FORMATION OF CHLOROFORM AND OTHER CHLORINATED BYPRODUCTS BY THE CHLORINATION OF ANTIBACTERIAL PRODUCTS

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Thesis submitted to the faculty of the Virginia Polytechnic Institute and State University in partial fulfillment of the requirements for the degree of

MASTER OF SCIENCE

in

Environmental Engineering

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August 3, 2006

Blacksburg, Virginia

Keywords: Triclosan, Antibacterial Soaps, Free Chlorine, Chloroform, Drinking Water

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(ABSTRACT)

Triclosan is a widely used antibacterial agent found in many personal hygiene products. While it has been established that pure triclosan and free chlorine readily react, interactions between triclosan-containing products and free chlorine have not previously been analyzed. Sixteen double-blinded solutions including both triclosan-containing (1.14-3.12 mg triclosan/g product) and triclosan-free products were contacted with free chlorine. Products detected included (chlorophenoxy)phenols, 2,4-dichlorophenol, 2,4,6-trichlorophenol, and chloroform. The daughter product yields were found to be highly variable and were dependent on the antimicrobial product investigated, the free chlorine to triclosan ratio, and the temperature at which the study was conducted. Lowering the temperature from 40 to 30 oC resulted in a decreased yield from 0.50 to 0.37 moles chloroform/mole triclosan after 1 minute of reaction time with [HOCl]initial = 4.0 mg/L as Cl2. Chloroform molar yields decreased to 0.29 when the initial chlorine concentration was reduced to 2.0 mg/L for a constant temperature of 40 oC. Field experiments, in which Atlanta and Danville tap waters were augmented with various soap products, exhibited differential results from the laboratory experiments in that different product yields were observed. These differences are attributed to the chlorine demand of constituents in the tap water. Higher chlorine to triclosan ratios tend to produce high levels of chloroform, while lower chlorine to triclosan ratios tend to form higher amounts of chlorophenols and (chlorophenoxy)phenol intermediates. The results from this study suggest that the chloroform produced by these reactions can be substantial under some conditions.

Acknowledgements

I would like to thank the American Water Works Association Research Foundation for funding this project, and the project advisory committee (Paul Westerhoff, Chad Jafvert, and Cordelia Hwang) for their advice and guidance.

I would like to thank my Advisor, Dr. Peter Vikesland, for allowing me the chance to work on this project. Your time and guidance throughout this process has been invaluable. Thank you for your patience and for having faith in my abilities from the start.

My deepest gratitude goes to Krista Rule. You have taught me so much and I would not be where I am at without your help.

I would finally like to thank the EWR laboratory technician, Jody Smiley, and my committee members, Dr. Nancy Love and Dr. Marc Edwards, for your input and assistance throughout my work.

This thesis is dedicated to my father, whose passion for engineering and insistence on education has influenced my life immeasurably.

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Chapter 1: Literature Review

1.1: Background

Triclosan (5-chloro-2-(2,4- dichlorophenoxy)phenol) is an antimicrobial agent found in many common household hygienic products to prevent bacterial infections and for oral applications (1). Triclosan is a synthetic, nonionic, broad spectrum antimicrobial agent that takes the form of an off-white, odorless, tasteless, crystalline powder (1). It is insoluble in water and has a molecular weight of 289.5 g/mole (1). Although triclosan was introduced for use in health care settings over 30 years ago, its use dramatically expanded over the last decade as a result of increased concern about microbial pathogens. Many companies currently add triclosan to products such as hand soaps, surgical scrubs, deodorants, dish soaps, body washes, and toothpastes at concentrations of up to 0.3%. Although its actual effectiveness is a topic of some debate, triclosan has been added to many personal care products because it exhibits antibacterial as well as some antifungal and antiviral properties (2).

1.2: Mode of Action

Bisphenols such as triclosan are a class of compounds that exhibit a broad spectrum of antimicrobial activity. The two most widely used members of this group are triclosan and hexachlorophene, although use of the latter in consumer products has been limited due to toxicity concerns (3). Historically, it was thought that triclosan worked as a non-specific biocide that disturbs membrane functionality in bacteria by preventing RNA and protein synthesis (4,5) Proponents of triclosan have also suggested that high triclosan concentrations, such as those observed with normal antibacterial product use, cause a multitude of different effects on numerous targets resulting in cell lysis (6). During the last decade, however, it was found that triclosan works as a site-specific biocide that inhibits a defined bacterial target in the bacterial fatty acid biosynthetic pathway. Studies have shown that triclosan can prevent fatty acid synthesis by inhibition of the NADH-dependent enoyl acyl carrier protein reductase enzyme

(FabI) in *E. coli* (7), *P. aeruginosa* (8), *S. aureus* (9) or its homolog InhA in *M. smegmatis* (10) and *M. tuberculosis* (11).

1.3: Triclosan Usage and Effectiveness

In the US, over 75% of liquid soaps and nearly 30% of bar soaps currently on the market contain some type of antibacterial product (12). An estimated 700 antibacterial products, the vast majority of which contain triclosan as the active ingredient, entered the consumer market between 1992 and 1999 (3). On average, a typical American uses approximately 5 mg of triclosan each day, resulting in a total nationwide usage of almost 1500 kg/day (13). When coupled with its relative chemical stability, the wide-spread use of triclosan has led to its presence in nearly every aquatic environment. Triclosan is washed down consumer's drains during product use and is present in wastewater treatment plant (WWTP) influents. Triclosan is common in WWTP biosolids (14), and due to incomplete removal by biological treatment processes, it is also detected in treatment plant effluents (15,16). Incomplete removal by treatment plants and land-application of triclosan containing biosolids result in its continued release into lake and river waters (14,17). A comprehensive study by the U.S. Geological Survey detected triclosan in 57.6% of 139 highly susceptible streams (18). Triclosan has even been detected in drinking water source waters (19).

Many European countries, such as Denmark and Germany, have limited the use of triclosan-containing products because of increasing fears about the acute toxicity of the compound, its potential to lead to bacterial resistance, and other long-term ill effects (20). Several recent studies have shown that some bacteria, such as *Escherichia coli* and *Mycobacterium smegmatis*, can readily build resistance to triclosan (10,21). *Pseudomonas putida* and *Alcaligenes xylosoxidans* bacteria that have been exposed to triclosan for a long period of time will even adopt triclosan as their sole carbon source (22).

In a household environment, it is not clear that the use of triclosan containing products provides enhanced antibacterial protection relative to triclosan-free products (20). The minimum

inhibitory concentration of triclosan varies from 0.01 to over 1000 mg/L depending on the organism in question (23). The wide range in effective concentrations, when combined with the large variability of tolerance within an individual species, has resulted in weak statistical findings in studies analyzing triclosan's effectiveness. Because of this, no study to date has been able to definitively show that antibacterial products work any better than regular soap and water. In fact, several studies have claimed that triclosan-containing soap use does not provide any prolonged antibacterial effect when compared to non-medicated soap, although it did cause skin irritation in several cases (24,25). Larson et al. showed that there was no statistically significant advantage to washing hands with triclosan-containing soap over triclosan-free soap, and that there was no reduction of an individual's risk of acquiring an infectious household disease. After performing a risk analysis, Larson instead argues in favor of the use of plain soap and water (26,27).

1.4: Implications from Product Use

Many of the triclosan containing antibacterial products that are currently on the market are designed to be used during activities such as showering and dish washing. As such, these products will be in contact with a consumer's skin for extended periods of time at water temperatures that can range from 21-46 ^{o}C (28,29). In the US, water used for household activities generally contains a disinfectant residual and is maintained at a circumneutral pH to prevent corrosion. A 1996 American Water Works Association survey determined that over 70% of all drinking water utilities in the United States use free chlorine for this residual disinfectant and almost 90% of utilities maintain the water pH between 7 and 9.5 (30).

Studies have shown that triclosan and free chlorine readily react to form several different byproducts including chlorinated phenoxy-phenols, chlorinated phenols, and trihalomethanes with an optimal pH ranging from 7 to 9 (31-34). It has also been shown that these and other phenols can act as trihalomethane precursors when they come in contact with free-chlorine (35-41). In a past study by Rule et al. (34), a reaction scheme was proposed that illustrates the

products that form during the free chlorine-triclosan reaction. From this study, and subsequent work by Canosa et al.(33), it is apparent that, when triclosan reacts in the presence of free chlorine, a number of simultaneous reaction pathways result in production of several byproducts. Chlorine substitution into triclosan can result in formation of 5,6-dichloro-2-(2,4-dichlorophenoxy)phenol, 4,5-dichloro-2-(2,4-dichlorophenoxy)phenol, and 4,5,6-trichloro-2-(2,4-dichlorophenoxy)phenol intermediates. Any of these products, or triclosan itself, react to produce 2,4-dichlorophenol and then 2,4,6-trichlorophenol after an ether cleavage. Additionally, triclosan and all byproducts mentioned above can form chloroform directly by ring cleavage and chlorination.

Due to the fact that most drinking water utilities maintain significant free chlorine concentrations within the optimal pH range for the triclosan-free chlorine reaction, considerable rates of product formation will likely be observed. The additional possibility that elevated reaction temperatures increase reaction rates will multiply these effects. It has also been shown that triclosan also reacts with chloramines, the most widely employed alternative to free chlorine, though it does so at an extremely slow rate and thus would not form significant byproduct concentrations over the timeframe of a shower or dishwashing (42).

1.5: Reaction Product Analysis

Repeatedly, chloroform has been shown to form from the chlorination of organic compounds such as fulvic and humic substances during drinking water treatment. These aromatic precursors are converted into several trichloromethyl-substituted intermediates that subsequently decompose to chloroform through a series of hydrolysis and decarboxylation steps (43,44). It was found that the phenolic cores of humic substances react with chlorine, and that reaction rates were proportional to chlorine concentration, TOC concentration, temperature, and pH (45), with the optimal reaction pH ranging from 8 to 10 (43). The reaction between humic or fulvic acids and low chlorine concentrations yielded substantial amounts of polyhalogenated intermediates, while reactions performed at high chlorine levels did not (43). Later studies have shown that

Resorcinol-type structures in NOM are responsible for the fast reacting THM precursors (k>100 $M^{-1}s^{-1}$, pH=8.0) while the slowly reacting precursors consist of phenolic compounds (k=0.026 $M^{-1}s^{-1}$, pH=8.0) (38,39). Triclosan exhibits some similar structural properties as NOM and can respond in similar ways.

The EPA has set a maximum contaminant level of 80 μg/L for total trihalomethanes since these volatile byproducts have been established as potentially carcinogenic compounds (46). The MCL was set by extrapolating a dose-response curve created by testing acute high-level exposure effects on animals to the estimated human effects from chronic, low-level exposure. Though the risk assessment method likely results in high levels of error, the evaluation is necessary since only 20 chemicals have adequate epidemiological exposure data to prove human carcinogenicity. Both 2,4-dichlorophenol and 2,4,6-trichlorophenol have been placed on the EPA Drinking Water Contaminant Candidate list since they are suspected carcinogens and are thus suspected to increase an individual's risk of cancer by their presence in drinking water, but at this time are not regulated due to an insufficient amount of data. The EPA is currently researching all 51 contaminants on the candidate list to determine if they need to be regulated (47). The (chlorophenoxy)phenol intermediates resulting from the triclosan-free chlorine reaction have unknown toxicity.

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Chapter 2: Chlorination of the Antibacterial Agent Triclosan

2.1: Introduction

Triclosan (5-chloro-2-(2,4- dichlorophenoxy)phenol) is an antimicrobial agent found in many common household hygienic products. Although triclosan was introduced over 30 years ago, its use dramatically expanded over the last decade as a result of increased concern about microbial pathogens. Many companies currently add triclosan to products such as hand soaps, dish soaps, body washes, and toothpastes at concentrations up to 0.3%. Although its actual effectiveness is a topic of some debate, triclosan has been added to many personal care products because it exhibits antibacterial as well as antifungal and antiviral properties (1). Historically, it was thought that triclosan worked as a non-specific biocide that disturbs membrane functionality in bacteria by preventing RNA and protein synthesis (2,3). Proponents of triclosan had also suggested that higher triclosan concentrations, as observed with normal antibacterial product use, caused a multitude of different effects on multiple targets resulting in cell lysis (4). It was only in the last decade that studies have shown that triclosan works as a site-specific biocide that inhibits the enoyl acyl carrier protein reductase enzyme, thus preventing fatty acid synthesis and causing cell death (5-7).

In the US, over 75% of liquid soaps and nearly 30% of bar soaps currently on the market contain some type of antibacterial product (8). On average, a typical American uses ~5 mg of triclosan each day, resulting in a total nationwide usage of ~1500 kg/day. Because of the wide-spread use of triclosan, it can be found in nearly every aquatic environment, including wastewater treatment plant effluents (9,10), stream waters (11), lakes, and river sediments (10,12,13). Many European countries, such as Denmark and Germany, have limited the use of triclosan-containing products because of increasing fears of acute toxicity, bacterial resistance, and other long-term ill effects (14). Several recent studies have shown that some bacteria, such

as *Escherichia coli* and *Mycobacterium smegmatis*, can readily build resistance to triclosan (15,16). *Pseudomonas putida* and *Alcaligenes xylosoxidans* bacteria that have been exposed to triclosan for a long period of time will even adopt triclosan as their sole carbon source (17).

In a household environment, it is not clear that the use of triclosan containing products provides enhanced antibacterial protection relative to triclosan-free products (14). No study to date has been able to show that antibacterial products work any better than regular soap and water. In fact, studies have shown that triclosan-containing soap use does not provide any prolonged antibacterial effect when compared to non-medicated soap, although it did cause skin irritation in several cases (18,19). Larson et al. showed that there was no statistically significant advantage to washing hands with triclosan-containing soap over triclosan-free soap, and that there was no reduction of an individual's risk of acquiring an infectious household disease. After performing a risk analysis, Larson instead argues in favor of the use of plain soap and water (20,21).

Many of the triclosan containing antibacterial products that are currently on the market are designed to be used during activities such as showering and dish washing. As such, these products will be in contact with a consumer's skin for extended periods of time at water temperatures that can range from 21-46 ^{o}C (22,23). In the US, water used for household activities generally contains a disinfectant residual. A 1996 American Water Works Association survey determined that over 70% of all drinking water utilities in the United States use free chlorine for this residual disinfectant (24). Because of this fact, the reactions that occur when triclosan products are exposed to free chlorine can be extremely important. Triclosan also reacts with chloramines, the most widely employed alternative to free chlorine, though it does so at an extremely slow rate and thus would not form significant byproduct concentrations over the timeframe of a shower or dishwashing (25).

Studies have shown that triclosan and free chlorine readily react to form several different byproducts including chlorinated phenoxy-phenols, chlorinated phenols, and trihalomethanes (26-29). It has been shown that these and other phenols can act as trihalomethane precursors when they come in contact with free-chlorine (30-36). In a past study by Rule et al. (29), a reaction scheme was proposed that illustrates the products that form during the free chlorine-triclosan reaction (Figure 1). From this study, and subsequent work by Canosa et al. (28), it is apparent that a number of byproducts can be produced when triclosan reacts in the presence of free chlorine. These byproducts include 5,6-dichloro-2-(2,4-dichlorophenoxy)phenol, 4,5-dichloro-2-(2,4-dichlorophenoxy)phenol, 4,5,6-trichloro-2-(2,4-dichlorophenoxy)phenol, 2,4-dichlorophenol, 2,4,6-trichlorophenol, and chloroform. Some of the chlorinated intermediates and products are reportedly carcinogenic, although insufficient studies have been performed to date to determine if that is the case for each compound.

The potentially hazardous products formed when triclosan is exposed to free chlorine suggest that these reactions could have implications on consumer exposure to these chemicals. Despite this fact, no study has closely analyzed the reaction rates and corresponding product formation potentials that likely will result from chlorination of antibacterial hygiene products at elevated temperatures. Thus, the purpose of the present study was to test the hypothesis that high temperature conditions, such as those observed during tasks such as showering and washing dishes, would enhance chloroform and other byproduct formation resulting from the reactions between free chlorine and triclosan in antibacterial products.

2.2: Experimental Methods

2.2.1: General Laboratory Procedures.

Reagent grade water was purified by deionization and distillation. Glassware was cleaned by consecutively soaking it in a 10% nitric acid water bath and a concentrated chlorine bath. Chlorophenol and trihalomethane standards were obtained from Chem Service Inc. and triclosan was supplied by Aldrich (>98% purity). Triclosan stock solutions were prepared by dissolving 100 mg of triclosan in reagent grade methanol and diluting to 50 mL. Free chlorine stock solutions were prepared with a solution of purified grade sodium hypochlorite (4-6%; Fisher Scientific). A Fisher Scientific model 60 pH meter coupled with a Thermo-Orion Ross PerpHect Combination Electrode was utilized for pH measurements. Seven common triclosan-containing hygienic products and five triclosan-free products (e.g., lotions, soaps, and bodywash) were purchased at a local discount store. See Supporting Information for a list of the tested products and their ingredients.

2.2.2: Preparation of Experimental Solutions.

To eliminate potential biases, all products to be tested (both triclosan-containing and triclosan-free, several in duplicate) were placed in 40 mL amber screw top vials and labeled using an alphabetical code. To further reduce bias and to ensure anonymity, each vial was relabeled by a second individual using Roman numerals. Both code-keys were kept confidential by the individuals responsible for the vial labeling. Using GC-MS analysis, ten vials were shown to contain triclosan-laden products, while six vials contained triclosan-free products that served as negative controls.

Experimental solutions were made by mixing a given unknown product at a concentration of 0.25 g/L with reagent grade water containing 2 mM $NaHCO_3$ buffer. This concentration is fairly conservative since a single pump from a typical household hand soap dispenser dispenses ~7× this amount of soap with a single pump (1.84 ± 0.002 g/pump average). H_2SO_4 and NaOH were used to adjust the solution to pH 7. Triplicate 40 mL amber screw top vials were filled

headspace free with soap solutions and were used to perform experiments. Prior to the start of an experiment, temperature was controlled by submerging sealed reactors in a water bath until temperature was stabilized. Reactions were initiated by spiking an aliquot of chlorine stock into a reaction vial using a Cheney Adaptor equipped syringe. Solutions were then immediately removed from the water bath to enable continuous mixing for a given reaction period. Reaction periods of less than five minutes were used and this period was insufficient for any measurable temperature change to occur.

2.2.3: Discussion of Experimental Parameters.

For laboratory experiments, a reaction pH of 7 was chosen since it falls in the range of typical drinking water pH values of 6.5-9 (24,37). An initial chlorine concentration of 4.0 mg/L represented the maximum amount allowed in drinking water (38). Additional experiments used an initial chlorine concentration of 2.0 mg/L, a value more typical of values found in at a consumer's tap (24). The reaction temperature was varied between 30 and 40 ^{o}C and the reaction period was set to 1 min. Reaction temperatures were chosen in order to simulate typical shower temperature ranges (39), and one minute of contact time was used to mimic short-term exposures (40).

2.2.4: Triclosan, Chlorophenol and (Chlorophenoxy)phenol Analysis.

In experiments where triclosan decay and daughter-product formation were monitored, reactions were quenched using a 3× molar excess of sodium sulfite. Quenched solutions were solid phase extracted using 3M Empore High Performance SDBS extraction cartridges after the sample pH was adjusted to pH 2 using 0.1 M HCl. Prior to use, each cartridge was rinsed with 1 mL acetone and dried under vacuum, followed by sequential additions of 0.5 mL methanol and 1.0 mL reagent water for cartridge conditioning. Care was taken to avoid drying out the solid phase during the conditioning process. A 20 mL sample was subsequently drawn through the

cartridge at a rate of 5 mL/min followed by elution with 1 mL acetone. The extracted sample was derivatized by addition of 100 µL of 5% pentafluorobenzyl bromide and 100 µL of 10% aqueous potassium carbonate. Reaction vials were crimp-sealed and submerged in an 80 ^{o}C water bath for 45 minutes to ensure complete derivatization. After cooling, samples were dried under nitrogen until volumes were reduced by ~85%. Each vial was then injected with 1.0 mL methylene chloride and 5 µL 1040 mg/L 1,3,5-tribromobenzene internal standard.

GC-MS analysis of samples was performed with an Agilent 6890/5973 system containing a DB-5ms GC-column (Agilent Technologies) in full scan mode (range *m/z* = 80-550). Upon injection of 1 µL of sample solution, the column was held at 70 ^{o}C for 1.5 minute followed by a temperature ramp of 20 ^{o}C/min to 160 ^{o}C. This was followed by a second temperature ramp of 8 ^{o}C/min to 280 ^{o}C, where the temperature was held for 1 minute. The helium carrier gas flow rate was 1.3 mL/min. Derivatized triclosan and chlorophenols were identified based on their mass spectra and their elution time as compared to the standards. The (chlorophenoxy)phenol daughter products were identified based on elution times and confirmed with mass spectral analysis. The (chlorophenoxy)phenol concentrations were not quantified because analytical standards were not available.

An initial control experiment was run to determine how triclosan recovery was affected by the various hygiene product solutions and by addition of the quenching agent (Appendix A). A soap solution containing 0.25 g/L of a triclosan containing product was made up and transferred into several 40 mL amber vials. In three of the vials, an aliquot of pure triclosan was injected so that each vial contained an additional 0.5 mg/L of triclosan. Three vials contained the initial soap solution without added triclosan, and three vials contained soap solution with an added aliquot of sodium sulfite. The final 3 vials contained soap solution that had been contacted with 2.0 mg/L of free chlorine and quenched after 1 minute of reaction time.

2.2.5: Trihalomethane Analysis.

Samples were analyzed for chloroform, bromoform, bromodichloromethane, and dibromochloromethane after quenching the reactions with sodium sulfite. A 5 mL aliquot was transferred from each reaction vessel and crimp sealed in a 20 mL headspace vial. Trihalomethanes (THMs) were quantified on a Thermo-Finnegan TraceGC Ultra with a HS2000 Headspace autosampler using an Agilent Technologies GS-GASPRO column. Each sample was incubated for 30 minutes at 60 ^{o}C. Upon injection, samples were held at 4 ^{o}C for 4 minutes followed by a temperature ramp of 10 ^{o}C per minute up to 225 ^{o}C where samples were held for 5 min. The helium carrier gas flow rate was 2 mL/min and the ECD detector makeup flow of nitrogen gas had a rate of 30 mL/min. THMs were identified based on elution times and quantified by comparison to standards.

2.2.6: Free Chlorine Analysis.

In product formation experiments, chlorine concentrations were determined by the DPD/FAS titrimetric method (41). A modified version of the same method was utilized for chlorine decay experiments. For analysis, 1 mL of N,N-dimethyl-p-phenylenediamine (DPD) indicator (4.19 mM) and 1 mL of phosphate buffer (0.507 M PO_4^{3-}) was added to each of six 20 mL amber vials. An aliquot of concentrated chlorine stock was injected to each soap solution making the initial chlorine concentration equal 4.0 mg/L. At 0, 0.5, 1, 2, 3, and 5 minutes, a 5 mL aliquot of each soap solution was transferred from the 40 mL reaction vessel to a corresponding 20 mL vial to quench the reaction and 5 minutes was allowed for color development. Each solution was transferred to a 1 cm cell and absorbance readings were taken on a UV-Vis spectrophotometer at a wavelength of 515 nm. A calibration curve was formed by serial dilution of concentrated chlorine stock and periodically verified by manual titrations.

2.2.7: Soap VII Spike Recovery Experiments.

To quantify the effects of changing triclosan to chlorine ratios on product formation, experiments were performed in which varying amounts of triclosan were spiked into a soap solution containing 0.25 g/L of soap VII. Triplicate vials containing solution VII with no additional triclosan, soap VII with an additional 0.25 mg/L, and solution VII with 2.0 mg/L additional triclosan were contacted with 2.0 mg/L free chlorine for 1 minute at 40 ^{o}C and a pH of 7.0. Chlorine-free vials containing the various soap solutions were also analyzed for controls. Samples were analyzed for chlorine decay, triclosan consumption, and for chlorophenol and intermediate formation as described previously.

2.2.8: Pure Triclosan Experiments.

To determine the triclosan reaction rate dependence on temperature and reaction time, independent from the effects of other constituents in the hygiene products, solutions were made by diluting pure triclosan to 0.285 and 0.780 mg/L with reagent-grade water containing 2mM bicarbonate buffer. Solutions were adjusted to a pH of 7.0. Both experimental solutions were transferred into amber vials and spiked with 2.0 mg/L free chlorine after regulating vials to temperatures of 24, 30, and 40 ^{o}C, respectively. Triplicate samples were analyzed for chlorine decay at all three temperatures after quenching triplicate vials at 0.0, 0.25, 0.50, 1, 2, and 3 minute reaction times to allow for reaction rate analysis. Triclosan consumption and chlorophenol and chloroform formation were analyzed at 40 ^{o}C.

2.2.9: Atlanta and Danville Field Experiments.

Chlorine concentrations were measured using a Hach field chlorine kit and pH was determined using a Fisher Scientific portable pH probe. The accuracy of field measurements was verified by comparisons to methods used in the laboratory (Appendix D). Reactions were initiated by addition of a given volume of soap using an auto-pipetter into 1 liter of tap water. The solution was well mixed and the reaction was quenched by pouring the soap solution into 40 mL amber

vials containing excess sulfite after 1 and 4 minutes of reaction time. Samples were refrigerated and shipped to Virginia Tech for triclosan, THM, and phenol analysis.

2.3: Results and Discussion

2.3.1: Background

Although only four of the tested experimental antibacterial products had the triclosan content published, the triclosan concentrations in the tested set of products varied from 0.12% to 0.3% of the product by weight (1.2–3.0 mg triclosan/g product) as reported by the manufacturer. Actual initial triclosan concentrations were quantified in each soap solution and compared to the reported range. Similar to the range reported by the manufacturers, the measured triclosan concentrations in the soaps ranged from 0.29 to 0.78 mg/L in solution containing 0.25 g of soap, or 1.14 to 3.12 mg triclosan/g product (Figure 2 and Figure 3).

The measured triclosan concentrations were used in conjunction with a model developed by Rule et al. (29) to predict triclosan consumption over time at 25 ^{o}C (refer to the Appendix for an explanation of the model). As illustrated in the Supplemental Materials, it is expected that 65% of the initial triclosan concentration would be removed after 1 minute of reaction time (pH=7, $[HOCl]_{initial}$ = 2.0 mg/L). This result suggests that rapid triclosan consumption can be expected at room temperature and that even higher triclosan consumption rates will be observed for the elevated temperatures common to activities such as showering and washing dishes.

Rule et al. ((29)) determined a 0.61 molar yield for chloroform (molar yield = product formed (mole/L) / initial triclosan present (mole/L)) after 48 hours of reaction with a 10-fold excess of free chlorine (temperature = 25 ^{o}C, pH = 7.0). Due to the extremely long reaction time period, this yield was assumed to represent the maximum amount of chloroform that could be produced from the triclosan precursor. Using this yield, the maximum amount of chloroform that could be

theoretically produced from the tested products was determined to be between 127 and 345 µg/L for an initial soap of 0.25 g/L. Rule observed a 0.022 molar yield of 2,4-dichlorophenol after one minute of reaction time (excess free chlorine, pH = 7.0, temperature = 25^{o}C), though no 2,4,6-trichlorophenol was observed over the time period. The soap solution experiments at higher temperatures are expected to result in dichlorophenol concentrations ranging from 3.5 to 9.7 µg/L, at the least, since the higher temperatures again will increase reaction rates. Despite the lack of detection of trichlorophenol in previous experiments, the increased temperatures may elevate reaction rates enough so that it is quickly formed.

2.3.2: Laboratory Experiments.

Triclosan consumption was quantified for seven randomly chosen samples (solutions: II, III (control), IV, VI (control), VII, IX, XII). For the five soaps that contained triclosan, over half of the initial triclosan was consumed within 1 minute of reaction time for an initial chlorine concentration of 2.0 mg/L at 40 ^{o}C (Figure 4). For three of the five tested soaps (II, VII, IX), all of the triclosan was consumed within one minute. This result indicates that triclosan readily reacts with free chlorine, even in the presence of other soap components. These other components exert a chlorine demand, as demonstrated by chlorine consumption experiments for both the triclosan-containing and triclosan-free soaps; however, the measure chlorine demand tended to be more rapidly exerted for the triclosan-containing soaps than for the non-triclosan soaps (Figure 5). The more rapid loss of free chlorine in the triclosan-containing samples suggests that the reaction rates for triclosan are high enough that this chemical out-competes other potential reactants.

2.3.2.1: Product Formation.

