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NMR-Based Sensors for *In Situ* Monitoring of Changes in Groundwater Chemistry

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The objective of this project is to explore the applicability of nuclear magnetic resonance relaxation-based sensors to determine key chemical parameters related to the natural attenuation of chlorinated ethenes. Recent progress in the development of chemical sensors based on nuclear magnetic resonance relaxation in the biomedical field may present opportunities for the development of chemical sensors based on similar principles for environmental applications. Small, portable sensors capable of measuring changes in chemical parameters related to the degradation of chlorinated ethenes may improve the ability to monitor the progress of remedial strategies based on monitored natural attenuation.

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Abstract

Objectives

The objective of this project is to explore the applicability of nuclear magnetic resonance relaxation-based sensors to determine key chemical parameters related to the natural attenuation of chlorinated ethenes. Recent progress in the development of chemical sensors based on nuclear magnetic resonance relaxation in the biomedical field may present opportunities for the development of chemical sensors based on similar principles for environmental applications. Small, portable sensors capable of measuring changes in chemical parameters related to the degradation of chlorinated ethenes may improve the ability to monitor the progress of remedial strategies based on monitored natural attenuation. The objective of this limited scope study is to explore the viability of a nuclear magnetic resonance relaxation approach to measure variation in key chemical parameters indicative of the attenuation of chlorinated ethenes in groundwater.

This project focused on three key research questions:

1) Can nuclear magnetic resonance sensor designs previously developed to study changes in pH, dissolved oxygen, and oxidative-reductive potential in biological organisms be used to perform the same measurements in groundwater under environmental conditions?
2) Can polymer materials be identified that have potential to exhibit measurable changes in relaxation properties upon exposure to chlorinated ethenes?
3) Can relaxation contrast agents be activated by exposure to chlorinated ethenes and thus be used to induce observable changes in polymer sensor materials?

Technical Approach

The scientific principle exploited by these sensors is the relaxation of the nuclear magnetic resonance signals from these sensor materials in response to changes in their physical or electronic structure resulting from interactions with the chemical parameters of interest. Nuclear magnetic resonance is a physical property intrinsic to many common stable isotopes, including hydrogen-1 nucleus. When placed into a strong external magnetic field, the individual nuclear magnetic moments of a sensor material align and can be manipulated using radiofrequency radiation. Once excited, a nuclear magnetic resonance signal is easily observed; the rate of decay of this signal is highly sensitive to variations in the structural mobility of the material being studied (e.g., binding of water to a polymer surface or rigidity of a polymer) and by the presence of magnetic materials, including ferromagnetic and paramagnetic species.

Here, a variety of potential sensor materials were screened for sensitivity to key chemical parameters, including pH, oxidation-reduction potential, dissolved oxygen, tetrachloroethene, trichloroethene, 1,1-dichloroethene, and ethene by placing the sensor material in contact with

prepared standard solutions using deionized water and then measuring the nuclear magnetic relaxation response. The sensor sensitivity for "natural" waters (i.e., groundwater) was also tested in a similar manner to investigate potential interferences not found in ideal standard solutions.

Results

The proof-of-concept experiments conducted achieved partial success in meeting the key research objectives. For example, sensor materials were identified that produced a measurable response in the T_2 relaxation properties upon exposure to changes in pH and dissolved oxygen, and upon exposure to chlorinated ethenes. Similarly, polymer sensor materials embedded with relaxation contrast agents were found to be activated by exposure to chlorinated ethenes. No sensor materials were identified that interacted with oxidation-reduction potential changes. Several other limitations were identified that limit the utility of magnetic relaxation sensors in field settings, including limited range in pH sensitivity (limited to the region of the pKa of the sensor material), non-unique T_2 response for changes in dissolved oxygen, similar responses in T_2 to individual chlorinated ethenes (i.e., cannot differentiate between constituents), and interference from naturally-occurring paramagnetic constituents such as iron and manganese found in groundwater.

For most measurements with any sensor material, the presence of iron and manganese in native groundwater is likely to prevent a simple correlation between measurements made in controlled (laboratory) and uncontrolled (field) environments. Any magnetic relaxation sensor employed in the field would need to be calibrated against a non-contaminated water sample taken from the same source, and calibrations would have to somehow account for natural variability in the site groundwater. Due to their paramagnetic properties, which strongly influence the response of paramagnetic sensor materials, variations in iron and/or manganese concentrations over time would interfere with the reliability of any measurements of the targeted chemical parameters, including pH, dissolved oxygen, and the concentration of chlorinated ethenes.

While the applications of relaxation-based sensors may not be well suited for the characterization of chlorinated ethenes in groundwater, other environmental contaminants may prove more fruitful. For example, the original development of these sensors was aimed at detecting trace concentrations of specific biomarkers of disease in biological samples; similar approaches could be developed to detect specific biomarkers of pathogens in water systems, or to detect contaminants such as heavy metals (i.e. mercury) that are able to form unique and specific interactions with structural moieties bound to magnetic nanoparticles (e.g. mercury binding to sulfur) in ways that chlorinated ethenes can not.

Benefits

This study has demonstrated some of the unique considerations and limitations for use of magnetic relaxation sensors in environmental applications. If further research is considered, it should focus on compounds that form unique and specific interactions with sensor materials, unlike the interactions of chlorinated ethenes.

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List of Acronyms

Acac	Acetylacetonate
CPMG	Carr-Purcell-Meiboom-Gill
DCE	Dichloroethene
DO	Dissolved Oxygen
EMNA	Enhanced Monitored Natural Attenuation
FY	Fiscal Year
^{1}H	Hydrogen-1 Nucleus
LDPE	Low-density Polyethylene
MNA	Monitored Natural Attenuation
MRI	Magnetic Resonance Imaging
MRS	Magnetic Relaxation Switches
NMR	Nuclear Magnetic Resonance
ORP	Oxidation Reduction Potential
PCE	Tetrachloroethene
PDMS	Polydimethylsiloxane
PEO	Polyethylene Oxide
PETP	Polyethylene Terephthalate
PMP	Polymethylpentene
PPS	Polyphenylene Sulfide
PSF	Polysulfone
PVC	Polyvinyl Chloride
SERDP	Strategic Environmental Research and Development Program
SAN	Styrene Acrylonitrile
SON	Statement of Need
T_1	Longitudinal Relaxation
T_2	Transverse Relaxation
TCE	Trichloroethene
VC	Vinyl Chloride

Objective

The objective of this limited scope project was to explore the applicability of nuclear magnetic resonance (NMR) relaxation-based sensors to monitor key chemical parameters indicative of the attenuation of chlorinated ethenes. This research builds upon recent progress in the development of chemical sensors based on variations in the NMR relaxation behavior for specific chemical analytes in the biomedical field. The development of similar chemical sensors for environmental applications may provide a novel approach for monitoring changes in the groundwater environment at low cost. Small, portable sensors capable of measuring changes in chemical parameters related to the degradation of chlorinated ethenes will improve the ability to monitor the progress of remedial strategies based on natural attenuation and enhanced natural attenuation.

