | + | 1.42E-03 | 7.70E-06 | 65.31 |
| 10 | + | - | + | + | - | + | 4.41E-05 | 2.39E-07 | 6.53 |
| 11 | + | + | - | + | - | + | 2.65E-03 | 1.44E-05 | 65.31 |
| 12 | + | - | - | + | - | + | 3.92E-03 | 2.13E-05 | 6.48 |
| 13 | + | + | + | - | - | + | 1.40E-04 | 7.59E-07 | 6.48 |
| 14 | + | - | + | - | - | + | 1.69E-03 | 9.18E-06 | 16.71 |
| 15 | + | + | - | - | - | + | 4.42E-03 | 2.40E-05 | 6.48 |
| 16 | + | - | - | - | - | + | 5.68E-04 | 3.09E-06 | 16.71 |
| 17 | + | + | + | + | + | - | 1.49E-03 | 8.09E-06 | 65.31 |
| 18 | + | - | + | + | + | - | 5.01E-04 | 2.72E-06 | 6.48 |
| 19 | + | + | - | + | + | - | 2.84E-03 | 1.54E-05 | 64.81 |
| 20 | + | - | - | + | + | - | 4.10E-03 | 2.23E-05 | 6.48 |
| 21 | + | + | + | - | + | - | 3.99E-04 | 2.17E-06 | 6.48 |
| 22 | + | - | + | - | + | - | 1.51E-03 | 8.20E-06 | 1.62 |
| 23 | + | + | - | - | + | - | 3.58E-04 | 1.94E-06 | 6.48 |
| 24 | + | - | - | - | + | - | 3.14E-03 | 1.71E-05 | 1.63 |
| 25 | + | + | + | + | - | - | 1.42E-03 | 7.70E-06 | 65.31 |
| 26 | + | - | + | + | - | - | 4.41E-05 | 2.39E-07 | 6.53 |
| 27 | + | + | - | + | - | - | 2.65E-03 | 1.44E-05 | 65.31 |
| 28 | + | - | - | + | - | - | 3.92E-03 | 2.13E-05 | 6.48 |
| 29 | + | + | + | - | - | - | 4.79E-04 | 2.60E-06 | 6.48 |
| 30 | + | - | + | - | - | - | 1.36E-05 | 7.39E-08 | 1.62 |
| 31 | + | + | - | - | - | - | 2.67E-03 | 1.45E-05 | 6.48 |
| 32 | + | - | - | - | - | - | 3.18E-03 | 1.73E-05 | 16.71 |
| 33 | - | + | + | + | + | + | 3.26E-05 | 4.71E-07 | 65.31 |
| 34 | - | - | + | + | + | + | 1.74E-04 | 2.52E-06 | 6.49 |
| 35 | - | + | - | + | + | + | 5.30E-04 | 7.66E-06 | 64.81 |
| 36 | - | - | - | + | + | + | 1.42E-03 | 2.05E-05 | 6.48 |
| 37 | - | + | + | - | + | + | 4.41E-04 | 6.37E-06 | 6.48 |
| 38 | - | - | + | - | + | + | 5.11E-04 | 7.39E-06 | 1.62 |
| 39 | - | + | - | - | + | + | 5.05E-04 | 7.30E-06 | 6.48 |
| 40 | - | - | - | - | + | + | 7.71E-04 | 1.11E-05 | 1.63 |
| 41 | - | + | + | + | - | + | 4.62E-04 | 6.68E-06 | 65.31 |
| 42 | - | - | + | + | - | + | 1.52E-05 | 2.20E-07 | 6.53 |
| 43 | - | + | - | + | - | + | 9.17E-04 | 1.33E-05 | 65.31 |

Continuation of above table

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH | Conc at groundwater (µg/L) | Adsorbed Conc (µg/g) | Maximum pollutant depth (m) |
|---|---|---|---|---|---|---|---|---|---|
| 44 | - | - | - | + | - | + | 1.36E-03 | 1.96E-05 | 6.48 |
| 45 | - | + | + | - | - | + | 4.83E-05 | 6.98E-07 | 6.48 |
| 46 | - | - | + | - | - | + | 5.84E-04 | 8.45E-06 | 16.71 |
| 47 | - | + | - | - | - | + | 1.53E-03 | 2.21E-05 | 6.48 |
| 48 | - | - | - | - | - | + | 1.96E-04 | 2.84E-06 | 16.71 |
| 49 | - | + | + | + | + | - | 5.15E-04 | 7.45E-06 | 65.31 |
| 50 | - | - | + | + | + | - | 1.74E-04 | 2.52E-06 | 6.48 |
| 51 | - | + | - | + | + | - | 9.83E-04 | 1.42E-05 | 64.81 |
| 52 | - | - | - | + | + | - | 1.42E-03 | 2.05E-05 | 6.48 |
| 53 | - | + | + | - | + | - | 1.38E-04 | 1.99E-06 | 6.48 |
| 54 | - | - | + | - | + | - | 5.22E-04 | 7.55E-06 | 1.62 |
| 55 | - | + | - | - | + | - | 1.24E-04 | 1.79E-06 | 6.48 |
| 56 | - | - | - | - | + | - | 1.09E-03 | 1.57E-05 | 1.63 |
| 57 | - | + | + | + | - | - | 4.90E-04 | 7.09E-06 | 65.31 |
| 58 | - | - | + | + | - | - | 1.52E-05 | 2.20E-07 | 6.53 |
| 59 | - | + | - | + | - | - | 9.17E-04 | 1.33E-05 | 65.31 |
| 60 | - | - | - | + | - | - | 1.36E-03 | 1.96E-05 | 6.48 |
| 61 | - | + | + | - | - | - | 1.65E-04 | 2.39E-06 | 6.48 |
| 62 | - | - | + | - | - | - | 4.70E-06 | 6.80E-08 | 16.71 |
| 63 | - | + | - | - | - | - | 9.22E-04 | 1.33E-05 | 6.48 |
| 64 | - | - | - | - | - | - | 1.10E-03 | 1.59E-05 | 16.71 |

Table C.30 SESOIL out put values for Triclosan (10 yrs of simulation)

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH | Conc at groundwater (µg/L) | Adsorbed Conc (µg/g) | Maximum pollutant depth (m) |
|---|---|---|---|---|---|---|---|---|---|
| 1 | + | + | + | + | + | + | 2.03E-03 | 1.60E-05 | 0.96 |
| 2 | + | - | + | + | + | + | 1.09E-02 | 8.54E-05 | 0.96 |
| 3 | + | + | - | + | + | + | 3.31E-02 | 2.60E-04 | 9.60 |
| 4 | + | - | - | + | + | + | 8.84E-02 | 6.95E-04 | 0.96 |
| 5 | + | + | + | - | + | + | 2.75E-02 | 2.16E-04 | 0.97 |
| 6 | + | - | + | - | + | + | 3.19E-02 | 2.51E-04 | 0.24 |
| 7 | + | + | - | - | + | + | 3.15E-02 | 2.48E-04 | 0.96 |
| 8 | + | - | - | - | + | + | 4.81E-02 | 3.78E-04 | 0.24 |
| 9 | + | + | + | + | - | + | 3.06E-02 | 2.41E-04 | 9.68 |
| 10 | + | - | + | + | - | + | 9.51E-04 | 7.47E-06 | 0.97 |
| 11 | + | + | - | + | - | + | 5.73E-02 | 4.50E-04 | 9.68 |
| 12 | + | - | - | + | - | + | 8.47E-02 | 6.65E-04 | 0.96 |
| 13 | + | + | + | - | - | + | 3.02E-03 | 2.37E-05 | 0.96 |
| 14 | + | - | + | - | - | + | 3.65E-02 | 2.87E-04 | 2.48 |
| 15 | + | + | - | - | - | + | 9.54E-02 | 7.50E-04 | 0.96 |
| 16 | + | - | - | - | - | + | 1.23E-02 | 9.64E-05 | 2.48 |
| 17 | + | + | + | + | + | - | 3.22E-02 | 2.53E-04 | 9.68 |
| 18 | + | - | + | + | + | - | 1.08E-02 | 8.51E-05 | 0.95 |
| 19 | + | + | - | + | + | - | 6.13E-02 | 4.82E-04 | 9.60 |
| 20 | + | - | - | + | + | - | 8.84E-02 | 6.95E-04 | 0.96 |
| 21 | + | + | + | - | + | - | 8.61E-03 | 6.76E-05 | 0.94 |
| 22 | + | - | + | - | + | - | 3.26E-02 | 2.56E-04 | 0.24 |
| 23 | + | + | - | - | + | - | 7.72E-03 | 6.06E-05 | 0.96 |
| 24 | + | - | - | - | + | - | 6.79E-02 | 5.33E-04 | 0.24 |
| 25 | + | + | + | + | - | - | 3.06E-02 | 2.41E-04 | 9.69 |
| 26 | + | - | + | + | - | - | 9.51E-04 | 7.47E-06 | 0.97 |
| 27 | + | + | - | + | - | - | 5.73E-02 | 4.50E-04 | 9.68 |
| 28 | + | - | - | + | - | - | 8.47E-02 | 6.65E-04 | 0.96 |
| 29 | + | + | + | - | - | - | 1.03E-02 | 8.12E-05 | 0.96 |
| 30 | + | - | + | - | - | - | 2.93E-04 | 2.31E-06 | 0.24 |
| 31 | + | + | - | - | - | - | 5.75E-02 | 4.52E-04 | 0.96 |
| 32 | + | - | - | - | - | - | 6.86E-02 | 5.40E-04 | 2.48 |
| 33 | - | + | + | + | + | + | 9.04E-05 | 1.92E-06 | 9.59 |
| 34 | - | - | + | + | + | + | 4.83E-04 | 1.02E-05 | 0.96 |
| 35 | - | + | - | + | + | + | 1.47E-03 | 3.12E-05 | 9.60 |
| 36 | - | - | - | + | + | + | 3.93E-03 | 8.33E-05 | 0.96 |
| 37 | - | + | + | - | + | + | 1.22E-03 | 2.59E-05 | 0.96 |
| 38 | - | - | + | - | + | + | 1.42E-03 | 3.00E-05 | 0.24 |
| 39 | - | + | - | - | + | + | 1.40E-03 | 2.97E-05 | 0.96 |
| 40 | - | - | - | - | + | + | 2.14E-03 | 4.53E-05 | 0.24 |
| 41 | - | + | + | + | - | + | 1.28E-03 | 2.72E-05 | 9.68 |
| 42 | - | - | + | + | - | + | 4.22E-05 | 8.96E-07 | 0.97 |

Continuation of above table

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH | Conc at groundwater (μg/L) | Adsorbed Conc (μg/g) | Maximum pollutant depth (m) |
|---|---|---|---|---|---|---|---|---|---|
| 43 | - | + | - | + | - | + | 2.54E-03 | 5.39E-05 | 9.68 |
| 44 | - | - | - | + | - | + | 3.76E-03 | 7.97E-05 | 0.96 |
| 45 | - | + | + | - | - | + | 1.34E-04 | 2.84E-06 | 0.96 |
| 46 | - | - | + | - | - | + | 1.62E-03 | 3.44E-05 | 2.48 |
| 47 | - | + | - | - | - | + | 4.24E-03 | 8.99E-05 | 0.96 |
| 48 | - | - | - | - | - | + | 5.45E-04 | 1.16E-05 | 2.48 |
| 49 | - | + | + | + | + | - | 1.43E-03 | 3.03E-05 | 9.62 |
| 50 | - | - | + | + | + | - | 4.83E-04 | 1.02E-05 | 0.96 |
| 51 | - | + | - | + | + | - | 2.73E-03 | 5.78E-05 | 9.60 |
| 52 | - | - | - | + | + | - | 3.93E-03 | 8.33E-05 | 0.96 |
| 53 | - | + | + | - | + | - | 3.82E-04 | 8.11E-06 | 0.96 |
| 54 | - | - | + | - | + | - | 1.45E-03 | 3.07E-05 | 0.24 |
| 55 | - | + | - | - | + | - | 3.43E-04 | 7.27E-06 | 0.96 |
| 56 | - | - | - | - | + | - | 3.01E-03 | 6.39E-05 | 0.24 |
| 57 | - | + | + | + | - | - | 1.36E-03 | 2.88E-05 | 9.68 |
| 58 | - | - | + | + | - | - | 4.22E-05 | 8.96E-07 | 0.97 |
| 59 | - | + | - | + | - | - | 2.54E-03 | 5.39E-05 | 9.68 |
| 60 | - | - | - | + | - | - | 3.76E-03 | 7.97E-05 | 0.96 |
| 61 | - | + | + | - | - | - | 4.59E-04 | 9.73E-06 | 0.96 |
| 62 | - | - | + | - | - | - | 1.30E-05 | 2.76E-07 | 2.48 |
| 63 | - | + | - | - | - | - | 2.56E-03 | 5.42E-05 | 0.96 |
| 64 | - | - | - | - | - | - | 3.05E-03 | 6.47E-05 | 2.48 |

Table C.31 SESOIL out put values for Ciprofloxacin (10 yrs of simulation)

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH | Conc at groundwater (µg/L) | Adsorbed Conc (µg/g) | Maximum pollutant depth (m) |
|---|---|---|---|---|---|---|---|---|---|
| 1 | + | + | + | + | + | + | 2.11E-03 | 1.75E-05 | 1.14 |
| 2 | + | - | + | + | + | + | 1.13E-02 | 9.33E-05 | 1.14 |
| 3 | + | + | - | + | + | + | 3.44E-02 | 2.84E-04 | 11.40 |
| 4 | + | - | - | + | + | + | 9.19E-02 | 7.59E-04 | 1.14 |
| 5 | + | + | + | - | + | + | 2.86E-02 | 2.36E-04 | 1.15 |
| 6 | + | - | + | - | + | + | 3.31E-02 | 2.74E-04 | 0.29 |
| 7 | + | + | - | - | + | + | 3.28E-02 | 2.71E-04 | 1.14 |
| 8 | + | - | - | - | + | + | 5.00E-02 | 4.13E-04 | 0.29 |
| 9 | + | + | + | + | - | + | 3.18E-02 | 2.63E-04 | 11.49 |
| 10 | + | - | + | + | - | + | 9.88E-04 | 8.17E-06 | 1.15 |
| 11 | + | + | - | + | - | + | 5.95E-02 | 4.92E-04 | 11.49 |
| 12 | + | - | - | + | - | + | 8.80E-02 | 7.27E-04 | 1.14 |
| 13 | + | + | + | - | - | + | 3.14E-03 | 2.59E-05 | 1.14 |
| 14 | + | - | + | - | - | + | 3.79E-02 | 3.13E-04 | 2.94 |
| 15 | + | + | - | - | - | + | 9.92E-02 | 8.20E-04 | 1.14 |
| 16 | + | - | - | - | - | + | 1.27E-02 | 1.05E-04 | 2.94 |
| 17 | + | + | + | + | + | - | 3.34E-02 | 2.76E-04 | 11.43 |
| 18 | + | - | + | + | + | - | 1.13E-02 | 9.29E-05 | 1.14 |
| 19 | + | + | - | + | + | - | 6.38E-02 | 5.27E-04 | 11.40 |
| 20 | + | - | - | + | + | - | 9.19E-02 | 7.59E-04 | 1.14 |
| 21 | + | + | + | - | + | - | 8.95E-03 | 7.39E-05 | 1.14 |
| 22 | + | - | + | - | + | - | 3.39E-02 | 2.80E-04 | 0.29 |
| 23 | + | + | - | - | + | - | 8.02E-03 | 6.63E-05 | 1.14 |
| 24 | + | - | - | - | + | - | 7.06E-02 | 5.83E-04 | 0.29 |
| 25 | + | + | + | + | - | - | 3.18E-02 | 2.63E-04 | 11.49 |
| 26 | + | - | + | + | - | - | 9.88E-04 | 8.17E-06 | 1.15 |
| 27 | + | + | - | + | - | - | 5.95E-02 | 4.92E-04 | 11.49 |
| 28 | + | - | - | + | - | - | 8.80E-02 | 7.27E-04 | 1.14 |
| 29 | + | + | + | - | - | - | 1.07E-02 | 8.87E-05 | 1.14 |
| 30 | + | - | + | - | - | - | 3.05E-04 | 2.52E-06 | 0.29 |
| 31 | + | + | - | - | - | - | 5.98E-02 | 4.94E-04 | 1.14 |
| 32 | + | - | - | - | - | - | 7.14E-02 | 5.90E-04 | 2.94 |
| 33 | - | + | + | + | + | + | 9.42E-05 | 1.36E-06 | 11.39 |
| 34 | - | - | + | + | + | + | 5.04E-04 | 7.25E-06 | 1.14 |
| 35 | - | + | - | + | + | + | 1.53E-03 | 2.21E-05 | 11.40 |
| 36 | - | - | - | + | + | + | 4.10E-03 | 5.90E-05 | 1.14 |
| 37 | - | + | + | - | + | + | 1.27E-03 | 1.84E-05 | 1.14 |
| 38 | - | - | + | - | + | + | 1.48E-03 | 2.13E-05 | 0.29 |
| 39 | - | + | - | - | + | + | 1.46E-03 | 2.10E-05 | 1.14 |