Prior studies have shown that (chlorophenoxy)phenols, chlorophenols, and chloroform are produced when triclosan reacts with excess free chlorine (26-29). The formation of chloroform

was monitored for all soap products at a pH of 7 with varying reaction temperatures and initial free chlorine concentrations. Formation of (chlorophenoxy)phenols and chlorophenols was monitored for 7 of the 16 products at pH 7, 40 ^{o}C, and with an initial free chlorine concentration of 2 mg/L as Cl_2.

Chloroform formation was quantified for sixteen soap samples for a pH of 7 with initial free chlorine concentrations of 4.0 and 2.0 mg/L as Cl_2 and temperatures of 40 and 30 ^{o}C (Figure 6). For this entire set of conditions, chloroform concentrations ranging from 21-152 μg/L (0-1.3 μM) with an average of 75.2 ± 37.6 μg/L for the soaps containing triclosan, and 0-39 μg/L (0-0.33 μM) with an average of 4.12 ± 10.3 μg/L for the triclosan-free controls were measured after 1 minute of contact between free chlorine and a given sample. With the exception of soap IX at 40 ^{o}C and 2 mg/L free chlorine, every sample that initially contained triclosan produced chloroform under all reaction conditions. At 40 ^{o}C and 4 mg/L free chlorine, the average chloroform yield for the soaps that contained triclosan was 0.50 moles chloroform/mole triclosan. Lowering both the initial free chlorine concentration to 2.0 mg/L (average chloroform yield = 0.29) and the reaction temperature to 30 ^{o}C (average chloroform yield = 0.37) caused the chloroform yield to decrease. Lower concentrations of chloroform were measured under these reaction conditions than are predicted using the yield of 0.612 moles chloroform/mole triclosan from Rule et al (29). This result is likely due to the shorter reaction period used herein and to the presence of other constituents that exert a chlorine demand. There was little to no formation of THMs other than chloroform, a result that is not unexpected since the solutions did not contain measurable quantities of bromide. Despite this, the EPA set maximum contaminant level (MCL) of 80 μg/L (38) for total trihalomethanes was exceeded by chloroform formation alone in 7 out of the 10 triclosan containing samples when exposed to 4.0 mg/L free chlorine at a temperature of 40 ^{o}C. The MCL was never exceeded for the control samples.

Chlorophenol and intermediate formation was quantified for solutions II, III (control), IV, VI (control), VII, IX, and XII following reactions at 40 ^{o}C with an initial chlorine concentration of 2.0 mg/L. 2,4-dichlorophenol levels ranging from 4.2 to 62.3 μg/L were measured in three of the five soap solutions, while no dichlorophenol was detected in either of the other soaps (Figure 7). The odor threshold for 2,4-dichlorophenol of 0.3 μg/L was exceeded in each case where it was detected (42). Soaps VII and IX produced 2,4,6-trichlorophenol at a concentration of around 8 μg/L. The lack of chlorophenol formation in two of the triclosan-containing sample solutions is likely the result of reactions with other constituents in the soaps. The "inactive" ingredients present in some of the soaps may exert a disinfectant demand and change the reaction mechanisms, selecting for or against the formation of chloroform rather than alternative reaction paths. Additionally, the wide range of triclosan content between different products changes the amount of chlorine available to each triclosan molecule. This contention is supported by the observation that of the triclosan containing products, only soap IX had measurable quantities of the three (chlorophenoxy)phenols [5,6-dichloro-2-(2,4-dichlorophenoxy)phenol, 4,5-dichloro-2-(2,4-dichlorophenoxy)phenol, and 4,5,6-trichloro-2-(2,4-dichlorophenoxy)phenol].

Molar yields calculated for chloroform and chlorophenols are shown in Figure 8. Chloroform yields were 0.36, 0.22, and 0.32 moles chloroform/mole triclosan for soaps II, IV, and XII, respectively in reactions initially containing 2.0 mg/L free chlorine. Of the three, dichlorophenol was only detected in solution II, with a yield of about 0.01, and trichlorophenol was not detected in any. Soap VII had yields of 0.069, 0.037, and 0.012 for chloroform, dichlorophenol, and trichlorophenol, respectively. Soap IX did not produce any chloroform, but had much higher yields of 0.25 and 0.027 for dichlorophenol and trichlorophenol, respectively. In the three solutions with chlorophenol formation, increasing chlorophenol yields were observed in the solutions as the chloroform yields decreased, and the only solution which failed to produce

detectable amounts of chloroform was also the only solution for which intermediate (chlorophenoxy)phenols were detected. These apparent inconsistencies are likely due to changes in reaction dynamics caused by reactions occurring with the other soap constituents.

Variations in the initial triclosan concentrations and the corresponding product formation had no immediately apparent relationship to one another. As stated previously, the large variability between different product solutions was likely the result of other ingredients present in the soaps. The increased chlorine demand of other ingredients decreases the amount of chlorine available to react with triclosan and likely promotes the formation of chlorophenols and (chlorophenoxy)phenols, rather than a chloroform end product. These other ingredients (included in Appendix A) may affect the reactivity of free chlorine towards triclosan or may even act as chloroform precursors, a hypothesis which was further supported by the observation of chloroform formation in two of the six control soap solutions.

2.3.3: Soap VII Spike Recovery Experiments.

A reagent-spike experiment was conducted to examine how a variation in the free chlorine to triclosan ratio alters product yields. For this purpose, a 0.25 g/L solution of soap VII was produced and split into three subsamples. One of these subsamples was left alone, while 0.25 mg/L (0.86 μM) and 2.0 mg/L (6.91 μM) of pure triclosan were added to the other subsamples, respectively. By adding pure triclosan to these subsamples, it was possible to vary the triclosan content, while keeping the total soap concentration constant. The initial total triclosan concentrations in the three samples were 0.78, 1.03, and 2.78 mg/L (2.78, 3.56, and 9.60 μM), respectively. As illustrated in Figure 9, for solutions treated with 2 mg/L free chlorine as Cl_2 at 40 ^oC, all of the triclosan present in the 0.78 and 1.03 mg/L samples was consumed within 1 minute, whereas 0.37 mg/L (2.28 μM) of triclosan remained after 1 minute for the 2.78 mg/L solution. Examining the product yield as a function of the free chlorine to triclosan ratio, it

was determined that the chloroform yield was the smallest at low free chlorine to triclosan ratios. Conversely, the chlorophenol yields increase with a decrease in the free chlorine to triclosan ratio (Figure 10). This result supports the hypothesis that the increased chlorine demand exerted by the additional triclosan affects the product yields. When ample free chlorine is present, triclosan is readily degraded to produce chloroform and chlorophenol accumulation is diminished; however, when free chlorine is limiting, the intermediate byproducts, such as the chlorophenols, are detected.

2.3.4: Pure Triclosan Experiments.

Solutions containing 0.780 and 0.285 mg/L pure triclosan at a pH of 7.0 and 2 mM buffer were spiked with 2.0 mg/L chlorine at temperatures of 40, 30, and 24 ^{o}C and monitored over time. As shown in Figure 11, the samples containing higher concentrations of triclosan consumed more chlorine than the solutions with lesser triclosan concentrations for all reactions, though changing the temperatures did not seem to have significant effects.

Chloroform, triclosan, and chlorophenol concentrations were quantified for the reaction over time at 40 ^{o}C. Triclosan was completely consumed in both solutions within the first 15 seconds of reaction. Figure 12 shows that the solution with a high free chlorine to triclosan ratio (= 28.66 μM free chlorine/ μM triclosan) quickly forms 81.8, 94.4 and 220.6 μg/L of chloroform, dichlorophenol, and trichlorophenol, respectively, within 15 seconds of reaction time. The chloroform concentration remains constant for the remainder of the reaction time. Trichlorophenol continues to form over the next 15 seconds to a concentration of 273.1 μg/L, likely the result of continued degradation of dichlorophenol, apparent from the concentration decrease to 52.5 μg/L during the same time period. Trichlorophenol concentrations began to taper off after 30 seconds as it continued to be degraded. For the solution with a low free chlorine to triclosan ratio (= 28.66 μM free chlorine/ μM triclosan), no chlorophenols were

detected though almost 50 μg/L of chloroform formed over the initial 15 seconds. The chloroform concentrations stabilized for the remaining reaction period.

Again, chlorophenol formation only occurs in the solution containing higher levels of triclosan, further supporting the hypothesis that increasing competition for triclosan to react with free chlorine (a.k.a. decreasing the free chlorine to triclosan ratio) results in preference towards the intermediate phenol products. And as before, high concentrations of byproducts, such as chlorophenols and chloroform, form very quickly when triclosan is exposed to free chlorine. So, not only do high amounts of products form quickly, the soap constituents and free chlorine to triclosan ratio determines what specific products result.

2.3.5: Field Experiments.

The observed variations in the product yields suggest that *a priori* predictions of product formation that are based solely on the triclosan content of a given soap may be difficult if not impossible. Furthermore, differences in the composition of the water are also expected to affect the product yields. To examine product formation under real world conditions, field experiments were performed by augmenting Atlanta, GA and Danville, VA tap waters with antibacterial products. For these experiments, water was obtained from distribution system taps after running the water for more than a half-hour to flush the pipes and reduce fluctuations in water quality. Atlanta tap water had an average free chlorine concentration of 1.0 mg/L, a pH of 6.35, and a temperature of 33 ^{o}C over the experimental time period. Danville maintained a 1.6 mg/L free chlorine residual as Cl_2 with an average pH of 7.22 and a temperature of 38 ^{o}C. Experiments were conducted immediately after obtaining the tap water with products VI (control), VII, IX, and XII. Chloroform and phenol product yields for each field site are illustrated in Figure 13 and triclosan consumption and (chlorophenoxy)phenol production is illustrated in Figure 14.

In the water from the Atlanta distribution system, there was minimal loss of triclosan from soaps IX and XII, but complete consumption for soap VII. In contrast, triclosan was completely consumed from all of the soaps in the experiments with Danville water. While all three (chlorophenoxy)phenol intermediates were detected following the chlorination of Atlanta water, only one dichlorinated intermediate was detected with soap IX in Danville water. In contrast, 2.4-dichlorophenol and 2,4,6-trichlorophenol yields were considerably higher in the Danville water than in the Atlanta water and significant quantities of chloroform above the baseline level were produced in the Danville water. The experiments in Atlanta water resulted in little chloroform formation above the baseline level of 37.6 μg/L (0.31 μM) present in the water coming from the tap.

Relative to the results in laboratory water, the Atlanta and Danville waters generally produced lower levels of chloroform, but higher levels of (chlorophenoxy)phenol intermediates. For the Danville water, although chloroform production was lower than observed in the laboratory, it was still produced at high yield for two of the soaps (0.07-0.17 moles chloroform/mole triclosan; Figure 13). The lower chloroform yields and the lack of triclosan consumption for two of the Atlanta water may be partially attributed to the low pH of the water. As the water pH decreases, the oxidizing power of the residual free chlorine increases and enhances the surface dissolution of copper on the pipe surfaces. The copper oxidation exerts a significant chlorine demand (43) that reduces the reactivity of triclosan towards free chlorine. The resulting interactions between copper and other increased concentration of constituents may significantly decrease the reactivity of chlorine towards triclosan and explains the inconsistencies in the results. In the case of Atlanta water, the pH of 6.35 resulted in increased levels of dissolved constituents, such as copper and zinc, due to the corrosion of pipe materials, as shown by an ICP analysis of the

water (Appendix D). These dissolved constituents may have affected the reactivity of free chlorine and triclosan in an unforeseen manner.

2.4: Potential Health Significance.

The present study has shown that under some circumstances, chloroform levels in excess of the MCL can be detected shortly after triclosan comes into contact with chlorinated water. The ramifications of this previously unidentified chloroform exposure pathway are not known, but require careful evaluation. In an effort to provide insight for future epidemiological studies that examine these exposures, we used a simple exposure model to estimate the potential increase in a person's chloroform exposure that occurs through the use of antibacterial soap.

The exposure model was developed by modification of the Soap and Detergent Association (SDA) model typically used to estimate exposures to volatile contaminants present within soap products (44). The standard SDA model was modified to incorporate the molar yield of chloroform determined from the experiments described herein. For this purpose, the soap weight was modified by the yield of triclosan (Y_{CF}) to obtain an estimated inhalational exposure:

$$\text{Inhalational Exposure}\left(\frac{\text{mg}}{\text{yr}}\right) = \frac{A \times FQ \times TC \times MW_{CF} \times Y_{CF} \times IR \times F \times ED \times T}{MW_{Tric} \times V} \qquad (1)$$

where A = amount of soap used (12.0 g body wash and 1.7 g liquid soap used per use), FQ =frequency (1.07 and 8 uses per day for body wash and liquid soap, repectively), IR = inhalation rate (546 L/hr), F = respirable fraction (0.257), ED = exposure duration (10 minutes for showering, 1 minute for washing hands), T = time correlation factor (365 days/year), V = effective breathing air space (2000 L) and MW_{CF} and MW_{Tric} are the molecular weights of chloroform and triclosan, respectively. Using chloroform yields (Y_{CF}) ranging from 0.07-0.29 (the range observed experimentally) and a triclosan mass concentration (TC) of 2.0 mg triclosan/g soap, the calculated inhalational exposure of chloroform was estimated to range from

5.8-24.2 mg/yr. Neglecting ingestional exposures, but accounting for the expected dermal exposure (typically 15% of an individual's total exposure; ref. (40)), total exposure ranges from 7.5-31.1 mg/yr.

It was possible to estimate how the triclosan-mediated pathway contributes to an individual's overall exposure by assuming an individual's only other chloroform exposure results from the chloroform present in disinfected tap water. For this purpose, a comprehensive model developed by Kim et al (40,45) that estimates an individual's exposure to a variety of drinking water contaminants was utilized. The model uses average values found in literature for a variety of input parameters (such as contaminant properties, shower size, house air exchange rates, etc) to estimate annual chloroform exposures. It predicted that an individual's exposure to chloroform per year as a result of normal water use alone is 0.65 mg per μg/L of chloroform present in the water at the tap. Using this value and the 7.5-31.1 mg chloroform/yr range calculated for the triclosan-mediated pathway, it was possible to construct a graph examining the percentage of an individual's exposure that can be attributed to the use of triclosan-containing antibacterial products. As shown in Figure 15, a person's overall exposure is predicted to be significantly enhanced by their use of antibacterial products that contain triclosan. For tap waters with a chloroform concentration at the MCL of 80 μg/L, the use of triclosan-containing products could increase an individual's overall exposure by 15-40% if the chloroform yield is within the tested range. For waters below the MCL, the percentage of an individual's exposure due to triclosan-use is even higher. The simulations indicate that for those conditions where triclosan reacts to produce chloroform, that the resulting exposure may be significant. We stress, however, that this is a model simulation based on a limited number of laboratory studies and needs to be verified at full scale as can only be done through well-designed epidemiologic studies.

In a household environment, it is not clear that the use of triclosan-containing products provides enhanced antibacterial protection relative to triclosan-free products and accordingly some have argued for the use of plain soap and water in lieu of triclosan-containing soaps (14,18-21). The laboratory and modeling studies described herein indicate that formation of chloroform and other chlorinated daughter products can occur when triclosan-containing antimicrobial products react with free chlorine and that these reactions can potentially lead to enhanced chloroform exposures. Even under conditions where chloroform is limited, other products of potential health concern are produced. This observation, when coupled with the general lack of evidence clearly illustrating the efficacy of triclosan-containing products in the home suggests that these products should be used with caution.

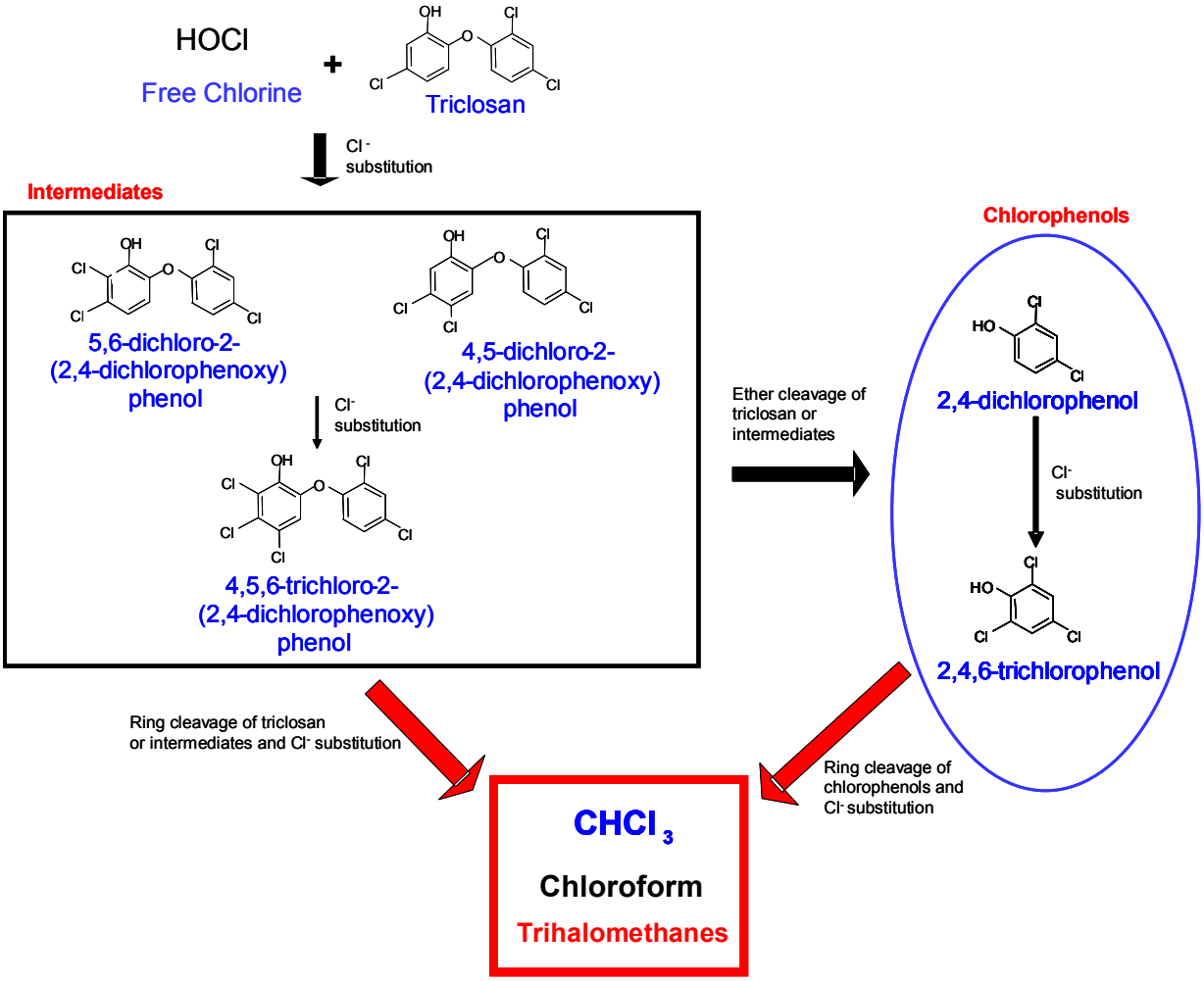

Figure 1: Reaction scheme showing reaction mechanisms and chemical structures for triclosan and its decay products. As detailed in Rule et al. (Environ. Sci. Tech. 2004, 38, 3176-3185), all species were identified either by mass spectral analysis (chlorinated triclosans and chlorophenols) or comparison of retention times of the analyte to known standards (chloroform).

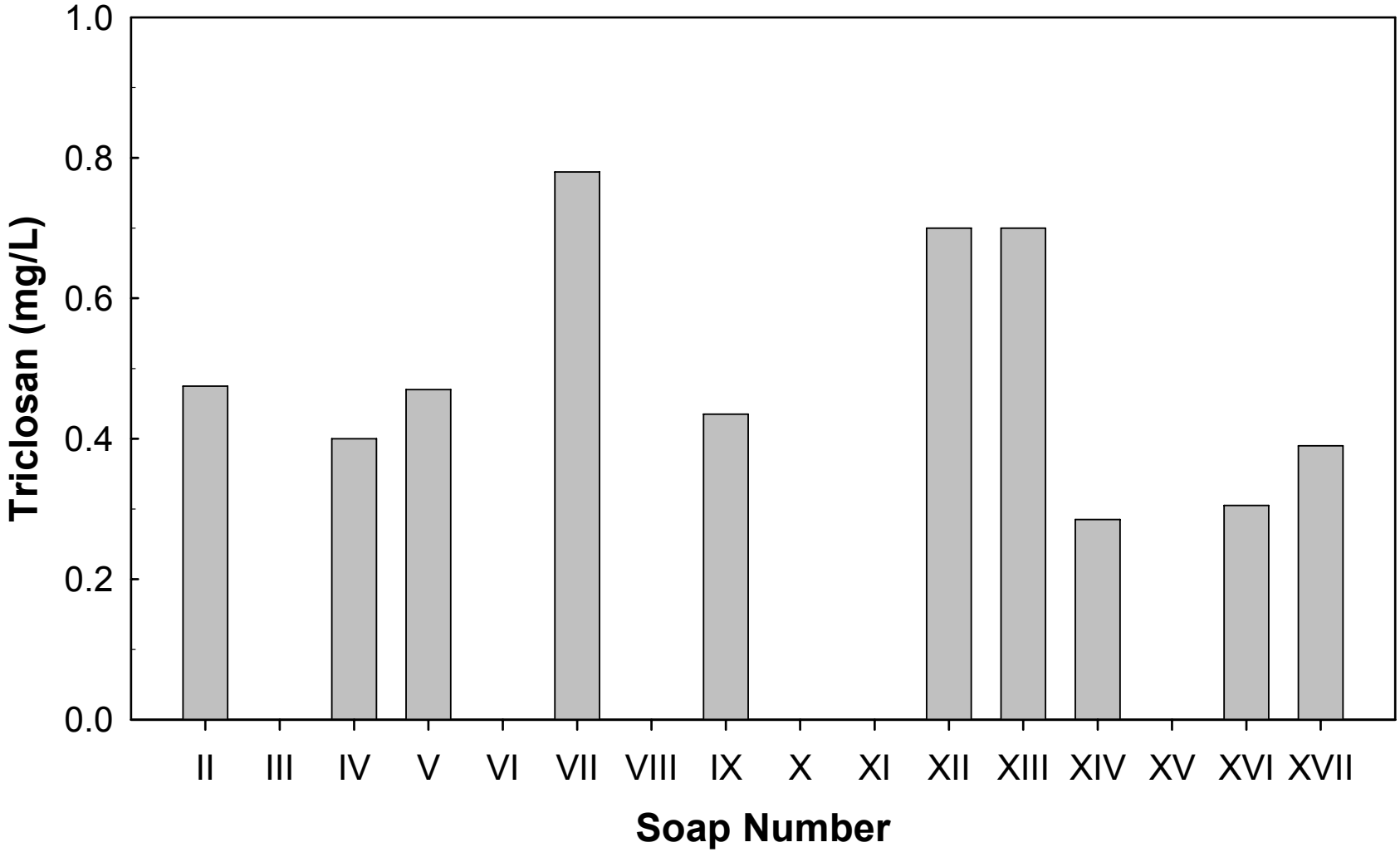

Figure 2: Initial triclosan concentrations in unknown soap solutions where 0.25 g/L of a given soap is added to 1 L of water.

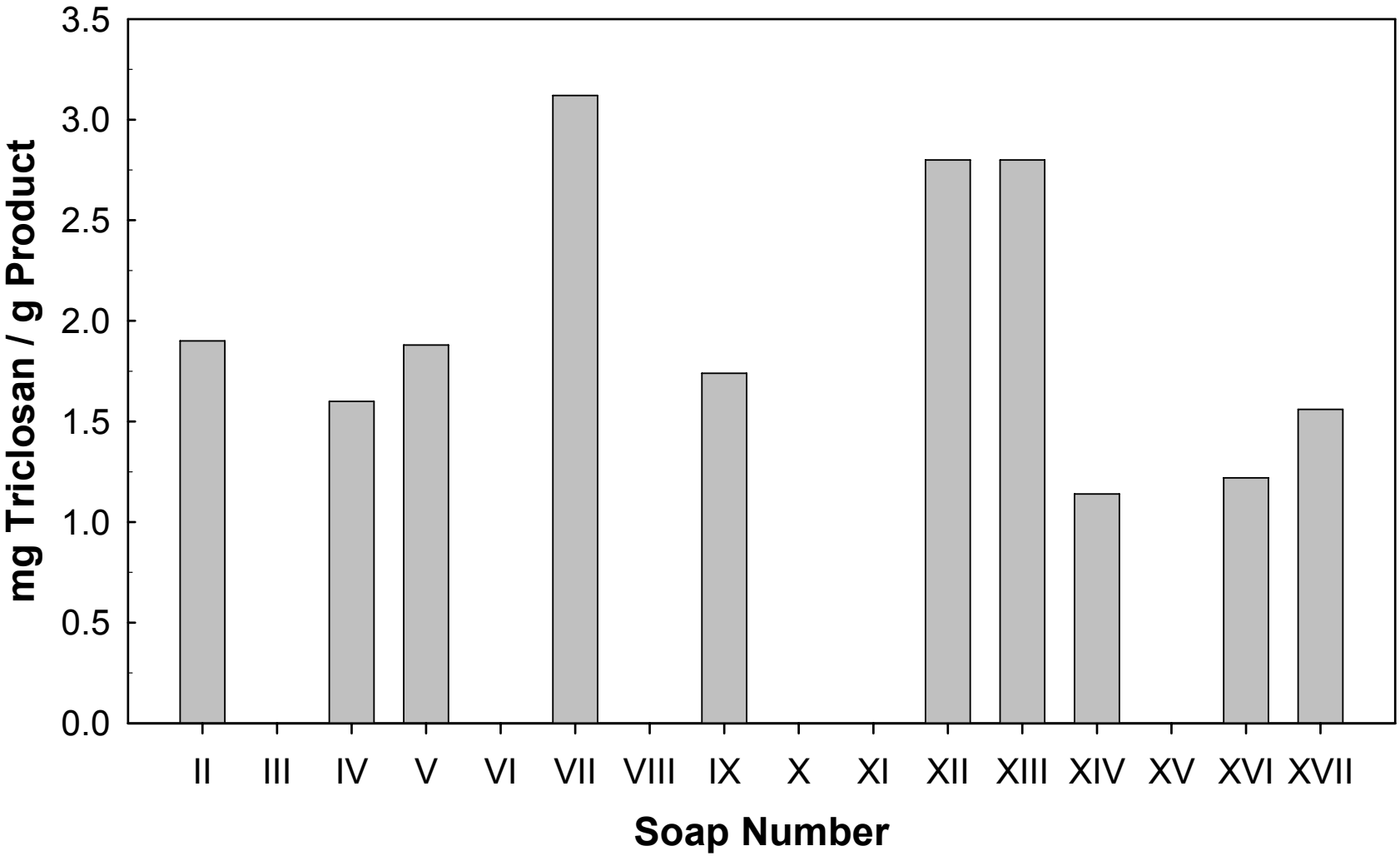

Figure 3: Initial triclosan content in unknown soap products. Soap solutions contain 0.25 g/L of a given soap. Product manufacturers report triclosan content as the percent of the total product weight is triclosan.