This limited scope study explored the viability of an NMR relaxation approach to measure variations in key chemical parameters indicative of the attenuation of chlorinated ethenes in groundwater. Key chemical parameters of interest included: decreases in the concentration of targeted chlorinated ethenes, including trichloroethene (TCE) and tetrachloroethene (PCE); the emergence of degradation products, including dichloroethene (DCE), vinyl chloride (VC), and ethene; and other geochemical parameters including pH, dissolved oxygen (DO), and oxidative-reductive potential (ORP) that are indicative of optimal environmental conditions for anaerobic dehalogenating microbial communities.

The specific research objectives of this project are related to the assessment of materials with properties desired for the potential construction of NMR-based sensors for deployment in groundwater wells in order to provide *in situ* monitoring of key indicators of natural attenuation processes. The general idea behind these proposed sensors are outlined in Figure 1. Specific technical questions that were to be addressed include:

- Will NMR relaxation-based approaches for sensors previously developed to monitor pH and DO conditions in biological settings be suitable for the monitoring of these same parameters under environmental conditions?

- Can polymer materials be identified that will exhibit sensitivity to chlorinated ethenes as measured by NMR relaxation?

- Can interactions between chlorinated ethenes and paramagnetic materials be used to induce measurable responses in the NMR properties of a bulk polymer material?

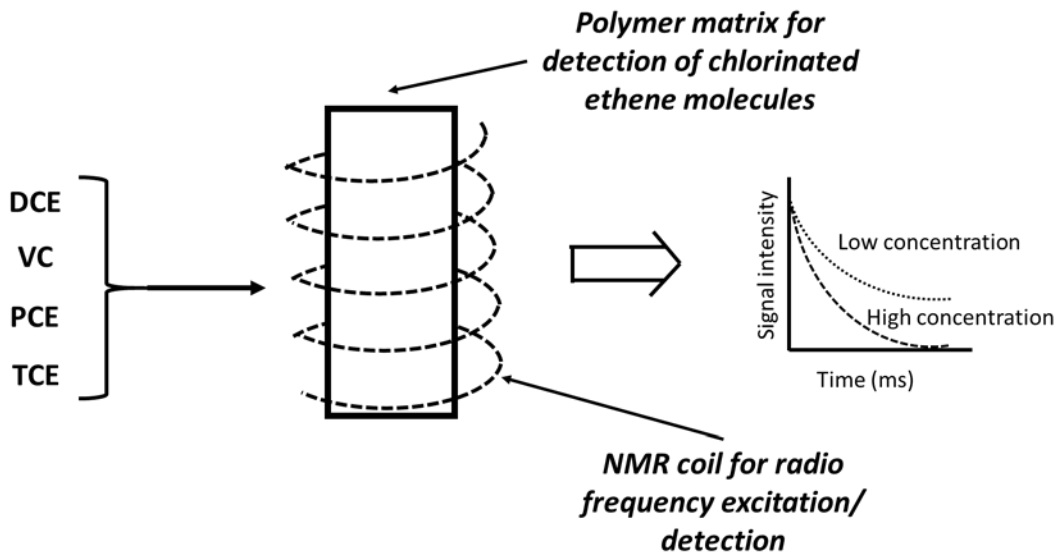

Figure 1: A graphical overview of the use of magnetic relaxation sensors to detect chlorinated ethene molecules in groundwater.

The investigations needed to address these questions have been performed in a laboratory setting and represent the initial stages in the development of NMR-based sensors for monitoring natural attenuation processes in the environment.

Background

This research was completed in response to the Strategic Environmental Research and Development Program (SERDP) fiscal year (FY) 2015 statement of need (SON) for "Improved Understanding of Long Term Natural Attenuation Processes on Contaminants in Groundwater." The objective of this SON was to improve the ability to estimate and understand the impact of natural attenuation processes on the fate and transport of contaminants in groundwater, with a particular focus on common chlorinated solvents, including PCE, TCE, and their degradation products, including DCE and VC. This project responds to the specific stated objective of the development of cost-effective diagnostic methods to determine whether natural attenuation processes are still occurring and the development of sensors for key contaminant attenuation indicators, including changes in pH, DO, ORP, and dissolved-phase concentrations of selected chlorinated ethenes.

Monitored Natural Attenuation

Monitored natural attenuation (MNA) and enhanced monitored natural attenuation (EMNA) are often desired as a long-term remediation option for contaminated groundwater after the initial removal of the source of contamination.[1] In general, MNA and EMNA options are lower cost, less environmentally invasive and more sustainable than more aggressive remedies for the removal of contamination from a site. Nevertheless, significant monitoring is often required over the life of a MNA/EMNA remedy in order to establish that attenuation processes are occurring and to assess the need to adjust the application of amendments that increases rates of attenuation in EMNA remedies, such as the addition of electron donors to stimulate *in situ* biodegradation.

Naturally occurring attenuation processes that can act to reduce the concentrations of contamination present in groundwater include: sorption, biotic degradation, abiotic degradation, volatilization, dispersion, and dilution. The relative influence of each of these processes on the overall natural attenuation of groundwater contaminants are typically assessed through multiple lines of evidence. Direct measurements of changes in contaminant and daughter product levels over time assist in elucidating the mechanism responsible for natural attenuation and the state of progress towards site closure. Sorption, volatilization, diffusion, advection, and dispersion of PCE, as an example, will result in a reduction in the concentration of that compound in groundwater, whereas degradation of PCE will result not only in a decrease in PCE levels, but also corresponding transient increases in TCE, DCE, VC, and ethene concentrations. Real-time monitoring using *in situ* NMR sensors may provide detailed temporal trend data that can provide valuable insight into the changing relative contributions of degradation, sorption, diffusion, advection, and dispersion transport mechanisms that control long-term plume behavior over time.