Continuation of above table

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH | Conc at groundwater (µg/L) | Adsorbed Conc (µg/g) | Maximum pollutant depth (m) |
|---|---|---|---|---|---|---|---|---|---|
| 40 | - | - | - | - | + | + | 2.23E-03 | 3.21E-05 | 0.29 |
| 41 | - | + | + | + | - | + | 1.34E-03 | 1.92E-05 | 11.49 |
| 42 | - | - | + | + | - | + | 4.41E-05 | 6.34E-07 | 1.15 |
| 43 | - | + | - | + | - | + | 2.65E-03 | 3.82E-05 | 11.49 |
| 44 | - | - | - | + | - | + | 3.92E-03 | 5.65E-05 | 1.14 |
| 45 | - | + | + | - | - | + | 1.40E-04 | 2.01E-06 | 1.14 |
| 46 | - | - | + | - | - | + | 1.69E-03 | 2.43E-05 | 2.94 |
| 47 | - | + | - | - | - | + | 4.42E-03 | 6.37E-05 | 1.14 |
| 48 | - | - | - | - | - | + | 5.68E-04 | 8.18E-06 | 2.94 |
| 49 | - | + | + | + | + | - | 1.49E-03 | 2.15E-05 | 11.49 |
| 50 | - | - | + | + | + | - | 5.04E-04 | 7.25E-06 | 1.14 |
| 51 | - | + | - | + | + | - | 2.84E-03 | 4.09E-05 | 11.40 |
| 52 | - | - | - | + | + | - | 4.10E-03 | 5.90E-05 | 1.14 |
| 53 | - | + | + | - | + | - | 3.99E-04 | 5.74E-06 | 1.14 |
| 54 | - | - | + | - | + | - | 1.51E-03 | 2.17E-05 | 0.29 |
| 55 | - | + | - | - | + | - | 3.58E-04 | 5.15E-06 | 1.14 |
| 56 | - | - | - | - | + | - | 3.14E-03 | 4.53E-05 | 0.29 |
| 57 | - | + | + | + | - | - | 1.42E-03 | 2.04E-05 | 11.49 |
| 58 | - | - | + | + | - | - | 4.41E-05 | 6.34E-07 | 1.15 |
| 59 | - | + | - | + | - | - | 2.65E-03 | 3.82E-05 | 11.49 |
| 60 | - | - | - | + | - | - | 3.92E-03 | 5.65E-05 | 1.14 |
| 61 | - | + | + | - | - | - | 4.79E-04 | 6.89E-06 | 1.14 |
| 62 | - | - | + | - | - | - | 1.36E-05 | 1.96E-07 | 2.94 |
| 63 | - | + | - | - | - | - | 2.67E-03 | 3.84E-05 | 1.14 |
| 64 | - | - | - | - | - | - | 3.18E-03 | 4.58E-05 | 2.94 |

Table C.32 SESOIL out put values for Metoprolol (10 yrs of simulation)

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH | Conc at groundwater (μg/L) | Adsorbed Conc (μg/g) | Maximum pollutant depth (m) |
|---|---|---|---|---|---|---|---|---|---|
| 1 | + | + | + | + | + | + | 6.60E-04 | 2.59E-06 | 5.35 |
| 2 | + | - | + | + | + | + | 3.53E-03 | 1.39E-05 | 5.35 |
| 3 | + | + | - | + | + | + | 1.07E-02 | 4.22E-05 | 53.41 |
| 4 | + | - | - | + | + | + | 2.87E-02 | 1.13E-04 | 5.34 |
| 5 | + | + | + | - | + | + | 8.92E-03 | 3.51E-05 | 5.38 |
| 6 | + | - | + | - | + | + | 1.03E-02 | 4.06E-05 | 1.34 |
| 7 | + | + | - | - | + | + | 1.02E-02 | 4.02E-05 | 5.34 |
| 8 | + | - | - | - | + | + | 1.56E-02 | 6.13E-05 | 1.34 |
| 9 | + | + | + | + | - | + | 9.93E-03 | 3.90E-05 | 53.82 |
| 10 | + | - | + | + | - | + | 3.08E-04 | 1.21E-06 | 5.38 |
| 11 | + | + | - | + | - | + | 1.86E-02 | 7.30E-05 | 53.82 |
| 12 | + | - | - | + | - | + | 2.75E-02 | 1.08E-04 | 5.34 |
| 13 | + | + | + | - | - | + | 9.78E-04 | 3.84E-06 | 5.34 |
| 14 | + | - | + | - | - | + | 1.18E-02 | 4.65E-05 | 13.77 |
| 15 | + | + | - | - | - | + | 3.10E-02 | 1.22E-04 | 5.34 |
| 16 | + | - | - | - | - | + | 3.98E-03 | 1.56E-05 | 13.77 |
| 17 | + | + | + | + | + | - | 1.04E-02 | 4.10E-05 | 53.80 |
| 18 | + | - | + | + | + | - | 3.51E-03 | 1.38E-05 | 5.34 |
| 19 | + | + | - | + | + | - | 1.99E-02 | 7.82E-05 | 53.41 |
| 20 | + | - | - | + | + | - | 2.87E-02 | 1.13E-04 | 5.34 |
| 21 | + | + | + | - | + | - | 2.79E-03 | 1.10E-05 | 5.34 |
| 22 | + | - | + | - | + | - | 1.06E-02 | 4.15E-05 | 1.34 |
| 23 | + | + | - | - | + | - | 2.50E-03 | 9.84E-06 | 5.34 |
| 24 | + | - | - | - | + | - | 2.20E-02 | 8.65E-05 | 1.34 |
| 25 | + | + | + | + | - | - | 9.93E-03 | 3.90E-05 | 53.82 |
| 26 | + | - | + | + | - | - | 3.08E-04 | 1.21E-06 | 5.38 |
| 27 | + | + | - | + | - | - | 1.86E-02 | 7.30E-05 | 53.82 |
| 28 | + | - | - | + | - | - | 2.75E-02 | 1.08E-04 | 5.34 |
| 29 | + | + | + | - | - | - | 3.35E-03 | 1.32E-05 | 5.34 |
| 30 | + | - | + | - | - | - | 9.52E-05 | 3.74E-07 | 1.34 |
| 31 | + | + | - | - | - | - | 1.87E-02 | 7.33E-05 | 5.34 |
| 32 | + | - | - | - | - | - | 2.23E-02 | 8.75E-05 | 13.77 |
| 33 | - | + | + | + | + | + | 8.62E-05 | 1.03E-06 | 53.69 |
| 34 | - | - | + | + | + | + | 4.61E-04 | 5.48E-06 | 5.35 |
| 35 | - | + | - | + | + | + | 1.40E-03 | 1.67E-05 | 53.41 |
| 36 | - | - | - | + | + | + | 3.75E-03 | 4.46E-05 | 5.34 |
| 37 | - | + | + | - | + | + | 1.17E-03 | 1.39E-05 | 5.34 |
| 38 | - | - | + | - | + | + | 1.35E-03 | 1.61E-05 | 1.34 |
| 39 | - | + | - | - | + | + | 1.34E-03 | 1.59E-05 | 5.34 |
| 40 | - | - | - | - | + | + | 2.04E-03 | 2.43E-05 | 1.34 |
| 41 | - | + | + | + | - | + | 1.22E-03 | 1.45E-05 | 53.82 |
| 42 | - | - | + | + | - | + | 4.03E-05 | 4.80E-07 | 5.38 |

Continuation of above table

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH | Conc at groundwater (µg/L) | Adsorbed Conc (µg/g) | Maximum pollutant depth (m) |
|---|---|---|---|---|---|---|---|---|---|
| 43 | - | + | - | + | - | + | 2.43E-03 | 2.89E-05 | 53.82 |
| 44 | - | - | - | + | - | + | 3.59E-03 | 4.27E-05 | 5.34 |
| 45 | - | + | + | - | - | + | 1.28E-04 | 1.52E-06 | 5.34 |
| 46 | - | - | + | - | - | + | 1.55E-03 | 1.84E-05 | 13.77 |
| 47 | - | + | - | - | - | + | 4.05E-03 | 4.82E-05 | 5.34 |
| 48 | - | - | - | - | - | + | 5.20E-04 | 6.19E-06 | 13.77 |
| 49 | - | + | + | + | + | - | 1.36E-03 | 1.62E-05 | 53.76 |
| 50 | - | - | + | + | + | - | 4.61E-04 | 5.48E-06 | 5.34 |
| 51 | - | + | - | + | + | - | 2.60E-03 | 3.10E-05 | 53.41 |
| 52 | - | - | - | + | + | - | 3.75E-03 | 4.46E-05 | 5.34 |
| 53 | - | + | + | - | + | - | 3.65E-04 | 4.34E-06 | 5.34 |
| 54 | - | - | + | - | + | - | 1.38E-03 | 1.64E-05 | 1.34 |
| 55 | - | + | - | - | + | - | 3.27E-04 | 3.89E-06 | 5.34 |
| 56 | - | - | - | - | + | - | 2.88E-03 | 3.42E-05 | 1.34 |
| 57 | - | + | + | + | - | - | 1.30E-03 | 1.54E-05 | 53.82 |
| 58 | - | - | + | + | - | - | 4.03E-05 | 4.80E-07 | 5.38 |
| 59 | - | + | - | + | - | - | 2.43E-03 | 2.89E-05 | 53.82 |
| 60 | - | - | - | + | - | - | 3.59E-03 | 4.27E-05 | 5.34 |
| 61 | - | + | + | - | - | - | 4.38E-04 | 5.21E-06 | 5.34 |
| 62 | - | - | + | - | - | - | 1.24E-05 | 1.48E-07 | 13.77 |
| 63 | - | + | - | - | - | - | 2.44E-03 | 2.90E-05 | 5.34 |
| 64 | - | - | - | - | - | - | 2.91E-03 | 3.46E-05 | 13.77 |

Table C.33 SESOIL out put values for Salicylic acid (10 yrs of simulation)

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH | Conc at groundwater (µg/L) | Adsorbed Conc (µg/g) | Maximum pollutant depth (m) |
|---|---|---|---|---|---|---|---|---|---|
| 1 | + | + | + | + | + | + | 6.05E-04 | 7.12E-06 | 2.70 |
| 2 | + | - | + | + | + | + | 3.23E-03 | 3.81E-05 | 2.70 |
| 3 | + | + | - | + | + | + | 9.84E-03 | 1.16E-04 | 27.00 |
| 4 | + | - | - | + | + | + | 2.63E-02 | 3.10E-04 | 2.70 |
| 5 | + | + | + | - | + | + | 8.18E-03 | 9.64E-05 | 2.72 |
| 6 | + | - | + | - | + | + | 9.48E-03 | 1.12E-04 | 0.68 |
| 7 | + | + | - | - | + | + | 9.37E-03 | 1.10E-04 | 2.70 |
| 8 | + | - | - | - | + | + | 1.43E-02 | 1.68E-04 | 0.68 |
| 9 | + | + | + | + | - | + | 9.10E-03 | 1.07E-04 | 27.21 |
| 10 | + | - | + | + | - | + | 2.83E-04 | 3.33E-06 | 2.72 |
| 11 | + | + | - | + | - | + | 1.70E-02 | 2.01E-04 | 27.21 |
| 12 | + | - | - | + | - | + | 2.52E-02 | 2.97E-04 | 2.70 |
| 13 | + | + | + | - | - | + | 8.97E-04 | 1.06E-05 | 2.70 |
| 14 | + | - | + | - | - | + | 1.08E-02 | 1.28E-04 | 6.96 |
| 15 | + | + | - | - | - | + | 2.84E-02 | 3.34E-04 | 2.70 |
| 16 | + | - | - | - | - | + | 3.65E-03 | 4.30E-05 | 6.96 |
| 17 | + | + | + | + | + | - | 9.56E-03 | 1.13E-04 | 27.21 |
| 18 | + | - | + | + | + | - | 3.22E-03 | 3.79E-05 | 2.70 |
| 19 | + | + | - | + | + | - | 1.82E-02 | 2.15E-04 | 27.00 |
| 20 | + | - | - | + | + | - | 2.63E-02 | 3.10E-04 | 2.70 |
| 21 | + | + | + | - | + | - | 2.56E-03 | 3.02E-05 | 2.70 |
| 22 | + | - | + | - | + | - | 9.69E-03 | 1.14E-04 | 0.68 |
| 23 | + | + | - | - | + | - | 2.29E-03 | 2.70E-05 | 2.70 |
| 24 | + | - | - | - | + | - | 2.02E-02 | 2.38E-04 | 0.68 |
| 25 | + | + | + | + | - | - | 9.10E-03 | 1.07E-04 | 27.21 |
| 26 | + | - | + | + | - | - | 2.83E-04 | 3.33E-06 | 2.72 |
| 27 | + | + | - | + | - | - | 1.70E-02 | 2.01E-04 | 27.21 |
| 28 | + | - | - | + | - | - | 2.52E-02 | 2.97E-04 | 2.70 |
| 29 | + | + | + | - | - | - | 3.07E-03 | 3.62E-05 | 2.70 |
| 30 | + | - | + | - | - | - | 8.72E-05 | 1.03E-06 | 0.68 |
| 31 | + | + | - | - | - | - | 1.71E-02 | 2.02E-04 | 2.70 |
| 32 | + | - | - | - | - | - | 2.04E-02 | 2.41E-04 | 6.96 |
| 33 | - | + | + | + | + | + | 2.60E-05 | 7.21E-07 | 27.21 |
| 34 | - | - | + | + | + | + | 1.39E-04 | 3.86E-06 | 2.70 |
| 35 | - | + | - | + | + | + | 4.23E-04 | 1.17E-05 | 27.00 |
| 36 | - | - | - | + | + | + | 1.13E-03 | 3.14E-05 | 2.70 |
| 37 | - | + | + | - | + | + | 3.51E-04 | 9.76E-06 | 2.70 |
| 38 | - | - | + | - | + | + | 4.07E-04 | 1.13E-05 | 0.68 |
| 39 | - | + | - | - | + | + | 4.03E-04 | 1.12E-05 | 2.70 |