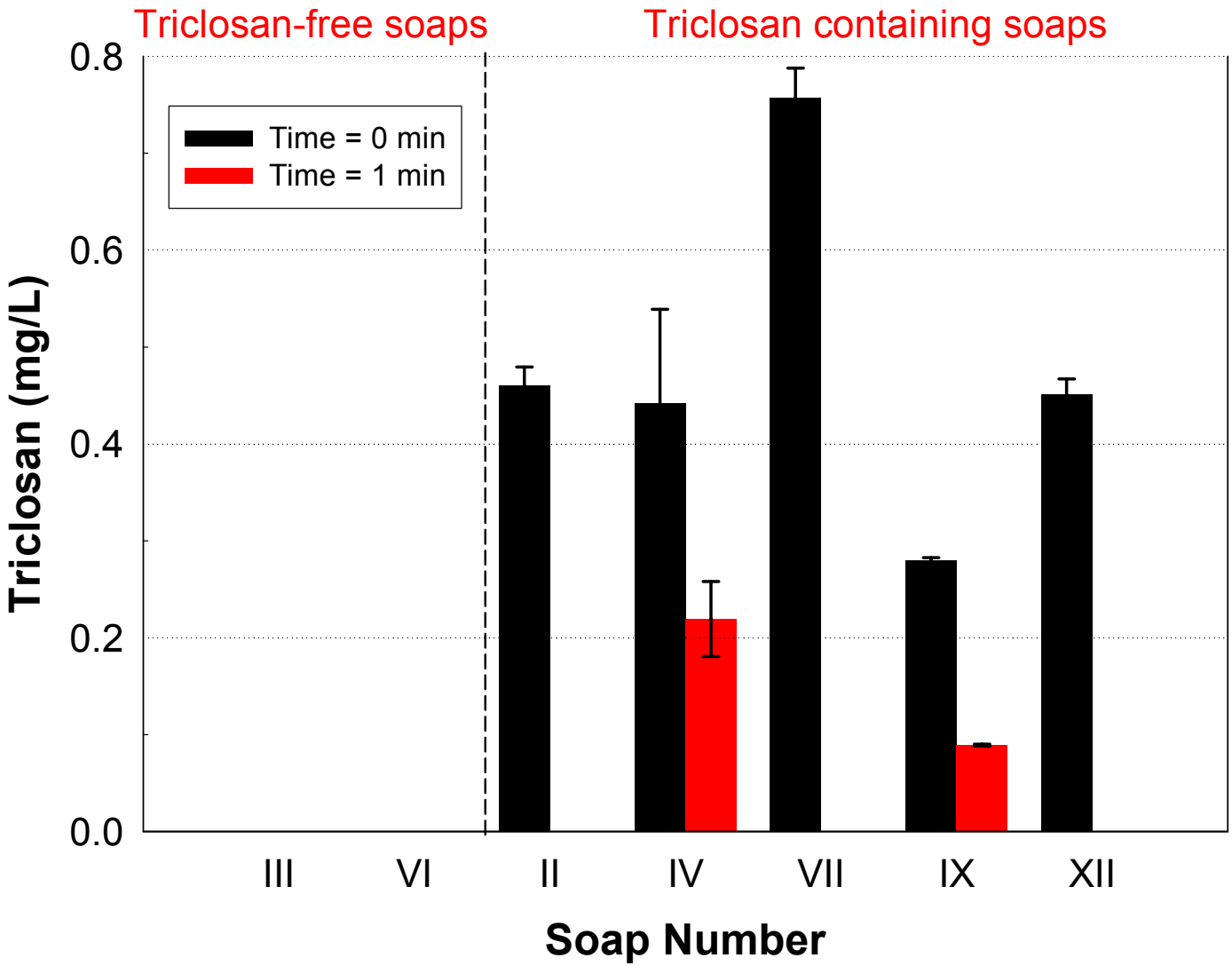

Figure 4: Initial and final triclosan concentrations for several unknown product solutions after one minute of reaction time with free chlorine. Conditions: $[HOCl]_{initial}$ = 2.0 mg/L, $[NaHCO_3]$ = 2 mM, [Soap] = 0.25 g/L, pH = 7.0, T = 40 ^{o}C.

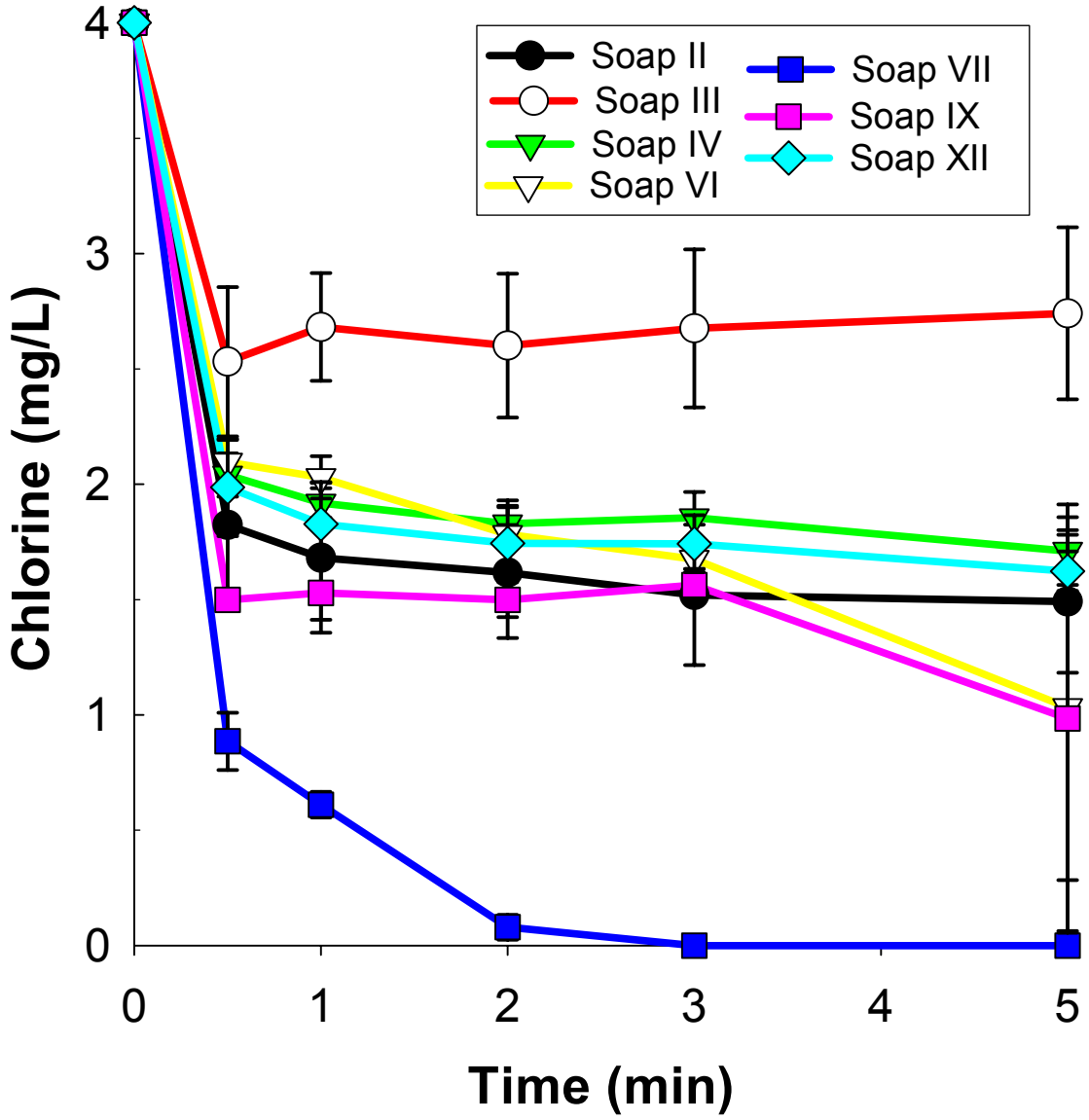

Figure 5: Chlorine consumption when several unknown product solutions are contacted with free chlorine (triclosan containing products=●,▲; triclosan free products=○,Δ). Conditions: $[HOCl]_{initial}$ = 4.0 mg/L, $[NaHCO_3]$ = 2 mM, [Soap] = 0.25 g/L, pH = 7.0, T = 40 °C.

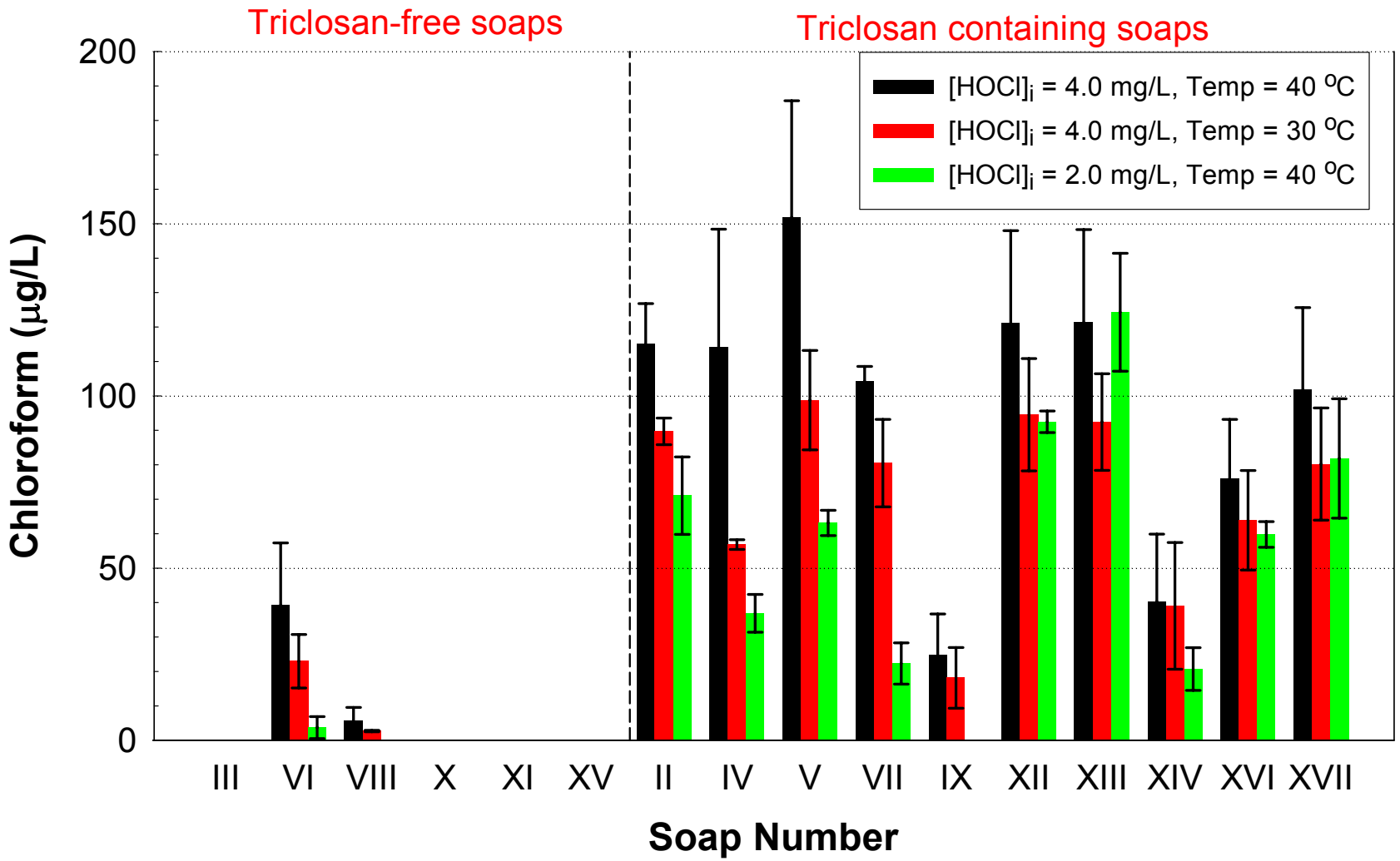

Figure 6: Effects of varying temperature and initial chlorine concentration on chloroform formation in all unknown soaps after 1 minute of contact with free chlorine. Conditions: [$NaHCO_3$] = 2 mM, pH = 7.0, [Soap] = 0.25 g/L, Temperature and [$HOCl]_{initial}$ included in legend.

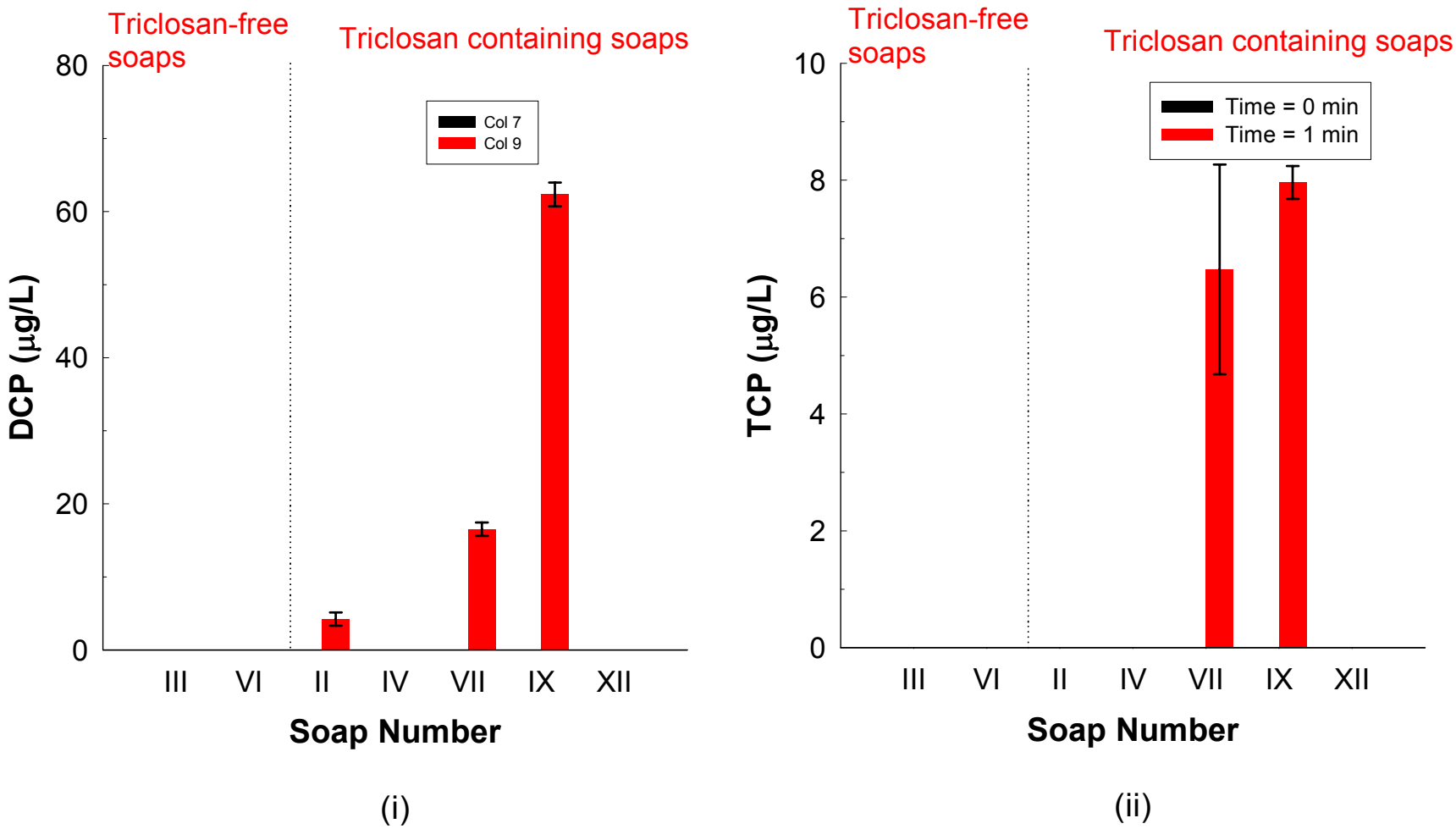

Figure 7: 2,4-dichlorophenol (i) and 2,4,6-trichlorophenol (ii) formation after 1 minute of contact with free chlorine. No products were detected at time zero. Conditions: $[HOCl]_{initial}$ = 2.0 mg/L, $[NaHCO_3]$ = 2 mM, [Soap] = 0.25 g/L, pH = 7.0, T = 40 °C.

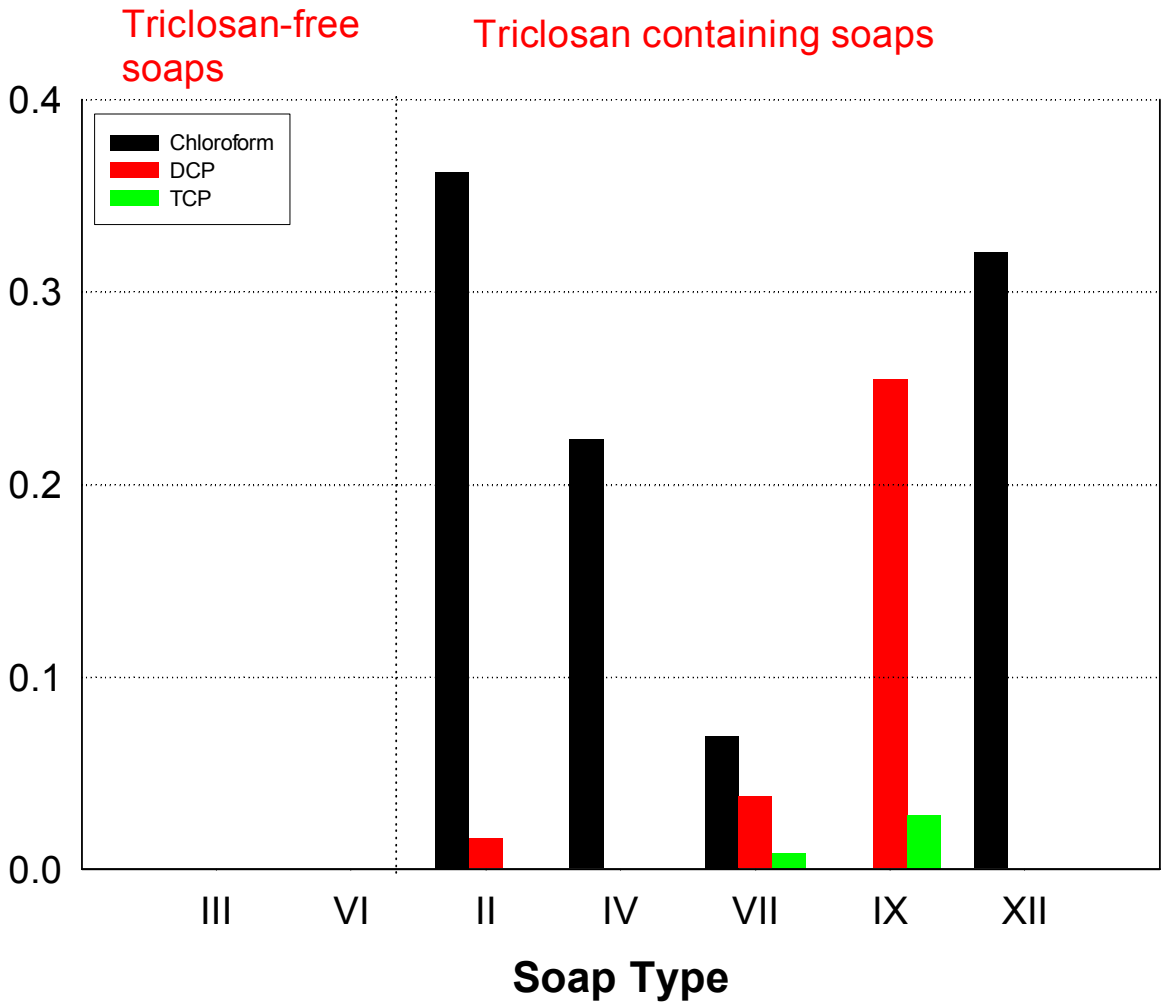

Figure 8: Yields of chloroform, 2,4-dichlorophenol, and 2,4,6-trichlorophenol after 1 minute of exposure to free chlorine. Conditions: $[HOCl]_{initial}$=2.0 mg/L, $[NaHCO_3]$ = 2 mM, [Soap] = 0.25 g/L, pH = 7.0, T = 40 ^{o}C.

$$Yield = \frac{[product](moles)}{[triclosan]_{initial}(moles)}$$

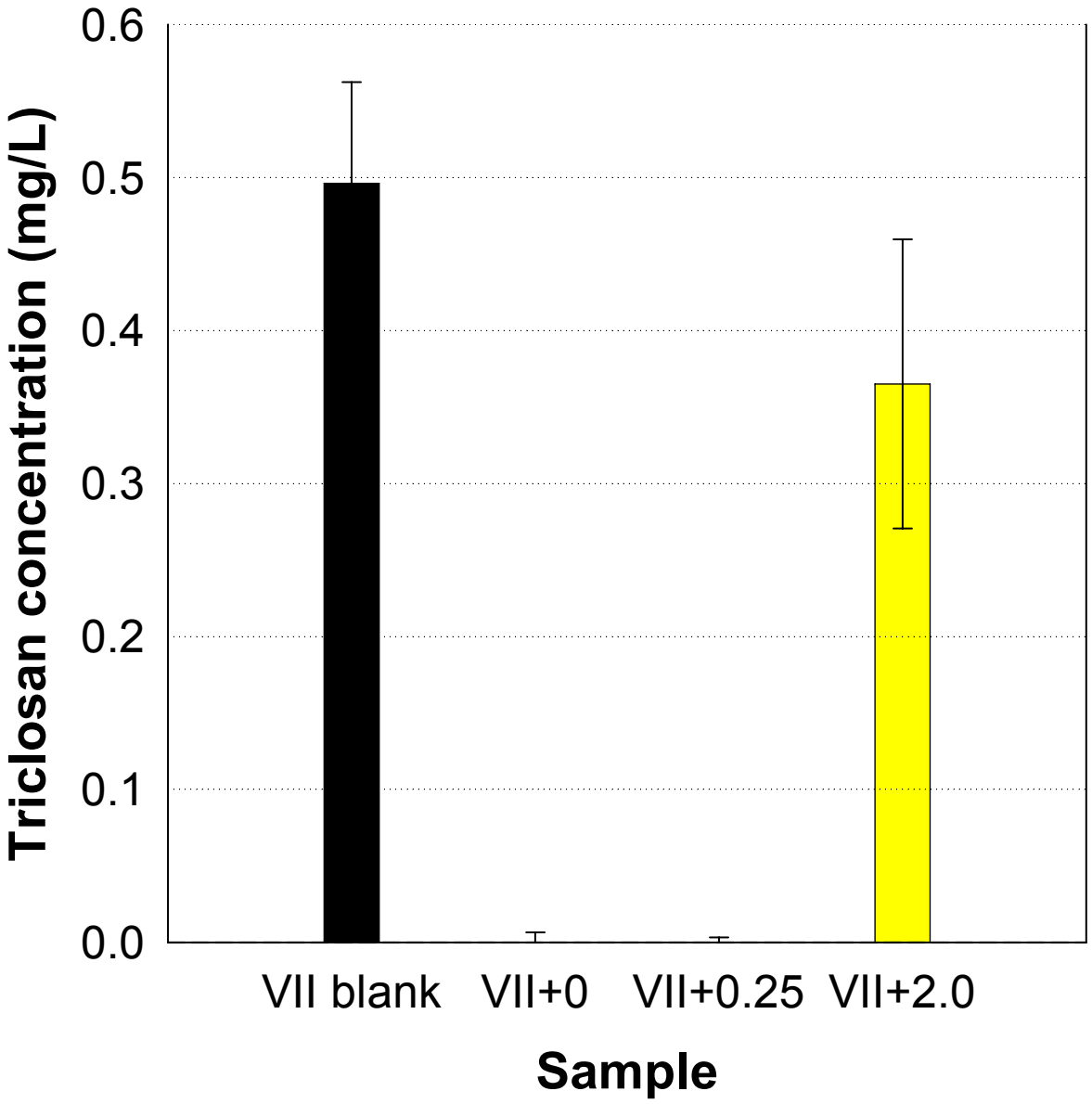

Figure 9: Initial triclosan concentration (blank) compared with triclosan concentrations after 1 minute of reaction time for soap VII solutions spiked with varying additional triclosan concentrations. Conditions: $[HOCl]_{initial}$ = 2.0 mg/L, [Soap] = 0.25 g/L, pH = 7.0, T = 40 ^{o}C. Triclosan only remained in after 1 minute when 2.0 mg/L of triclosan was added and free chlorine was completely consumed in all cases for the reaction period.

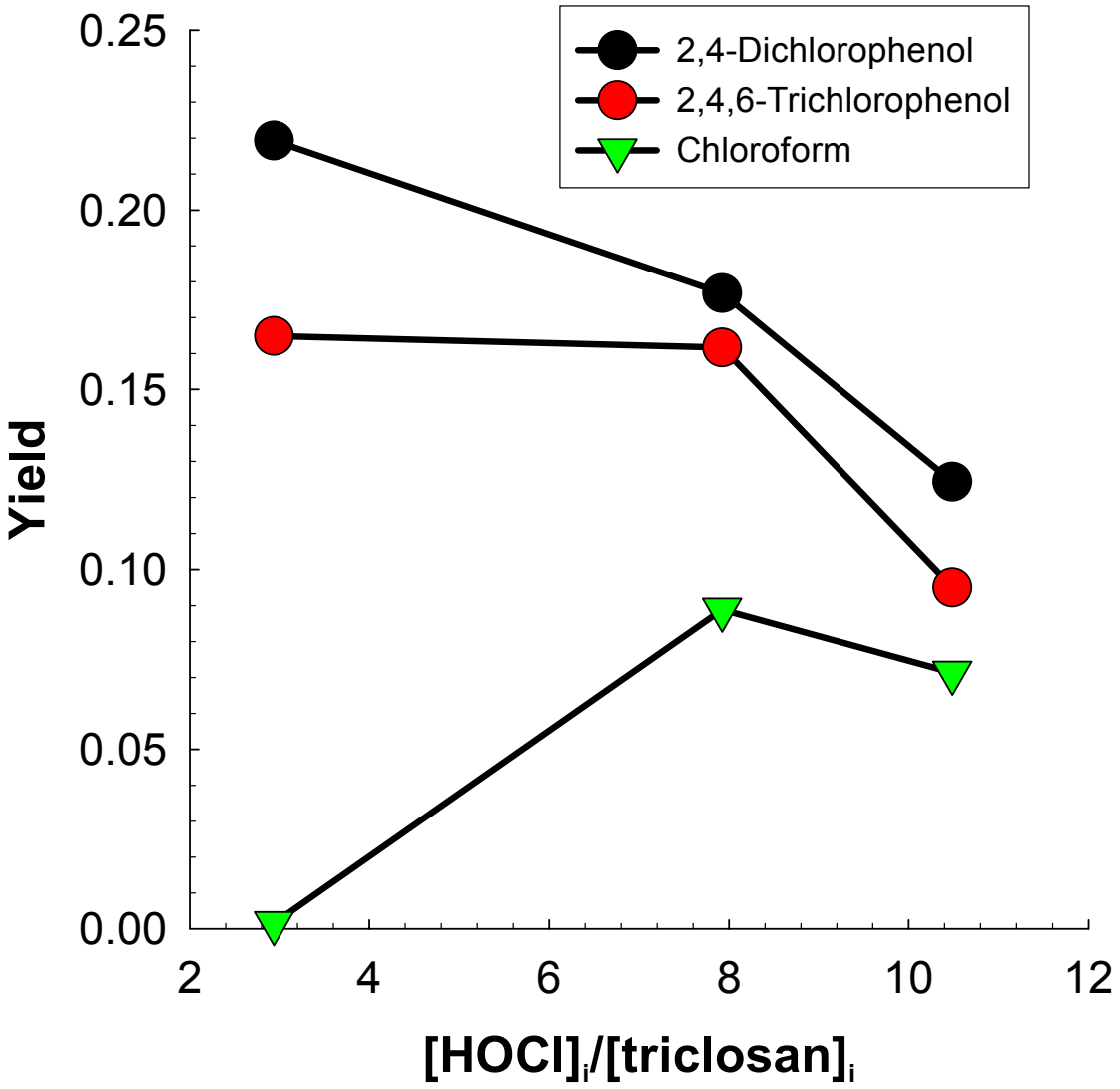

Figure 10: Product yields versus the free chlorine to triclosan ratio for Soap VII spiked with varying amounts of triclosan. Soap VII with no spike represented by $[HOCl]_i/[triclosan]_i = 10.5$; Soap VII with a spike of 0.25 mg/L represented by $[HOCl]_i/[triclosan]_i = 7.9$; Soap VII with a 2.0 mg/L spike denoted by $[HOCl]_i/[triclosan]_i = 2.9$. Conditions: $[HOCl]_i = 2.0$ mg/L, $[NaHCO_3] = 2$ mM, [Soap VII] = 0.25 g/L, Temperature = 40 ^oC, reaction time = 1 minute.