Measurements of general chemical parameters *in situ* can provide proxy information on the occurrences of both abiotic and biotic degradation activity and ensure that geochemical conditions are conducive to the processes degrading the contaminants. Chlorinated ethenes can be degraded

under oxidizing and/or reducing conditions (depending on the constituent) either biotically or abiotically. These processes are sensitive to the redox conditions as well as pH. Bacteria carrying out the degradation reactions are also sensitive to the presence/absence of dissolved oxygen. Higher chlorinated ethenes, for example, generally biodegrade under only anaerobic conditions, whereas lower chlorinated ethenes such as VC can biodegrade under either aerobic or anaerobic conditions. Suitable conditions are not always encountered naturally in the subsurface. *In situ* measurements of pH, DO, and ORP can indicate if conditions for these reactions are favorable. Real-time measurements of changes in other chemical indicators such as the concentration of chloride, ethene, or the chlorinated ethenes themselves, can indicate if the rates of biotic or abiotic activity are changing and thus if natural attenuation processes have accelerated, slowed, or stopped.

Groundwater Monitoring

Current technologies for monitoring remediation progress include collection of water samples through pumping or using diffusion-based passive samplers. These sample collection techniques have an associated high labor and analytical cost; as a result, monitoring is typically only completed one to four times a year. The low temporal resolution of plume concentrations reduces our ability to identify changes in chemical kinetics in a timely manner or to optimize sampling events to reduce costs or capture changes in plume behavior that may otherwise be missed. There are also challenges in analyzing labile parameters, such as DO and ORP, which are difficult to measure accurately by these methods.

Imbedded or *in situ* sensors designed to monitor changes in key indicators of natural attenuation processes in real-time have the potential to provide improved capabilities for monitoring changes in groundwater chemistry by providing detailed temporal data and more accurate analysis of labile parameters. As examples, the benefits of incorporating real-time monitoring of MNA/EMNA indicators using sensors into these programs could include:

- Sensors could be developed such that changes in plume behavior outside of “normal” parameters trigger an “alarm” condition sent remotely to site owners (e.g., reductions of groundwater pH below neutral in EMNA programs where the amendment of electron donor may trigger transient pH reductions below neutral, adversely impacting microbial activity), allowing for timely response to changes (e.g., buffering of groundwater) and limiting the need for frequent checking of sensor data records;

- High-cost sampling programs could be optimized to provide maximum information for lowest cost. For example, when coupled with continual monitoring using NMR-based sensors, sampling of stable plumes could be reduced to once per year or every two years as an independent check on the sensor accuracy. Alternatively, sampling of plumes with temporally variable behavior (e.g., seasonal changes in groundwater flow direction, etc.)

may require more frequent sampling to capture temporal changes, and optimal sample collection timing could be identified from the sensor records;

- The enhanced detail and timely indications of changes in plume behavior will encourage both public and regulatory support for MNA/EMNA as a viable and preferred remediation method at many sites.

Features required in a field sensor deployed for extended periods of time include:

- The sensor should be able to be permanently or semi-permanently deployed inside a monitoring well and capable of real-time measurements, providing improved kinetic measurements;

- Remote access of measurement data or alarm capabilities should be incorporated as features, to limit field time for downloading of data records;

- The sensor needs to be durable and unaffected by environmental matrices (opaqueness, turbidity, biofilms, corrosive environments, well materials, changes in non-target geochemical parameters, etc.);

- Power requirements should be low and/or operable using alternative power (e.g., solar-powered);

- The mode of measurement and data downloads should be simple and user-friendly.

A Review of Magnetic Relaxation Contrast

NMR relaxation is a physical phenomenon that involves the polarization and manipulation of the spin states of atomic nuclei.[2] NMR properties are intrinsic for many atomic nuclei, termed NMR-active nuclei, and are useful for the study of the chemical and physical parameters of many types of materials. NMR presents many potentially useful attributes for the development of sensors for the real-time and *in situ* measurements of chemical parameters in the environment and NMR relaxation was the approach investigated in this study.

The phenomenon underlying NMR measurements arise from the interactions that occur between the magnetic moment of many types of atomic nuclei, including hydrogen (^{1}H), and an applied magnetic field. When placed inside a magnetic field, NMR-active nuclei exhibit two basic phenomena: (i) they polarize so that there is an excess of nuclear magnetic moments in a bulk sample that are aligned with the applied magnetic field, and (ii) they precess about the axis of the applied field at a rate that is intrinsic to each type of nuclei and proportional to the strength of the applied field. These phenomena are illustrated in Figure 2. This precession frequency, termed the Larmor frequency, corresponds to the same bandwidth as radiofrequency radiation, and it is thus

through the application of radiofrequency radiation that NMR can be probed using tuned radiofrequency circuits.