Continuation of above table

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH | Conc at groundwater (μg/L) | Adsorbed Conc (μg/g) | Maximum pollutant depth (m) |
|---|---|---|---|---|---|---|---|---|---|
| 40 | - | - | - | - | + | + | 6.15E-04 | 1.71E-05 | 0.68 |
| 41 | - | + | + | + | - | + | 3.68E-04 | 1.02E-05 | 27.21 |
| 42 | - | - | + | + | - | + | 1.21E-05 | 3.37E-07 | 2.72 |
| 43 | - | + | - | + | - | + | 7.32E-04 | 2.03E-05 | 27.21 |
| 44 | - | - | - | + | - | + | 1.08E-03 | 3.00E-05 | 2.70 |
| 45 | - | + | + | - | - | + | 3.85E-05 | 1.07E-06 | 2.70 |
| 46 | - | - | + | - | - | + | 4.66E-04 | 1.29E-05 | 6.96 |
| 47 | - | + | - | - | - | + | 1.22E-03 | 3.39E-05 | 2.70 |
| 48 | - | - | - | - | - | + | 1.57E-04 | 4.35E-06 | 6.96 |
| 49 | - | + | + | + | + | - | 4.11E-04 | 1.14E-05 | 27.21 |
| 50 | - | - | + | + | + | - | 1.39E-04 | 3.86E-06 | 2.70 |
| 51 | - | + | - | + | + | - | 7.84E-04 | 2.18E-05 | 27.00 |
| 52 | - | - | - | + | + | - | 1.13E-03 | 3.14E-05 | 2.70 |
| 53 | - | + | + | - | + | - | 1.10E-04 | 3.05E-06 | 2.70 |
| 54 | - | - | + | - | + | - | 4.16E-04 | 1.16E-05 | 0.68 |
| 55 | - | + | - | - | + | - | 9.86E-05 | 2.74E-06 | 2.70 |
| 56 | - | - | - | - | + | - | 8.67E-04 | 2.41E-05 | 0.68 |
| 57 | - | + | + | + | - | - | 3.91E-04 | 1.09E-05 | 27.21 |
| 58 | - | - | + | + | - | - | 1.21E-05 | 3.37E-07 | 2.72 |
| 59 | - | + | - | + | - | - | 7.32E-04 | 2.03E-05 | 27.21 |
| 60 | - | - | - | + | - | - | 1.08E-03 | 3.00E-05 | 2.70 |
| 61 | - | + | + | - | - | - | 1.32E-04 | 3.66E-06 | 2.70 |
| 62 | - | - | + | - | - | - | 3.75E-06 | 1.04E-07 | 6.96 |
| 63 | - | + | - | - | - | - | 7.35E-04 | 2.04E-05 | 2.70 |
| 64 | - | - | - | - | - | - | 8.77E-04 | 2.43E-05 | 6.96 |

Table C.34 Factorial Design for simulations of PPCPs

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH |
|---|---|---|---|---|---|---|
| 1 | + | + | + | + | + | + |
| 2 | + | - | + | + | + | + |
| 3 | + | + | - | + | + | + |
| 4 | + | - | - | + | + | + |
| 5 | + | + | + | - | + | + |
| 6 | + | - | + | - | + | + |
| 7 | + | + | - | - | + | + |
| 8 | + | - | - | - | + | + |
| 9 | + | + | + | + | - | + |
| 10 | + | - | + | + | - | + |
| 11 | + | + | - | + | - | + |
| 12 | + | - | - | + | - | + |
| 13 | + | + | + | - | - | + |
| 14 | + | - | + | - | - | + |
| 15 | + | + | - | - | - | + |
| 16 | + | - | - | - | - | + |
| 17 | + | + | + | + | + | - |
| 18 | + | - | + | + | + | - |
| 19 | + | + | - | + | + | - |
| 20 | + | - | - | + | + | - |
| 21 | + | + | + | - | + | - |
| 22 | + | - | + | - | + | - |
| 23 | + | + | - | - | + | - |
| 24 | + | - | - | - | + | - |
| 25 | + | + | + | + | - | - |
| 26 | + | - | + | + | - | - |
| 27 | + | + | - | + | - | - |
| 28 | + | - | - | + | - | - |
| 29 | + | + | + | - | - | - |
| 30 | + | - | + | - | - | - |
| 31 | + | + | - | - | - | - |
| 32 | + | - | - | - | - | - |
| 33 | - | + | + | + | + | + |
| 34 | - | - | + | + | + | + |
| 35 | - | + | - | + | + | + |
| 36 | - | - | - | + | + | + |
| 37 | - | + | + | - | + | + |
| 38 | - | - | + | - | + | + |
| 39 | - | + | - | - | + | + |
| 40 | - | - | - | - | + | + |
| 41 | - | + | + | + | - | + |
| 42 | - | - | + | + | - | + |
| 43 | - | + | - | + | - | + |

Continuation of above table

| Run | Concentration | Rainfall | Vadose zone Thickness | Intrinsic Permeability | Organic Content | pH |
|---|---|---|---|---|---|---|
| 44 | - | - | - | + | - | + |
| 45 | - | + | + | - | - | + |
| 46 | - | - | + | - | - | + |
| 47 | - | + | - | - | - | + |
| 48 | - | - | - | - | - | + |
| 49 | - | + | + | + | + | - |
| 50 | - | - | + | + | + | - |
| 51 | - | + | - | + | + | - |
| 52 | - | - | - | + | + | - |
| 53 | - | + | + | - | + | - |
| 54 | - | - | + | - | + | - |
| 55 | - | + | - | - | + | - |
| 56 | - | - | - | - | + | - |
| 57 | - | + | + | + | - | - |
| 58 | - | - | + | + | - | - |
| 59 | - | + | - | + | - | - |
| 60 | - | - | - | + | - | - |
| 61 | - | + | + | - | - | - |
| 62 | - | - | + | - | - | - |
| 63 | - | + | - | - | - | - |
| 64 | - | - | - | - | - | - |

Table C.35 Calculated Effects of Factors and their Interactions on migration depth of Nystatin

| Factors/ Interactions | Effect on migration depth | Factors/ Interactions | Effect on migration depth |
|---|---|---|---|
| A | -9.29E-01 | BCE | -9.22E-01 |
| B | 1.09E+01 | BCF | -9.40E-01 |
| C | -9.12E-01 | BDE | -2.11E+00 |
| D | 1.09E+01 | BDF | -5.57E-01 |
| E | -2.11E+00 | BEF | -5.51E-01 |
| F | -5.38E-01 | CDE | -9.33E-01 |
| AB | -5.42E-01 | CDF | -9.53E-01 |
| AC | -9.35E-01 | CEF | -9.49E-01 |
| AD | -5.55E-01 | DEF | -5.56E-01 |
| AE | -5.55E-01 | ABCD | -9.44E-01 |
| AF | -5.73E-01 | ABCE | -9.43E-01 |
| BC | -5.33E-01 | ABCF | -9.14E-01 |
| BD | 1.16E+01 | ABDE | -5.54E-01 |
| BE | 5.82E-01 | ABDF | -5.83E-01 |
| BF | -9.27E-01 | ABEF | -5.81E-01 |
| CD | -5.37E-01 | ACDE | -9.48E-01 |
| CE | -5.46E-01 | ACDF | -9.22E-01 |
| CF | -5.55E-01 | ACEF | -1.14E+00 |
| DE | 5.73E-01 | ADEF | -5.82E-01 |
| DF | -9.36E-01 | BCDE | -5.39E-01 |
| EF | -9.33E-01 | BCDF | -5.70E-01 |
| ABC | -5.50E-01 | BCEF | -5.71E-01 |
| ABD | -9.35E-01 | BDEF | -9.42E-01 |
| ABE | -9.34E-01 | CDEF | -5.72E-01 |
| ABF | -9.54E-01 | ABCDE | -5.62E-01 |
| ACD | -5.61E-01 | ABCDF | -5.44E-01 |
| ACE | -5.63E-01 | ABCEF | -5.37E-01 |
| ACF | -5.23E-01 | ABDEF | -9.73E-01 |
| ADE | -9.41E-01 | ACDEF | -5.44E-01 |
| ADF | -9.71E-01 | BCDEF | -9.62E-01 |
| AEF | -9.60E-01 | ABCDEF | -9.29E-01 |
| BCD | -9.28E-01 | | |

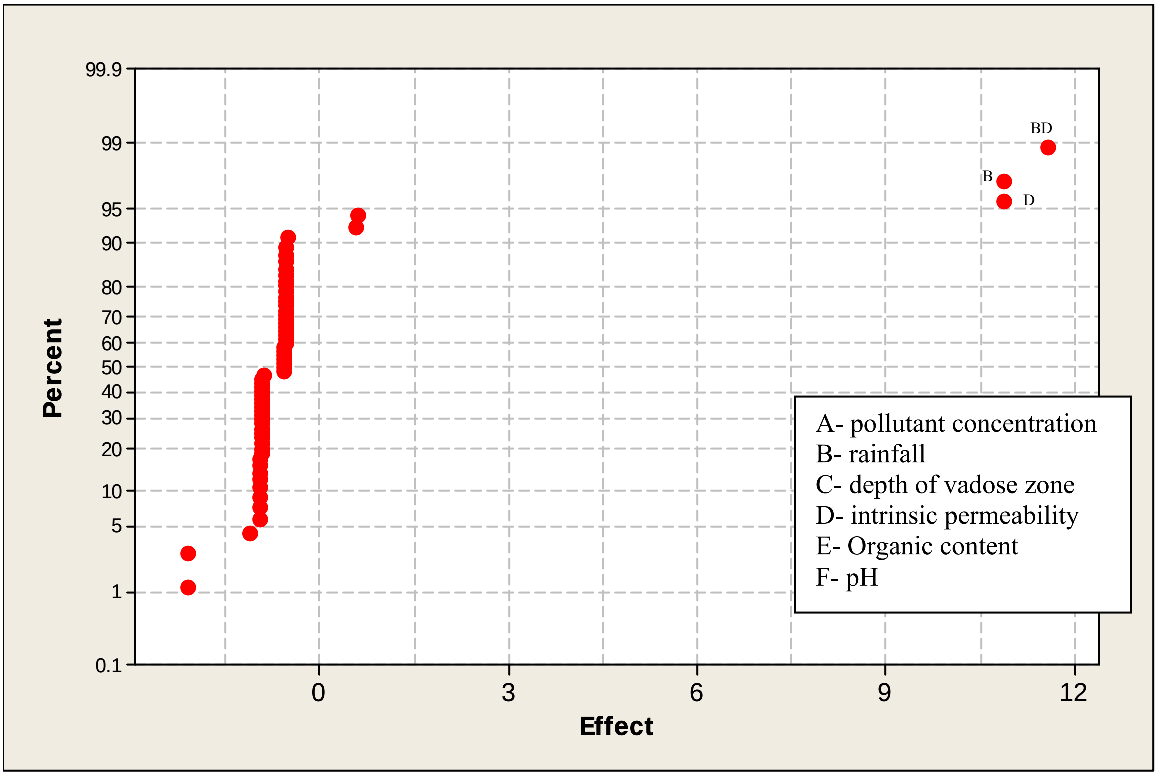


Figure C.1 Estimated main effects and effect interactions on nystatin migration in vadose zone

Table C.36 Calculated Effects of Factors and their Interactions on migration depth of Dexamethasone

| Factors/ Interactions | Effect on migration depth | Factors/ Interactions | Effect on migration depth |
|---|---|---|---|
| A | -1.05E+00 | BCE | -1.02E+00 |
| B | 1.21E+01 | BCF | -1.05E+00 |
| C | -1.02E+00 | BDE | -2.35E+00 |
| D | 1.21E+01 | BDF | -6.20E-01 |
| E | -2.36E+00 | BEF | -6.18E-01 |
| F | -6.17E-01 | CDE | -1.02E+00 |
| AB | -6.23E-01 | CDF | -1.05E+00 |
| AC | -1.04E+00 | CEF | -1.05E+00 |
| AD | -6.25E-01 | DEF | -6.19E-01 |
| AE | -6.22E-01 | ABCD | -1.05E+00 |
| AF | -6.21E-01 | ABCE | -1.04E+00 |
| BC | -5.95E-01 | ABCF | -1.04E+00 |
| BD | 1.29E+01 | ABDE | -6.23E-01 |
| BE | 6.43E-01 | ABDF | -6.23E-01 |
| BF | -1.04E+00 | ABEF | -6.23E-01 |
| CD | -5.91E-01 | ACDE | -1.05E+00 |
| CE | -5.95E-01 | ACDF | -1.05E+00 |
| CF | -6.23E-01 | ACEF | -1.27E+00 |
| DE | 6.36E-01 | ADEF | -6.24E-01 |
| DF | -1.05E+00 | BCDE | -5.92E-01 |
| EF | -1.05E+00 | BCDF | -6.24E-01 |
| ABC | -6.17E-01 | BCEF | -6.25E-01 |
| ABD | -1.05E+00 | BDEF | -1.05E+00 |
| ABE | -1.05E+00 | CDEF | -6.26E-01 |
| ABF | -1.05E+00 | ABCDE | -6.19E-01 |
| ACD | -6.18E-01 | ABCDF | -6.18E-01 |
| ACE | -6.16E-01 | ABCEF | -6.15E-01 |
| ACF | -6.17E-01 | ABDEF | -1.05E+00 |
| ADE | -1.05E+00 | ACDEF | -6.17E-01 |
| ADF | -1.05E+00 | BCDEF | -1.05E+00 |
| AEF | -1.05E+00 | ABCDEF | -1.04E+00 |
| BCD | -1.03E+00 | | |