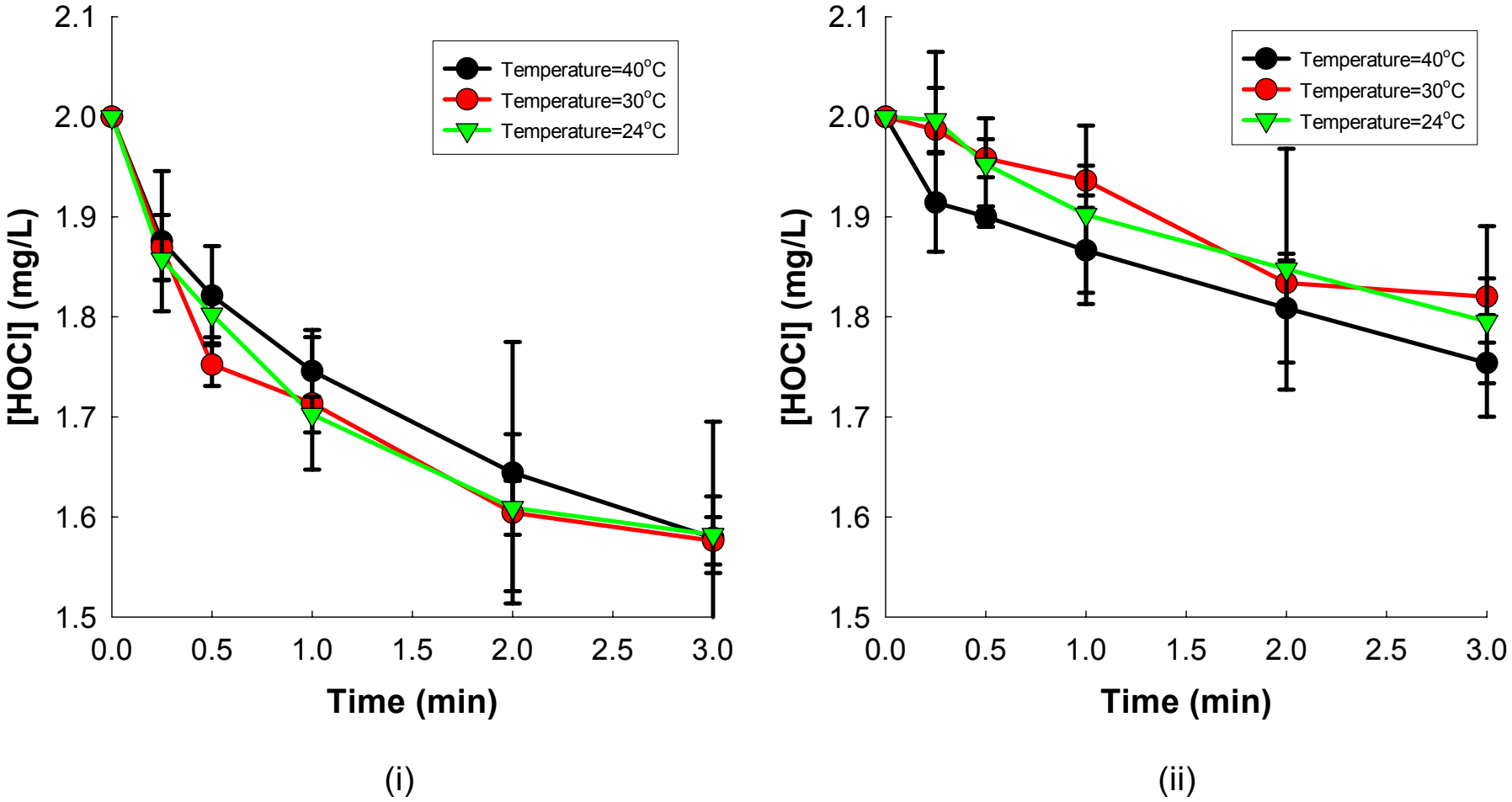

Figure 11: Free chlorine consumption varying with temperature in pure triclosan experiments. Conditions: $[HOCl]_i$=2.0 mg/L, $[NaHCO_3]$=2 mM, pH=7.0, $[triclosan]_i$= 0.780 mg/L (i) and 0.285 mg/L (ii). Triclosan was completely consumed by the first sampling time (15 sec) for both cases.

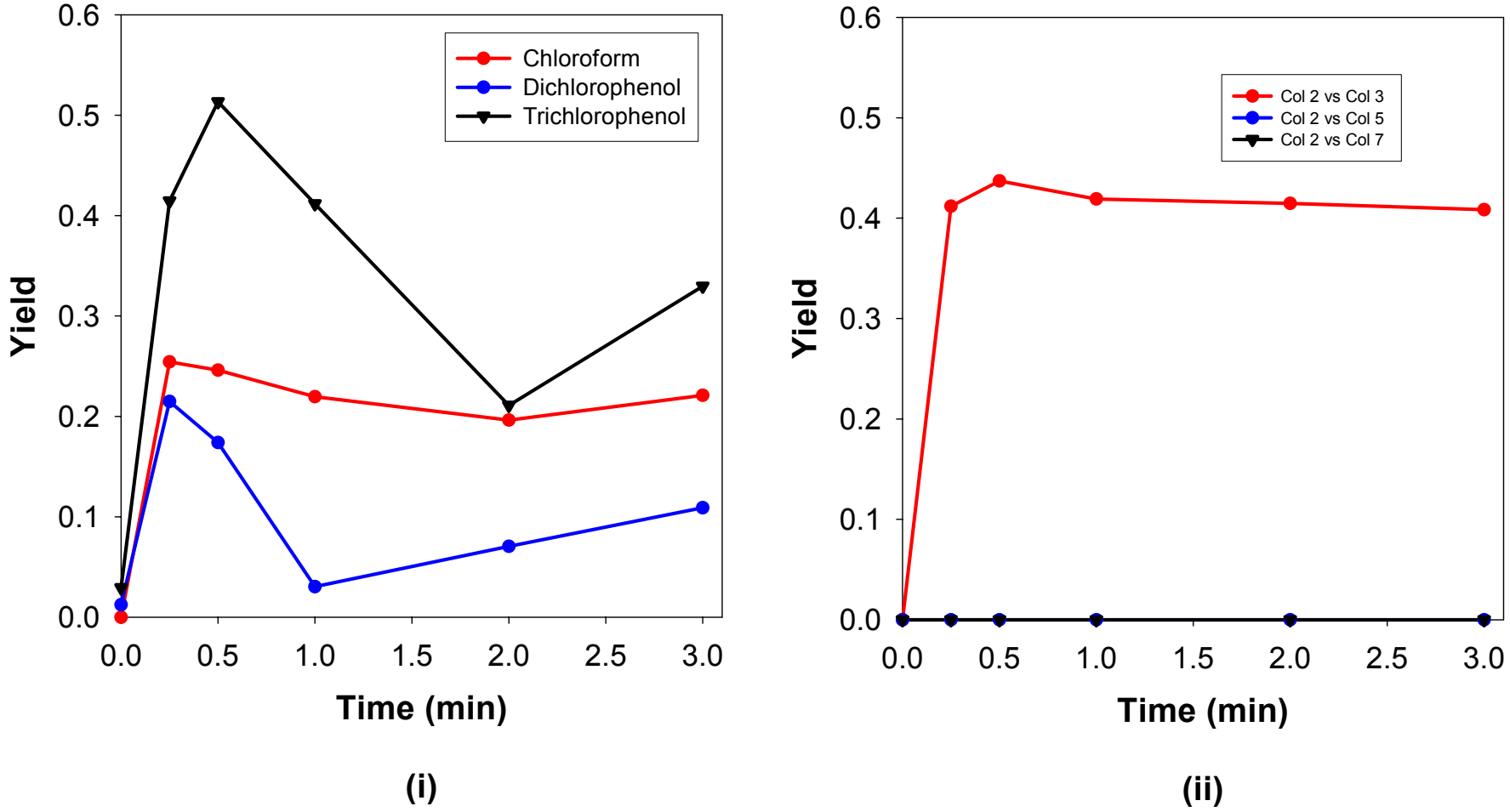

Figure 12: Chloroform, 2,4-dichlorophenol, and 2,4,6-trichlorophenol formation yields in pure triclosan experiments with $[triclosan]_i$= 0.780 mg/L (i) and 0.285 mg/L(ii). Experiments ran with $[triclosan]_i$= 0.285 mg/L did not have any chlorophenols detected during the reaction time. Conditions: $[HOCl]_i$=2.0 mg/L, $[NaHCO_3]$=2 mM, pH=7.0.

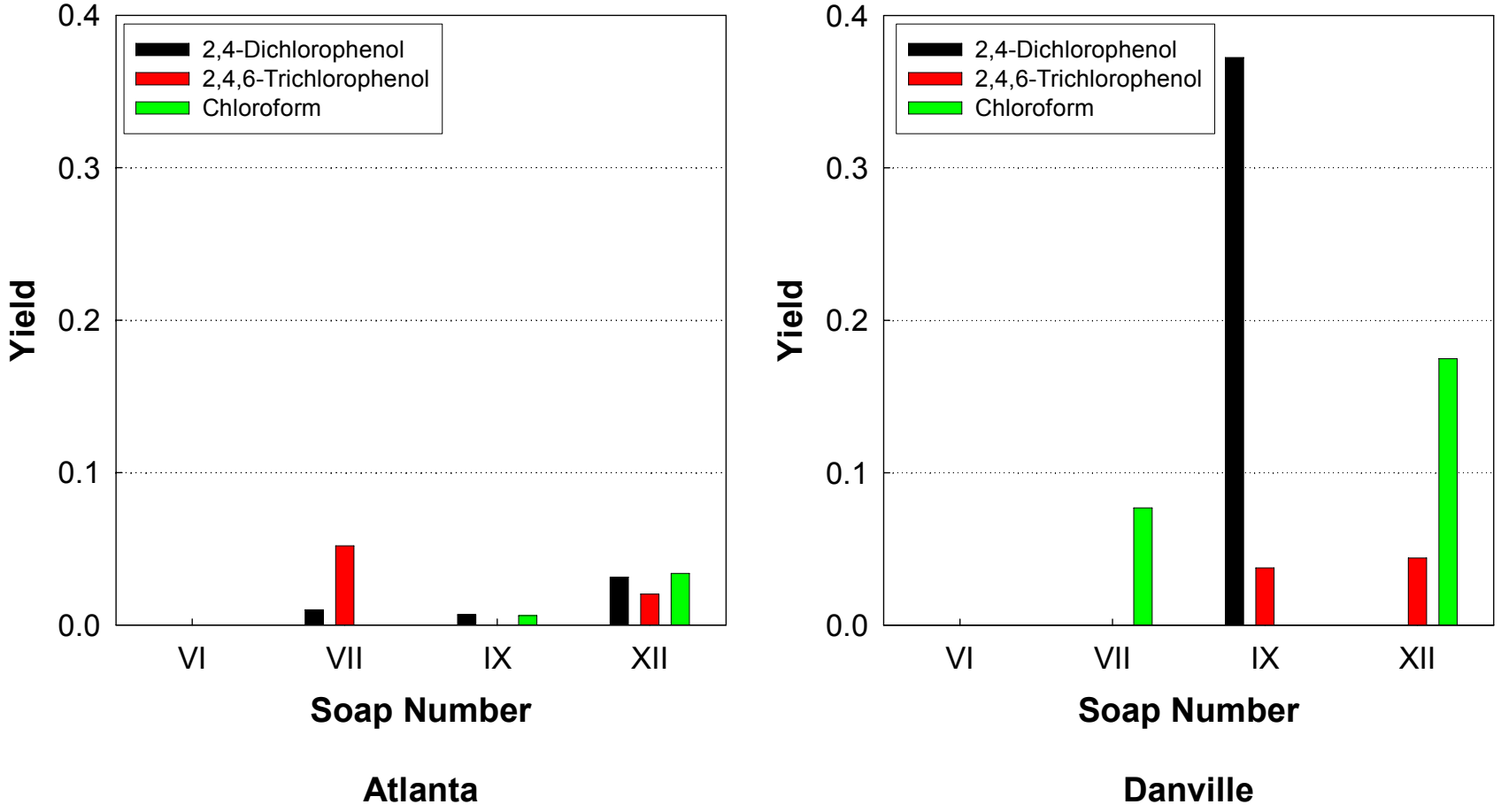

Figure 13: Product yield comparisons between Atlanta and Danville field experiments after 1 minute of reaction time. Atlanta conditions: $[HOCl]_i$ = 1.0 mg/L, [Soap] = 0.25 g/L, Temperature = 33 °C, pH = 6.35. Danville conditions: $[HOCl]_i$ = 1.6 mg/L, [Soap] = 0.25 g/L, Temperature = 38 °C, pH = 7.22.

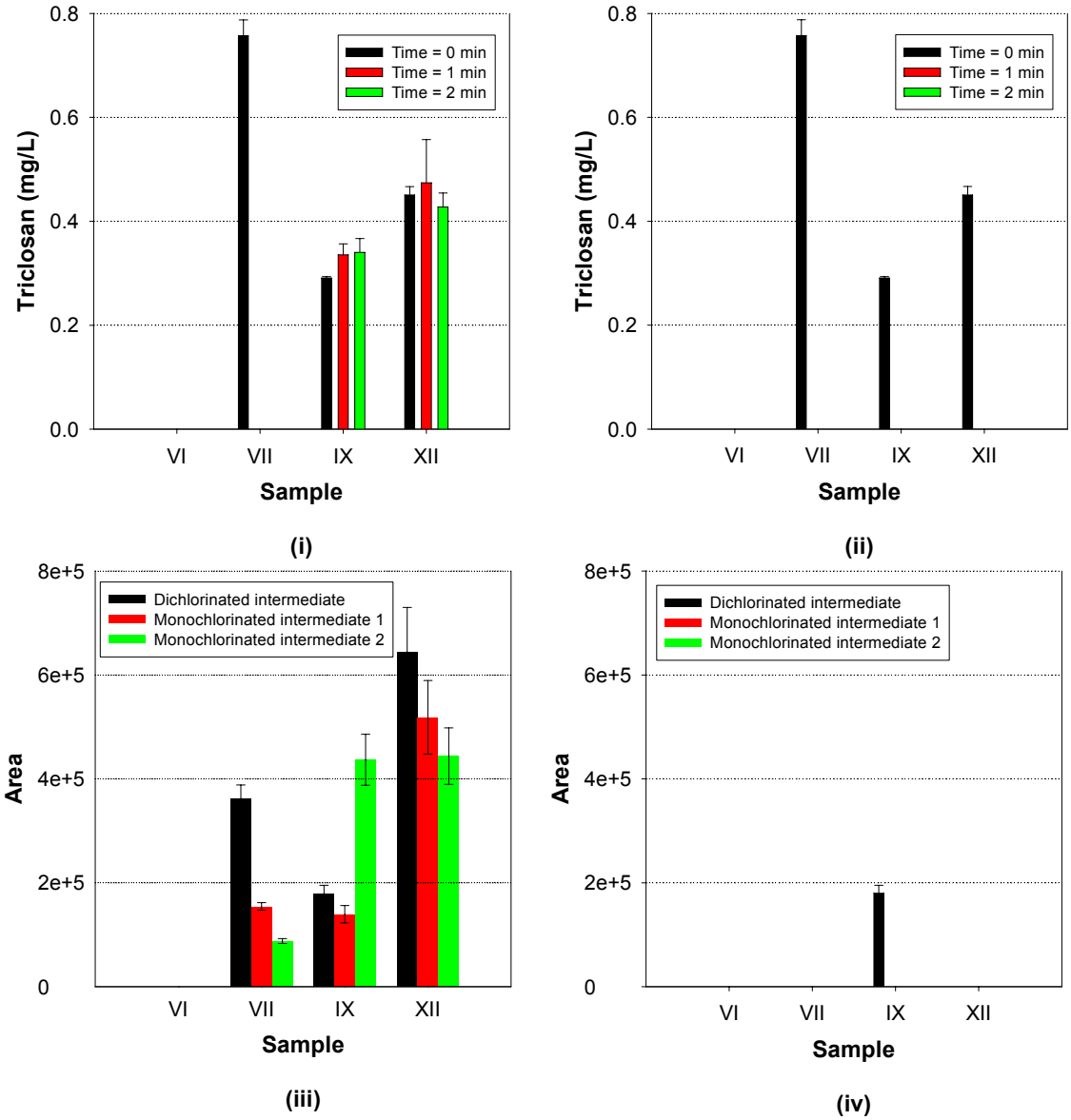

Figure 14: Triclosan consumption and (chlorophenoxy)phenol formation in Atlanta and Danville experiments: (i) = triclosan consumption in Atlanta, (ii) = triclosan consumption in Danville, (iii) intermediate formation in Atlanta, (iv) = intermediate formation in Danville.

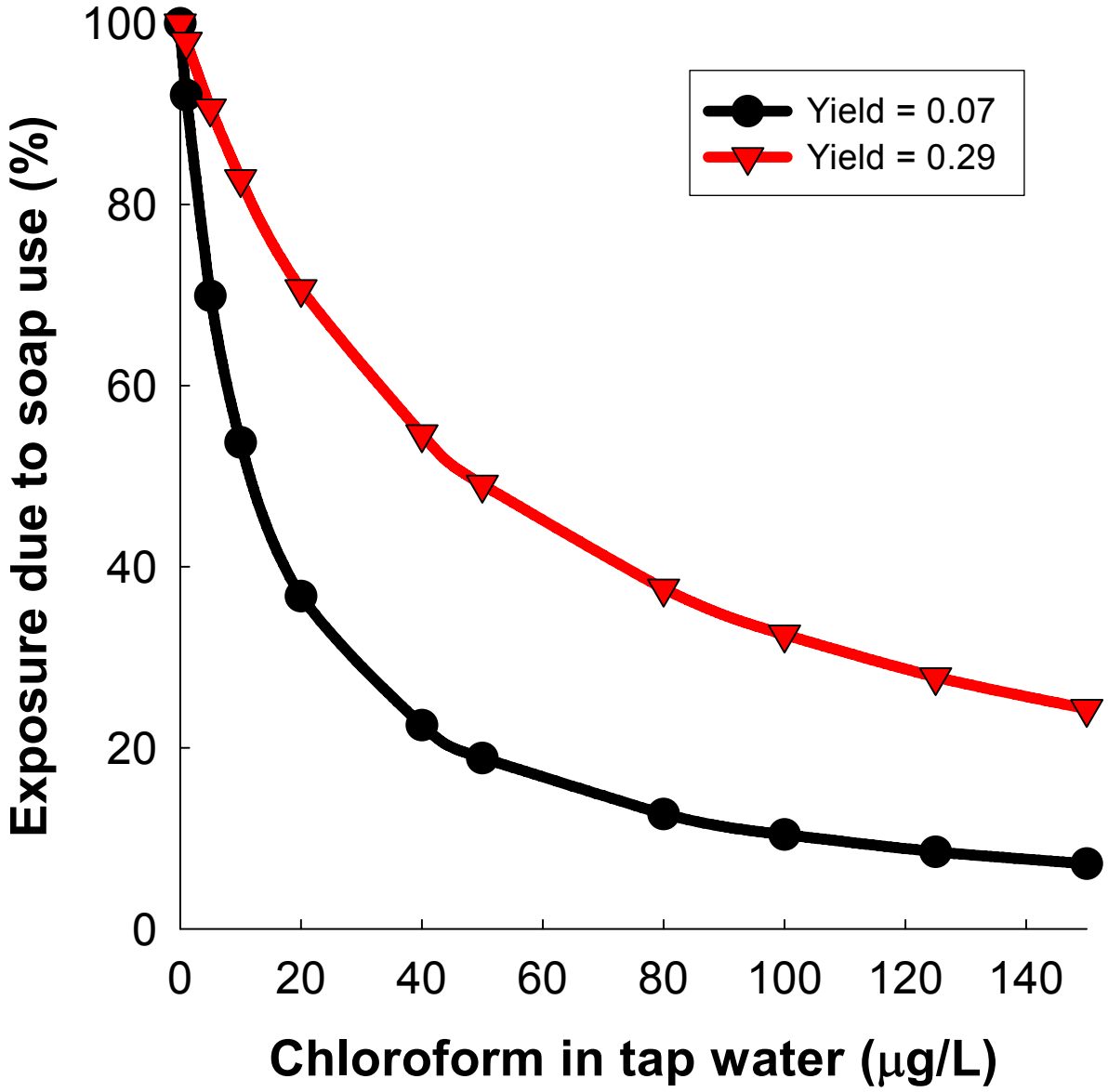

Figure 15: Estimated exposure due to chloroform formation from normal antibacterial soap use as predicted by the comparison of the SDA model to the output of the computerized model from Kim et al [22]. The figure illustrates the percentage of an individual's exposure that results from the use of different soaps as a function of the chloroform concentration already present at the tap.

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Supplementary Information

Formation of Chloroform and Other Chlorinated Byproducts Due to the Chlorination of Antibacterial Products

E. Matthew Fiss, Krista L. Rule, and Peter J. Vikesland

Appendix A

Experimental Products and Ingredients

Table A 1: List of products various products tested and their corresponding triclosan concentrations. The predicted solution triclosan concentrations were also included for soaps where the manufacturer published ingredient information.

Product	Triclosan content	Predicted Solution Triclosan Concentration
Antibacterial Products	**%**	**(mg/L)**
Dial Mountain Fresh Antibacterial Body Wash	0.15	0.375
Equate Island Spring Antibacterial Body Wash	??	
Softsoap Antibacterial plus Real Moisturizing Lotion Hand Soap	0.125	0.3125
Dial Berry Splash Antibacterial Hand Soap	??	
Bath and Body Works Moonlight Path Antibacterial Deep Cleansing Hand Soap	0.3	0.75
Body Essence Cucumber Melon Antibacterial Hand Lotion	??	
Ultra Palmolive Antibacterial Dish Soap	0.12	0.3
Control Products		
Ultra Palmolive Oxy-Plus Dish Soap	0	
Ultra Concentrated Natural Citrus Joy Dish Soap	0	
Seventh Generation Natural Dish Soap	0	
Softsoap Naturals Milk and Honey Liquid Hand Soap	0	
Gojo Lotion Skin Cleaner (Durham Hall's bathroom soap)	0	

Table A 2: Ingredients found in product tested other than triclosan. (* denotes that ingredient information was not available)

Dial Mountain Fresh Antibacterial Body Wash	Equate Island Spring Antibacterial Body Wash	Softsoap Antibacterial plus Real Moisturizing Lotion Hand Soap	Dial Berry Splash Antibacterial Hand Soap
triclosan	triclosan	triclosan	triclosan
water	water	water	water
sodium laureth sulfate	sodium laureth sulfate	sodium laureth sulfate	sodium laureth sulfate
cocamidopropyl betaine	cocamidolpropyl betaine	cocamidopropyl betaine	decyl glucoside
PEG-8	PET-8	petrolatum	cocamidopropyl betaine
fragrance	glycerin	dimethicone	sodium chloride
glycerin	disodium laureth sulfosuccinate	lauric acid	cocamide MEA
isostearamidopropyl morpholine lactate	fragrance	decyl glucoside	fragrance
polyquaternium-10	polyquaternium-10	acrylates/C10-30 alkyl acrylate crosspolymer	PEG-120 methyl glucose dioleate
cocamidopropyl PG-dimonium chloride	PEG-7 glyceryl cocoate	hydroxypropyl methylcellulose	PEG-18 glyceryl oleate/cocoate
DMDM hydantoin	DMDM hydantoin	fragrance	aloe barbadensis leaf juice
citric acid	iodopropynyl butyl carbamate	triethanolamine	polyquaternium-7
tetrasodium EDTA	citric acid	DMDM hydantoin	DMDM hydantoin
sodium chloride	tetrasodium EDTA	polyquaternium-39	tetrasodium EDTA
red 33	FD&C blue #1	tetrasodium EDTA	citric acid
blue 1	D&C red #33	polyquaternium-7	sodium sulfate
		D&C orange #4	red 33
		FD&C red #40	red 4

Bath and Body Works Moonlight Path Antibacterial Deep Cleansing Hand Soap	Body Essence Cucumber Melon Antibacterial Hand Lotion	Ultra Palmolive Antibacterial Dish Soap	* Ultra Palmolive Oxy-Plus Dish Soap
triclosan	triclosan	triclosan	water
water	water	water	sodium dodecylbenzene sulfonate
sodium trideceth sulfate	stearic acid	ammonium C12-15 pareth sulfate	ethanol
hydrogenated soybean oil	sunflower seed oil	magnesium dodecylbenzenesulfonate	methanol
sodium lauroamphoacetate	C12-15 alkyl ethylhexanoate	lauramidopropylamine oxide	sulfuric acid
petrolatum	cetyl alcohol	SD alcohol 3-A	sodium bisulfite
cocamide MEA	dimethicone	sodium xylenesulfonate	hydrogen peroxide
glycerin	triethanolamine	sodium chloride	
ammonium chloride	cucucumber fruit extract	fragrace	
fragrace	aloe barbadensis leaf extract	pentasodium pentetate	
propylene glycol	hydrolyzed silk	DMDM hydantoin	
tocopheryl acetate (vitamin E acetate)	panthenol (pro vitamin B5)	sodium bisulfite	
artemia extract	tocopheryl acetate (vitamin E)	D&C orange #4	
echinacea purpurea (coneflower) extract	retinyl palmitate (vitamin A)		
butyrospermum parkii (shea butter)	wheat germ oil		
cellulose	DEA-cetyl phosphate		
hydroxypropyl methylcellulose	fragrance		
guar hydroxypropyltrimonium chloride	jojoba esters		
tetinyl palmitate (vitamin A palmitate)	nylon 12		
benzophenone-4	glyceryl stearate		
citric acid	PEG-100 stearate		
imidazolidinyl urea	polyacrylamide		
DMDM hydantion	C13-14 isoparaffin		
tetrasodium EDTA	laureth-7		
mica	carbomer		
titanium dioxide	xanthan gum		
ultramaries	BHT		
yellow 5	phenoxyethanol		
red 4	methylparaben		
	ethylparaben		
	propylparaben		
	butylparaben		
	ultramarines		
	FD&C yellow #5		

* Ultra Concentrated Natural Citrus Joy Dish Soap	Seventh Generation Natural Dish Soap	Softsoap Naturals Milk and Honey Liquid Hand Soap	* Gojo Lotion Skin Cleaner (Durham Hall's bathroom soap)
water	water	water	water
protease	natural fragrance (citrus oil)	sodium C14-16 olefin sulfonate	ammonium chloride
ethanol	preservative	lauramide DEA	sodium lauryl sulfate
	corn and/or coconut-based surfactants	glycol stearate	
		sodium chloride	
		cocamidopropyl betaine	
		fragrance	
		DMDM hydantoin	
		polyquaternium-7	
		citric acid	
		aloe barbadensis gel	
		tetrasodium EDTA	
		honey	
		lactose	
		milk protein	
		glycerin	
		silk peptide	
		hydrolyzed silk protein	
		D&C yellow #10	
		FD&C red #40	

Appendix B

Quality Assurance/Quality Control

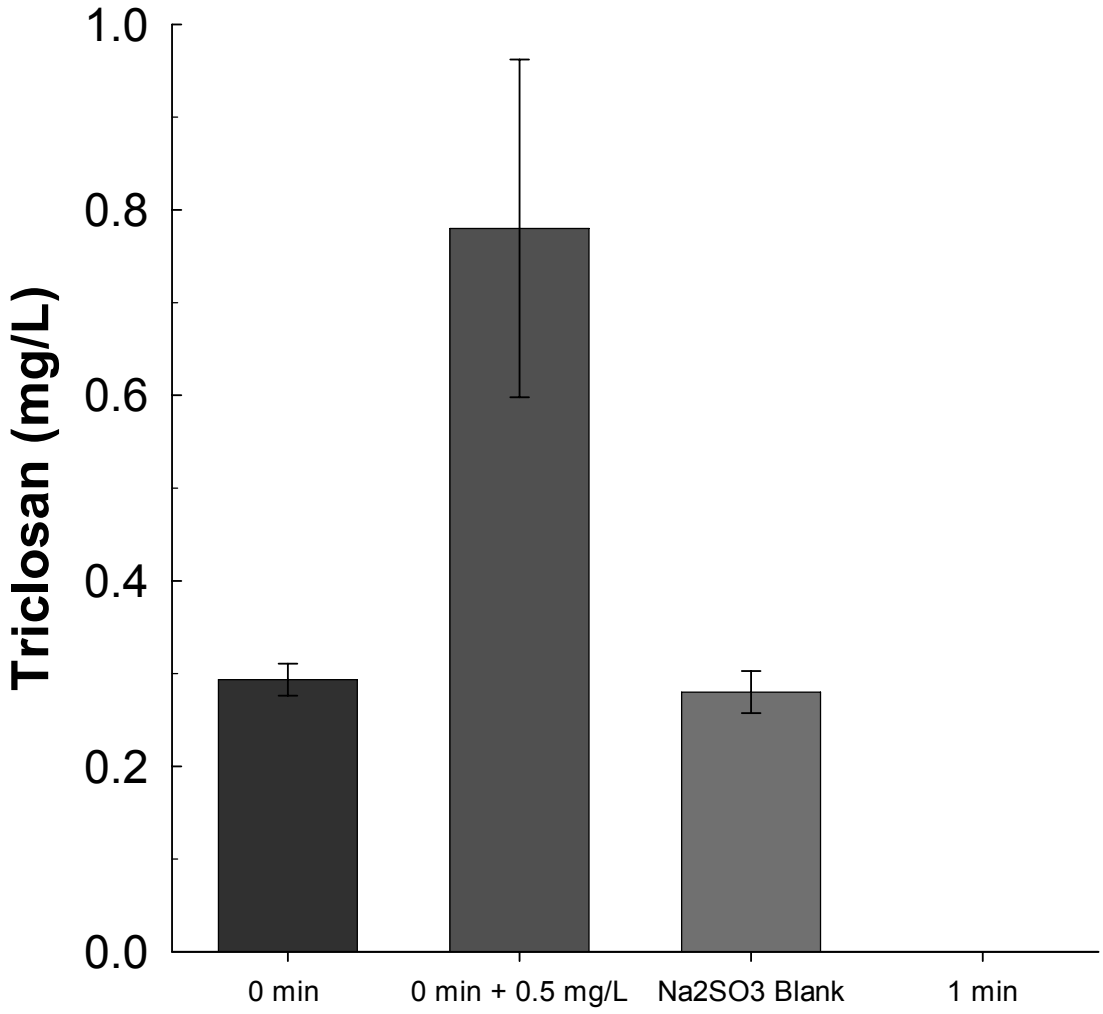

Figure B 1: Spike recovery experiments where 0.5 mg/L of triclosan was added to a soap solution initially containing 0.30 mg/L of triclosan and the amount of triclosan recovered was recorded. A second comparison was made to a soap sample when an equivalent aliquot of sodium sulfite solution was added. The spiked triclosan was completely recovered, and sodium sulfite had no affect on the recovery amount.