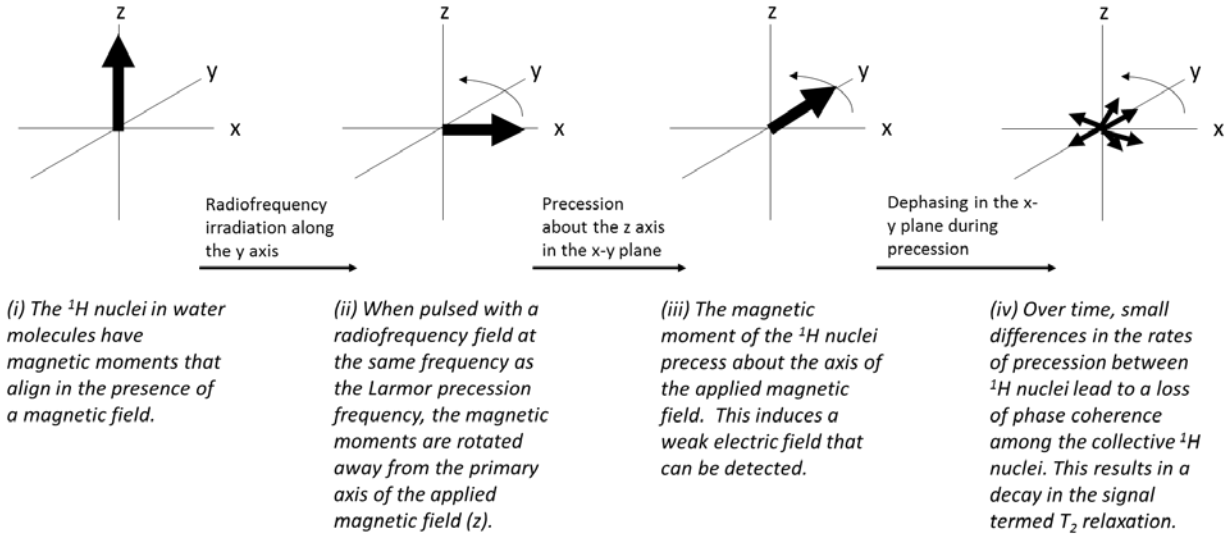

Figure 2: A graphical overview of the T_2 relaxation.

In general, NMR can be applied to derive two very different types of information. First, by measuring small variations in the precession frequency of atomic nuclei, a molecular spectrum detailing the chemical composition of a substance may be acquired (NMR spectroscopy). This application requires finely tuned and stable magnetic fields and as such is ill-suited for use as an *in situ* chemical sensor.

The second type of NMR application is based on measurement of the rate of decay, or relaxation, of the NMR signals in a bulk material in response to pulsed radiofrequency radiation. The lifetime of an NMR signal is typically on the order of 100's of milliseconds to seconds, and thus it is relatively easy to measure small variations in this parameter.[3] This type of measurement does not require the same quality of magnetic field as NMR spectroscopy, and thus can be performed with small, robust, and portable instrumentation. As such, NMR relaxometry may be used to make *in situ* measurements in the sub-surface environment.[4]

In general, during an NMR measurement, radiofrequency radiation is applied to shift the alignment of polarized nuclear spins away from their equilibrium position such that they may be observed as an oscillating electric field, as illustrated in Figure 2.[2] These excited NMR states decay exponentially with rates that are sensitive to variations in local chemical environments, including molecular mobility and strong magnetic dipole interactions, particularly with paramagnetic materials (i.e., materials that contain molecular structures with one or more unpaired electrons).[3] Two distinct types of NMR signal decay occur: the return of nuclear spin states to their equilibrium position in alignment with the applied magnetic field is termed longitudinal, or T_1 relaxation, while

the loss of phase coherence within a bulk sample about the plane perpendicular to the applied magnetic field is termed transverse, or T_2 relaxation (see Figure 2).

The mechanisms behind both T_1 and T_2 are complex but are, in general, affected by the local chemical and physical environment surrounding an observed nucleus, albeit in slightly different manners and to different degrees.[3] Factors that affect relaxation include changes in molecular dynamics, such as boundary interactions and material mobility, and local fluctuations in the strength of dipole-dipole interactions, such as the type that occur when the strong magnetic moments of unpaired electron spins are in close proximity. The information provided by T_1 and T_2 relaxation are not the same. In general, the measurement of T_2 can be made more rapidly than measurements of T_1. For direct monitoring of *dissolved* species, measuring both T_1 and T_2 responses can provide an enhanced measurement of changes in the physical properties of these dissolved species. However, for a *bulk material* such as the porous network in the polymer matrices studied here, the T_1 responses will not vary significantly, T_2 provides a more meaningful measurement as it is more sensitive to the type of structural variations being exploited. Therefore, this study was confined to investigation into the T_2 response of the polymers tested.

NMR tools are being used increasingly in a variety of practical applications to correlate measurements of changes in NMR properties to key physical and chemical parameters of interest. A significant advantage of NMR over optical methods for analyte detection, such as fluorescence or infra-red spectroscopy, is that NMR is capable of detecting signals through opaque media. Furthermore, NMR is able to analyze bulk material and is restricted only by the need for those materials to have a high density of NMR-active nuclei (i.e. ^1H) for rapid detection, such as organic polymers. Examples of NMR tools used strictly for relaxation measurements include geophysical profilers for down-bore measurements of rock porosity and fluid parameters,[4] tools for measuring fat and moisture content in food products, and Magnetic Resonance Imaging (MRI) for medical diagnostic applications.[5]

Small NMR sensors have previously been developed to monitor small changes in key biochemical indicators, including pH, dissolved oxygen and specific chemical markers resulting from disease[6-11] in a simple and minimally invasive manner. These sensors are implanted into an organism permanently and then scanned wirelessly using a handheld NMR tool similar in design and function to a down-bore NMR well-logger to measure T_2 values.[5] The sensors consist primarily of a polymer matrix enclosed by a size-selective permeable membrane.

In order to detect changes in local chemistry, an NMR–based sensor must respond to these changes by producing a measurable and predictable change in the relaxation properties of the sensor material. Several mechanisms are possible to accomplish this goal; however, one approach that is becoming more common in biomedical applications involves the use of Magnetic Relaxation Switches (MRS).[8-11] The general design of an MRS sensor is a polymer matrix with paramagnetic nanoparticles dispersed throughout its volume. These nanoparticles are functionalized such that

they are sensitive to interactions with specific analytes and chemical properties. Changes in the conformation of these nanoparticles result in changes in the NMR relaxation properties of the polymer material; these changes are then used to quantify the sensor's exposure to the targeted chemical agents. MRS sensors can be tuned to measure cumulative exposure to these molecules over a set time period.[8] In this way, intermediate compounds that exist only fleetingly can be both identified and quantified. MRS materials have been previously developed to detect a variety of analytes, including proteins, antibodies, peptides, nucleic acids, and other small molecules.[7] Many magnetic nanoparticles are also sensitive to pH and DO as they are usually comprised of iron oxides that are sensitive to these parameters.