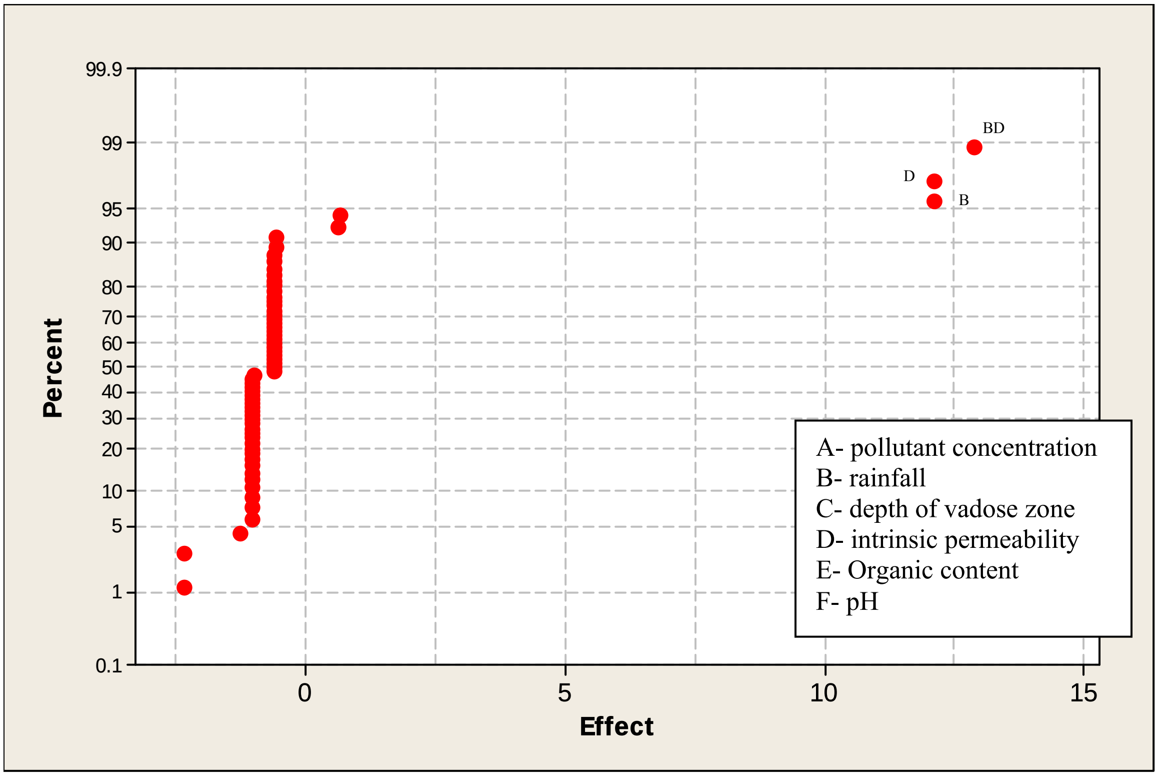


Figure C.2 Estimated main effects and effect interactions on dexamethasone migration in vadose zone

Table C.37 Calculated Effects of Factors and their Interactions on migration depth of Methoprene

| Factors/ Interactions | Effect on migration depth | Factors/ Interactions | Effect on migration depth |
|---|---|---|---|
| A | -2.77E-01 | BCE | -2.69E-01 |
| B | 3.21E+00 | BCF | -2.78E-01 |
| C | -2.69E-01 | BDE | -6.26E-01 |
| D | 3.21E+00 | BDF | -1.64E-01 |
| E | -6.26E-01 | BEF | -1.64E-01 |
| F | -1.64E-01 | CDE | -2.71E-01 |
| AB | -1.65E-01 | CDF | -2.78E-01 |
| AC | -2.77E-01 | CEF | -2.78E-01 |
| AD | -1.65E-01 | DEF | -1.64E-01 |
| AE | -1.65E-01 | ABCD | -2.78E-01 |
| AF | -1.64E-01 | ABCE | -2.77E-01 |
| BC | -1.58E-01 | ABCF | -2.78E-01 |
| BD | 3.42E+00 | ABDE | -1.65E-01 |
| BE | 1.70E-01 | ABDF | -1.65E-01 |
| BF | -2.78E-01 | ABEF | -1.64E-01 |
| CD | -1.56E-01 | ACDE | -2.78E-01 |
| CE | -1.58E-01 | ACDF | -2.79E-01 |
| CF | -1.64E-01 | ACEF | -3.39E-01 |
| DE | 1.68E-01 | ADEF | -1.65E-01 |
| DF | -2.79E-01 | BCDE | -1.57E-01 |
| EF | -2.78E-01 | BCDF | -1.65E-01 |
| ABC | -1.65E-01 | BCEF | -1.64E-01 |
| ABD | -2.78E-01 | BDEF | -2.79E-01 |
| ABE | -2.78E-01 | CDEF | -1.64E-01 |
| ABF | -2.78E-01 | ABCDE | -1.65E-01 |
| ACD | -1.65E-01 | ABCDF | -1.65E-01 |
| ACE | -1.65E-01 | ABCEF | -1.64E-01 |
| ACF | -1.64E-01 | ABDEF | -2.78E-01 |
| ADE | -2.78E-01 | ACDEF | -1.64E-01 |
| ADF | -2.78E-01 | BCDEF | -2.78E-01 |
| AEF | -2.78E-01 | ABCDEF | -2.79E-01 |
| BCD | -2.71E-01 | | |

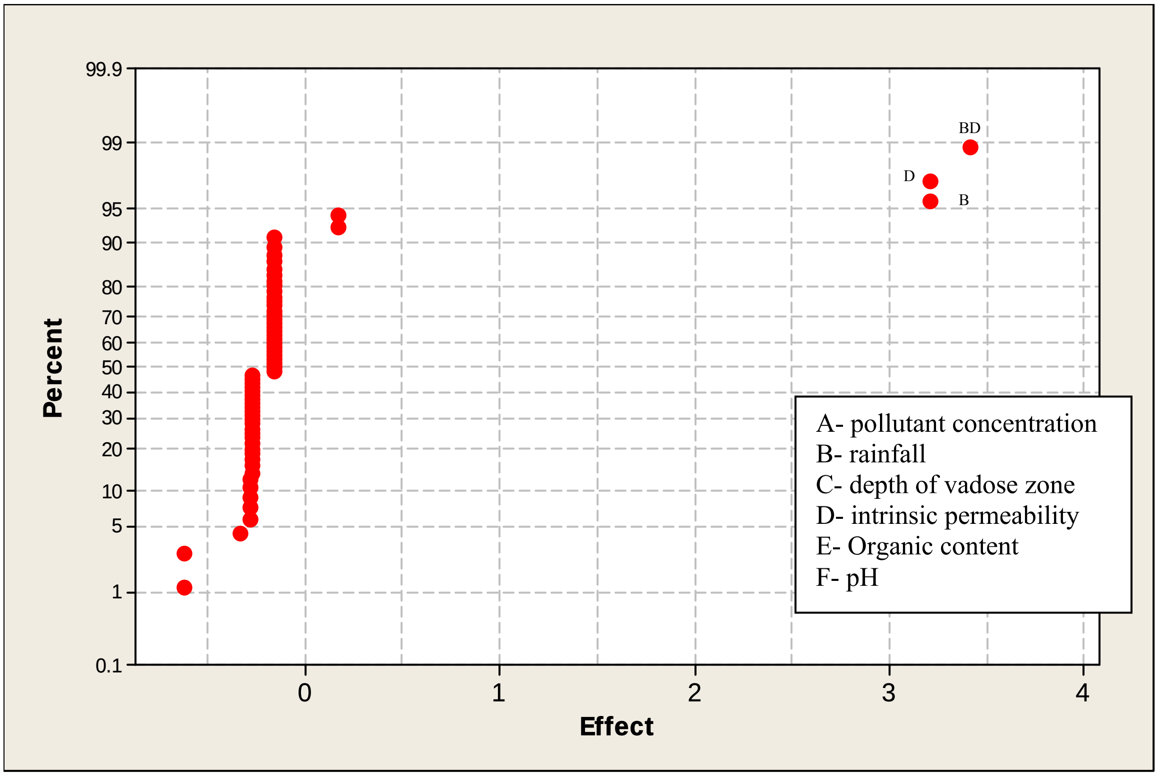


Figure C.3 Estimated main effects and effect interactions on methoprene migration in vadose zone

Table C.38 Calculated Effects of Factors and their Interactions on migration depth of Prednisone

| Factors/ Interactions | Effect on migration depth | Factors/ Interactions | Effect on migration depth |
|---|---|---|---|
| A | -1.82E+00 | BCE | -1.76E+00 |
| B | 2.10E+01 | BCF | -1.82E+00 |
| C | -1.76E+00 | BDE | -4.09E+00 |
| D | 2.10E+01 | BDF | -1.08E+00 |
| E | -4.10E+00 | BEF | -1.07E+00 |
| F | -1.07E+00 | CDE | -1.77E+00 |
| AB | -1.07E+00 | CDF | -1.82E+00 |
| AC | -1.82E+00 | CEF | -1.82E+00 |
| AD | -1.08E+00 | DEF | -1.08E+00 |
| AE | -1.07E+00 | ABCD | -1.82E+00 |
| AF | -1.07E+00 | ABCE | -1.82E+00 |
| BC | -1.03E+00 | ABCF | -1.82E+00 |
| BD | 2.23E+01 | ABDE | -1.08E+00 |
| BE | 1.11E+00 | ABDF | -1.08E+00 |
| BF | -1.82E+00 | ABEF | -1.07E+00 |
| CD | -1.02E+00 | ACDE | -1.82E+00 |
| CE | -1.03E+00 | ACDF | -1.82E+00 |
| CF | -1.07E+00 | ACEF | -2.22E+00 |
| DE | 1.10E+00 | ADEF | -1.08E+00 |
| DF | -1.82E+00 | BCDE | -1.02E+00 |
| EF | -1.82E+00 | BCDF | -1.08E+00 |
| ABC | -1.07E+00 | BCEF | -1.07E+00 |
| ABD | -1.82E+00 | BDEF | -1.82E+00 |
| ABE | -1.82E+00 | CDEF | -1.08E+00 |
| ABF | -1.82E+00 | ABCDE | -1.08E+00 |
| ACD | -1.08E+00 | ABCDF | -1.08E+00 |
| ACE | -1.07E+00 | ABCEF | -1.07E+00 |
| ACF | -1.07E+00 | ABDEF | -1.82E+00 |
| ADE | -1.82E+00 | ACDEF | -1.08E+00 |
| ADF | -1.82E+00 | BCDEF | -1.82E+00 |
| AEF | -1.82E+00 | ABCDEF | -1.82E+00 |
| BCD | -1.78E+00 | | |

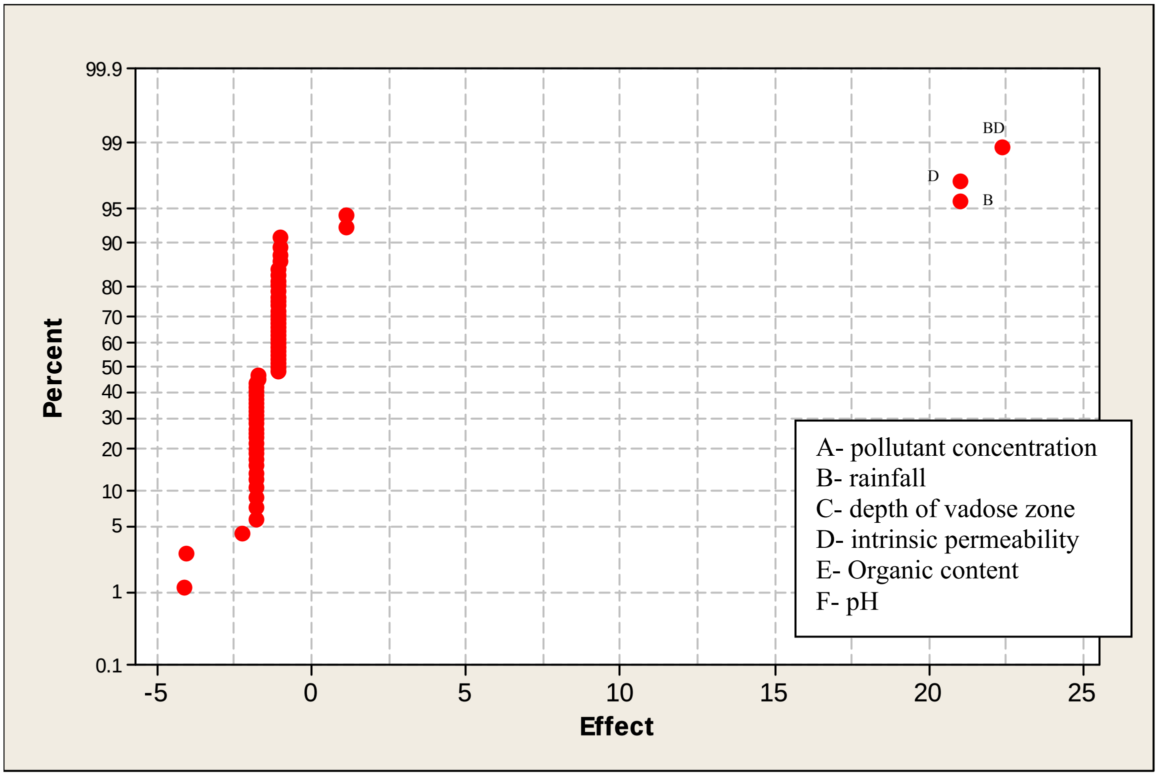


Figure C.4 Estimated main effects and effect interactions on prednisone migration in vadose zone

Table C.39 Calculated Effects of Factors and their Interactions on migration depth of Metronidazole

| Factors/ Interactions | Effect on migration depth | Factors/ Interactions | Effect on migration depth |
|---|---|---|---|
| A | -1.99E+00 | BCE | -1.93E+00 |
| B | 2.29E+01 | BCF | -1.99E+00 |
| C | -1.93E+00 | BDE | -4.47E+00 |
| D | 2.29E+01 | BDF | -1.18E+00 |
| E | -4.48E+00 | BEF | -1.18E+00 |
| F | -1.18E+00 | CDE | -1.94E+00 |
| AB | -1.18E+00 | CDF | -1.99E+00 |
| AC | -1.99E+00 | CEF | -1.99E+00 |
| AD | -1.18E+00 | DEF | -1.18E+00 |
| AE | -1.18E+00 | ABCD | -1.99E+00 |
| AF | -1.18E+00 | ABCE | -1.99E+00 |
| BC | -1.13E+00 | ABCF | -1.99E+00 |
| BD | 2.44E+01 | ABDE | -1.18E+00 |
| BE | 1.21E+00 | ABDF | -1.18E+00 |
| BF | -1.99E+00 | ABEF | -1.18E+00 |
| CD | -1.12E+00 | ACDE | -1.99E+00 |
| CE | -1.13E+00 | ACDF | -1.99E+00 |
| CF | -1.18E+00 | ACEF | -2.43E+00 |
| DE | 1.20E+00 | ADEF | -1.18E+00 |
| DF | -1.99E+00 | BCDE | -1.12E+00 |
| EF | -1.99E+00 | BCDF | -1.18E+00 |
| ABC | -1.18E+00 | BCEF | -1.18E+00 |
| ABD | -1.99E+00 | BDEF | -1.99E+00 |
| ABE | -1.99E+00 | CDEF | -1.18E+00 |
| ABF | -1.99E+00 | ABCDE | -1.18E+00 |
| ACD | -1.18E+00 | ABCDF | -1.18E+00 |
| ACE | -1.18E+00 | ABCEF | -1.18E+00 |
| ACF | -1.18E+00 | ABDEF | -1.99E+00 |
| ADE | -1.99E+00 | ACDEF | -1.18E+00 |
| ADF | -1.99E+00 | BCDEF | -1.99E+00 |
| AEF | -1.99E+00 | ABCDEF | -1.99E+00 |
| BCD | -1.94E+00 | | |