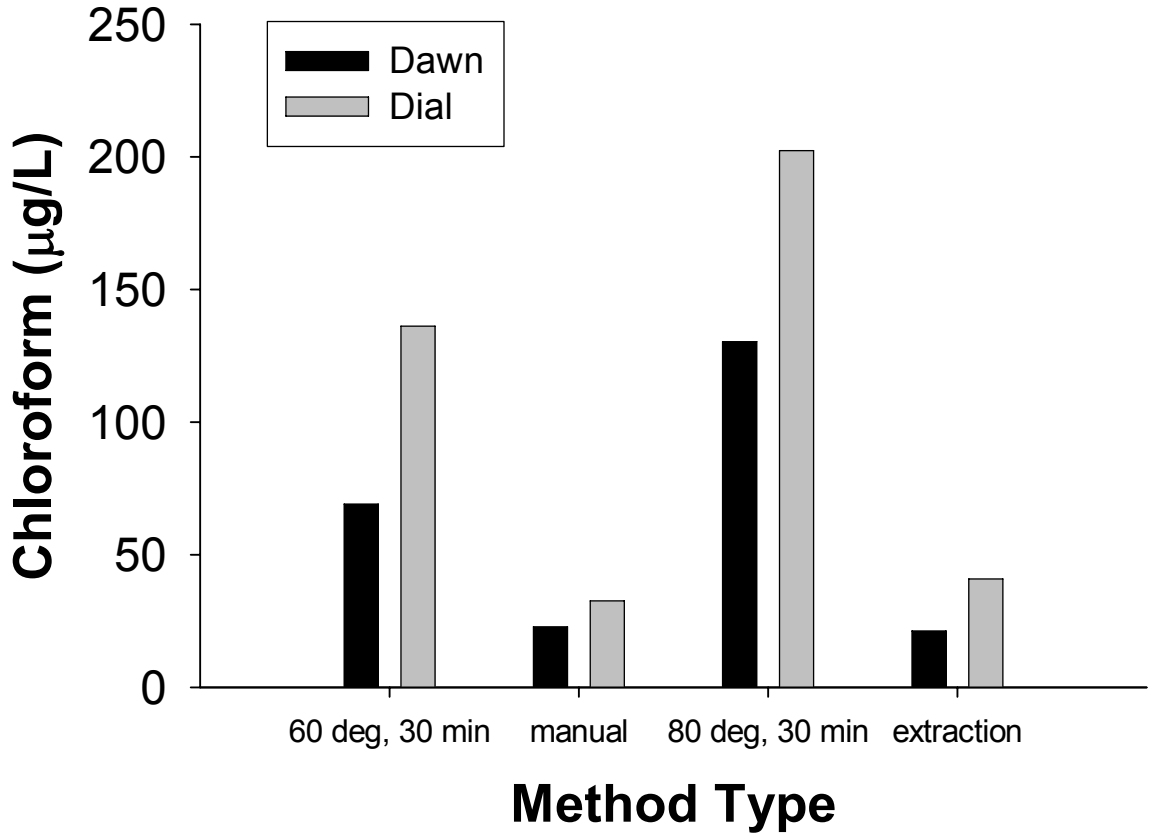

Figure B 2: Method comparison for different chloroform analysis methods. Using a GC-ECD incubation temperature of 60 °C for 30 minutes was determined to be the best method. The other GC-ECD method with higher incubation temperature was inadequate since 80 °C is higher than the boiling temperature for chloroform, so all of the byproduct was being boiled out of the solution. The emulsion formed by the soaps while using the extraction method prevented the chloroform from being totally removed efficiently. Using manual injections was also determined to be a poor predictor since leaks from punctures in the injection valve septa failed to close fully after injections and resulted in a loss of chloroform.

Appendix C

Laboratory Experiment Data Summary

Table C 1: Summary table for calibration curve equation values for all laboratory experiments. The regression equation is in the form y=ax+b.

Curve Reference Number	Calibration Constituent	Regression Values		
		a	b	r^2
1	chloroform	153542.461	498634.539	0.995
2	chloroform	111128.702	627457.462	0.996
3	chloroform	84115.904	285412.462	0.996
4	chloroform	337714.677	1069993.462	0.996
5	chloroform	226381.931	1939417.692	0.994
6	chloroform	74544.085	943556.624	0.984
7	chloroform	68943.352	1147537.892	0.978
8	chloroform	59128.186	598092.571	0.980
9	chloroform	46742.617	414207.649	0.992
10	chloroform	59125.186	598092.571	0.980
11	free chlorine	0.122	0.074	0.988
12	triclosan	7.094	-0.298	0.995
13	triclosan	8.665	-0.269	0.995
14	dichlorophenol	0.034	-0.171	0.989
15	dichlorophenol	0.041	-0.251	0.994
16	trichlorophenol	0.035	-0.143	0.993
17	trichlorophenol	0.037	-0.157	0.995

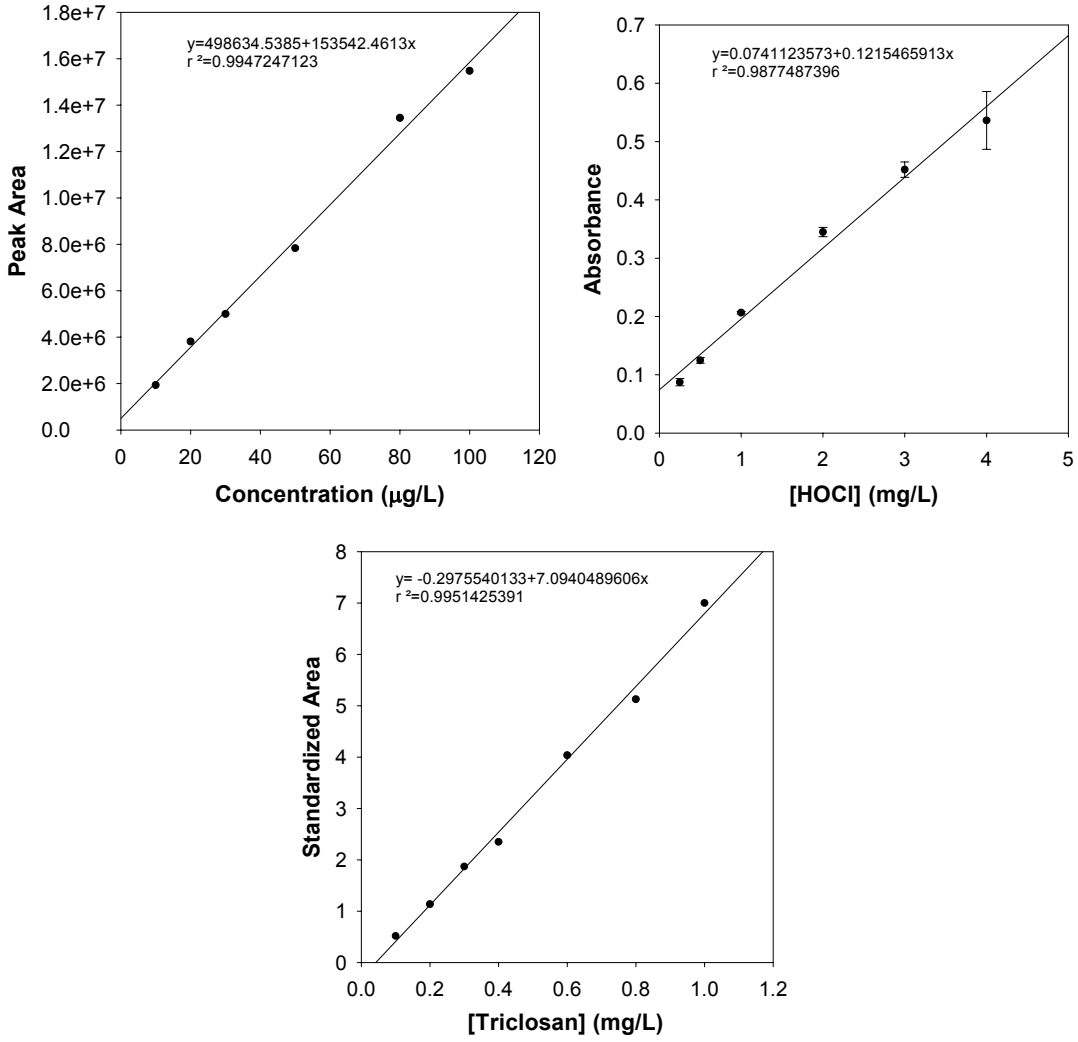

Figure C 1: Example calibration curves for chloroform, free chlorine, and triclosan, respectively. All calibration curve equation values are included in Table C 1.

Table C 2: Summary of data obtained during experiments with Product II. Initial laboratory conditions.

Product II

Trihalomethane Analysis

Incubation Temperature 60 °C
Incubation Time 30 min
pH 7.0
[$NaHCO_3$] 2 mmol

Sample Date	$[HOCl]_i$ (mg/L)	Rxn. Temp. (°C)	Rxn. Time (min)	Repetition	Calibration Curve Reference	Chloroform Area	Chloroform Concentration (ppb)	Chloroform Average Concentration (ppb)	Chloroform Standard Deviation
1/30/2006	4.0	40	0		1			0.000	0.000
1/31/2006	4.0	40	1	1	1	16764166	105.935		
1/31/2006	4.0	40	1	2	2	14886835	128.314	115.005	11.776
2/1/2006	4.0	40	1	3	3	9602573	110.766		
2/9/2006	4.0	30	0		4			0.000	0.000
2/10/2006	4.0	30	1	1	4	47424425	137.259		
2/12/2006	4.0	30	1	2		GC ERROR		134.535	3.853
2/13/2006	4.0	30	1	3	5	31778908	131.810		
2/22/2006	2.0	40	0		6			0.000	0.000
2/23/2006	2.0	40	1	1	6	7177194	83.624		
2/23/2006	2.0	40	1	2	7	5791158	67.354	71.017	11.232
2/24/2006	2.0	40	1	3	8	4268366	62.073		
2/27/2006	2.0	30			9			0.000	0.000
2/27/2006	2.0	30	1	1	9	5062255	99.439		
2/28/2006	2.0	30	1	2	10	3837515	82.165	90.802	12.215
3/1/2006	2.0	30	1	3		GC ERROR			

Chlorine Decay Analysis

Calibration Curve Reference 11
Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol

Repetition	Time (min)	Abs.	Cell #	Cell Abs.	Soap Blank Abs.	Corrected Abs.	Chlorine Concentration (mg/L)	Time (min)	Average [HOCl] (mg/L)	Standard Deviation
1	0		1	0.0026			4.00	0	4.00	0.00
	0.5	0.3806	2	0.0023	0.0911	0.2898	1.77	0.5	1.82	0.31
	1	0.3646	3	0.0056	0.0911	0.2705	1.61	1	1.68	0.32
	2	0.3461	4	0.0011	0.0911	0.2565	1.50	2	1.62	0.28
	3	0.3183	5	-0.0005	0.0911	0.2303	1.28	3	1.52	0.30
	5	0.3256	6	-0.0001	0.0911	0.2372	1.34	5	1.49	0.31
2	0		13	-0.0005			4.00			
	0.5	0.3608	14	0.0006	0.0979	0.2618	1.54			
	1	0.3447	15	0.0029	0.0979	0.2434	1.39			
	2	0.3483	16	0.0044	0.0979	0.2455	1.41			
	3	0.3427	17	-0.0013	0.0979	0.2456	1.41			
	5	0.3300	18	0.0012	0.0979	0.2304	1.29			
3	0		7	0.0030			4.00			
	0.5	0.4157	8	0.0031	0.0800	0.3356	2.15			
	1	0.3994	9	0.0012	0.0800	0.3212	2.03			
	2	0.3834	10	-0.0035	0.0800	0.3099	1.94			
	3	0.3826	11	0.0050	0.0800	0.3006	1.86			
	5	0.3791	12	0.0035	0.0800	0.2986	1.85			

Product II Continued…

Triclosan Concentration

Calibration Curve Reference n/a
Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol
$[HOCl]_i$ 4.0 mg/L

Run Number	(mg triclosan / L)	(mg triclosan / g soap)
1	0.49	1.96
2	0.46	1.84
AVERAGE	0.48	1.90
Standard Deviation	0.02	0.08

Triclosan Consumption and Phenol Formation

Calibration Curve Reference Triclosan 12 DCP 14 TCP 16
Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol
$[HOCl]_i$ 4.0 mg/L

			Area				Concentration		
Reaction Time (min)	Date/Time	File Name	Internal Std.	Triclosan	DCP	TCP	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)
0	3/31/2006 3:04	10.D	142980	402482	1426	2376	0.4387	0.3117	0.5431
	3/31/2006 3:39	11.D	147647	444086	2225	1113	0.4659	0.4709	0.2463
	3/31/2006 4:13	12.D	140929	433561	1923	1390	0.4756	0.4264	0.3223
1	3/31/2006 4:48	13.D	146113	1998	18551	982	0.0439	3.9676	0.2196
	3/31/2006 5:23	14.D	142511	772	23841	710	0.0427	5.2279	0.1628
	3/31/2006 5:57	15.D	128828	246	14272	1106	0.0422	3.4620	0.2806
5	3/31/2006 6:32	16.D	148776	399	32120	1117	0.0423	6.7467	0.2454
	3/31/2006 7:06	17.D	142761	373	18042	754	0.0423	3.9493	0.1726
	3/31/2006 7:41	18.D	147315	171	26706	500	0.0421	5.6652	0.1109

	Average			Standard Deviation		
Reaction Time (min)	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)
0	**0.4601**	**0.4030**	**0.3706**	**0.0191**	**0.0822**	**0.1541**
1	**0.0429**	**4.2192**	**0.2210**	**0.0009**	**0.9094**	**0.0589**
5	**0.0422**	**5.4537**	**0.1763**	**0.0001**	**1.4106**	**0.0673**

Table C 3: Summary of data obtained during experiments with Product III. Initial laboratory conditions.

Product III

Trihalomethane Analysis

Incubation Temperature 60 °C
Incubation Time 30 min
pH 7.0
[$NaHCO_3$] 2 mmol

Sample Date	$[HOCl]_i$ (mg/L)	Rxn. Temp. (°C)	Rxn. Time (min)	Repetition Number	Calibration Curve Reference	Chloroform Area	Chloroform Concentration (ppb)	Chloroform Average Concentration (ppb)	Chloroform Standard Deviation
1/30/2006	**4.0**	**40**	0		1	ND	ND	**0.000**	**0.000**
1/31/2006	**4.0**	**40**	1	1	1	ND	ND		
2/1/2006	**4.0**	**40**	1	2	2	362479	-2.384	**0.000**	**0.000**
2/1/2006	**4.0**	**40**	1	3	3	ND	ND		
2/9/2006	**4.0**	**30**	0		4	ND	ND	**0.000**	**0.000**
2/10/2006	**4.0**	**30**	1	1	4	ND	ND		
2/12/2006	**4.0**	**30**	1	2		GC ERROR	ND	**0.000**	**0.000**
2/13/2006	**4.0**	**30**	1	3	5	351183	-7.016		
2/22/2006	**2.0**	**40**	0		6	ND	ND	**0.000**	**0.000**
2/23/2006	**2.0**	**40**	1	1	6	ND	ND		
2/23/2006	**2.0**	**40**	1	2	7	ND	ND	**#DIV/0!**	**#DIV/0!**
2/24/2006	**2.0**	**40**	1	3	8	ND	ND		
2/27/2006	**2.0**	**30**			9	ND	ND	**0.000**	**0.000**
2/27/2006	**2.0**	**30**	1	1	9	ND	ND		
2/28/2006	**2.0**	**30**	1	2	10	ND	ND	**#DIV/0!**	**#DIV/0!**
3/1/2006	**2.0**	**30**	1	3		GC ERROR	ND		

Chlorine Decay Analysis

Calibration Curve Reference 11
Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol

Repetition	Time (min)	Abs.	Cell #	Cell Abs.	Soap Blank Abs.	Corrected Abs.	Chlorine Concentration (mg/L)	Time (min)	Average [HOCl] (mg/L)	Standard Deviation
1	0		7	0.0030			4.00	0	**4.00**	**0.00**
	0.5	0.4418	8	0.0031	0.0925	0.3492	2.26	0.5	**2.53**	**0.32**
	1	0.4821	9	0.0012	0.0925	0.3914	2.61	1	**2.68**	**0.23**
	2	0.4442	10	-0.0035	0.0925	0.3582	2.34	2	**2.60**	**0.31**
	3	0.4606	11	0.0050	0.0925	0.3661	2.40	3	**2.67**	**0.34**
	5	0.4574	12	0.0035	0.0925	0.3644	2.39	5	**2.74**	**0.37**
2	0		1	0.0026			4.00			
	0.5	0.4490	2	0.0023	0.0788	0.3705	2.44			
	1	0.4587	3	0.0056	0.0788	0.3769	2.49			
	2	0.4578	4	0.0011	0.0788	0.3805	2.52			
	3	0.4614	5	-0.0005	0.0788	0.3857	2.56			
	5	0.4787	6	-0.0001	0.0788	0.4026	2.70			
3	0		13	-0.0005			4.00			
	0.5	0.4796	14	0.0006	0.0530	0.4255	2.89			
	1	0.4881	15	0.0029	0.0530	0.4317	2.94			
	2	0.49	16	0.0044	0.0530	0.4321	2.94			
	3	0.4983	17	-0.0013	0.0530	0.4461	3.06			
	5	0.5093	18	0.0012	0.0530	0.4546	3.13			

Product III continued…

Triclosan Concentration

Calibration Curve Reference n/a
Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol
$[HOCl]_i$ 4.0 mg/L

Run Number	(mg triclosan / L)	(mg triclosan / g soap)
1	0.00	0.00
2	0.00	0.00
AVERAGE	0.00	0.00
Standard Deviation	0.00	0.00

Triclosan Consumption and Phenol Formation

Calibration Curve Reference Triclosan 12 DCP 14 TCP 16
Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol
$[HOCl]_i$ 4.0 mg/L

Reaction Time			Area				Concentration		
min	Date/Time	File Name	Internal Std.	Triclosan	DCP	TCP	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)
0	3/31/2006 8:15	19.D	153930	1982	1009	1281	0.0438	0.2048	0.2720
	3/31/2006 8:50	20.D	162252	1851	1282	1459	0.0436	0.2469	0.2939
	3/31/2006 9:24	21.D	137457	1775	1232	1574	0.0438	0.2801	0.3742
1	3/31/2006 9:59	22.D	171212	159	1560	509	0.0421	0.2847	0.0972
	3/31/2006 10:33	23.D	154505	636	514	947	0.0425	0.1040	0.2003
	3/31/2006 11:08	24.D	154094	351	325	440	0.0423	0.0659	0.0933
5	3/31/2006 11:43	25.D	162378	130	2212	474	0.0421	0.4257	0.0954
	4/1/2006 12:17	26.D	153379	200	373	167	0.0421	0.0760	0.0356
	4/1/2006 12:52	27.D	168835	431	1750	323	0.0423	0.3239	0.0625

Reaction Time	Average			Standard Deviation		
(min)	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)
0	**0.0437**	**0.2439**	**0.3133**	**0.0001**	**0.0377**	**0.0538**
1	**0.0423**	**0.1515**	**0.1303**	**0.0002**	**0.1169**	**0.0607**
5	**0.0422**	**0.2752**	**0.0645**	**0.0001**	**0.1799**	**0.0300**

Table C 4: Summary of data obtained during experiments with Product IV. Initial laboratory conditions.

Product IV

Trihalomethane Analysis

Incubation Temperature 60 °C
Incubation Time 30 min
pH 7.0
[$NaHCO_3$] 2 mmol

Sample Date	$[HOCl]_i$ (mg/L)	Rxn. Temp. (°C)	Rxn. Time (min)	Repetition Number	Calibration Curve Reference	Chloroform Area	Chloroform Concentration (ppb)	Chloroform Average Concentration (ppb)	Chloroform Standard Deviation
1/30/2006	4.0	40	0		1			0.000	0.000
1/31/2006	4.0	40	1	1	1	15889073	100.236		
2/1/2006	4.0	40	1	2	2	17649009	153.170	114.182	34.217
2/1/2006	4.0	40	1	3	3	7783551	89.141		
2/9/2006	4.0	30	0		4			0.000	0.000
2/10/2006	4.0	30	1	1	4	29516085	84.231		
2/12/2006	4.0	30	1	2		GC ERROR		85.226	1.408
2/13/2006	4.0	30	1	3	5	21458441	86.222		
2/22/2006	2.0	40	0		6			0.000	0.000
2/23/2006	2.0	40	1	1	6	3912976	39.834		
2/23/2006	2.0	40	1	2	7	3253453	30.546	36.869	5.480
2/24/2006	2.0	40	1	3	8	2976601	40.226		
2/27/2006	2.0	30			9			0.000	0.000
2/27/2006	2.0	30	1	1	9	2111762	36.317		
2/28/2006	2.0	30	1	2	10	1972447	41.677	38.997	3.790
3/1/2006	2.0	30	1	3		GC ERROR			

Chlorine Decay Analysis

Calibration Curve Reference 11
Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol

Repetition	Time (min)	Abs.	Cell #	Cell Abs.	Soap Blank Abs.	Corrected Abs.	Chlorine Concentration (mg/L)	Time (min)	Average [HOCl] (mg/L)	Standard Deviation
1	0		13	-0.0005			4.00	0	4.00	0.00
	0.5	0.4346	14	0.0006	0.1108	0.3227	2.04	0.5	2.04	0.09
	1	0.4139	15	0.0029	0.1108	0.2997	1.86	1	1.92	0.06
	2	0.4031	16	0.0044	0.1108	0.2874	1.75	2	1.83	0.10
	3	0.4137	17	-0.0013	0.1108	0.3037	1.89	3	1.85	0.11
	5	0.3764	18	0.0012	0.1108	0.2639	1.56	5	1.71	0.15
2	0		7	0.0030			4.00			
	0.5	0.4313	8	0.0031	0.1210	0.3102	1.94			
	1	0.4261	9	0.0012	0.1210	0.3069	1.92			
	2	0.4058	10	-0.0035	0.1210	0.2913	1.79			
	3	0.4075	11	0.0050	0.1210	0.2845	1.73			
	5	0.4040	12	0.0035	0.1210	0.2825	1.71			
3	0		1	0.0026			4.00			
	0.5	0.4081	2	0.0023	0.0754	0.3330	2.13			
	1	0.3936	3	0.0056	0.0754	0.3152	1.98			
	2	0.3843	4	0.0011	0.0754	0.3104	1.94			
	3	0.3828	5	-0.0005	0.0754	0.3105	1.95			
	5	0.3722	6	-0.0001	0.0754	0.2995	1.85			

Product IV continued…

Triclosan Concentration

Calibration Curve Reference n/a
Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol
$[HOCl]_i$ 4.0 mg/L

Run Number	(mg triclosan / L)	(mg triclosan / g soap)
1	0.39	1.56
2	0.41	1.64
AVERAGE	0.40	1.60
Standard Deviation	0.01	0.06

Triclosan Consumption and Phenol Formation

Calibration Curve Reference Triclosan 12 DCP 14 TCP 16
Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol
$[HOCl]_i$ 4.0 mg/L

Reaction Time			Area				Concentration		
min	Date/Time	File Name	Internal Std.	Triclosan	DCP	TCP	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)
0	4/1/2006 1:26	28.D	167069	369870	412	282	0.3540	0.0771	0.0552
	4/1/2006 2:01	29.D	163399	444505	871	255	0.4254	0.1666	0.0510
	4/1/2006 2:35	30.D	155956	557701	578	420	0.5460	0.1158	0.0880
1	4/1/2006 3:10	31.D	162733	254683	639	826	0.2626	0.1227	0.1659
	4/1/2006 3:44	32.D	136784	141573	2409	602	0.1878	0.5504	0.1438
	4/1/2006 4:19	33.D	162459	190661	616	3042	0.2074	0.1185	0.6119
5	4/1/2006 4:53	34.D	172305	210229	7584	2853	0.2139	1.3755	0.5411
	4/1/2006 5:28	35.D	167724	229985	748	2466	0.2352	0.1394	0.4805
	4/1/2006 6:03	36.D	160393	172396	5996	742	0.1935	1.1682	0.1512

	Average			Standard Deviation		
Reaction Time (min)	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)
0	0.4418	0.1198	0.0647	0.0971	0.0449	0.0203
1	0.2193	0.2639	0.3072	0.0387	0.2481	0.2641
5	0.2142	0.8944	0.3909	0.0209	0.6620	0.2098

Table C 5: Summary of data obtained during experiments with Product V. Initial laboratory conditions.

Product V

Trihalomethane Analysis

Incubation Temperature 60 °C
Incubation Time 30 min
pH 7.0
[$NaHCO_3$] 2 mmol

Sample Date	$[HOCl]_i$ (mg/L)	Rxn. Temp. (°C)	Rxn. Time (min)	Repetition Number	Calibration Curve Reference	Chloroform Area	Chloroform Concentration (ppb)	Chloroform Average Concentration (ppb)	Chloroform Standard Deviation
1/30/2006	4.0	40	0		1			0.000	0.000
1/31/2006	4.0	40	1	1	1	18736304	118.779		
2/1/2006	4.0	40	1	2	2	21354487	186.514	151.801	33.899
2/1/2006	4.0	40	1	3	3	12912109	150.111		
2/9/2006	4.0	30	0		4			0.000	0.000
2/10/2006	4.0	30	1	1	4	47643023	137.906		
2/12/2006	4.0	30	1	2		GC ERROR		148.107	14.426
2/13/2006	4.0	30	1	3	5	37777576	158.308		
2/22/2006	2.0	40	0		6			0.000	0.000
2/23/2006	2.0	40	1	1	6	5906225	66.574		
2/23/2006	2.0	40	1	2	7	5230863	59.227	63.092	3.688
2/24/2006	2.0	40	1	3	8	4351226	63.475		
2/27/2006	2.0	30			9			0.000	0.000
2/27/2006	2.0	30	1	1	9	5864093	116.594		
2/28/2006	2.0	30	1	2	10	3590915	76.812	96.703	28.130
3/1/2006	2.0	30	1	3		GC ERROR			

Chlorine Decay Analysis

Calibration Curve Reference 11
Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol

Repetition	Time (min)	Abs.	Cell #	Cell Abs.	Soap Blank Abs.	Corrected Abs.	Chlorine Concentration (mg/L)	Time (min)	Average [HOCl] (mg/L)	Standard Deviation
1	0		1	0.0026			4.00	0	4.00	0.00
	0.5	0.3772	2	0.0023	0.0744	0.3031	1.88	0.5	1.75	0.15
	1	0.396	3	0.0056	0.0744	0.3186	2.01	1	1.80	0.28
	2	0.3852	4	0.0011	0.0744	0.3123	1.96	2	1.76	0.31
	3	0.3643	5	-0.0005	0.0744	0.2930	1.80	3	1.69	0.23
	5	0.3624	6	-0.0001	0.0744	0.2907	1.78	5	1.63	0.23
2	0		13	-0.0005			4.00			
	0.5	0.3912	14	0.0006	0.1220	0.2681	1.60			
	1	0.3808	15	0.0029	0.1220	0.2554	1.49			
	2	0.3707	16	0.0044	0.1220	0.2438	1.40			
	3	0.3687	17	-0.0013	0.1220	0.2475	1.43			
	5	0.3644	18	0.0012	0.1220	0.2407	1.37			
3	0		7	0.0030			4.00			
	0.5	0.3761	8	0.0031	0.0855	0.2905	1.78			
	1	0.3901	9	0.0012	0.0855	0.3064	1.91			
	2	0.3866	10	-0.0035	0.0855	0.3076	1.92			
	3	0.3866	11	0.0050	0.0855	0.2991	1.85			
	5	0.373	12	0.0035	0.0855	0.2870	1.75			

Product V continued…

Triclosan Concentration

Calibration Curve Reference	**n/a**	
Temperature	**40**	°C
pH	**7.0**	
[$NaHCO_3$]	**2**	**mmol**
$[HOCl]_i$	**4.0**	**mg/L**

Run Number	(mg triclosan / L)	(mg triclosan / g soap)
1	0.47	1.88
2	0.47	1.88
AVERAGE	0.47	1.88
Standard Deviation	0.00	0.00

Table C 6: Summary of data obtained during experiments with Product VI. Initial laboratory conditions.