To date, the NMR sensors described above have only been developed and tested for biomedical applications. The research described in this report explores the applicability of recent advancements in the use of NMR-based sensors to monitor changes in chemical markers of disease, including DO, [6] pH,[7] and the concentration of small organic molecules *in vivo*,[8-11] to develop similar sensors to monitor chemical markers of natural attenuation in groundwater. Ideally, future environmental NMR sensors will be deployed into groundwater monitoring wells as tools similar in design and function to wire-line NMR well-loggers or permanently embedded in the subsurface using direct push methods and then monitored in real time using surface-based electronics. Based on the size of similar medical-based NMR sensors, which are often only several millimeters in diameter,[12] NMR sensors for environmental monitoring may potentially be of similarly small size, leading to the opportunity to reduce the size of monitoring wells (cost savings) and increasing the ability to deploy three-dimensional arrays of sensors to improve spatial resolution in measurements of groundwater chemistry at small incremental costs.

Materials and Methods

Sensor Preparation

Both untreated polymers and polymers doped with paramagnetic salts and iron oxide (Fe_2O_3) nanoparticles were prepared. In the case of untreated polymers, ~ 80 mg of polymer material was added to the bottom of a 5 mm diameter glass NMR tube and thoroughly mixed with 300 µL of the water sample to be tested. For the doped polymers, polydimethyl siloxane (PDMS) was prepared using the Sylgard 184 (Aldrich, USA) kit with a set amount of Fe_2O_3 nanoparticles (<100 nm particles, 20 wt% in H_2O, Sigma Aldrich, USA), iron sulfate ($FeSO_4$; Heptahydrate, ≥99.0% pure, Sigma Aldrich, USA), manganese (Mn) (III) Acetylacetonate (acac) (>99.99%, Sigma Aldrich, USA), or potassium permanganate ($KMnO_4$; Monohydrate, ≥97% pure, Sigma Aldrich, USA) present. This polymer was allowed to cure in a vacuum before ~80 mg was placed into a 5 mm NMR tube and mixed with 300 µL of the water sample to be tested.[14,15]

Preparation of Control Water Samples

"Control" water samples were prepared with deionized water to assess the ability of different sensor materials to measure pH, DO, ORP, TCE, PCE, and 1,1 DCE. These are further described below.

pH

The pH of samples of deionized water were set using a buffer prepared from sodium phosphate monobasic (decahydrate, ≥99.0%, Sigma Aldrich, USA) and sodium phosphate dibasic (≥99.0%, Sigma Aldrich, USA). pH values were determined using a pH electrode. Tested polymer materials are not expected to interact with the sodium phosphate directly (only pH).

Dissolved Oxygen

Samples were prepared with high concentrations of dissolved oxygen by bubbling compressed gas through samples of deionized water. Samples with lower concentrations of DO were prepared by adding small amounts of ascorbic acid (≥99.0 %, Sigma Aldrich, USA) to remove DO. DO values were determined using Horiba handheld dissolved optical oxygen meter (Horiba Scientific, Japan).

Oxidative-Reductive Potential

Samples with low ORP values were prepared by the addition of small amounts of sodium bisulfite (Reagent grade, Sigma Aldrich). Samples with high ORP values were prepared by the addition of small amounts of sodium persulfate (≥98%, Sigma Aldrich, USA). ORP values were determined using a Horiba handheld ORP meter (Horiba Scientific, Japan).

Chlorinated Ethenes and Ethene

Standard solutions of PCE (anhydrous, ≥99%, Sigma Aldrich, USA), TCE (anhydrous, contains 40 parts per million [ppm] diisopropylamine as stabilizer, ≥99%, Sigma Aldrich, USA), 1,1 DCE

(with 200 ppm Mequinol as inhibitor, 99%, Aldrich, USA), and ethene (≥99.5%, Aldrich, USA) were prepared at saturated concentrations. Individual solutions were prepared as needed by diluting the stock solutions.

To test for the effects of cumulative exposure, samples were spiked with a set amount of stock solution of PCE, TCE, 1,1 DCE, and ethene every couple of days. The amended contaminant will absorb into the polymer matrix, removing it from solution. Re-spiking of the samples simulates a real-world situation where fresh analyte continually diffuses towards the polymer material in situ, replacing mass that absorbs to the polymer. In this way, the sensor material is allowed to be exposed to a cumulative mass of chlorinated ethene greater than it would be under instantaneous conditions, which are limited by the water solubility of the specific analyte and the volume of water used for the test.

Preparation of Uncontrolled Water Samples

Aerobic and anaerobic "natural" groundwater samples were collected from the Arboretum at the University of Guelph (referred to herein as "uncontrolled" samples). Anaerobic samples were stored under a nitrogen environment. These natural samples were used for testing of sensor response to changes in pH and DO in waters containing other trace materials (e.g., paramagnetic materials such as dissolved iron or manganese) that may interact with and alter the sensor response.

The pH and DO of these samples were explored in their natural state and with modifications of pH and DO concentrations (referred to herein as "stimulated" samples). pH was modified through the addition of small amounts of sodium phosphate salts. The pH and DO of these samples were also tested after stimulation to create synthetic high DO environments through the bubbling of compressed air, and through the preparation of synthetic low DO environments through the use of ascorbic acid to strip out any DO. The stimulation of these environments was designed to simulate changes observed through enhanced remedial activity.

While the amendment of ascorbic acid will affect the pH, which would affect the oxidation state of Fe_2O_3, the pH change affects the polymer to a lesser degree than the presence or absence of DO.

NMR Analysis

The response of each sensor material to the set chemical parameters was tested by measuring variations in transverse relaxation (T_2) using the Carr-Purcell-Meiboom-Gill (CPMG) pulse train.[3] For all measurements, an Oxford Instruments Pulsar Benchtop NMR spectrometer was employed, operating at a ^1H precession frequency of 60 MHz. Each measurement consisted of 16 sequential experiments that involved a train of spin echo pulses, with a delay of 1000 microseconds (μs) between each pulse. This combination of echo delay and pulses were optimized so that in most samples the signal intensity had been attenuated to ~10% its initial intensity by the end of the final experiment. Here, the use of the CPMG sequence allows for the effects of all non-T_2 related dephasing over the period of the experiment to be removed such that all signal loss over the period

of the experiment is due entirely to transverse relaxation (T_2). In general, the more pulses allowed in an experiment, the longer the time period allowed for T_2 signal relaxation. Over this time period, the strength of the NMR signal decays based on the following equation,

$$I(t) = I(0)e^{-t/T_2} \quad (1)$$

Where I(t) is the intensity of the signal after a set pulse train (i.e. after 2, 4, 6, …32 pulses), I(0) is the extrapolated signal intensity at time 0, t is the total time allowed for relaxation, and T_2 is the relaxation value to be determined (see Figure 3 for an example illustrating the decay of signal intensity over time).