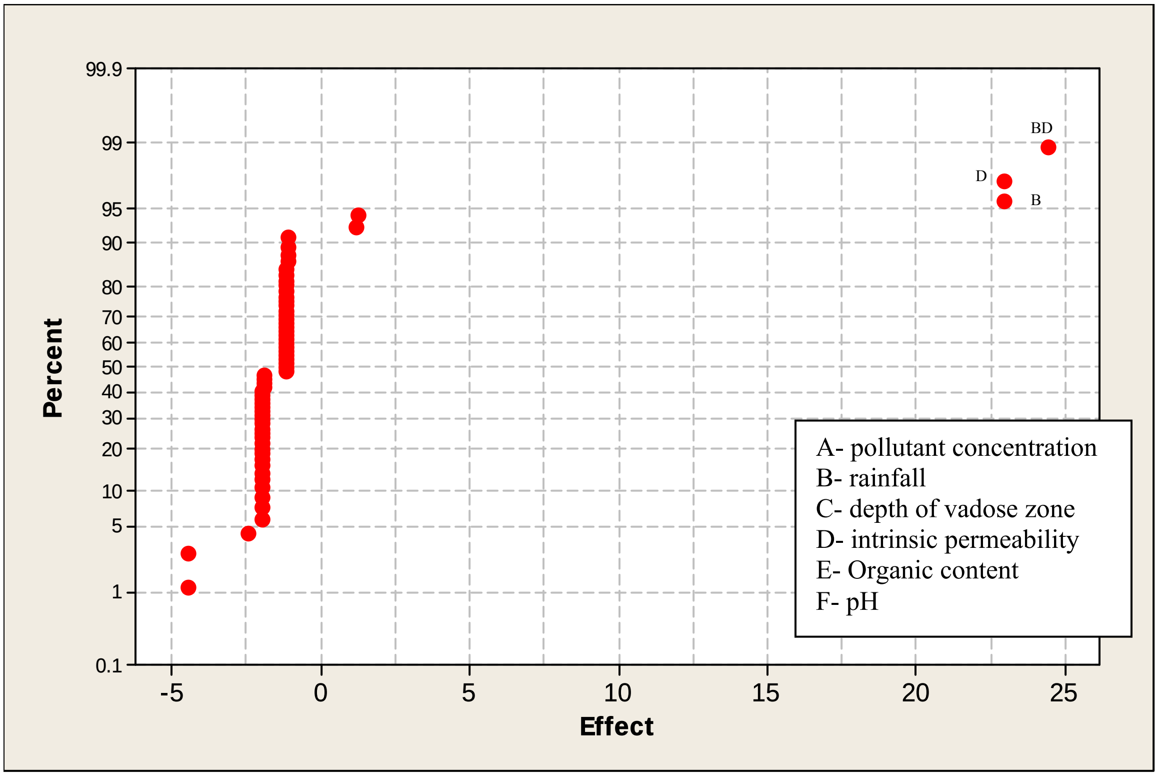


Figure C.5 Estimated main effects and effect interactions on metronidazole migration in vadose zone

Table C.40 Calculated Effects of Factors and their Interactions on migration depth of Clindamycin

| Factors/ Interactions | Effect on migration depth | Factors/ Interactions | Effect on migration depth |
|---|---|---|---|
| A | -1.13E+00 | BCE | -1.10E+00 |
| B | 1.31E+01 | BCF | -1.13E+00 |
| C | -1.10E+00 | BDE | -2.55E+00 |
| D | 1.31E+01 | BDF | -6.72E-01 |
| E | -2.55E+00 | BEF | -6.70E-01 |
| F | -6.70E-01 | CDE | -1.11E+00 |
| AB | -6.70E-01 | CDF | -1.13E+00 |
| AC | -1.13E+00 | CEF | -1.13E+00 |
| AD | -6.71E-01 | DEF | -6.71E-01 |
| AE | -6.70E-01 | ABCD | -1.13E+00 |
| AF | -6.70E-01 | ABCE | -1.13E+00 |
| BC | -6.42E-01 | ABCF | -1.13E+00 |
| BD | 1.39E+01 | ABDE | -6.71E-01 |
| BE | 6.90E-01 | ABDF | -6.71E-01 |
| BF | -1.13E+00 | ABEF | -6.70E-01 |
| CD | -6.37E-01 | ACDE | -1.13E+00 |
| CE | -6.43E-01 | ACDF | -1.13E+00 |
| CF | -6.70E-01 | ACEF | -1.38E+00 |
| DE | 6.83E-01 | ADEF | -6.71E-01 |
| DF | -1.13E+00 | BCDE | -6.39E-01 |
| EF | -1.13E+00 | BCDF | -6.72E-01 |
| ABC | -6.70E-01 | BCEF | -6.70E-01 |
| ABD | -1.13E+00 | BDEF | -1.13E+00 |
| ABE | -1.13E+00 | CDEF | -6.71E-01 |
| ABF | -1.13E+00 | ABCDE | -6.71E-01 |
| ACD | -6.71E-01 | ABCDF | -6.71E-01 |
| ACE | -6.70E-01 | ABCEF | -6.70E-01 |
| ACF | -6.70E-01 | ABDEF | -1.13E+00 |
| ADE | -1.13E+00 | ACDEF | -6.71E-01 |
| ADF | -1.13E+00 | BCDEF | -1.13E+00 |
| AEF | -1.13E+00 | ABCDEF | -1.13E+00 |
| BCD | -1.11E+00 | | |

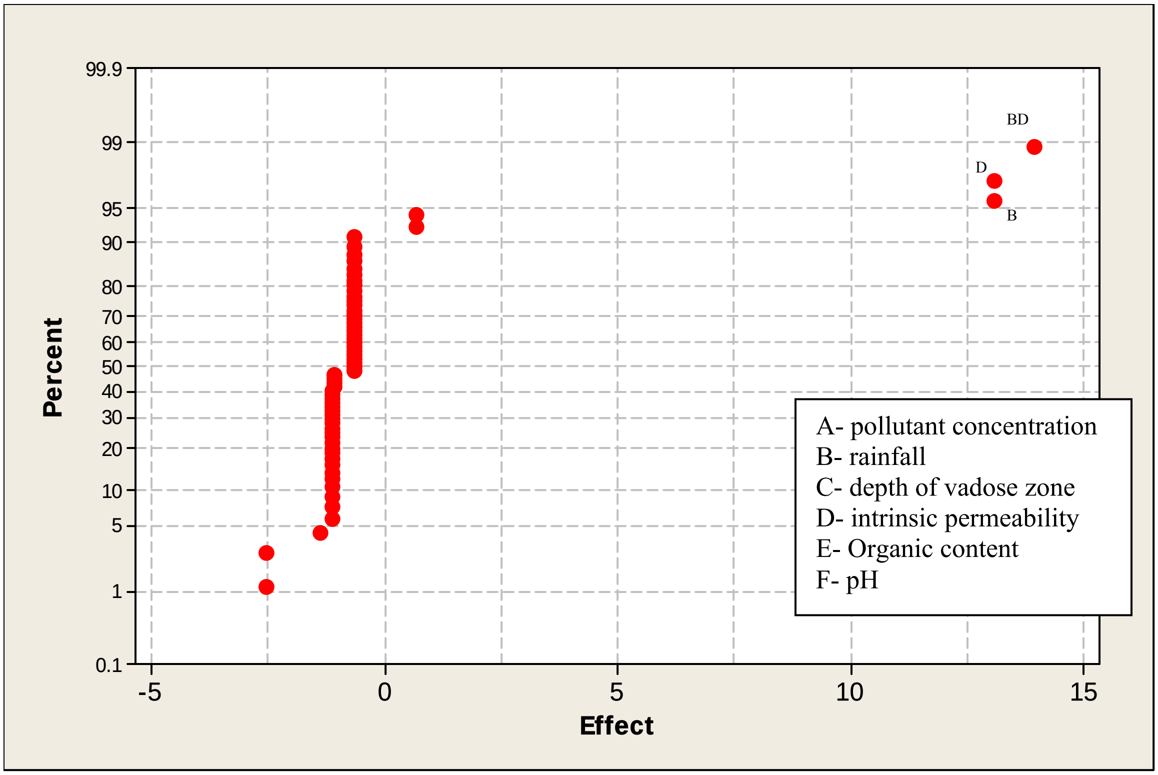


Figure C.6 Estimated main effects and effect interactions on clindamycin migration in vadose zone

Table C.41 Calculated Effects of Factors and their Interactions on migration depth of Ketoconazole

| Factors/ Interactions | Effect on migration depth | Factors/ Interactions | Effect on migration depth |
|---|---|---|---|
| A | -1.35E+00 | BCE | -1.31E+00 |
| B | 1.55E+01 | BCF | -1.35E+00 |
| C | -1.31E+00 | BDE | -3.03E+00 |
| D | 1.55E+01 | BDF | -7.98E-01 |
| E | -3.04E+00 | BEF | -7.97E-01 |
| F | -7.96E-01 | CDE | -1.31E+00 |
| AB | -7.96E-01 | CDF | -1.35E+00 |
| AC | -1.35E+00 | CEF | -1.35E+00 |
| AD | -7.98E-01 | DEF | -7.98E-01 |
| AE | -7.96E-01 | ABCD | -1.35E+00 |
| AF | -7.96E-01 | ABCE | -1.35E+00 |
| BC | -7.64E-01 | ABCF | -1.35E+00 |
| BD | 1.66E+01 | ABDE | -7.98E-01 |
| BE | 8.20E-01 | ABDF | -7.98E-01 |
| BF | -1.35E+00 | ABEF | -7.96E-01 |
| CD | -7.58E-01 | ACDE | -1.35E+00 |
| CE | -7.64E-01 | ACDF | -1.35E+00 |
| CF | -7.96E-01 | ACEF | -1.64E+00 |
| DE | 8.12E-01 | ADEF | -7.98E-01 |
| DF | -1.35E+00 | BCDE | -7.59E-01 |
| EF | -1.35E+00 | BCDF | -7.98E-01 |
| ABC | -7.96E-01 | BCEF | -7.97E-01 |
| ABD | -1.35E+00 | BDEF | -1.35E+00 |
| ABE | -1.35E+00 | CDEF | -7.98E-01 |
| ABF | -1.35E+00 | ABCDE | -7.98E-01 |
| ACD | -7.98E-01 | ABCDF | -7.98E-01 |
| ACE | -7.96E-01 | ABCEF | -7.96E-01 |
| ACF | -7.96E-01 | ABDEF | -1.35E+00 |
| ADE | -1.35E+00 | ACDEF | -7.98E-01 |
| ADF | -1.35E+00 | BCDEF | -1.35E+00 |
| AEF | -1.35E+00 | ABCDEF | -1.35E+00 |
| BCD | -1.32E+00 | | |

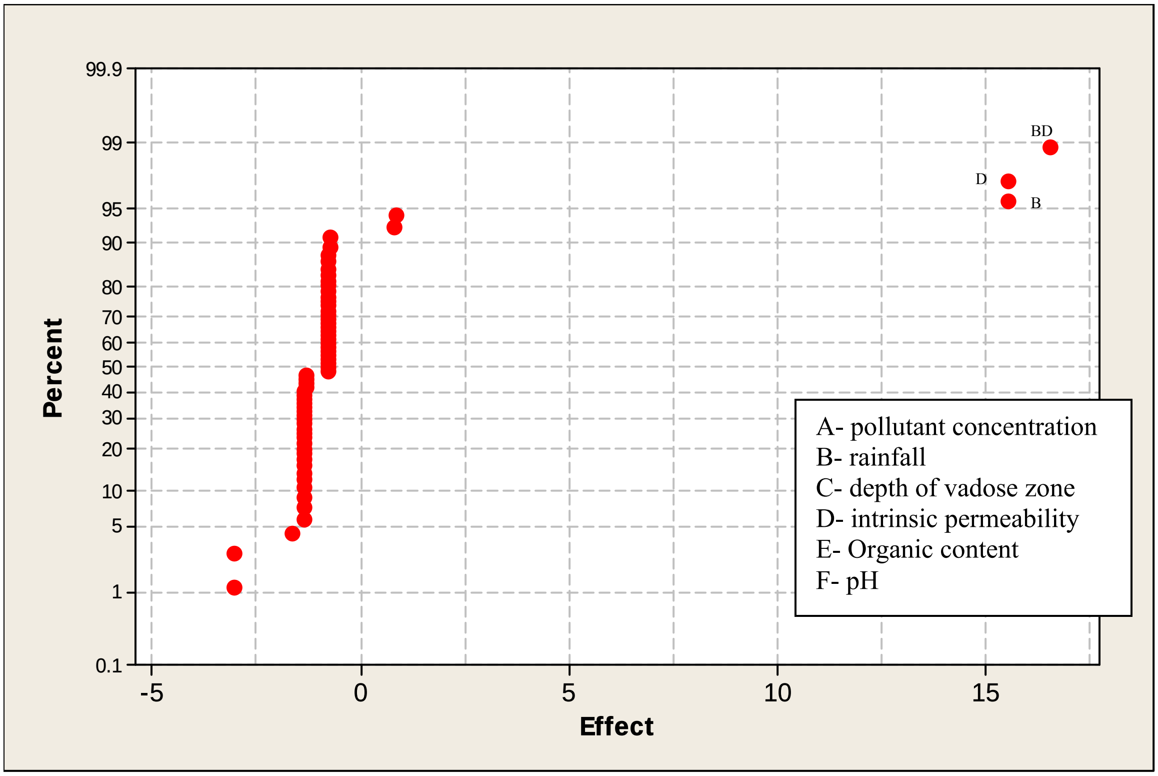


Figure C.7 Estimated main effects and effect interactions on ketoconazole migration in vadose zone

Table C.42 Calculated Effects of Factors and their Interactions on migration depth of Carbamazepine

| Factors/ Interactions | Effect on migration depth | Factors/ Interactions | Effect on migration depth |
|---|---|---|---|
| A | -1.26E+00 | BCE | -1.22E+00 |
| B | 1.46E+01 | BCF | -1.26E+00 |
| C | -1.22E+00 | BDE | -2.84E+00 |
| D | 1.46E+01 | BDF | -7.48E-01 |
| E | -2.84E+00 | BEF | -7.46E-01 |
| F | -7.46E-01 | CDE | -1.23E+00 |
| AB | -7.46E-01 | CDF | -1.26E+00 |
| AC | -1.26E+00 | CEF | -1.26E+00 |
| AD | -7.47E-01 | DEF | -7.47E-01 |
| AE | -7.46E-01 | ABCD | -1.26E+00 |
| AF | -7.46E-01 | ABCE | -1.26E+00 |
| BC | -7.15E-01 | ABCF | -1.26E+00 |
| BD | 1.55E+01 | ABDE | -7.47E-01 |
| BE | 7.68E-01 | ABDF | -7.47E-01 |
| BF | -1.26E+00 | ABEF | -7.46E-01 |
| CD | -7.09E-01 | ACDE | -1.26E+00 |
| CE | -7.15E-01 | ACDF | -1.26E+00 |
| CF | -7.46E-01 | ACEF | -1.54E+00 |
| DE | 7.60E-01 | ADEF | -7.47E-01 |
| DF | -1.26E+00 | BCDE | -7.11E-01 |
| EF | -1.26E+00 | BCDF | -7.48E-01 |
| ABC | -7.46E-01 | BCEF | -7.46E-01 |
| ABD | -1.26E+00 | BDEF | -1.26E+00 |
| ABE | -1.26E+00 | CDEF | -7.47E-01 |
| ABF | -1.26E+00 | ABCDE | -7.47E-01 |
| ACD | -7.47E-01 | ABCDF | -7.47E-01 |
| ACE | -7.46E-01 | ABCEF | -7.46E-01 |
| ACF | -7.46E-01 | ABDEF | -1.26E+00 |
| ADE | -1.26E+00 | ACDEF | -7.47E-01 |
| ADF | -1.26E+00 | BCDEF | -1.26E+00 |
| AEF | -1.26E+00 | ABCDEF | -1.26E+00 |
| BCD | -1.23E+00 | | |