Product VI

Trihalomethane Analysis

Incubation Temperature 60 °C
Incubation Time 30 min
pH 7.0
[$NaHCO_3$] 2 mmol

Sample Date	$[HOCl]_i$ (mg/L)	Rxn. Temp. (°C)	Rxn. Time (min)	Repetition Number	Calibration Curve Reference	Chloroform Area	Chloroform Concentration (ppb)	Chloroform Average Concentration (ppb)	Chloroform Standard Deviation
1/30/2006	4.0	40	0		1			0.000	0.000
1/31/2006	4.0	40	1	1	1	3638898	20.452		
2/1/2006	4.0	40	1	2	2	6889044	56.345	39.288	18.013
2/1/2006	4.0	40	1	3	3	3739764	41.067		
2/9/2006	4.0	30	0		4			0.000	0.000
2/10/2006	4.0	30	1	1	4	10843983	28.942		
2/12/2006	4.0	30	1	2		GC ERROR		34.421	7.749
2/13/2006	4.0	30	1	3	5	10972090	39.900		
2/22/2006	2.0	40	0		6			0.000	0.000
2/23/2006	2.0	40	1	1	6	1350475	5.459		
2/23/2006	2.0	40	1	2	7	1149499	0.028	3.684	3.167
2/24/2006	2.0	40	1	3	8	927202	5.566		
2/27/2006	2.0	30			9			0.000	0.000
2/27/2006	2.0	30	1	1	9	846643	9.251		
2/28/2006	2.0	30	1	2	10	680541	13.632	11.442	3.098
3/1/2006	2.0	30	1	3		GC ERROR			

Chlorine Decay Analysis

Calibration Curve Reference 11
Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol

Repetition	Time (min)	Abs.	Cell #	Cell Abs.	Soap Blank Abs.	Corrected Abs.	Chlorine Concentration (mg/L)	Time (min)	Average [HOCl] (mg/L)	Standard Deviation
1	0		7	0.0030			4.00	0	4.00	0.00
	0.5	0.428	8	0.0031	0.0917	0.3362	2.16	0.5	2.10	0.10
	1	0.4105	9	0.0012	0.0917	0.3206	2.03	1	2.03	0.09
	2	0.3804	10	-0.0035	0.0917	0.2952	1.82	2	1.78	0.04
	3	0.3759	11	0.0050	0.0917	0.2822	1.71	3	1.67	0.04
	5	0.1868	12	0.0035	0.0917	0.0946	0.17	5	1.03	0.75
2	0		7	0.0030			4.00			
	0.5	0.4256	8	0.0031	0.0907	0.3348	2.15			
	1	0.4209	9	0.0012	0.0907	0.3320	2.12			
	2	0.3758	10	-0.0035	0.0907	0.2916	1.79			
	3	0.3711	11	0.0050	0.0907	0.2784	1.68			
	5	0.3454	12	0.0035	0.0907	0.2542	1.48			
3	0		13	-0.0005			4.00			
	0.5	0.3987	14	0.0006	0.0822	0.3154	1.98			
	1	0.3953	15	0.0029	0.0822	0.3097	1.94			
	2	0.3727	16	0.0044	0.0822	0.2856	1.74			
	3	0.3536	17	-0.0013	0.0822	0.2722	1.63			
	5	0.3339	18	0.0012	0.0822	0.2500	1.45			

Product VI continued…

Triclosan Concentration

Calibration Curve Reference n/a
Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol
$[HOCl]_i$ 4.0 mg/L

Run Number	(mg triclosan / L)	(mg triclosan / g soap)
1	0.00	0.00
2	0.00	0.00
AVERAGE	0.00	0.00
Standard Deviation	0.00	0.00

Triclosan Consumption and Phenol Formation

Calibration Curve Reference Triclosan 13 DCP 15 TCP 17
Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol
$[HOCl]_i$ 4.0 mg/L

Reaction Time			Area				Concentration		
min	Date/Time	File Name	Internal Std.	Triclosan	DCP	TCP	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)
0	4/27/2006 7:12	10.D	142735	10331	879	723	0.0394	0.1621	0.1447
1	4/27/2006 7:47	11.D	138625	836	611	1149	0.0317	0.1160	0.2368
5	4/27/2006 8:22	12.D	136089	649	719	577	0.0316	0.1390	0.1211

	Average			Standard Deviation		
Reaction Time (min)	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)
0	0.0394	0.1621	0.1447	NA	NA	NA
1	0.0317	0.1160	0.2368	NA	NA	NA
5	0.0316	0.1390	0.1211	NA	NA	NA

Table C 7: Summary of data obtained during experiments with Product VII. Initial laboratory conditions.

Product VII

Trihalomethane Analysis

Incubation Temperature 60 °C
Incubation Time 30 min
pH 7.0
[$NaHCO_3$] 2 mmol

Sample Date	$[HOCl]_i$ (mg/L)	Rxn. Temp. (°C)	Rxn. Time (min)	Repetition Number	Calibration Curve Reference	Chloroform Area	Chloroform Concentration (ppb)	Chloroform Average Concentration (ppb)	Chloroform Standard Deviation
1/30/2006	4.0	40	0		1			0.000	0.000
1/31/2006	4.0	40	1	1	1	16338289	103.161		
2/1/2006	4.0	40	1	2	2	11805648	100.588	104.238	4.290
2/1/2006	4.0	40	1	3	3	9450980	108.964		
2/9/2006	4.0	30	0		4			0.000	0.000
2/10/2006	4.0	30	1	1	4	38806354	111.740		
2/12/2006	4.0	30	1	2		GC ERROR		120.729	12.712
2/13/2006	4.0	30	1	3	5	31305102	129.717		
2/22/2006	2.0	40	0		6			0.000	0.000
2/23/2006	2.0	40	1	1	6	3095073	28.862		
2/23/2006	2.0	40	1	2	7	2323951	17.063	22.306	6.008
2/24/2006	2.0	40	1	3	8	1839288	20.992		
2/27/2006	2.0	30			9			0.000	0.000
2/27/2006	2.0	30	1	1	9	3521786	66.483		
2/28/2006	2.0	30	1	2	10	2665099	56.714	61.598	6.908
3/1/2006	2.0	30	1	3		GC ERROR			

Chlorine Decay Analysis

Calibration Curve Reference 11
Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol

Repetition	Time (min)	Abs.	Cell #	Cell Abs.	Soap Blank Abs.	Corrected Abs.	Chlorine Concentration (mg/L)	Time (min)	Average [HOCl] (mg/L)	Standard Deviation
1	0		1	0.0026			4.00	0	4.00	0.00
	0.5	0.2475	2	0.0023	0.0573	0.1905	0.96	0.5	0.89	0.12
	1	0.2094	3	0.0056	0.0573	0.1491	0.62	1	0.61	0.06
	2	0.1406	4	0.0011	0.0573	0.0848	0.09	2	0.08	0.05
	3	0.1015	5	-0.0005	0.0573	0.0473	-0.22	3	-0.21	0.03
	5	0.0791	6	-0.0001	0.0573	0.0245	-0.41	5	-0.41	0.06
2	0		13	-0.0005			4.00			
	0.5	0.2250	14	0.0006	0.0596	0.1643	0.74			
	1	0.2042	15	0.0029	0.0596	0.1412	0.55			
	2	0.1413	16	0.0044	0.0596	0.0768	0.02			
	3	0.1046	17	-0.0013	0.0596	0.0458	-0.23			
	5	0.0774	18	0.0012	0.0596	0.0161	-0.48			
3	0		1	0.0026			4.00			
	0.5	0.2465	2	0.0023	0.0565	0.1903	0.96			
	1	0.2141	3	0.0056	0.0565	0.1546	0.66			
	2	0.1448	4	0.0011	0.0565	0.0898	0.13			
	3	0.1063	5	-0.0005	0.0565	0.0529	-0.17			
	5	0.0852	6	-0.0001	0.0565	0.0314	-0.35			

Product VII continued…

Triclosan Concentration

Calibration Curve Reference n/a
Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol
$[HOCl]_i$ 4.0 mg/L

Run Number	(mg triclosan / L)	(mg triclosan / g soap)
1	0.87	3.48
2	0.87	3.48
AVERAGE	0.87	3.48
Standard Deviation	0.00	0.00

Triclosan Consumption and Phenol Formation

Calibration Curve Reference Triclosan 13 DCP 15 TCP 17
Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol
$[HOCl]_i$ 4.0 mg/L

Reaction Time			Area				Concentration		
min	Date/Time	File Name	Internal Std.	Triclosan	DCP	TCP	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)
0	4/27/2006 8:57	13.D	126490	830376	998	370	0.7886	0.2076	0.0836
	4/27/2006 9:31	14.D	127223	768319	522	814	0.7279	0.1080	0.1828
	4/27/2006 10:06	15.D	126967	797177	178	461	0.7556	0.0369	0.1037
1	4/27/2006 10:41	16.D	127762	8564	84530	26393	0.0387	17.4111	5.9023
	4/27/2006 11:16	17.D	129113	11737	81295	38337	0.0415	16.5695	8.4836
	4/27/2006 11:50	18.D	126712	7369	75050	22321	0.0377	15.5865	5.0330
5	4/28/2006 12:25	19.D	114078	607	70611	22807	0.0316	16.2887	5.7121
	4/28/2006 1:00	20.D	133016	2965	66111	23089	0.0336	13.0794	4.9594
	4/28/2006 1:35	21.D	124723	2885	65198	26288	0.0337	13.7564	6.0220

	Average			Standard Deviation		
Reaction Time (min)	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)
0	0.7574	0.1175	0.1234	0.0304	0.0858	0.0524
1	0.0393	16.5224	6.4730	0.0020	0.9132	1.7947
5	0.0330	14.3748	5.5645	0.0012	1.6917	0.5465

Table C 8: Summary of data obtained during experiments with Product VIII. Initial laboratory conditions.

Product VIII

Trihalomethane Analysis

Incubation Temperature 60 °C
Incubation Time 30 min
pH 7.0
[$NaHCO_3$] 2 mmol

Sample Date	$[HOCl]_i$ (mg/L)	Rxn. Temp. (°C)	Rxn. Time (min)	Repetition Number	Calibration Curve Reference	Chloroform Area	Chloroform Concentration (ppb)	Chloroform Average Concentration (ppb)	Chloroform Standard Deviation
1/30/2006	4.0	40	0		1			0.000	0.000
1/31/2006	4.0	40	1	1	1	704302	1.339		
2/1/2006	4.0	40	1	2	2	1627514	8.999	5.634	3.913
2/1/2006	4.0	40	1	3	3	837464	6.563		
2/9/2006	4.0	30	0		4			0.000	0.000
2/10/2006	4.0	30	1	1	4	2371222	3.853		
2/12/2006	4.0	30	1	2		GC ERROR		4.018	0.234
2/13/2006	4.0	30	1	3	5	2886438	4.183		
2/22/2006	2.0	40	0		6			0.000	0.000
2/23/2006	2.0	40	1	1	6				
2/23/2006	2.0	40	1	2	7			#DIV/0!	#DIV/0!
2/24/2006	2.0	40	1	3	8				
2/27/2006	2.0	30			9			0.000	0.000
2/27/2006	2.0	30	1	1	9				
2/28/2006	2.0	30	1	2	10			#DIV/0!	#DIV/0!
3/1/2006	2.0	30	1	3		GC ERROR			

Chlorine Decay Analysis

Calibration Curve Reference 11
Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol

Repetition	Time (min)	Abs.	Cell #	Cell Abs.	Soap Blank Abs.	Corrected Abs.	Chlorine Concentration (mg/L)	Time (min)	Average [HOCl] (mg/L)	Standard Deviation
1	0		7	0.0030			4.00	0	4.00	0.00
	0.5	0.2536	8	0.0031	0.0806	0.1729	0.81	0.5	0.85	0.04
	1	0.2393	9	0.0012	0.0806	0.1605	0.71	1	0.71	0.02
	2	0.2118	10	-0.0035	0.0806	0.1377	0.52	2	0.51	0.01
	3	0.2131	11	0.0050	0.0806	0.1305	0.46	3	0.43	0.04
	5	0.1836	12	0.0035	0.0806	0.1025	0.23	5	0.25	0.04
2	0		1	0.0026			4.00			
	0.5	0.2616	2	0.0023	0.0792	0.1827	0.89			
	1	0.2398	3	0.0056	0.0792	0.1576	0.69			
	2	0.2147	4	0.0011	0.0792	0.1370	0.52			
	3	0.2026	5	-0.0005	0.0792	0.1265	0.43			
	5	0.1860	6	-0.0001	0.0792	0.1095	0.29			
3	0		7	0.0030			4.00			
	0.5	0.2631	8	0.0031	0.0872	0.1758	0.84			
	1	0.2473	9	0.0012	0.0872	0.1619	0.72			
	2	0.215	10	-0.0035	0.0872	0.1343	0.50			
	3	0.2107	11	0.0050	0.0872	0.1215	0.39			
	5	0.1879	12	0.0035	0.0872	0.1002	0.21			

Product VIII continued…

Triclosan Concentration

Calibration Curve Reference	**n/a**	
Temperature	**40**	°C
pH	**7.0**	
[$NaHCO_3$]	**2**	**mmol**
$[HOCl]_i$	**4.0**	**mg/L**

Run Number	(mg triclosan / L)	(mg triclosan / g soap)
1	0.00	0.00
2	0.00	0.00
AVERAGE	0.00	0.00
Standard Deviation	0.00	0.00

Table C 9: Summary of data obtained during experiments with Product IX. Initial laboratory conditions.

Product IX

Trihalomethane Analysis

Incubation Temperature 60 °C
Incubation Time 30 min
pH 7.0
[$NaHCO_3$] 2 mmol

Sample Date	$[HOCl]_i$ (mg/L)	Rxn. Temp. (°C)	Rxn. Time (min)	Repetition Number	Calibration Curve Reference	Chloroform Area	Chloroform Concentration (ppb)	Chloroform Average Concentration (ppb)	Chloroform Standard Deviation
1/30/2006	4.0	40	0		1			0.000	0.000
1/31/2006	4.0	40	1	1	1	2165312	10.855		
2/1/2006	4.0	40	1	2	2	4254216	32.636	24.658	12.002
2/1/2006	4.0	40	1	3	3	2849548	30.483		
2/9/2006	4.0	30	0		4			0.000	0.000
2/10/2006	4.0	30	1	1	4	8143720	20.946		
2/12/2006	4.0	30	1	2		GC ERROR		27.181	8.818
2/13/2006	4.0	30	1	3	5	9504353	33.417		
2/22/2006	2.0	40	0		6			0.000	0.000
2/23/2006	2.0	40	1	1	6	763489	-2.416		
2/23/2006	2.0	40	1	2	7	386216	-11.043	0.000	5.805
2/24/2006	2.0	40	1	3	8	445095	0.000		
2/27/2006	2.0	30			9			0.000	0.000
2/27/2006	2.0	30	1	1	9	909027	10.586		
2/28/2006	2.0	30	1	2	10	697625	14.003	12.294	2.416
3/1/2006	2.0	30	1	3		GC ERROR			

Chlorine Decay Analysis

Calibration Curve Reference 11
Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol

Repetition	Time (min)	Abs.	Cell #	Cell Abs.	Soap Blank Abs.	Corrected Abs.	Chlorine Concentration (mg/L)	Time (min)	Average [HOCl] (mg/L)	Standard Deviation
1	0		13	-0.0005			4.00	0	4.00	0.00
	0.5	0.3295	14	0.0006	0.0766	0.2518	1.46	0.5	1.50	0.03
	1	0.3351	15	0.0029	0.0766	0.2551	1.49	1	1.53	0.12
	2	0.3379	16	0.0044	0.0766	0.2564	1.50	2	1.50	0.08
	3	0.3454	17	-0.0013	0.0766	0.2696	1.61	3	1.56	0.07
	5	0.1417	18	0.0012	0.0766	0.0634	-0.09	5	0.98	0.93
2	0		7	0.0030			4.00			
	0.5	0.3016	8	0.0031	0.0433	0.2582	1.51			
	1	0.3174	9	0.0012	0.0433	0.2759	1.66			
	2	0.3022	10	-0.0035	0.0433	0.2654	1.57			
	3	0.3137	11	0.0050	0.0433	0.2684	1.60			
	5	0.3067	12	0.0035	0.0433	0.2629	1.55			
3	0		13	-0.0005			4.00			
	0.5	0.3064	14	0.0006	0.0465	0.2588	1.52			
	1	0.2986	15	0.0029	0.0465	0.2487	1.44			
	2	0.2985	16	0.0044	0.0465	0.2471	1.42			
	3	0.3	17	-0.0013	0.0465	0.2543	1.48			
	5	0.303	18	0.0012	0.0465	0.2548	1.49			

Product IX continued…

Triclosan Concentration

Calibration Curve Reference n/a
Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol
[$HOCl]_i$ 4.0 mg/L

Run Number	(mg triclosan / L)	(mg triclosan / g soap)
1	0.44	1.76
2	0.43	1.72
AVERAGE	0.44	1.74
Standard Deviation	0.01	0.03

Triclosan Consumption and Phenol Formation

Calibration Curve Reference Triclosan 13 DCP 15 TCP 17
Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol
[$HOCl]_i$ 4.0 mg/L

Reaction Time			Area				Concentration		
min	Date/Time	File Name	Internal Std.	Triclosan	DCP	TCP	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)
0	4/28/2006 2:09	22.D	146083	316259	1196	725	0.2808	0.2155	0.1418
	4/28/2006 2:44	23.D	137273	298619	756	497	0.2820	0.1449	0.1034
	4/28/2006 3:19	24.D	138355	295110	681	484	0.2772	0.1295	0.0999
1	4/28/2006 3:54	25.D	141448	72388	325708	39029	0.0901	60.5966	7.8836
	4/28/2006 4:28	26.D	135587	67058	328876	39254	0.0881	63.8308	8.2718
	4/28/2006 5:03	27.D	139862	70805	332650	37809	0.0894	62.5899	7.7237
5	4/28/2006 5:38	28.D	142406	68109	353015	36259	0.0862	65.2351	7.2748
	4/28/2006 6:13	29.D	136151	60575	328928	42588	0.0823	63.5765	8.9371
	4/28/2006 6:47	30.D	138211	61160	324831	33236	0.0821	61.8488	6.8707

	Average			Standard Deviation		
Reaction Time (min)	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)
0	0.2800	0.1633	0.1151	0.0025	0.0458	0.0232
1	0.0892	62.3391	7.9597	0.0010	1.6317	0.2818
5	0.0835	63.5535	7.6942	0.0023	1.6933	1.0952

Intermediate (chlorophenoxy)phenol Formation

Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol
[$HOCl]_i$ 4.0 mg/L

Reaction Time			Area				Average		
min	Date/Time	File Name	Internal Std.	dichlorinated triclosan	monochlorinated triclosan 1	monochlorinated triclosan 2	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)
0	4/28/2006 2:09	22.D	146083	0	0	0	0.0000	0.0000	0.0000
	4/28/2006 2:44	23.D	137273	0	0	0			
	4/28/2006 3:19	24.D	138355	0	0	0			
1	4/28/2006 3:54	25.D	141448	234151	131222	224934	1.6860	0.8969	1.6824
	4/28/2006 4:28	26.D	135587	239296	111036	230870			
	4/28/2006 5:03	27.D	139862	229044	132031	245342			
5	4/28/2006 5:38	28.D	142406	255847	119472	251493	1.8497	0.8280	1.7635
	4/28/2006 6:13	29.D	136151	251093	100059	261292			
	4/28/2006 6:47	30.D	138211	263730	125775	221857			

Table C 10: Summary of data obtained during experiments with Product X. Initial laboratory conditions.

Product X

Trihalomethane Analysis

Incubation Temperature 60 °C
Incubation Time 30 min
pH 7.0
[$NaHCO_3$] 2 mmol

Sample Date	$[HOCl]_i$ (mg/L)	Rxn. Temp. (°C)	Rxn. Time (min)	Repetition Number	Calibration Curve Reference	Chloroform Area	Chloroform Concentration (ppb)	Chloroform Average Concentration (ppb)	Chloroform Standard Deviation
2/2/2006	4.0	40	0		2			0.000	0.000
2/1/2006	4.0	40	1	1	1				
2/2/2006	4.0	40	1	2	2			#DIV/0!	#DIV/0!
2/2/2006	4.0	40	1	3	3				
2/13/2006	4.0	30	0		5			0.000	0.000
2/10/2006	4.0	30	1	1	4				
2/12/2006	4.0	30	1	2		GC ERROR		0.000	#DIV/0!
2/13/2006	4.0	30	1	3	5	370576	-6.930		
2/23/2006	2.0	40	0		7			0.000	0.000
2/23/2006	2.0	40	1	1	6				
2/23/2006	2.0	40	1	2	7			#DIV/0!	#DIV/0!
2/24/2006	2.0	40	1	3	8				
2/28/2006	2.0	30			10			0.000	0.000
2/27/2006	2.0	30	1	1	9				
2/28/2006	2.0	30	1	2	10			#DIV/0!	#DIV/0!
3/1/2006	2.0	30	1	3		GC ERROR			

Chlorine Decay Analysis

Calibration Curve Reference 11
Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol

Repetition	Time (min)	Abs.	Cell #	Cell Abs.	Soap Blank Abs.	Corrected Abs.	Chlorine Concentration (mg/L)	Time (min)	Average [HOCl] (mg/L)	Standard Deviation
1	0		1	0.0026			4.00	0	4.00	0.00
	0.5	0.298	2	0.0023	0.0521	0.2462	1.42	0.5	1.56	0.13
	1	0.2954	3	0.0056	0.0521	0.2403	1.37	1	1.51	0.13
	2	0.2803	4	0.0011	0.0521	0.2297	1.28	2	1.46	0.16
	3	0.2918	5	-0.0005	0.0521	0.2428	1.39	3	1.51	0.13
	5	0.2804	6	-0.0001	0.0521	0.2310	1.29	5	1.43	0.12
2	0		13	-0.0005			4.00			
	0.5	0.3427	14	0.0006	0.0633	0.2783	1.68			
	1	0.3365	15	0.0029	0.0633	0.2698	1.61			
	2	0.3342	16	0.0044	0.0633	0.2660	1.58			
	3	0.3370	17	-0.0013	0.0633	0.2745	1.65			
	5	0.3246	18	0.0012	0.0633	0.2596	1.53			
3	0		1	0.0026			4.00			
	0.5	0.3197	2	0.0023	0.0541	0.2659	1.58			
	1	0.3196	3	0.0056	0.0541	0.2625	1.55			
	2	0.3129	4	0.0011	0.0541	0.2603	1.53			
	3	0.3059	5	-0.0005	0.0541	0.2549	1.49			
	5	0.3046	6	-0.0001	0.0541	0.2532	1.47			

Product X continued…

Triclosan Concentration

Calibration Curve Reference n/a
Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol
$[HOCl]_i$ 4.0 mg/L

Run Number	(mg triclosan / L)	(mg triclosan / g soap)
1	0.00	0.00
2	0.00	0.00
AVERAGE	0.00	0.00
Standard Deviation	0.00	0.00

Table C 11: Summary of data obtained during experiments with Product XI. Initial laboratory conditions.

Product XI

Trihalomethane Analysis

Incubation Temperature 60 °C
Incubation Time 30 min
pH 7.0
[$NaHCO_3$] 2 mmol

Sample Date	$[HOCl]_i$ (mg/L)	Rxn. Temp. (°C)	Rxn. Time (min)	Repetition Number	Calibration Curve Reference	Chloroform Area	Chloroform Concentration (ppb)	Chloroform Average Concentration (ppb)	Chloroform Standard Deviation
2/2/2006	4.0	40	0		2			0.000	0.000
2/1/2006	4.0	40	1	1	1			#DIV/0!	#DIV/0!
2/2/2006	4.0	40	1	2	2				
2/2/2006	4.0	40	1	3	3				
2/13/2006	4.0	30	0		5			0.000	0.000
2/10/2006	4.0	30	1	1	4			#DIV/0!	#DIV/0!
2/12/2006	4.0	30	1	2		GC ERROR			
2/13/2006	4.0	30	1	3	5				
2/23/2006	2.0	40	0		7			0.000	0.000
2/23/2006	2.0	40	1	1	6			#DIV/0!	#DIV/0!
2/23/2006	2.0	40	1	2	7				
2/24/2006	2.0	40	1	3	8				
2/28/2006	2.0	30			10			0.000	0.000
2/27/2006	2.0	30	1	1	9			#DIV/0!	#DIV/0!
2/28/2006	2.0	30	1	2	10				
3/1/2006	2.0	30	1	3		GC ERROR			

Chlorine Decay Analysis

Calibration Curve Reference 11
Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol

Repetition	Time (min)	Abs.	Cell #	Cell Abs.	Soap Blank Abs.	Corrected Abs.	Chlorine Concentration (mg/L)	Time (min)	Average [HOCl] (mg/L)	Standard Deviation
1	0		7	0.0030			4.00	0	4.00	0.00
	0.5	0.3659	8	0.0031	0.0924	0.2734	1.64	0.5	1.85	0.22
	1	0.3526	9	0.0012	0.0924	0.2620	1.55	1	1.78	0.21
	2	0.338	10	-0.0035	0.0924	0.2521	1.46	2	1.70	0.23
	3	0.3427	11	0.0050	0.0924	0.2483	1.43	3	1.67	0.22
	5	0.172	12	0.0035	0.0924	0.0791	0.04	5	1.22	1.02
2	0		1	0.0026			4.00			
	0.5	0.3745	2	0.0023	0.0477	0.3271	2.08			
	1	0.3622	3	0.0056	0.0477	0.3115	1.95			
	2	0.3538	4	0.0011	0.0477	0.3076	1.92			
	3	0.3464	5	-0.0005	0.0477	0.3018	1.87			
	5	0.3481	6	-0.0001	0.0477	0.3031	1.88			
3	0		7	0.0030			4.00			
	0.5	0.374	8	0.0031	0.0762	0.2977	1.84			
	1	0.3712	9	0.0012	0.0762	0.2968	1.83			
	2	0.3504	10	-0.0035	0.0762	0.2807	1.70			
	3	0.3587	11	0.0050	0.0762	0.2805	1.70			
	5	0.3608	12	0.0035	0.0762	0.2841	1.73			

Product XI continued…

Triclosan Concentration

Calibration Curve Reference n/a
Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol
$[HOCl]_i$ 4.0 mg/L

Run Number	(mg triclosan / L)	(mg triclosan / g soap)
1	0.00	0.00
2	0.00	0.00
AVERAGE	0.00	0.00
Standard Deviation	0.00	0.00

Table C 12: Summary of data obtained during experiments with Product XII. Initial laboratory conditions.