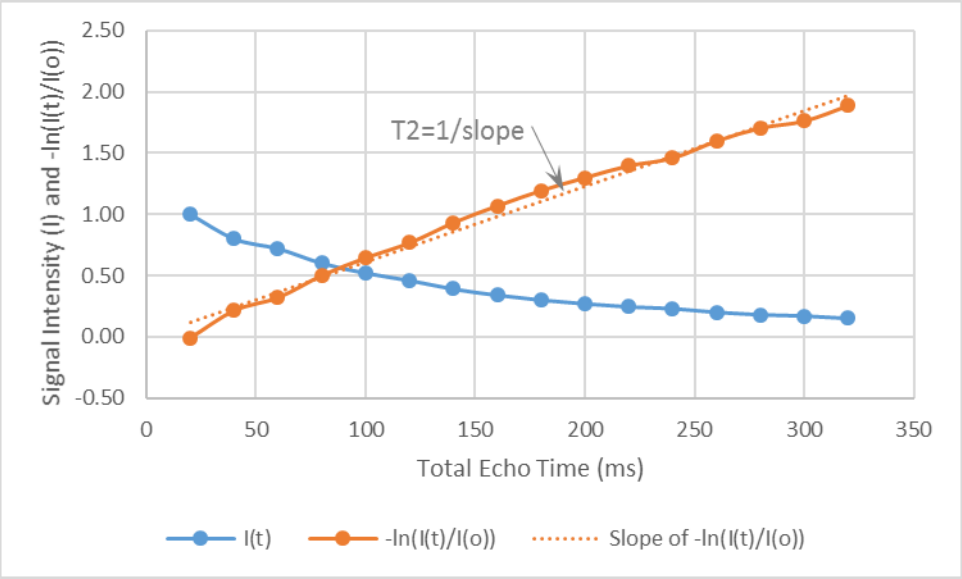

Figure 3: Example illustrating the linear decay of the NMR signal intensity (I_t) and the relationship to T_2, which is calculated as 1/slope of the -ln(I_t/I_o) relationship.

Signal intensities for each experiment were determined using Mestrenova NMR processing software. For linear decays, T_2 was calculated as 1/slope for plots of -ln(I_t/I_0) *versus* t (see Figure 3 for an example). Non-linear decay behavior was observed for pH-sensitive polymers due to the presence of multiple relaxation domains (i.e. the observed relaxation behaviour is the product of multiple processes, each with their own rate of T_2; see Figure 4 for an example of nonlinear decay). MatLab was used to decompose the decay curves into two components based on

$$I(t) = I(0)(A\, e^{-\frac{t}{T_{2\,fast}}} + B\, e^{-\frac{t}{T_{2\,slow}}}) \quad (2)$$

where T_{2fast} is the T_2 rate for the fast relaxation domain, T_{2slow} is the T_2 rate for the slow relaxation domain, $A = f\ T_{2fast}$, which is the fraction of the total signal due to the fast relaxation domain, and $B = f\ T_{2slow}$, which is the fraction of the total signal due to the slow relaxation domain and $A + B = 1$. Linear T_2 decay (i.e. all signals in the sample decay at the same rate) was observed for all other samples.

Results and Discussion

pH

pH tests were conducted under both controlled and uncontrolled conditions. The results of each set of tests are described further below.

Controlled Tests with pH-Sensitive Polymer Materials

Water samples were prepared across a wide range of pH values as described above using sodium monobasic phosphate and sodium dibasic phosphate. Small aliquots of these water samples were added to the polymer sensor materials being tested (chitosan, polyacrylic acid, polydimethyl siloxane (PDMS), and PDMS-Fe_2O_3) in 5mm NMR tubes and mixed thoroughly. A variety of molecular-weight distributions (low-, medium-, and high-molecular weight preparations) was tested for chitosan to explore the influence of particle size of the polymer on the observed relaxation properties. The pH of the water sample in the NMR tube was determined using a narrow H^+ electrode and compared to the T_2 decay behavior of the NMR signal of the polymer-water mixture in the NMR tube (See Appendix A).

First, the response of polymer materials with pH-sensitive structural moieties (i.e., low-, medium- and high-weight chitosan, and poly acrylic acid) was tested and compared to polymer materials that do not possess pH-sensitive functionality (i.e., PDMS). Table 1 compares the measured T_2 decays as a function of pH for the selected polymers. In general, polymers that are known to be pH sensitive, including chitosan and polyacrylic acid, exhibited variable T_2 decay behavior in response to differences in solution pH; whereas polymers that do not possess pH-sensitive functionality (i.e. PDMS) do not vary in their T_2 decay behavior in response to differences in solution pH.

Table 1: Decomposition of the T_2 behavior of pH-sensitive materials into a fast ($fT_{2(fast)}$) and slow-relaxing ($fT_{2(slow)}$) compartment for controlled samples.

Material	pH	$T_{2\,(fast)}$	$f\,T_{2(fast)}$	$T_{2\,(slow)}$	$f\,T_{2\,(slow)}$
Chitosan, Medium Molecular Weight	**4.28**	84.0	0.70	379.0	0.30
	5.47	77.0	0.69	376.0	0.31
	5.86	75.0	0.68	373.0	0.32
	6.21	83.0	0.66	372.0	0.34
	6.57	94.0	0.63	370.0	0.37
	6.87	93.0	0.58	367.0	0.42
	7.21	93.0	0.55	365.0	0.45
	7.63	94.0	0.54	368.0	0.46
	8.88	70.0	0.52	363.0	0.48
Chitosan, Low Molecular Weight	**4.26**	33.0	0.78	251.0	0.22
	5.89	43.0	0.81	241.0	0.19
	6.57	40.0	0.80	232.0	0.20
	7.40	47.0	0.70	244.0	0.30
	8.21	50.0	0.67	276.0	0.33
Chitosan, High Molecular Weight	**4.29**	87.0	0.68	430.0	0.32
	5.88	96.0	0.67	421.0	0.33
	6.58	97.0	0.60	421.0	0.40
	6.89	100.0	0.55	418.0	0.45
	8.89	101.0	0.49	411.0	0.51
Poly Acrylic Acid	**4.24**	85.0	0.72	331.0	0.28
	5.23	92.0	0.69	327.0	0.31
	5.86	94.0	0.60	325.0	0.40
	6.53	99.0	0.56	321.0	0.44
	6.80	103.0	0.53	317.0	0.47
	8.76	105.0	0.49	315.0	0.51
Polydimethyl Siloxane	**4.23**	221	1	--	0
	5.86	223	1	--	0
	6.54	221	1	--	0
	6.88	229	1	--	0
	8.92	225	1	--	0