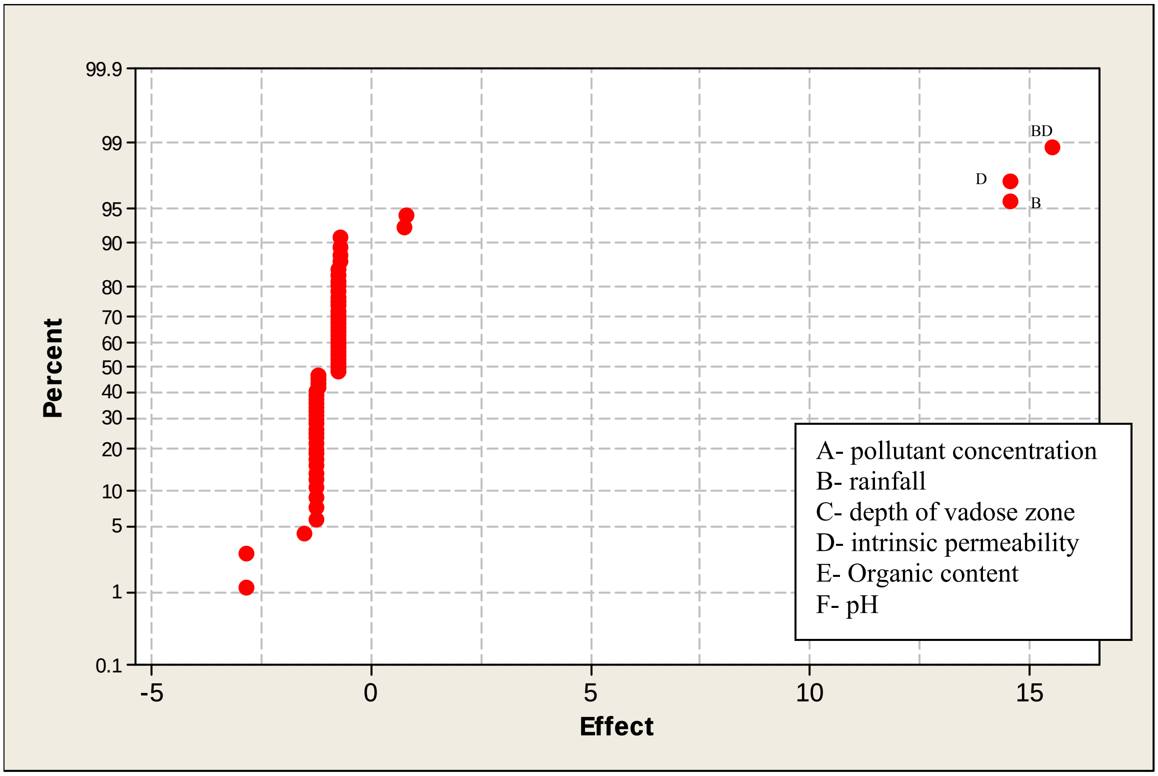


Figure C.8 Estimated main effects and effect interactions on carbamazepine migration in vadose zone

Table C.43 Calculated Effects of Factors and their Interactions on migration depth of Caffeine

| Factors/ Interactions | Effect on migration depth | Factors/ Interactions | Effect on migration depth |
|---|---|---|---|
| A | -2.22E+00 | BCE | -2.16E+00 |
| B | 2.57E+01 | BCF | -2.22E+00 |
| C | -2.16E+00 | BDE | -5.00E+00 |
| D | 2.57E+01 | BDF | -1.32E+00 |
| E | -5.01E+00 | BEF | -1.31E+00 |
| F | -1.31E+00 | CDE | -2.17E+00 |
| AB | -1.31E+00 | CDF | -2.23E+00 |
| AC | -2.22E+00 | CEF | -2.22E+00 |
| AD | -1.32E+00 | DEF | -1.32E+00 |
| AE | -1.31E+00 | ABCD | -2.23E+00 |
| AF | -1.31E+00 | ABCE | -2.22E+00 |
| BC | -1.26E+00 | ABCF | -2.22E+00 |
| BD | 2.73E+01 | ABDE | -1.32E+00 |
| BE | 1.35E+00 | ABDF | -1.32E+00 |
| BF | -2.22E+00 | ABEF | -1.31E+00 |
| CD | -1.25E+00 | ACDE | -2.23E+00 |
| CE | -1.26E+00 | ACDF | -2.23E+00 |
| CF | -1.31E+00 | ACEF | -2.71E+00 |
| DE | 1.34E+00 | ADEF | -1.32E+00 |
| DF | -2.23E+00 | BCDE | -1.25E+00 |
| EF | -2.22E+00 | BCDF | -1.32E+00 |
| ABC | -1.31E+00 | BCEF | -1.31E+00 |
| ABD | -2.23E+00 | BDEF | -2.23E+00 |
| ABE | -2.22E+00 | CDEF | -1.32E+00 |
| ABF | -2.22E+00 | ABCDE | -1.32E+00 |
| ACD | -1.32E+00 | ABCDF | -1.32E+00 |
| ACE | -1.31E+00 | ABCEF | -1.31E+00 |
| ACF | -1.31E+00 | ABDEF | -2.23E+00 |
| ADE | -2.23E+00 | ACDEF | -1.32E+00 |
| ADF | -2.23E+00 | BCDEF | -2.23E+00 |
| AEF | -2.22E+00 | ABCDEF | -2.23E+00 |
| BCD | -2.17E+00 | | |

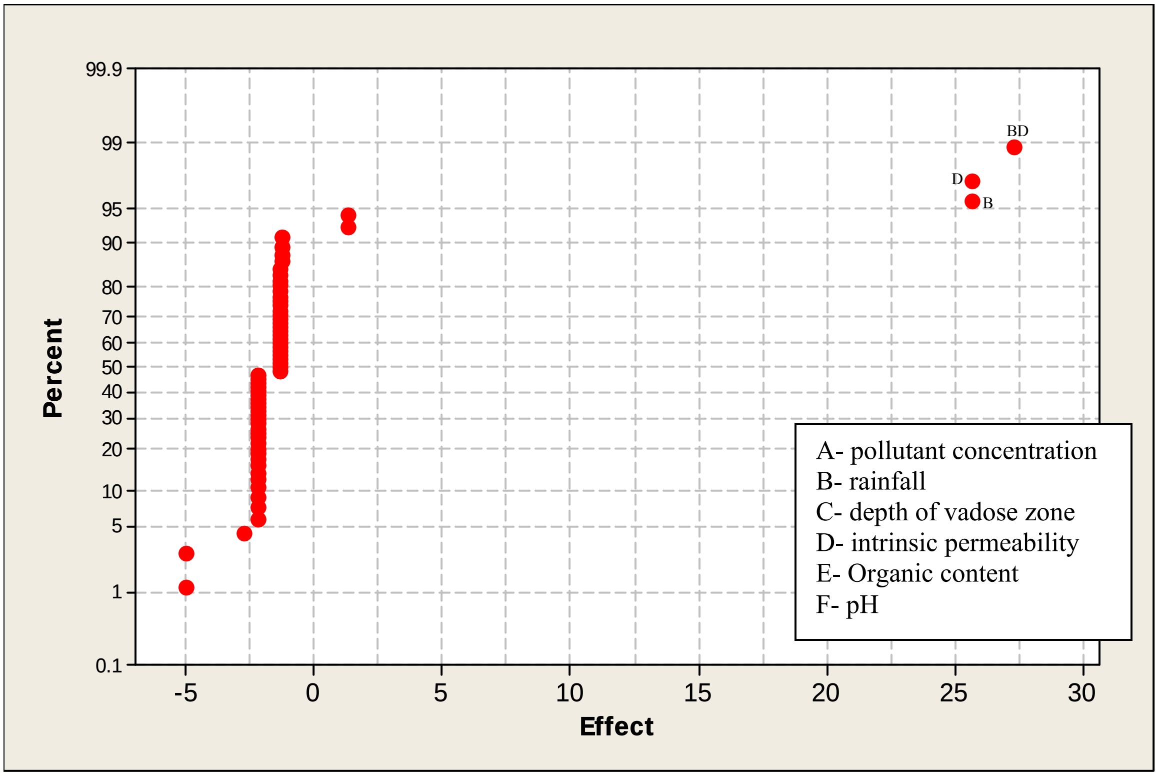


Figure C.9 Estimated main effects and effect interactions on caffeine migration in vadose zone

Table C.44 Calculated Effects of Factors and their Interactions on migration depth of Ibuprofen

| Factors/ Interactions | Effect on migration depth | Factors/ Interactions | Effect on migration depth |
|---|---|---|---|
| A | -4.70E-01 | BCE | -4.56E-01 |
| B | 5.43E+00 | BCF | -4.70E-01 |
| C | -4.56E-01 | BDE | -1.06E+00 |
| D | 5.43E+00 | BDF | -2.79E-01 |
| E | -1.06E+00 | BEF | -2.78E-01 |
| F | -2.78E-01 | CDE | -4.59E-01 |
| AB | -2.78E-01 | CDF | -4.71E-01 |
| AC | -4.70E-01 | CEF | -4.70E-01 |
| AD | -2.79E-01 | DEF | -2.79E-01 |
| AE | -2.78E-01 | ABCD | -4.71E-01 |
| AF | -2.78E-01 | ABCE | -4.70E-01 |
| BC | -2.67E-01 | ABCF | -4.70E-01 |
| BD | 5.78E+00 | ABDE | -2.79E-01 |
| BE | 2.87E-01 | ABDF | -2.79E-01 |
| BF | -4.70E-01 | ABEF | -2.78E-01 |
| CD | -2.65E-01 | ACDE | -4.71E-01 |
| CE | -2.67E-01 | ACDF | -4.71E-01 |
| CF | -2.78E-01 | ACEF | -5.74E-01 |
| DE | 2.84E-01 | ADEF | -2.79E-01 |
| DF | -4.71E-01 | BCDE | -2.65E-01 |
| EF | -4.70E-01 | BCDF | -2.79E-01 |
| ABC | -2.78E-01 | BCEF | -2.78E-01 |
| ABD | -4.71E-01 | BDEF | -4.71E-01 |
| ABE | -4.70E-01 | CDEF | -2.79E-01 |
| ABF | -4.70E-01 | ABCDE | -2.79E-01 |
| ACD | -2.79E-01 | ABCDF | -2.79E-01 |
| ACE | -2.78E-01 | ABCEF | -2.78E-01 |
| ACF | -2.78E-01 | ABDEF | -4.71E-01 |
| ADE | -4.71E-01 | ACDEF | -2.79E-01 |
| ADF | -4.71E-01 | BCDEF | -4.71E-01 |
| AEF | -4.70E-01 | ABCDEF | -4.71E-01 |
| BCD | -4.60E-01 | | |

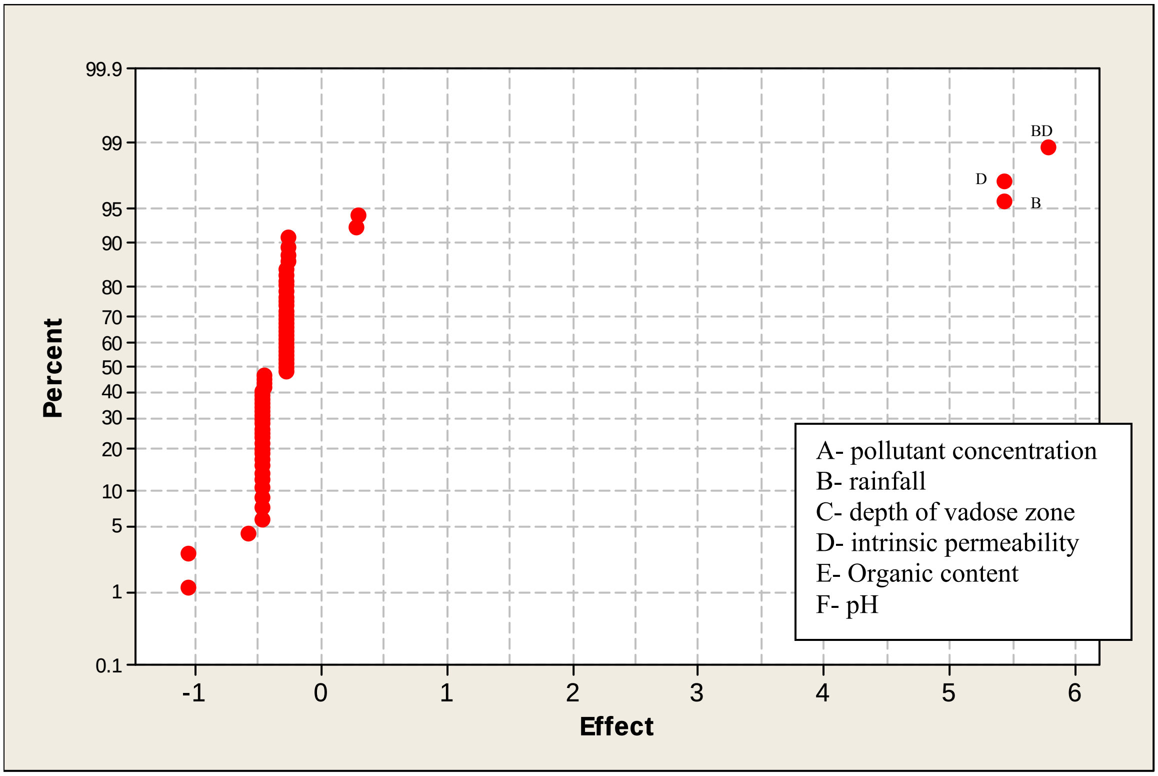


Figure C.10 Estimated main effects and effect interactions on ibuprofen migration in vadose zone

Table C.45 Calculated Effects of Factors and their Interactions on migration depth of Diclofenac

| Factors/ Interactions | Effect on migration depth | Factors/ Interactions | Effect on migration depth |
|---|---|---|---|
| A | -8.55E-01 | BCE | -8.29E-01 |
| B | 9.87E+00 | BCF | -8.55E-01 |
| C | -8.30E-01 | BDE | -1.92E+00 |
| D | 9.87E+00 | BDF | -5.07E-01 |
| E | -1.93E+00 | BEF | -5.06E-01 |
| F | -5.05E-01 | CDE | -8.35E-01 |
| AB | -5.06E-01 | CDF | -8.56E-01 |
| AC | -8.55E-01 | CEF | -8.55E-01 |
| AD | -5.07E-01 | DEF | -5.07E-01 |
| AE | -5.06E-01 | ABCD | -8.56E-01 |
| AF | -5.06E-01 | ABCE | -8.55E-01 |
| BC | -4.85E-01 | ABCF | -8.55E-01 |
| BD | 1.05E+01 | ABDE | -5.07E-01 |
| BE | 5.21E-01 | ABDF | -5.07E-01 |
| BF | -8.55E-01 | ABEF | -5.06E-01 |
| CD | -4.81E-01 | ACDE | -8.56E-01 |
| CE | -4.85E-01 | ACDF | -8.56E-01 |
| CF | -5.05E-01 | ACEF | -1.04E+00 |
| DE | 5.15E-01 | ADEF | -5.07E-01 |
| DF | -8.56E-01 | BCDE | -4.82E-01 |
| EF | -8.55E-01 | BCDF | -5.07E-01 |
| ABC | -5.06E-01 | BCEF | -5.06E-01 |
| ABD | -8.56E-01 | BDEF | -8.56E-01 |
| ABE | -8.55E-01 | CDEF | -5.07E-01 |
| ABF | -8.55E-01 | ABCDE | -5.07E-01 |
| ACD | -5.07E-01 | ABCDF | -5.07E-01 |
| ACE | -5.06E-01 | ABCEF | -5.06E-01 |
| ACF | -5.06E-01 | ABDEF | -8.56E-01 |
| ADE | -8.56E-01 | ACDEF | -5.07E-01 |
| ADF | -8.56E-01 | BCDEF | -8.56E-01 |
| AEF | -8.55E-01 | ABCDEF | -8.56E-01 |
| BCD | -8.36E-01 | | |