Product XII

Trihalomethane Analysis

Incubation Temperature 60 °C
Incubation Time 30 min
pH 7.0
[$NaHCO_3$] 2 mmol

Sample Date	$[HOCl]_i$ (mg/L)	Rxn. Temp. (°C)	Rxn. Time (min)	Repetition Number	Calibration Curve Reference	Chloroform Area	Chloroform Concentration (ppb)	Chloroform Average Concentration (ppb)	Chloroform Standard Deviation
2/2/2006	4.0	40	0		2			0.000	0.000
2/1/2006	4.0	40	1	1	1	14358211	90.265		
2/2/2006	4.0	40	1	2	2	16245290	140.538	121.025	26.957
2/2/2006	4.0	40	1	3	3	11411461	132.270		
2/13/2006	4.0	30	0		5			0.000	0.000
2/10/2006	4.0	30	1	1	4	45052630	130.236		
2/12/2006	4.0	30	1	2		GC ERROR		141.766	16.306
2/13/2006	4.0	30	1	3	5	36642869	153.296		
2/23/2006	2.0	40	0		7			0.000	0.000
2/23/2006	2.0	40	1	1	6	7681785	90.393		
2/23/2006	2.0	40	1	2	7	7773059	96.101	92.479	3.148
2/24/2006	2.0	40	1	3	8	5975484	90.945		
2/28/2006	2.0	30			10			0.000	0.000
2/27/2006	2.0	30	1	1	9	6281076	125.514		
2/28/2006	2.0	30	1	2	10	4223676	90.548	108.031	24.725
3/1/2006	2.0	30	1	3		GC ERROR			

Chlorine Decay Analysis

Calibration Curve Reference 11
Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol

Repetition	Time (min)	Abs.	Cell #	Cell Abs.	Soap Blank Abs.	Corrected Abs.	Chlorine Concentration (mg/L)	Time (min)	Average [HOCl] (mg/L)	Standard Deviation
1	0		13	-0.0005			4.00	0	4.00	0.00
	0.5	0.3822	14	0.0006	0.0939	0.2872	1.75	0.5	1.99	0.21
	1	0.3728	15	0.0029	0.0939	0.2755	1.66	1	1.83	0.18
	2	0.3655	16	0.0044	0.0939	0.2667	1.58	2	1.74	0.16
	3	0.3653	17	-0.0013	0.0939	0.2722	1.63	3	1.74	0.12
	5	0.36	18	0.0012	0.0939	0.2644	1.57	5	1.62	0.09
2	0		7	0.0030			4.00			
	0.5	0.4219	8	0.0031	0.0846	0.3372	2.16			
	1	0.4023	9	0.0012	0.0846	0.3195	2.02			
	2	0.3842	10	-0.0035	0.0846	0.3061	1.91			
	3	0.3885	11	0.0050	0.0846	0.3019	1.87			
	5	0.3684	12	0.0035	0.0846	0.2833	1.72			
3	0		13	-0.0005			4.00			
	0.5	0.4029	14	0.0006	0.0797	0.3221	2.04			
	1	0.3768	15	0.0029	0.0797	0.2937	1.81			
	2	0.3698	16	0.0044	0.0797	0.2852	1.74			
	3	0.3623	17	-0.0013	0.0797	0.2834	1.72			
	5	0.3477	18	0.0012	0.0797	0.2663	1.58			

Product XII continued…

Triclosan Concentration

Calibration Curve Reference n/a
Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol
$[HOCl]_i$ 4.0 mg/L

Run Number	(mg triclosan / L)	(mg triclosan / g soap)
1	0.72	2.88
2	0.68	2.72
AVERAGE	0.70	2.80
Standard Deviation	0.03	0.11

Triclosan Consumption and Phenol Formation

Calibration Curve Reference Triclosan 13 DCP 15 TCP 17
Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol
$[HOCl]_i$ 4.0 mg/L

Reaction Time min	Date/Time	File Name	Area				Concentration		
			Internal Std.	Triclosan	DCP	TCP	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)
0	4/28/2006 7:22	31.D	140468	498377	1207	303	0.4404	0.2261	0.0616
	4/28/2006 7:57	32.D	145521	518287	482	12226	0.4420	0.0872	2.4004
	4/28/2006 8:32	33.D	136385	518234	498	235	0.4695	0.0961	0.0492
1	4/28/2006 9:06	34.D	126239	828	39387	1398	0.0318	8.2106	0.3164
	4/28/2006 9:41	35.D	125963	1512	986	11291	0.0324	0.2060	2.5611
	4/28/2006 10:16	36.D	141226	173	825	1085	0.0311	0.1537	0.2195
5	4/28/2006 10:50	37.D	135185	732	93110	24848	0.0316	18.1253	5.2516
	4/28/2006 11:25	38.D	121950	210	76243	28246	0.0312	16.4526	6.6177
	4/28/2006 12:00	39.D	139562	232	95514	29356	0.0312	18.0101	6.0098

Reaction Time (min)	Average			Standard Deviation		
	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)
0	**0.4507**	**0.1365**	**0.8371**	**0.0163**	**0.0778**	**1.3539**
1	**0.0318**	**2.8568**	**1.0323**	**0.0006**	**4.6366**	**1.3248**
5	**0.0313**	**17.5293**	**5.9597**	**0.0002**	**0.9342**	**0.6844**

Table C 13: Summary of data obtained during experiments with Product XIII. Initial laboratory conditions.

Product XIII

Trihalomethane Analysis

Incubation Temperature 60 °C
Incubation Time 30 min
pH 7.0
[$NaHCO_3$] 2 mmol

Sample Date	$[HOCl]_i$ (mg/L)	Rxn. Temp. (°C)	Rxn. Time (min)	Repetition Number	Calibration Curve Reference	Chloroform Area	Chloroform Concentration (ppb)	Chloroform Average Concentration (ppb)	Chloroform Standard Deviation
2/2/2006	4.0	40	0		2			0.000	0.000
2/1/2006	4.0	40	1	1	1	14322566	90.033		
2/2/2006	4.0	40	1	2	2	15832694	136.825	121.246	27.031
2/2/2006	4.0	40	1	3	3	11799129	136.879		
2/13/2006	4.0	30	0		5			0.000	0.000
2/10/2006	4.0	30	1	1	4	44532454	128.696		
2/12/2006	4.0	30	1	2		GC ERROR		138.606	14.016
2/13/2006	4.0	30	1	3	5	35560972	148.517		
2/23/2006	2.0	40	0		7			0.000	0.000
2/23/2006	2.0	40	1	1	6	11654232	143.682		
2/23/2006	2.0	40	1	2	7	9262941	117.711	124.256	17.120
2/24/2006	2.0	40	1	3	8	7183398	111.373		
2/28/2006	2.0	30			10			0.000	0.000
2/27/2006	2.0	30	1	1	9	7006119	141.026		
2/28/2006	2.0	30	1	2	10	4556501	97.773	119.399	30.584
3/1/2006	2.0	30	1	3		GC ERROR			

Chlorine Decay Analysis

Calibration Curve Reference 11
Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol

Repetition	Time (min)	Abs.	Cell #	Cell Abs.	Soap Blank Abs.	Corrected Abs.	Chlorine Concentration (mg/L)	Time (min)	Average [HOCl] (mg/L)	Standard Deviation
1	0		1	0.0026			4.00	0	4.00	0.00
	0.5	0.3653	2	0.0023	0.0676	0.2980	1.84	0.5	1.97	0.11
	1	0.355	3	0.0056	0.0676	0.2844	1.73	1	1.79	0.05
	2	0.3331	4	0.0011	0.0676	0.2670	1.59	2	1.67	0.09
	3	0.3225	5	-0.0005	0.0676	0.2580	1.51	3	1.60	0.09
	5	0.3062	6	-0.0001	0.0676	0.2413	1.38	5	1.46	0.08
2	0		13	-0.0005			4.00			
	0.5	0.3813	14	0.0006	0.0573	0.3229	2.05			
	1	0.3527	15	0.0029	0.0573	0.2920	1.79			
	2	0.3510	16	0.0044	0.0573	0.2888	1.77			
	3	0.3368	17	-0.0013	0.0573	0.2803	1.70			
	5	0.3189	18	0.0012	0.0573	0.2599	1.53			
3	0		1	0.0026			4.00			
	0.5	0.3795	2	0.0023	0.0616	0.3182	2.01			
	1	0.3621	3	0.0056	0.0616	0.2975	1.84			
	2	0.3359	4	0.0011	0.0616	0.2758	1.66			
	3	0.3247	5	-0.0005	0.0616	0.2662	1.58			
	5	0.3123	6	-0.0001	0.0616	0.2534	1.48			

Product XIII continued…

Triclosan Concentration

Calibration Curve Reference n/a

Temperature 40 °C

pH 7.0

[$NaHCO_3$] 2 mmol

$[HOCl]_i$ 4.0 mg/L

Run Number	(mg triclosan / L)	(mg triclosan / g soap)
1	0.72	2.88
2	0.68	2.72
AVERAGE	0.70	2.80
Standard Deviation	0.03	0.11

Table C 14: Summary of data obtained during experiments with Product XIV. Initial laboratory conditions.

Product XIV

Trihalomethane Analysis

Incubation Temperature 60 °C
Incubation Time 30 min
pH 7.0
[$NaHCO_3$] 2 mmol

Sample Date	$[HOCl]_i$ (mg/L)	Rxn. Temp. (°C)	Rxn. Time (min)	Repetition Number	Calibration Curve Reference	Chloroform Area	Chloroform Concentration (ppb)	Chloroform Average Concentration (ppb)	Chloroform Standard Deviation
2/2/2006	4.0	40	0		2			0.000	0.000
2/1/2006	4.0	40	1	1	1	3381036	18.773		
2/2/2006	4.0	40	1	2	2	5625553	44.976	40.284	19.591
2/2/2006	4.0	40	1	3	3	5088719	57.103		
2/13/2006	4.0	30	0		5			0.000	0.000
2/10/2006	4.0	30	1	1	4	16439279	45.510		
2/12/2006	4.0	30	1	2		GC ERROR		58.532	18.416
2/13/2006	4.0	30	1	3	5	18137989	71.554		
2/23/2006	2.0	40	0		7			0.000	0.000
2/23/2006	2.0	40	1	1	6	2875828	25.921		
2/23/2006	2.0	40	1	2	7	2688973	22.358	20.704	6.212
2/24/2006	2.0	40	1	3	8	1415996	13.833		
2/28/2006	2.0	30			10			0.000	0.000
2/27/2006	2.0	30	1	1	9	1485279	22.914		
2/28/2006	2.0	30	1	2	10	1397597	29.198	26.056	4.443
3/1/2006	2.0	30	1	3		GC ERROR			

Chlorine Decay Analysis

Calibration Curve Reference 11
Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol

Repetition	Time (min)	Abs.	Cell #	Cell Abs.	Soap Blank Abs.	Corrected Abs.	Chlorine Concentration (mg/L)	Time (min)	Average [HOCl] (mg/L)	Standard Deviation
1	0		7	0.0030			4.00	0	4.00	0.00
	0.5	0.4218	8	0.0031	0.0905	0.3312	2.12	0.5	2.21	0.21
	1	0.4261	9	0.0012	0.0905	0.3374	2.17	1	2.27	0.18
	2	0.4158	10	-0.0035	0.0905	0.3318	2.12	2	2.18	0.15
	3	0.4128	11	0.0050	0.0905	0.3203	2.03	3	2.11	0.19
	5	0.4115	12	0.0035	0.0905	0.3205	2.03	5	2.07	0.16
2	0		1	0.0026			4.00			
	0.5	0.4489	2	0.0023	0.0769	0.3723	2.45			
	1	0.4554	3	0.0056	0.0769	0.3755	2.48			
	2	0.4360	4	0.0011	0.0769	0.3606	2.36			
	3	0.4311	5	-0.0005	0.0769	0.3573	2.33			
	5	0.4223	6	-0.0001	0.0769	0.3481	2.25			
3	0		7	0.0030			4.00			
	0.5	0.4128	8	0.0031	0.0870	0.3257	2.07			
	1	0.4225	9	0.0012	0.0870	0.3373	2.17			
	2	0.4058	10	-0.0035	0.0870	0.3253	2.07			
	3	0.4038	11	0.0050	0.0870	0.3148	1.98			
	5	0.3972	12	0.0035	0.0870	0.3097	1.94			

Product XIV continued…

Triclosan Concentration

Calibration Curve Reference	**n/a**	
Temperature	**40**	°C
pH	**7.0**	
[$NaHCO_3$]	**2**	**mmol**
$[HOCl]_i$	**4.0**	**mg/L**

Run Number	(mg triclosan / L)	(mg triclosan / g soap)
1	0.00	0.00
2	0.00	0.00
AVERAGE	0.00	0.00
Standard Deviation	0.00	0.00

Table C 15: Summary of data obtained during experiments with Product XV. Initial laboratory conditions.

Product XV

Trihalomethane Analysis

Incubation Temperature 60 °C
Incubation Time 30 min
pH 7.0
[$NaHCO_3$] 2 mmol

Sample Date	$[HOCl]_i$ (mg/L)	Rxn. Temp. (°C)	Rxn. Time (min)	Repetition Number	Calibration Curve Reference	Chloroform Area	Chloroform Concentration (ppb)	Chloroform Average Concentration (ppb)	Chloroform Standard Deviation
2/2/2006	4.0	40	0		2			0.000	0.000
2/1/2006	4.0	40	1	1	1				
2/2/2006	4.0	40	1	2	2	525933	-0.914	0.647	2.207
2/2/2006	4.0	40	1	3	3	471104	2.208		
2/13/2006	4.0	30	0		5			0.000	0.000
2/10/2006	4.0	30	1	1	4	855994	-0.634		
2/12/2006	4.0	30	1	2		GC ERROR		-1.529	1.266
2/13/2006	4.0	30	1	3	5	1390649	-2.424		
2/23/2006	2.0	40	0		7			0.000	0.000
2/23/2006	2.0	40	1	1	6				
2/23/2006	2.0	40	1	2	7			#DIV/0!	#DIV/0!
2/24/2006	2.0	40	1	3	8				
2/28/2006	2.0	30			10			0.000	0.000
2/27/2006	2.0	30	1	1	9				
2/28/2006	2.0	30	1	2	10			#DIV/0!	#DIV/0!
3/1/2006	2.0	30	1	3		GC ERROR			

Chlorine Decay Analysis

Calibration Curve Reference 11
Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol

Repetition	Time (min)	Abs.	Cell #	Cell Abs.	Soap Blank Abs.	Corrected Abs.	Chlorine Concentration (mg/L)	Time (min)	Average [HOCl] (mg/L)	Standard Deviation
1	0		13	-0.0005			4.00	0	4.00	0.00
	0.5	0.4178	14	0.0006	0.0765	0.3402	2.19	0.5	2.39	0.36
	1	0.4176	15	0.0029	0.0765	0.3377	2.17	1	2.38	0.36
	2	0.4134	16	0.0044	0.0765	0.3320	2.12	2	2.27	0.24
	3	0.3872	17	-0.0013	0.0765	0.3115	1.95	3	2.13	0.22
	5	0.3624	18	0.0012	0.0765	0.2842	1.73	5	1.97	0.28
2	0		7	0.0030			4.00			
	0.5	0.4603	8	0.0031	0.0451	0.4151	2.81			
	1	0.4577	9	0.0012	0.0451	0.4144	2.80			
	2	0.4224	10	-0.0035	0.0451	0.3838	2.55			
	3	0.4105	11	0.0050	0.0451	0.3634	2.38			
	5	0.3970	12	0.0035	0.0451	0.3514	2.28			
3	0		13	-0.0005			4.00			
	0.5	0.4022	14	0.0006	0.0613	0.3398	2.19			
	1	0.4029	15	0.0029	0.0613	0.3382	2.17			
	2	0.3988	16	0.0044	0.0613	0.3326	2.13			
	3	0.3837	17	-0.0013	0.0613	0.3232	2.05			
	5	0.3666	18	0.0012	0.0613	0.3036	1.89			

Product XV continued…

Triclosan Concentration

Calibration Curve Reference	**n/a**	
Temperature	**40**	°C
pH	**7.0**	
[$NaHCO_3$]	**2**	**mmol**
$[HOCl]_i$	**4.0**	**mg/L**

Run Number	(mg triclosan / L)	(mg triclosan / g soap)
1	0.26	1.04
2	0.31	1.24
AVERAGE	0.29	1.14
Standard Deviation	0.04	0.14

Table C 16: Summary of data obtained during experiments with Product XVI. Initial laboratory conditions.

Product XVI

Trihalomethane Analysis

Incubation Temperature 60 °C
Incubation Time 30 min
pH 7.0
[$NaHCO_3$] 2 mmol

Sample Date	$[HOCl]_i$ (mg/L)	Rxn. Temp. (°C)	Rxn. Time (min)	Repetition Number	Calibration Curve Reference	Chloroform Area	Chloroform Concentration (ppb)	Chloroform Average Concentration (ppb)	Chloroform Standard Deviation
2/2/2006	**4.0**	**40**	0		2			**0.000**	**0.000**
2/1/2006	**4.0**	**40**	1	1	1	9147909	56.331		
2/2/2006	**4.0**	**40**	1	2	2	10142328	85.620	**76.071**	**17.098**
2/2/2006	**4.0**	**40**	1	3	3	7541410	86.262		
2/13/2006	**4.0**	**30**	0		5			**0.000**	**0.000**
2/10/2006	**4.0**	**30**	1	1	4	29970785	85.578		
2/12/2006	**4.0**	**30**	1	2		GC ERROR		**95.800**	**14.457**
2/13/2006	**4.0**	**30**	1	3	5	25941031	106.023		
2/23/2006	**2.0**	**40**	0		7			**0.000**	**0.000**
2/23/2006	**2.0**	**40**	1	1	6	5651021	63.150		
2/23/2006	**2.0**	**40**	1	2	7	4990867	55.746	**59.769**	**3.743**
2/24/2006	**2.0**	**40**	1	3	8	4169982	60.409		
2/28/2006	**2.0**	**30**			10			**0.000**	**0.000**
2/27/2006	**2.0**	**30**	1	1	9	4057973	77.954		
2/28/2006	**2.0**	**30**	1	2	10	2746775	58.487	**68.220**	**13.765**
3/1/2006	**2.0**	**30**	1	3		GC ERROR			

Chlorine Decay Analysis

Calibration Curve Reference 11
Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol

Repetition	Time (min)	Abs.	Cell #	Cell Abs.	Soap Blank Abs.	Corrected Abs.	Chlorine Concentration (mg/L)	Time (min)	Average [HOCl] (mg/L)	Standard Deviation
1	0		1	0.0026			4.00	0	**4.00**	**0.00**
	0.5	0.3739	2	0.0023	0.0615	0.3127	1.96	0.5	**2.18**	**0.19**
	1	0.3724	3	0.0056	0.0615	0.3079	1.92	1	**2.14**	**0.18**
	2	0.3584	4	0.0011	0.0615	0.2984	1.85	2	**2.01**	**0.15**
	3	0.3501	5	-0.0005	0.0615	0.2917	1.79	3	**1.96**	**0.15**
	5	0.3505	6	-0.0001	0.0615	0.2917	1.79	5	**2.01**	**0.19**
2	0		13	-0.0005			4.00			
	0.5	0.4335	14	0.0006	0.0750	0.3574	2.33			
	1	0.4273	15	0.0029	0.0750	0.3489	2.26			
	2	0.4036	16	0.0044	0.0750	0.3237	2.05			
	3	0.3980	17	-0.0013	0.0750	0.3238	2.05			
	5	0.4055	18	0.0012	0.0750	0.3288	2.10			
3	0		1	0.0026			4.00			
	0.5	0.4226	2	0.0023	0.0751	0.3478	2.25			
	1	0.4224	3	0.0056	0.0751	0.3443	2.22			
	2	0.4068	4	0.0011	0.0751	0.3332	2.13			
	3	0.395	5	-0.0005	0.0751	0.3230	2.05			
	5	0.4069	6	-0.0001	0.0751	0.3345	2.14			

Product XVI continued…

Triclosan Concentration

Calibration Curve Reference	**n/a**	
Temperature	**40**	°C
pH	**7.0**	
[$NaHCO_3$]	**2**	**mmol**
$[HOCl]_i$	**4.0**	**mg/L**

Run Number	(mg triclosan / L)	(mg triclosan / g soap)
1	0.31	1.24
2	0.30	1.20
AVERAGE	0.31	1.22
Standard Deviation	0.01	0.03

Table C 17: Summary of data obtained during experiments with Product XVII. Initial laboratory conditions.

Product XVII

Trihalomethane Analysis

Incubation Temperature 60 °C
Incubation Time 30 min
pH 7.0
[$NaHCO_3$] 2 mmol

Sample Date	$[HOCl]_i$ (mg/L)	Rxn. Temp. (°C)	Rxn. Time (min)	Repetition Number	Calibration Curve Reference	Chloroform Area	Chloroform Concentration (ppb)	Chloroform Average Concentration (ppb)	Chloroform Standard Deviation
2/2/2006	**4.0**	**40**	0		2			**0.000**	**0.000**
2/1/2006	**4.0**	**40**	1	1	1	12094447	75.522		
2/2/2006	**4.0**	**40**	1	2	2	12616491	107.884	**101.790**	**23.813**
2/2/2006	**4.0**	**40**	1	3	3	10544416	121.963		
2/13/2006	**4.0**	**30**	0		5			**0.000**	**0.000**
2/10/2006	**4.0**	**30**	1	1	4	37800366	108.762		
2/12/2006	**4.0**	**30**	1	2		GC ERROR		**120.282**	**16.293**
2/13/2006	**4.0**	**30**	1	3	5	31777292	131.803		
2/23/2006	**2.0**	**40**	0		7			**0.000**	**0.000**
2/23/2006	**2.0**	**40**	1	1	6	8384555	99.820		
2/23/2006	**2.0**	**40**	1	2	7	5649630	65.301	**81.823**	**17.307**
2/24/2006	**2.0**	**40**	1	3	8	5348929	80.348		
2/28/2006	**2.0**	**30**			10			**0.000**	**0.000**
2/27/2006	**2.0**	**30**	1	1	9	5219230	102.797		
2/28/2006	**2.0**	**30**	1	2	10	3299723	70.490	**86.644**	**22.845**
3/1/2006	**2.0**	**30**	1	3		GC ERROR			

Chlorine Decay Analysis

Calibration Curve Reference n/a
Temperature 40 °C
pH 7.0
[$NaHCO_3$] 2 mmol

Repetition	Time (min)	Abs.	Cell #	Cell Abs.	Soap Blank Abs.	Corrected Abs.	Chlorine Concentration (mg/L)	Time (min)	Average [HOCl] (mg/L)	Standard Deviation
1	0		7	0.0030			4.00	0	**4.00**	**0.00**
	0.5	0.3526	8	0.0031	0.0808	0.2717	1.63	0.5	**1.93**	**0.27**
	1	0.345	9	0.0012	0.0808	0.2660	1.58	1	**1.86**	**0.25**
	2	0.3284	10	-0.0035	0.0808	0.2541	1.48	2	**1.75**	**0.24**
	3	0.3329	11	0.0050	0.0808	0.2501	1.45	3	**1.77**	**0.28**
	5	0.3304	12	0.0035	0.0808	0.2491	1.44	5	**1.74**	**0.27**
2	0		1	0.0026			4.00			
	0.5	0.3894	2	0.0023	0.0597	0.3300	2.11			
	1	0.3705	3	0.0056	0.0597	0.3078	1.92			
	2	0.3570	4	0.0011	0.0597	0.2988	1.85			
	3	0.3582	5	-0.0005	0.0597	0.3016	1.87			
	5	0.3572	6	-0.0001	0.0597	0.3002	1.86			
3	0		7	0.0030			4.00			
	0.5	0.3858	8	0.0031	0.0597	0.3260	2.07			
	1	0.3844	9	0.0012	0.0597	0.3265	2.08			
	2	0.3623	10	-0.0035	0.0597	0.3091	1.93			
	3	0.3775	11	0.0050	0.0597	0.3158	1.99			
	5	0.369	12	0.0035	0.0597	0.3088	1.93			

Product XVII continued…

Triclosan Concentration

Calibration Curve Reference	**n/a**	
Temperature	**40**	°C
pH	**7.0**	
[$NaHCO_3$]	**2**	**mmol**
[$HOCl]_i$	**4.0**	**mg/L**

Run Number	(mg triclosan / L)	(mg triclosan / g soap)
1	0.35	1.40
2	0.43	1.72
AVERAGE	0.39	1.56
Standard Deviation	0.06	0.23

Appendix D

Atlanta and Danville Experimental Data

Table D 1: Summary table for calibration curve equation values for Atlanta tap water, simulated Atlanta condition, and Danville tap water experiments. The regression equation is in the form y=ax+b.

Curve Reference Number	Calibration Constituent	Regression Values		
		a	b	r^2
18	chloroform	1020608.55	46341353.49	0.936909
19	triclosan	1237235.31	-5423.14978	0.993665
20	triclosan	8.66537706	-0.268671536	0.995252
21	dichlorophenol	5259.93823	-8547.4936	0.99069
22	dichlorophenol	0.04051385	-0.251045977	0.994103
23	trichlorophenol	5175.71889	-11763.05647	0.998161
24	trichlorophenol	0.0369316	-0.1569724	0.995323
25	chloroform	1045044.56	16115342.58	0.9806
26	triclosan	7.091262	-0.051406	0.980394
27	dichlorophenol	0.045178	-0.33427	0.99031
28	trichlorophenol	0.038016	0.129483	0.991367

Table D 2: Summary of Atlanta tap water experimental data.