For the pH-sensitive materials, the resulting decay of the NMR signal is not linear (see Figure 4) and can be decomposed into two components, one fast relaxing and one slow relaxing (see Table 1). In general, the fast-relaxing domain dominates the initial part of the curve, with the slow-

relaxing component dominating the latter part of the curve. This distribution produces the characteristic line shapes observed in Figure 4. In general, T_2 is calculated from the slope of each curve assuming a linear trend. The non-linear nature of the curves in Figure 4 require a deconstruction of the curve into two linear components. While the general trend of each individual decay curve is clearly influenced by pH, these variations appear to be mostly connected to changes in the relative contributions of the fast and slow relaxing components, rather than changes in the rate of T_2 relaxation of these components, which are relatively constant with respect to changes in pH (see Table 1 and Figure 5). The rate of T_2 relaxation with the tested polymer materials is thus not directly informative for predicting pH.

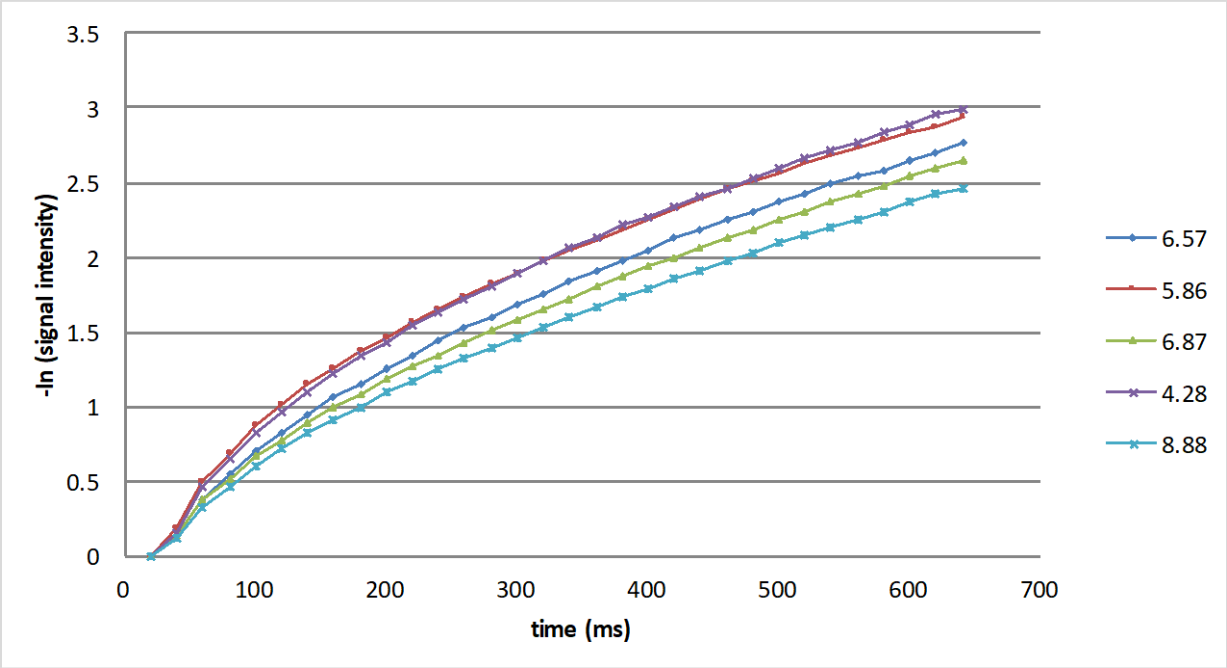

Figure 4: Example of the non-linear T_2 relaxation behavior for medium weight chitosan at a variety of pH value under controlled conditions.