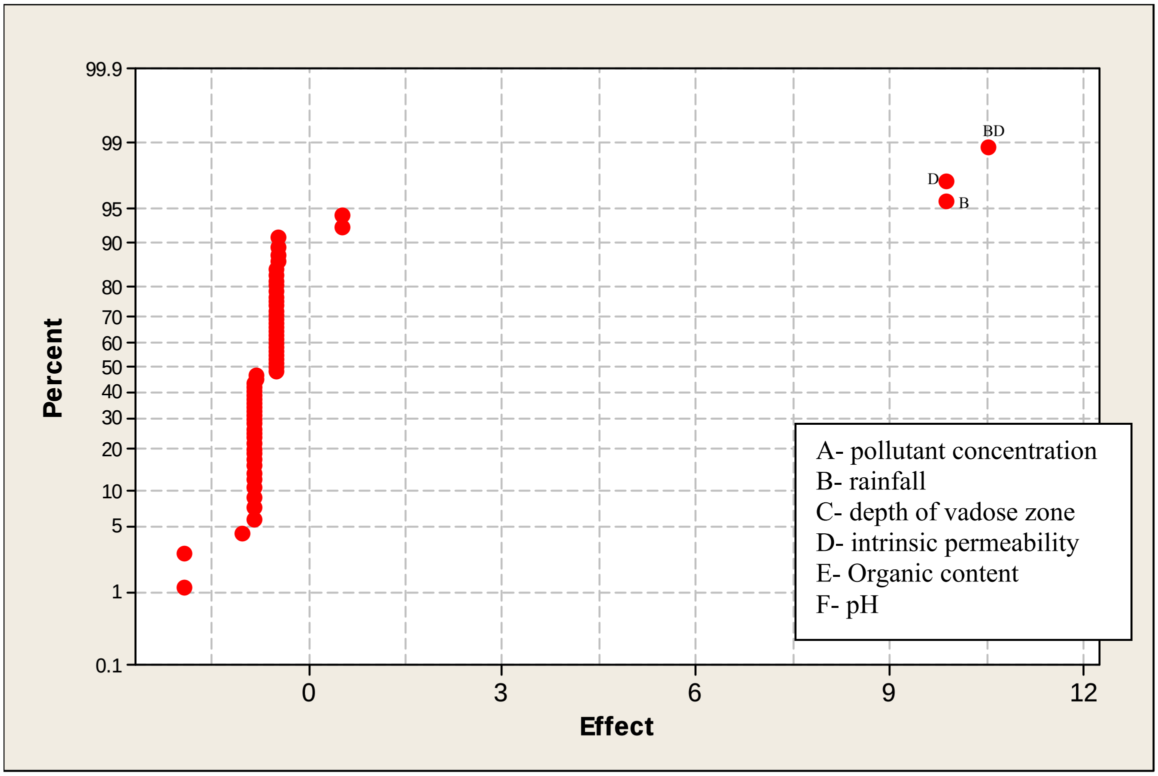


Figure C.11 Estimated main effects and effect interactions on diclofenac migration in vadose zone

Table C.46 Calculated Effects of Factors and their Interactions on migration depth of Acetaminophen

| Factors/ Interactions | Effect on migration depth | Factors/ Interactions | Effect on migration depth |
|---|---|---|---|
| A | -2.31E+00 | BCE | -2.24E+00 |
| B | 2.66E+01 | BCF | -2.31E+00 |
| C | -2.24E+00 | BDE | -5.20E+00 |
| D | 2.66E+01 | BDF | -1.37E+00 |
| E | -5.20E+00 | BEF | -1.37E+00 |
| F | -1.36E+00 | CDE | -2.25E+00 |
| AB | -1.37E+00 | CDF | -2.31E+00 |
| AC | -2.31E+00 | CEF | -2.31E+00 |
| AD | -1.37E+00 | DEF | -1.37E+00 |
| AE | -1.37E+00 | ABCD | -2.31E+00 |
| AF | -1.37E+00 | ABCE | -2.31E+00 |
| BC | -1.31E+00 | ABCF | -2.31E+00 |
| BD | 2.84E+01 | ABDE | -1.37E+00 |
| BE | 1.41E+00 | ABDF | -1.37E+00 |
| BF | -2.31E+00 | ABEF | -1.37E+00 |
| CD | -1.30E+00 | ACDE | -2.31E+00 |
| CE | -1.31E+00 | ACDF | -2.31E+00 |
| CF | -1.36E+00 | ACEF | -2.82E+00 |
| DE | 1.39E+00 | ADEF | -1.37E+00 |
| DF | -2.31E+00 | BCDE | -1.30E+00 |
| EF | -2.31E+00 | BCDF | -1.37E+00 |
| ABC | -1.37E+00 | BCEF | -1.37E+00 |
| ABD | -2.31E+00 | BDEF | -2.31E+00 |
| ABE | -2.31E+00 | CDEF | -1.37E+00 |
| ABF | -2.31E+00 | ABCDE | -1.37E+00 |
| ACD | -1.37E+00 | ABCDF | -1.37E+00 |
| ACE | -1.37E+00 | ABCEF | -1.37E+00 |
| ACF | -1.37E+00 | ABDEF | -2.31E+00 |
| ADE | -2.31E+00 | ACDEF | -1.37E+00 |
| ADF | -2.31E+00 | BCDEF | -2.31E+00 |
| AEF | -2.31E+00 | ABCDEF | -2.31E+00 |
| BCD | -2.26E+00 | | |

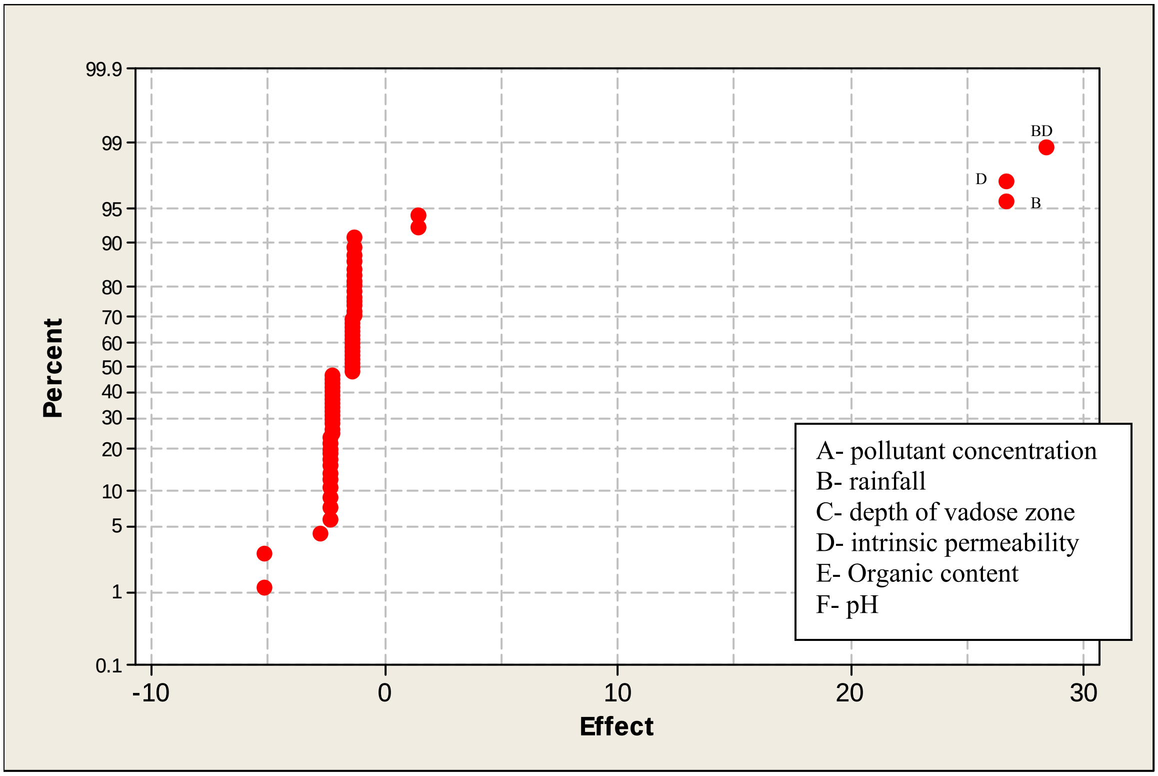


Figure C.12 Estimated main effects and effect interactions on acetaminophen migration in vadose zone

Table C.47 Calculated Effects of Factors and their Interactions on migration depth of Triclosan

| Factors/ Interactions | Effect on migration depth | Factors/ Interactions | Effect on migration depth |
|---|---|---|---|
| A | -3.42E-01 | BCE | -3.32E-01 |
| B | 3.95E+00 | BCF | -3.42E-01 |
| C | -3.32E-01 | BDE | -7.70E-01 |
| D | 3.95E+00 | BDF | -2.03E-01 |
| E | -7.71E-01 | BEF | -2.02E-01 |
| F | -2.02E-01 | CDE | -3.34E-01 |
| AB | -2.02E-01 | CDF | -3.42E-01 |
| AC | -3.42E-01 | CEF | -3.42E-01 |
| AD | -2.03E-01 | DEF | -2.03E-01 |
| AE | -2.02E-01 | ABCD | -3.42E-01 |
| AF | -2.02E-01 | ABCE | -3.42E-01 |
| BC | -1.94E-01 | ABCF | -3.42E-01 |
| BD | 4.20E+00 | ABDE | -2.03E-01 |
| BE | 2.08E-01 | ABDF | -2.03E-01 |
| BF | -3.42E-01 | ABEF | -2.02E-01 |
| CD | -1.92E-01 | ACDE | -3.42E-01 |
| CE | -1.94E-01 | ACDF | -3.42E-01 |
| CF | -2.02E-01 | ACEF | -4.17E-01 |
| DE | 2.06E-01 | ADEF | -2.03E-01 |
| DF | -3.42E-01 | BCDE | -1.93E-01 |
| EF | -3.42E-01 | BCDF | -2.03E-01 |
| ABC | -2.02E-01 | BCEF | -2.02E-01 |
| ABD | -3.42E-01 | BDEF | -3.42E-01 |
| ABE | -3.42E-01 | CDEF | -2.03E-01 |
| ABF | -3.42E-01 | ABCDE | -2.03E-01 |
| ACD | -2.03E-01 | ABCDF | -2.03E-01 |
| ACE | -2.02E-01 | ABCEF | -2.02E-01 |
| ACF | -2.02E-01 | ABDEF | -3.42E-01 |
| ADE | -3.42E-01 | ACDEF | -2.03E-01 |
| ADF | -3.42E-01 | BCDEF | -3.42E-01 |
| AEF | -3.42E-01 | ABCDEF | -3.42E-01 |
| BCD | -3.34E-01 | | |

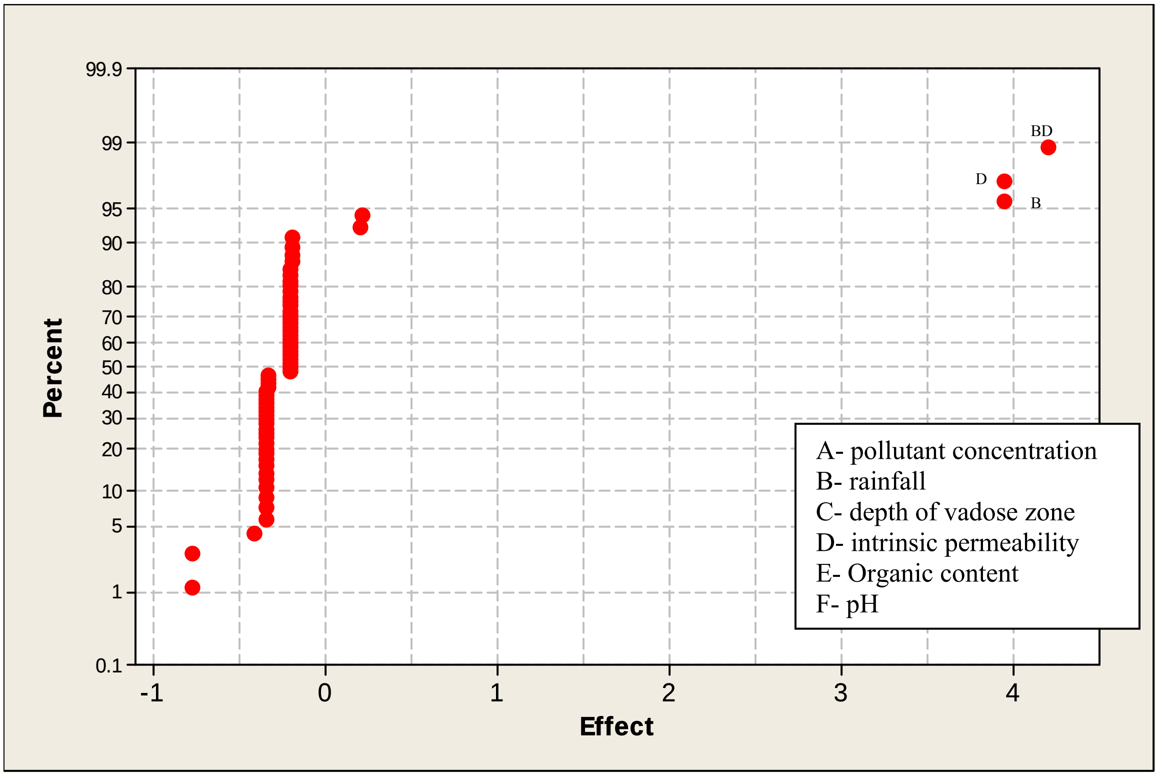


Figure C.13 Estimated main effects and effect interactions on triclosan migration in vadose zone