Atlanta Tap Water Experiments

$[HOCl]_i$ 1 mg/L
Temperature 33 °C
pH 6.35

Trihalomethane Analysis

Calibration Reference 18

		Chloroform			
Sample Date	Sample	Area	Concentration (ppb)	Average Concentration (ppb)	Standard Deviation
4/2/2006	t=0	90198119	42.9711916		
4/2/2006	t=0	83878241	36.77892719	**37.6162**	**4.9893**
4/2/2006	t=0	80121957	33.09849162		
4/2/2006	VI, t=1	85149863	38.02487207		
4/2/2006	VI, t=1	78512092	31.52113368	**35.9960**	**3.8809**
4/2/2006	VI, t=1	85575494	38.44190855		
4/2/2006	VI, t=4	81181932	34.13706317		
4/2/2006	VI, t=4	79636345	32.6226853	**34.5398**	**2.1471**
4/2/2006	VI, t=4	83960741	36.85976131		
4/2/2006	VII, t=1	86624224	39.46946217		
4/2/2006	VII, t=1	80706625	33.67135377	**36.5704**	**4.0999**
	VII, t=1	Broken Vial			
4/2/2006	VII, t=4	76424848	29.47603617		
4/2/2006	VII, t=4	82320931	35.25306303	**33.3736**	**3.3761**
4/3/2006	VII, t=4	82462334	35.39161077		
4/3/2006	IX, t=1	95079882	47.75438003		
4/3/2006	IX, t=1	74405937	27.49789186	**39.3374**	**10.5530**
4/3/2006	IX, t=1	89982533	42.75995881		
4/3/2006	IX, t=4	86374294	39.22457886		
4/3/2006	IX, t=4	78481151	31.49081746	**41.6733**	**11.6023**
4/3/2006	IX, t=4	101765095	54.30460245		
4/3/2006	XII, t=1	87607335	40.43272178		
4/3/2006	XII, t=1	96586762	49.23083249	**46.1494**	**4.9558**
4/3/2006	XII, t=1	96131305	48.78457226		
4/3/2006	XII, t=4	106801508	59.23931812		
4/3/2006	XII, t=4	105891115	58.34730815	**51.1803**	**13.1937**
4/3/2006	XII, t=4	83036588	35.95426919		

Atlanta Tap Water Experiments Continued…

Triclosan and Phenol Analysis

Calibration Reference	Triclosan	19	DCP	21	TCP	23						
	Area			Concentration			Average Concentration			Standard Deviation		
Sample	Triclosan	DCP	TCP	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)
t=0	421	1174	2507	0.004723557	0.18482138	2.757124179						
t=0	118	1367	415	0.004478656	0.188490625	2.352929129	**0.00453**	**0.18869**	**2.53951**	**0.00018**	**0.00397**	**0.20388**
t=0	0	1591	1220	0.004383282	0.19274923	2.508463075						
VI t=1	1860	1374	204	0.005886634	0.188623706	2.312161846						
VI t=1	0	278	186	0.004383282	0.167786959	2.308684069	**0.00490**	**0.17858**	**2.35100**	**0.00086**	**0.01044**	**0.07030**
VI t=1	55	885	825	0.004427736	0.179327019	2.432145176						
VI t=4	210	562	581	0.004553015	0.173186262	2.385001968						
VI t=4	192	1699	971	0.004538467	0.194802486	2.460353818	**0.00463**	**0.18670**	**2.40761**	**0.00015**	**0.01178**	**0.04583**
VI t=4	512	1558	542	0.004797108	0.192121846	2.377466783						
VII t=1	Vial Broken											
VII t=1	76744	203966	129198	0.066411919	4.040228041	27.23507594	**0.07905**	**3.50131**	**21.95977**	**0.01788**	**0.76214**	**7.46041**
VII t=1	108025	147273	74591	0.091694908	2.962401648	16.68446452						
VII t=4	73667	181814	141100	0.063924921	3.619082392	29.53465982						
VII t=4	62430	113800	82410	0.054842572	2.326025326	18.1951725	**0.06166**	**2.65426**	**20.77060**	**0.00601**	**0.84966**	**7.80195**
VII t=4	76490	97581	63709	0.066206622	2.017675684	14.5819547						
IX t=1	381031	103481	429	0.31235307	2.129844306	2.355634067						
IX t=1	415937	147586	1687	0.34056598	2.968352289	2.598692085	**0.33559**	**2.59942**	**2.51510**	**0.02119**	**0.42822**	**0.13815**
IX t=1	432358	133474	1647	0.353838317	2.700060153	2.59096369						
IX t=4	440802	140123	3199	0.360663213	2.826468487	2.89082541						
IX t=4	427849	918	3512	0.3501939	0.179954403	2.9513001	**0.34043**	**1.88789**	**2.90706**	**0.02650**	**1.48153**	**0.03877**
IX t=4	378655	131222	3138	0.310432658	2.65724596	2.879039608						
XII t=1	687410	490510	26962	0.559985088	9.487896816	7.482071573						
XII t=1	574329	597259	34448	0.46858693	11.51736941	8.928440667	**0.47424**	**10.82083**	**8.45759**	**0.08307**	**1.15474**	**0.84499**
XII t=1	482214	594095	34623	0.394134623	11.45721661	8.962252394						
XII t=4	499050	703993	33104	0.407742385	13.54655682	8.6687666						
XII t=4	510123	691582	45257	0.416692181	13.31060347	11.01684616	**0.42755**	**13.81067**	**10.46465**	**0.02693**	**0.67224**	**1.59325**
XII t=4	561489	758081	48836	0.45820895	14.57485792	11.70834429						

Intermediate (chlorophenoxy)phenol Formation

Sample	Area			Average			Standard Deviation		
Soap, time (min)	dichlorinated triclosan	monochlorinated triclosan 1	monochlorinated triclosan 2	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)
t=0	ND	ND	ND						
t=0	ND	ND	ND	**ND**	**ND**	**ND**	**ND**	**ND**	**ND**
t=0	ND	ND	ND						
VII t=1	343586	149425	84630						
VII t=1	380770	159533	91381	**362178.00**	**154479.00**	**88005.50**	**26293.06**	**7147.44**	**4773.68**
VII t=1	Broken Vial								
VII t=4	316545	111824	68995						
VII t=4	226872	102096	68534	**291601.00**	**123941.33**	**93038.00**	**56545.97**	**29812.00**	**42043.57**
VII t=4	331386	157904	141585						
IX t=1	175103	140280	391072						
IX t=1	168214	122481	430271	**180143.33**	**139556.67**	**436711.33**	**15094.43**	**16725.73**	**49176.82**
IX t=1	197113	155909	488791						
IX t=4	245424	166372	555036						
IX t=4	215481	174949	543382	**223124.33**	**170386.67**	**525279.00**	**19627.83**	**4314.65**	**41855.57**
IX t=4	208468	169839	477419						
XII t=1	718341	585075	503125						
XII t=1	664170	525992	432313	**644375.67**	**518419.33**	**443913.67**	**85596.62**	**70746.62**	**54347.65**
XII t=1	550616	444191	396303						
XII t=4	558296	456599	380467						
XII t=4	668949	477496	430191	**637793.67**	**482382.00**	**427762.33**	**69381.25**	**28541.41**	**46128.98**
XII t=4	686136	513051	472629						

Table D 3: Summary of experimental data from experiments ran in Atlanta conditions simulated in the lab.

Simulated Atlanta Tap Water Experiments

[HOCl],	1	mg/L
Temperature	33	°C
[$NaHCO_3$]	2	mmol/L
pH	6.35	

Triclosan and Phenol Analysis

Calibration Reference	Triclosan	20	DCP	22	TCP	24								
		Area			Concentration			Average Concentration			Standard Deviation		
Soap Type	Triclosan	DCP	TCP	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)
VI 0	14740	683	215	0.015470687	4.127973447	5.850538904	**0.015470687**	**4.127973447**	**5.850538904**	NA	NA	NA
VI 1	361	737	45374	0.003063371	4.137990909	14.76365893	**0.003063371**	**4.137990909**	**14.76365893**	NA	NA	NA
VI 5	219	73266	51499	0.002940842	17.59274083	15.97256214	**0.002940842**	**17.59274083**	**15.97256214**	NA	NA	NA
VII 0	513001	1570	1209	0.445408913	4.292519535	6.046726626						
VII 0	461848	1024	1065	0.401270138	4.191231864	6.018305064	**0.42915**	**4.37414**	**6.00580**	**0.02426**	**0.23463**	**0.04840**
VII 0	507631	3436	731	0.440775261	4.638678496	5.952382832						
VII 1	31555	360946	480367	0.029979973	70.95984166	100.6190769						
VII 1	40987	323117	402759	0.038118634	63.94223857	85.30143434	**0.03393**	**60.72911**	**79.12547**	**0.00407**	**12.15997**	**25.15674**
VII 1	35858	233326	231278	0.033692935	47.28523999	51.45589447						
VII 4	26982	265705	315931	0.026034034	53.29182147	68.16402241						
VII 4	63865	235706	180649	0.057859546	47.72675035	41.46314987	**0.03995**	**53.38952**	**59.03550**	**0.01628**	**5.71225**	**15.22196**
VII 4	38487	297284	312462	0.03596144	59.1499961	67.4793391						
IX 0	289622	568	245	0.252660191	4.106639963	5.856460063						
IX 0	303143	843	625	0.264327158	4.157654816	5.931461405	**0.26597**	**4.34081**	**5.88626**	**0.01421**	**0.36232**	**0.03980**
IX 0	322384	4080	318	0.280929785	4.758146005	5.870868216						
IX 1	54609	301043	23005	0.049872751	59.84732275	10.34864571						
IX 1	57434	312188	26949	0.052310381	61.91481559	11.1270807	**0.05231**	**64.05429**	**11.00201**	**0.00244**	**5.59254**	**0.60068**
IX 1	60255	357932	28992	0.054744558	70.40071888	11.5303116						
IX 5	55806	319989	27342	0.050905616	63.36196782	11.20464787						
IX 5	70703	336570	22872	0.063759903	66.43788515	10.32239524	**0.05674**	**67.16693**	**10.95510**	**0.00651**	**4.21702**	**0.55200**
IX 5	61196	364941	28019	0.055556526	71.70094834	11.33826868						
XII 0	521440	1735	406	0.452690737	4.323128446	5.888236947						
XII 0	Vial Broken						**0.41692**	**4.21600**	**6.10002**	**0.05059**	**0.15151**	**0.29950**
XII 0	438526	580	2552	0.381146108	4.108866066	6.311797158						
XII 1	1370	95610	868956	0.003934014	21.73774396	177.3156467						
XII 1	708	100467	808645	0.003362789	22.63875901	165.4119468	**0.00341**	**22.17734**	**163.48171**	**0.00050**	**0.45090**	**14.89316**
XII 1	220	97862	718995	0.002941705	22.15550922	147.7175513						
XII 5	93	162812	835200	0.002832119	34.20428981	170.6531591						
XII 5	422	156487	814341	0.003116006	33.03094821	166.5361775	**0.00293**	**38.98460**	**168.62990**	**0.00016**	**9.31437**	**2.05940**
XII 5	116	246443	825306	0.002851966	49.7185557	168.700361						

Intermediate (chlorophenoxy)phenol Formation

Sample	Area			Average			Standard Deviation		
Soap, time (min)	dichlorinated triclosan	monochlorinated triclosan 1	monochlorinated triclosan 2	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)
VI t=0	ND	ND	ND	**ND**	**ND**	**ND**	**ND**	**ND**	**ND**
VI t=1	ND	ND	ND	**ND**	**ND**	**ND**	**ND**	**ND**	**ND**
VI t=4	ND	ND	ND	**ND**	**ND**	**ND**	**ND**	**ND**	**ND**
VII t=0	ND	ND	ND						
VII t=0	ND	ND	ND	**#DIV/0!**	**#DIV/0!**	**#DIV/0!**	**#DIV/0!**	**#DIV/0!**	**#DIV/0!**
VII t=0	ND	ND	ND						
VII t=1	313193	80258	ND						
VII t=1	337241	124975	ND	**320175.33**	**106461.00**	**#DIV/0!**	**14860.41**	**23329.02**	**#DIV/0!**
VII t=1	310092	114150	ND						
VII t=4	298090	102590	ND						
VII t=4	447258	212762	120544	**365146.00**	**140120.33**	**120544.00**	**75715.16**	**62921.15**	**#DIV/0!**
VII t=4	350090	105009	ND						
IX t=0	ND	ND	ND						
IX t=0	ND	ND	ND	**#DIV/0!**	**#DIV/0!**	**#DIV/0!**	**#DIV/0!**	**#DIV/0!**	**#DIV/0!**
IX t=0	ND	ND	ND						
IX t=1	276989	108971	172364						
IX t=1	271378	111403	188923	**268454.00**	**110018.67**	**179419.33**	**10312.73**	**1250.47**	**8546.69**
IX t=1	256995	109682	176971						
IX t=4	286812	112136	199562						
IX t=4	271809	121305	186860	**276946.67**	**113966.33**	**189795.67**	**8546.09**	**6616.19**	**8679.21**
IX t=4	272219	108458	182965						
XII t=0	ND	ND	ND						
XII t=0	ND	ND	ND	**#DIV/0!**	**#DIV/0!**	**#DIV/0!**	**#DIV/0!**	**#DIV/0!**	**#DIV/0!**
XII t=0	ND	ND	ND						
XII t=1	ND	ND	ND						
XII t=1	ND	ND	ND	**#DIV/0!**	**#DIV/0!**	**#DIV/0!**	**#DIV/0!**	**#DIV/0!**	**#DIV/0!**
XII t=1	ND	ND	ND						
XII t=4	ND	ND	ND						
XII t=4	ND	ND	ND	**#DIV/0!**	**#DIV/0!**	**#DIV/0!**	**#DIV/0!**	**#DIV/0!**	**#DIV/0!**
XII t=4	ND	ND	ND						

Table D 4: Summary of Danville tap water experimental data.

Danville Tap Water Experiments

$[HOCl]_i$ 1.6 mg/L
Temperature 38 °C
pH 7.22

Trihalomethane Analysis

Calibration Reference 25

		Chloroform			
Sample Date	Sample	Area	Concentration (ppb)	Average Concentration (ppb)	Standard Deviation
8/1/2006	t=0	100100222	74.7992		
8/1/2006	t=0	97171361	69.85758	**72.4844**	**5.6375**
8/1/2006	t=0	97132913	72.79659		
8/1/2006	VI, t=1	86922721	67.75536786		
8/1/2006	VI, t=1	74227369	55.60722364	**61.6813**	**8.5900**
8/1/2006	VI, t=1				
8/1/2006	VI, t=4	78091495	59.30479421		
8/1/2006	VI, t=4	79208700	60.37384432	**59.8393**	**0.7559**
8/1/2006	VI, t=4				
8/1/2006	VII, t=1	94283882	107.1964		
8/1/2006	VII, t=1	89119629	97.45371	**100.0774**	**6.2359**
8/1/2006	VII, t=1	92191022	95.58209		
8/1/2006	VII, t=4	127950406	107.0146365		
8/1/2006	VII, t=4	128038487	107.0989209	**106.4996**	**0.9659**
8/1/2006	VII, t=4	126247768	105.3853873		
8/1/2006	IX, t=1	76907221	58.17156597		
8/1/2006	IX, t=1	74710529	56.06955799	**58.5342**	**2.6645**
8/1/2006	IX, t=1	80240850	61.36150555		
8/1/2006	IX, t=4	76715649	57.9882513		
8/1/2006	IX, t=4	75754610	57.06863597	**56.2644**	**2.2371**
8/1/2006	IX, t=4	72272277	53.73640197		
8/1/2006	XII, t=1	153678379	131.6336566		
8/1/2006	XII, t=1	137656486	116.3023553	**122.9482**	**7.8665**
8/1/2006	XII, t=1	142470101	120.908489		
8/1/2006	XII, t=4	146811768	125.0630171		
8/1/2006	XII, t=4	140770389	119.2820397	**116.0889**	**22.4900**
8/1/2006	XII, t=4	124718236	103.9217827		

Danville Tap Water Experiments Continued…

Triclosan and Phenol Analysis

Calibration Reference	Triclosan	26	DCP	27	TCP	28						
	Area			Concentration			Average Concentration			Standard Deviation		
Sample	Triclosan	DCP	TCP	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)	Triclosan (mg/L)	DCP (µg/L)	TCP (µg/L)
t=0	421	1174	2507	1298	1077	1206						
t=0	118	1367	415	64	746	715	**0.00000**	**7.71314**	**-3.11813**	**0.00000**	**0.20056**	**0.09003**
t=0	0	1591	1220	133	2626	1475						
VI t=1	1860	1374	204	405	2460	2892						
VI t=1	0	278	186				**0.00000**	**7.98189**	**-2.59143**			
VI t=1	55	885	825									
VI t=4	210	562	581	139	1429	1161						
VI t=4	192	1699	971				**0.00000**	**7.68652**	**-3.12822**			
VI t=4	512	1558	542									
VII t=1	Vial Broken			54	1644	2354						
VII t=1	76744	203966	129198	0	1810	2642	**0.00000**	**7.66529**	**-2.73210**	**0.00000**	**0.16737**	**0.08735**
VII t=1	108025	147273	74591	0	344	3060						
VII t=4	73667	181814	141100	0	410	3274						
VII t=4	62430	113800	82410	0	1863	1676	**0.00000**	**7.79797**	**-2.66747**	**0.00000**	**0.31017**	**0.13254**
VII t=4	76490	97581	63709	0	1880	2383						
IX t=1	381031	103481	429	3355	411375	58750						
IX t=1	415937	147586	1687	3863	416222	73119	**0.00000**	**92.24299**	**11.27625**	**0.00000**	**1.91559**	**3.08904**
IX t=1	432358	133474	1647	3655	1003	50299						
IX t=4	440802	140123	3199	4648	292270	63318						
IX t=4	427849	918	3512	3489	466986	72177	**0.00000**	**76.51811**	**10.36393**	**0.00000**	**17.12724**	**1.75467**
IX t=4	378655	131222	3138	3748	380732	56240						
XII t=1	687410	490510	26962	61	1896	64472						
XII t=1	574329	597259	34448	0	725	146371	**0.00000**	**7.66133**	**21.07526**	**0.00000**	**0.17452**	**12.56875**
XII t=1	482214	594095	34623									
XII t=4	499050	703993	33104	0	344	182886						
XII t=4	510123	691582	45257	0	661	25701	**0.00000**	**7.50536**	**15.16931**	**0.00000**	**0.03722**	**18.77265**
XII t=4	561489	758081	48836	0	643	40882						

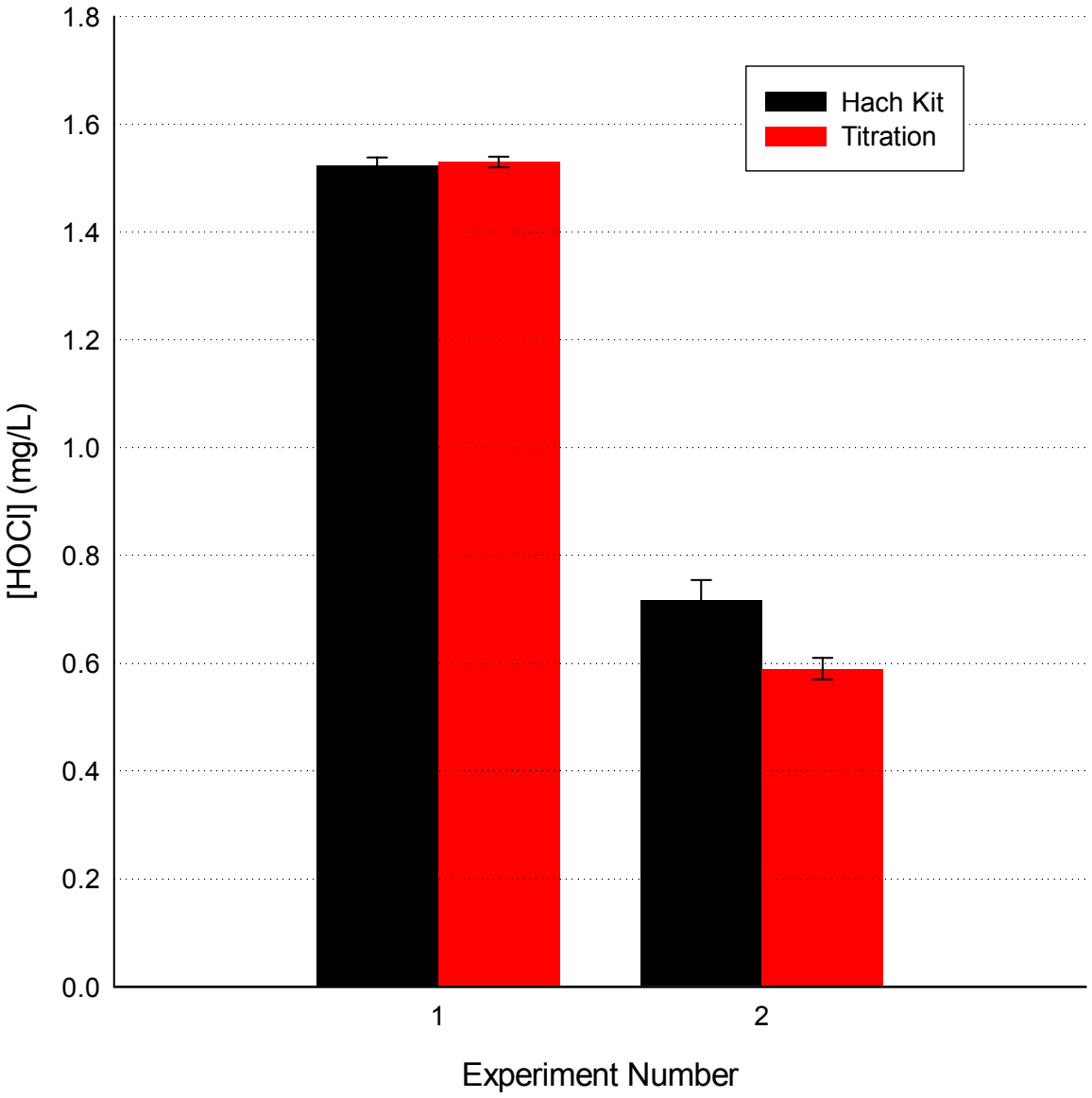

Figure D 1: Comparison between field chlorine Hach kit and manual DPD-FAS titrations performed in the lab.

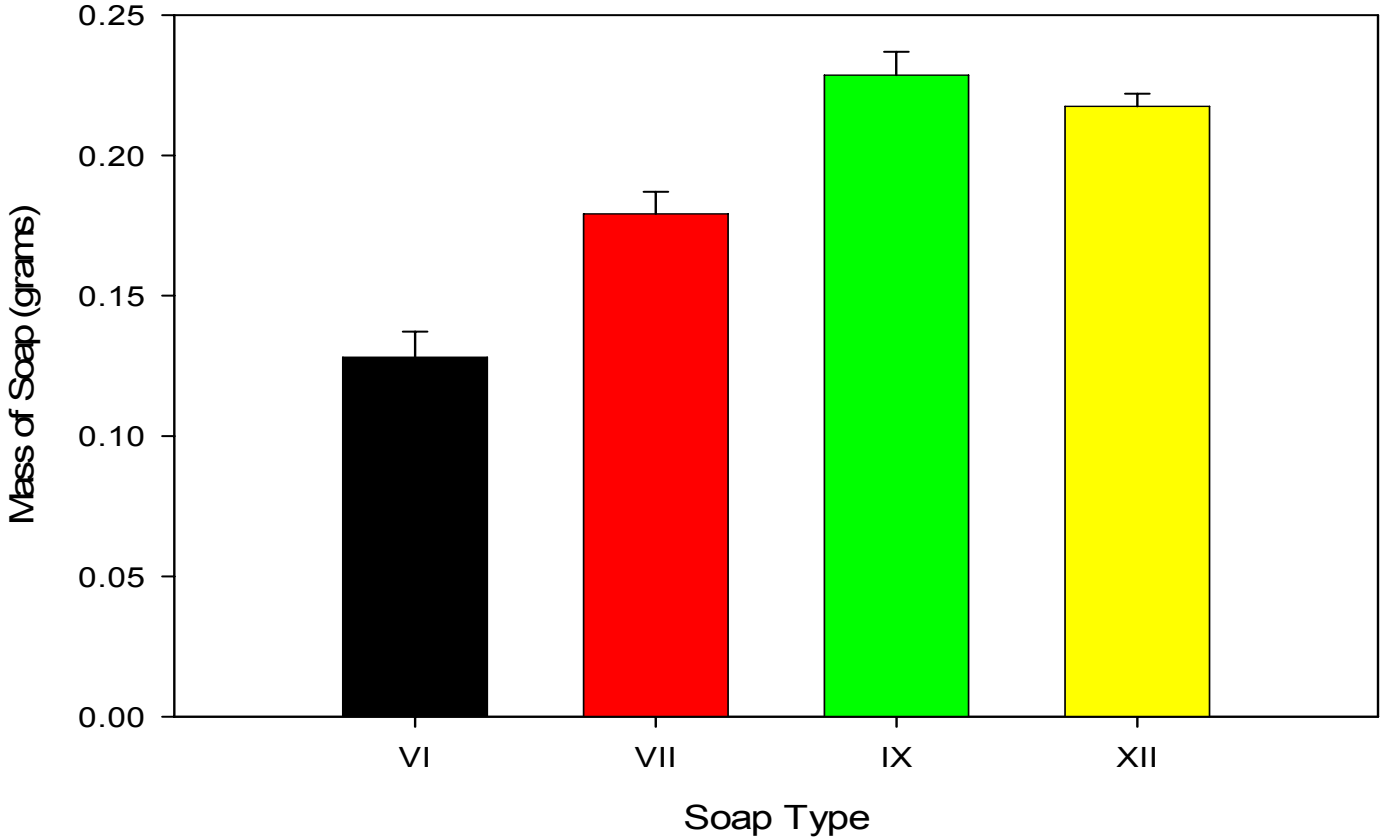

Figure D 2: Mass of each tested soap dispensed during field experiments by transferring a given aliquot of soap to the reaction vial. Each was compared to the 0.25 g mass of soap utilized in the laboratory and product levels were normalized to allow for comparisons.

Table D 5: Breakdown of ICP analysis for Atlanta tap water.

Constituent	Concentration (ppb)
Na	45,530.0
Mg	1,305.0
Al	9.8
Si	3,314.0
P	109.8
K	16,990.0
Ca	4,834.0
Cr	0.3
Fe	16.1
Mn	0.9
Co	0.1
Ni	1.0
Cu	117.6
Zn	59.0
As	0.1
Se	0.0
Sr	25.8
I	11.6
Ba	16.6
Pb	0.3

Appendix E

Discussion of Application of Model from Rule et al. (2005)

Discussion E 1: Discussion of model proposed by Rule et al which predicts consumption rates of free chlorine and triclosan during reactions at 25 °C.

Rule et al (33) developed the model shown below which predicts the observed rates of the pH dependent reaction between triclosan and free chlorine. The reaction rates are optimized when between a pH of 7 to 9, which also happens to be the pH range that encompasses the majority of drinking waters.

$$\frac{d[HOCl]}{dt} = \frac{d[triclosan]}{dt} = -k_{ArO^-}[phenolate - triclosan][HOCl] \quad (1)$$

where

$$HOCl \leftrightarrow phenolate - triclosan + H^+ \; K_A = 10^{-7.9} \quad (2)$$

The model can then be expressed as the pseudo first order equation

$$\frac{d[triclosan]_{total}}{dt} = k_{obs}[triclosan]_{total} \quad (3)$$

where

$$k_{obs} = -k_{ArO^-}\left(\frac{1}{1+\frac{[H^+]}{K_A}}\right)[HOCL]_{initial} \qquad k_{ArO^-} = 5.40x10^3 M^{-1}s^{-1} \quad (4)$$

when excess free chlorine is present, as was determined to be the case for soap reactions. The model can then be used to predict triclosan concentrations still present over time, as shown in Figure S 2 below.

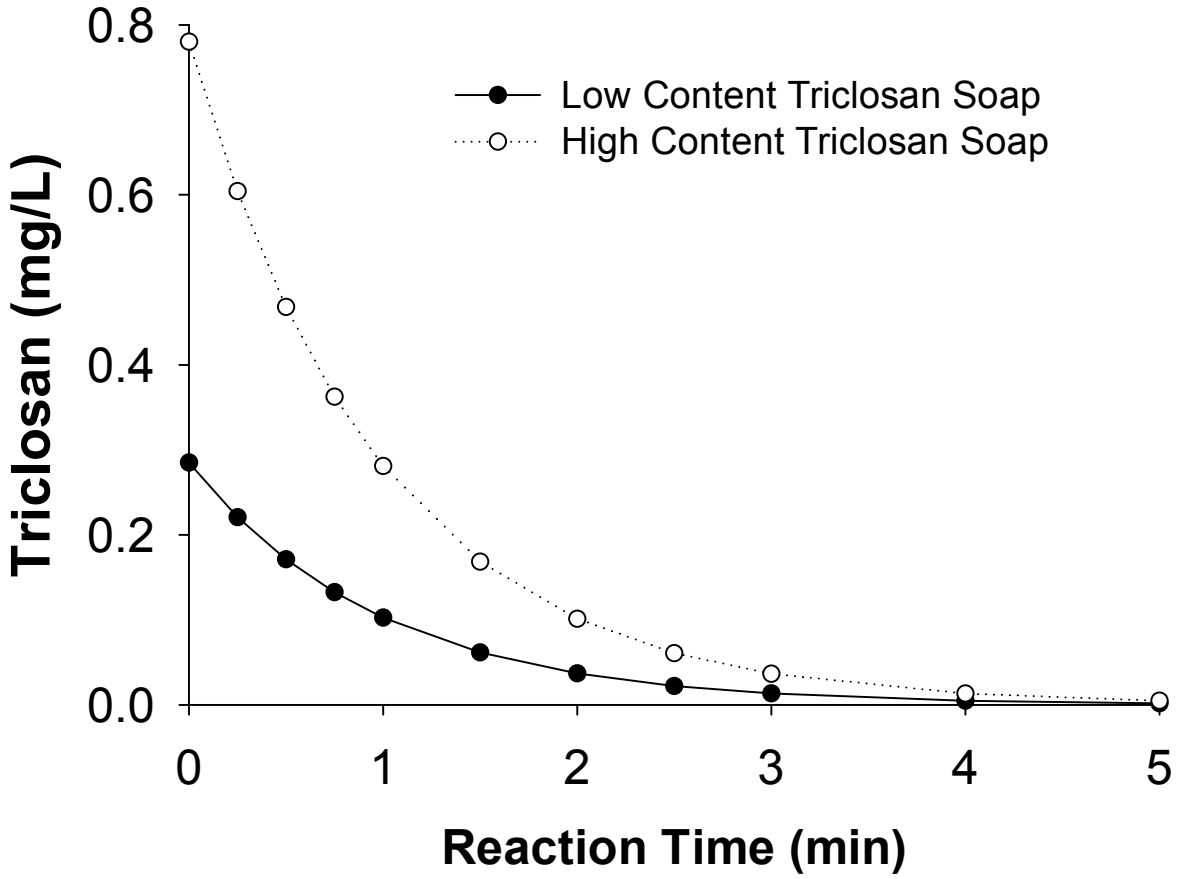

Figure E 1: Triclosan consumption over time as predicted by Rule et al model. The high and low content soap solutions have initial triclosan concentrations of 0.78 and 0.285 mg/L, respectively.

Vita

E. Matthew Fiss was born March 8, 1982 in Charlotte, NC. He graduated from Providence Day School in 2000 and received a Bachelor of Science of Public Health in Environmental Sciences and Engineering from the University of North Carolina at Chapel Hill in 2003. He completed his Masters graduate work in 2006 at Virginia Tech and is staying to continue his PhD work.