Table C.48 Calculated Effects of Factors and their Interactions on migration depth of Ciprofloxacin

| Factors/ Interactions | Effect on migration depth | Factors/ Interactions | Effect on migration depth |
|---|---|---|---|
| A | -4.06E-01 | BCE | -3.94E-01 |
| B | 4.69E+00 | BCF | -4.06E-01 |
| C | -3.94E-01 | BDE | -9.14E-01 |
| D | 4.69E+00 | BDF | -2.41E-01 |
| E | -9.15E-01 | BEF | -2.40E-01 |
| F | -2.40E-01 | CDE | -3.97E-01 |
| AB | -2.40E-01 | CDF | -4.07E-01 |
| AC | -4.06E-01 | CEF | -4.06E-01 |
| AD | -2.41E-01 | DEF | -2.41E-01 |
| AE | -2.40E-01 | ABCD | -4.07E-01 |
| AF | -2.40E-01 | ABCE | -4.06E-01 |
| BC | -2.30E-01 | ABCF | -4.06E-01 |
| BD | 4.99E+00 | ABDE | -2.41E-01 |
| BE | 2.47E-01 | ABDF | -2.41E-01 |
| BF | -4.06E-01 | ABEF | -2.40E-01 |
| CD | -2.28E-01 | ACDE | -4.07E-01 |
| CE | -2.30E-01 | ACDF | -4.07E-01 |
| CF | -2.40E-01 | ACEF | -4.96E-01 |
| DE | 2.45E-01 | ADEF | -2.41E-01 |
| DF | -4.07E-01 | BCDE | -2.29E-01 |
| EF | -4.06E-01 | BCDF | -2.41E-01 |
| ABC | -2.40E-01 | BCEF | -2.40E-01 |
| ABD | -4.07E-01 | BDEF | -4.07E-01 |
| ABE | -4.06E-01 | CDEF | -2.41E-01 |
| ABF | -4.06E-01 | ABCDE | -2.41E-01 |
| ACD | -2.41E-01 | ABCDF | -2.41E-01 |
| ACE | -2.40E-01 | ABCEF | -2.40E-01 |
| ACF | -2.40E-01 | ABDEF | -4.07E-01 |
| ADE | -4.07E-01 | ACDEF | -2.41E-01 |
| ADF | -4.07E-01 | BCDEF | -4.07E-01 |
| AEF | -4.06E-01 | ABCDEF | -4.07E-01 |
| BCD | -3.97E-01 | | |

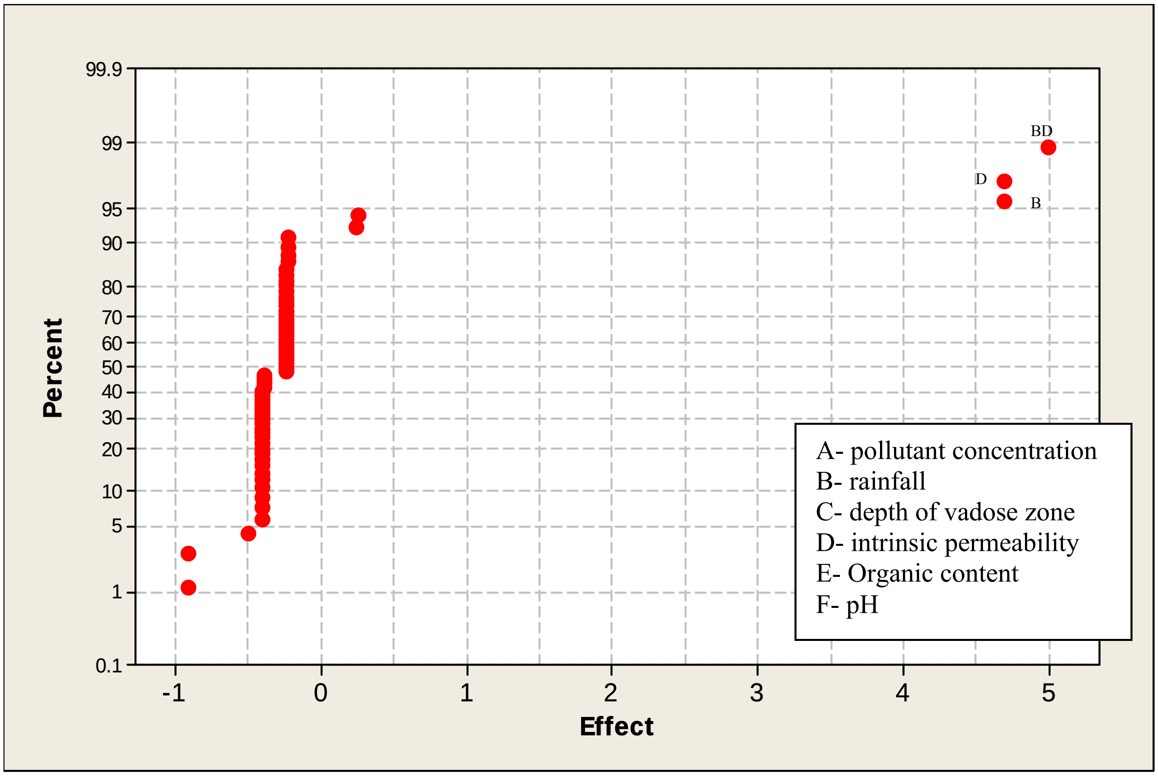


Figure C.14 Estimated main effects and effect interactions on ciprofloxacin migration in vadose zone

Table C.49 Calculated Effects of Factors and their Interactions on migration depth of Metoprolol

| Factors/ Interactions | Effect on migration depth | Factors/ Interactions | Effect on migration depth |
|---|---|---|---|
| A | -1.90E+00 | BCE | -1.85E+00 |
| B | 2.20E+01 | BCF | -1.90E+00 |
| C | -1.85E+00 | BDE | -4.28E+00 |
| D | 2.20E+01 | BDF | -1.13E+00 |
| E | -4.29E+00 | BEF | -1.13E+00 |
| F | -1.12E+00 | CDE | -1.86E+00 |
| AB | -1.12E+00 | CDF | -1.90E+00 |
| AC | -1.90E+00 | CEF | -1.90E+00 |
| AD | -1.13E+00 | DEF | -1.13E+00 |
| AE | -1.12E+00 | ABCD | -1.90E+00 |
| AF | -1.12E+00 | ABCE | -1.90E+00 |
| BC | -1.08E+00 | ABCF | -1.90E+00 |
| BD | 2.34E+01 | ABDE | -1.13E+00 |
| BE | 1.16E+00 | ABDF | -1.13E+00 |
| BF | -1.90E+00 | ABEF | -1.12E+00 |
| CD | -1.07E+00 | ACDE | -1.90E+00 |
| CE | -1.08E+00 | ACDF | -1.90E+00 |
| CF | -1.12E+00 | ACEF | -2.32E+00 |
| DE | 1.15E+00 | ADEF | -1.13E+00 |
| DF | -1.90E+00 | BCDE | -1.07E+00 |
| EF | -1.90E+00 | BCDF | -1.13E+00 |
| ABC | -1.12E+00 | BCEF | -1.13E+00 |
| ABD | -1.90E+00 | BDEF | -1.90E+00 |
| ABE | -1.90E+00 | CDEF | -1.13E+00 |
| ABF | -1.90E+00 | ABCDE | -1.13E+00 |
| ACD | -1.13E+00 | ABCDF | -1.13E+00 |
| ACE | -1.12E+00 | ABCEF | -1.12E+00 |
| ACF | -1.12E+00 | ABDEF | -1.90E+00 |
| ADE | -1.90E+00 | ACDEF | -1.13E+00 |
| ADF | -1.90E+00 | BCDEF | -1.90E+00 |
| AEF | -1.90E+00 | ABCDEF | -1.90E+00 |
| BCD | -1.86E+00 | | |

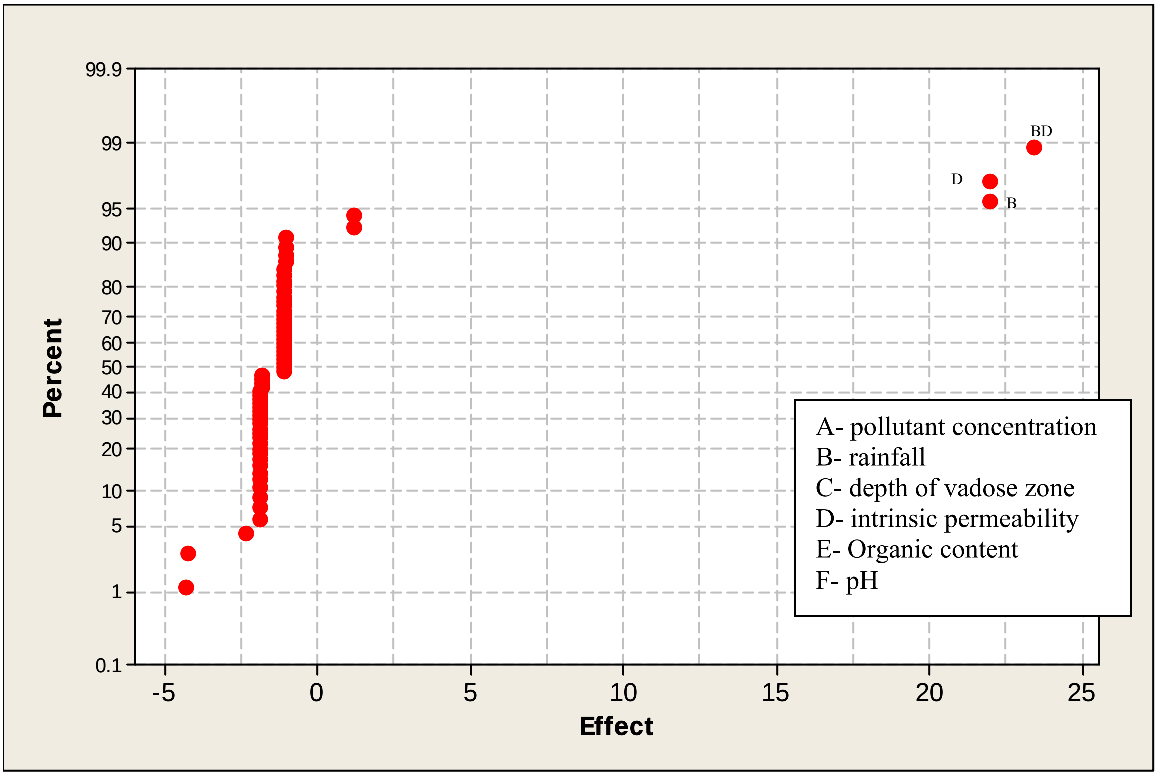


Figure C.15 Estimated main effects and effect interactions on metoprolol migration in vadose zone

Table C.50 Calculated Effects of Factors and their Interactions on migration depth of Salicylic acid

| Factors/ Interactions | Effect on migration depth | Factors/ Interactions | Effect on migration depth |
|---|---|---|---|
| A | -9.62E-01 | BCE | -9.33E-01 |
| B | 1.11E+01 | BCF | -9.62E-01 |
| C | -9.33E-01 | BDE | -2.16E+00 |
| D | 1.11E+01 | BDF | -5.70E-01 |
| E | -2.17E+00 | BEF | -5.69E-01 |
| F | -5.69E-01 | CDE | -9.39E-01 |
| AB | -5.69E-01 | CDF | -9.63E-01 |
| AC | -9.62E-01 | CEF | -9.62E-01 |
| AD | -5.70E-01 | DEF | -5.70E-01 |
| AE | -5.69E-01 | ABCD | -9.63E-01 |
| AF | -5.69E-01 | ABCE | -9.62E-01 |
| BC | -5.45E-01 | ABCF | -9.62E-01 |
| BD | 1.18E+01 | ABDE | -5.70E-01 |
| BE | 5.86E-01 | ABDF | -5.70E-01 |
| BF | -9.62E-01 | ABEF | -5.69E-01 |
| CD | -5.41E-01 | ACDE | -9.63E-01 |
| CE | -5.46E-01 | ACDF | -9.63E-01 |
| CF | -5.69E-01 | ACEF | -1.17E+00 |
| DE | 5.80E-01 | ADEF | -5.70E-01 |
| DF | -9.63E-01 | BCDE | -5.42E-01 |
| EF | -9.61E-01 | BCDF | -5.70E-01 |
| ABC | -5.69E-01 | BCEF | -5.69E-01 |
| ABD | -9.63E-01 | BDEF | -9.63E-01 |
| ABE | -9.62E-01 | CDEF | -5.70E-01 |
| ABF | -9.62E-01 | ABCDE | -5.70E-01 |
| ACD | -5.70E-01 | ABCDF | -5.70E-01 |
| ACE | -5.69E-01 | ABCEF | -5.69E-01 |
| ACF | -5.69E-01 | ABDEF | -9.63E-01 |
| ADE | -9.63E-01 | ACDEF | -5.70E-01 |
| ADF | -9.63E-01 | BCDEF | -9.63E-01 |
| AEF | -9.62E-01 | ABCDEF | -9.63E-01 |
| BCD | -9.40E-01 | | |

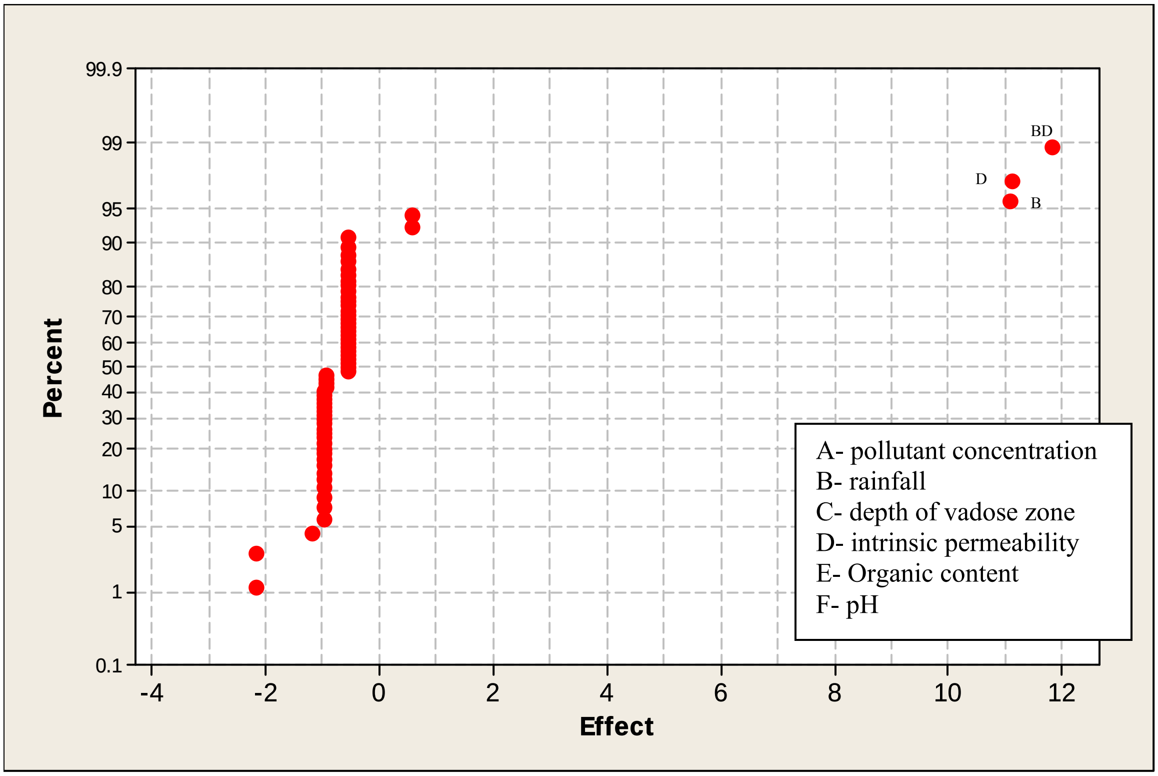


Figure C.16 Estimated main effects and effect interactions on salicylic acid migration in vadose zone