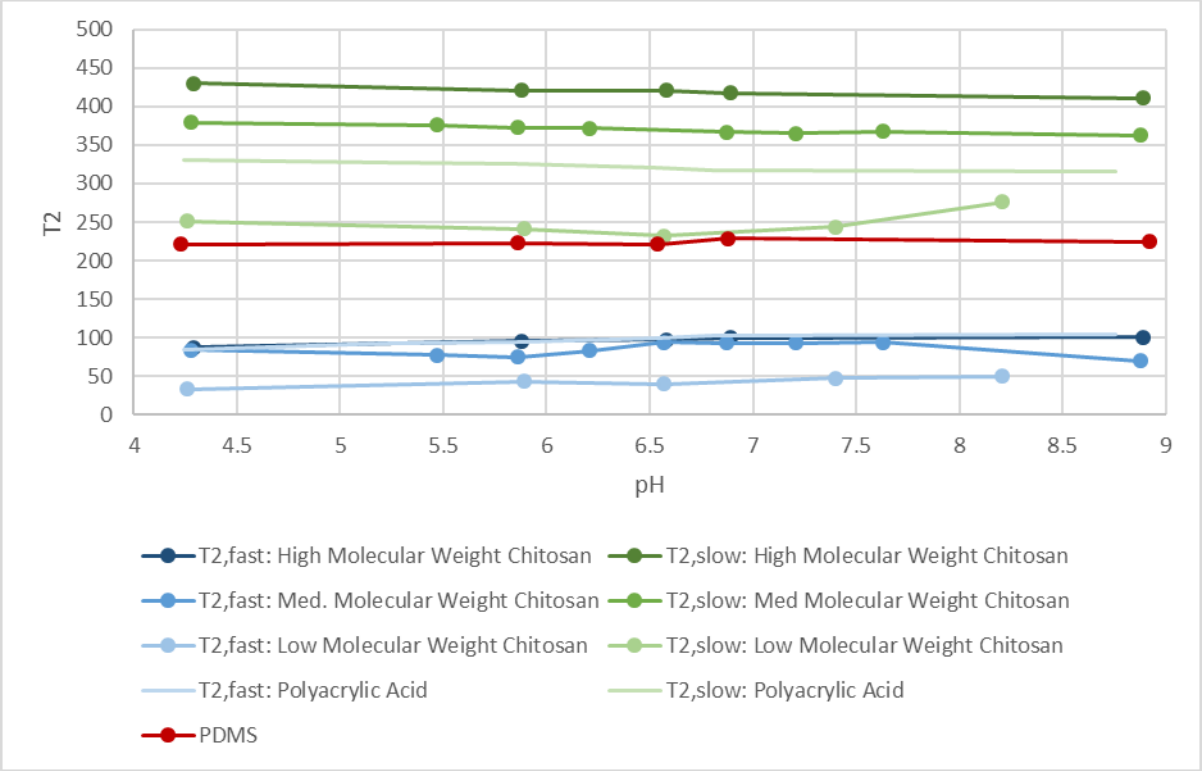

Figure 5: Variation in fast and slow relaxing components of T_2 with pH for various pH sensor materials.

Figure 6 and Table 1 compares the relative contribution of fast and slow relaxing components in the pH-sensitive polymers (chitosan and polyacrylic acid) to the sample pH. The observed trends are not linear, but instead display an "S" shaped profile characteristic of the titration analysis of a pH sensitive system. In general, there is a greater contribution of the slow relaxation domain as the pH increases. For pH-sensitive polymers, the observed changes in T_2 behavior occurs in response to changes in the conformational structure of the polymer matrix due to protonation or deprotonation of acidic functional groups. It is likely that at low pH, the protonated polymer surfaces are able to form a strong interaction with a layer of water through hydrogen bonding and that this layer of water is the source for the fast-relaxation domain. As the pH increases, hydrogen-bonding diminishes, resulting in a smaller relative contribution to the fast-relaxation domain.

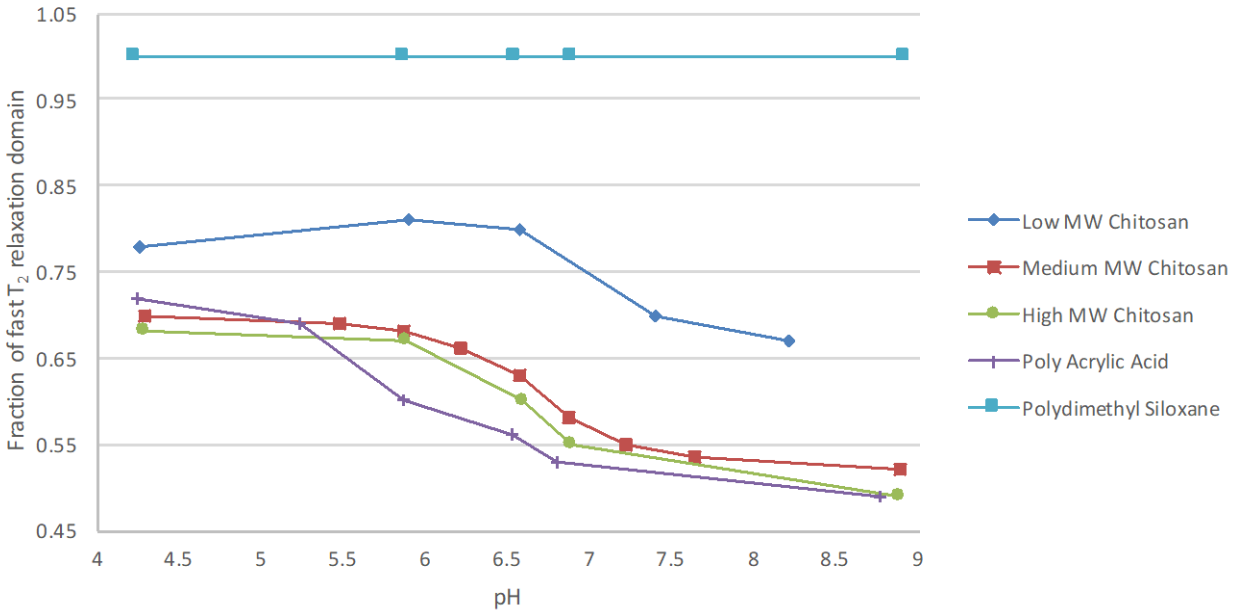

Figure 6: Variation in the fraction of the fast relaxation domain as a function of pH in control samples.

As seen in Figure 5, the sensitivity of the rate of T_2 relaxation to pH changes for the tested polymers is insufficient for accurately predicting pH. As seen in Figure 6, however, there is a greater degree of sensitivity to the ratio between the $T_{2,fast}$:$T_{2,slow}$ response for some polymers, in particular polyacrylic acid and high molecular weight chitosan. The $T_{2,fast}$:$T_{2,slow}$ response is most sensitive in the pH region surrounding the acid dissociation constant (p*K*a) of the polymer. In the case of chitosan, the higher molecular weight material is more sensitive to changes in pH, with a greater difference in measured $T_{2,fast}$:$T_{2,slow}$ response between the high and low pH systems. However, the range over which the $T_{2,fast}$:$T_{2,slow}$ response is sensitive to pH was limited to the neutral range (i.e., 6 to 7.5). As a result, sensors developed using these materials may be useful for monitoring for deviations from the neutral range (i.e., pH < 6 or pH > 7.5), but not for providing specific pH values outside of the neutral range.

Controlled Tests with Iron Oxide Nanoparticles

Also investigated was the T_2 response to a pH-insensitive polymer matrix (PDMS) doped with pH-sensitive Fe_2O_3 nanoparticles. Fe_2O_3 is sensitive to pH and provides an alternative mechanism through which to measure pH (see Appendix B). The T_2 behavior for these systems are linear and as such did not need to be decomposed into multiple domains. Figure 8 compares the measured T_2 as a function of sample pH. These samples were all prepared under low-DO conditions to ensure that the response is due to pH and not DO, as Fe_2O_3 will also react with DO.

Unlike the pH-sensitive polymers described above, the decay of the NMR signal is linear and there is no discernible difference between the NMR signal decay for all pH values below 7.8 (see Figure 7).

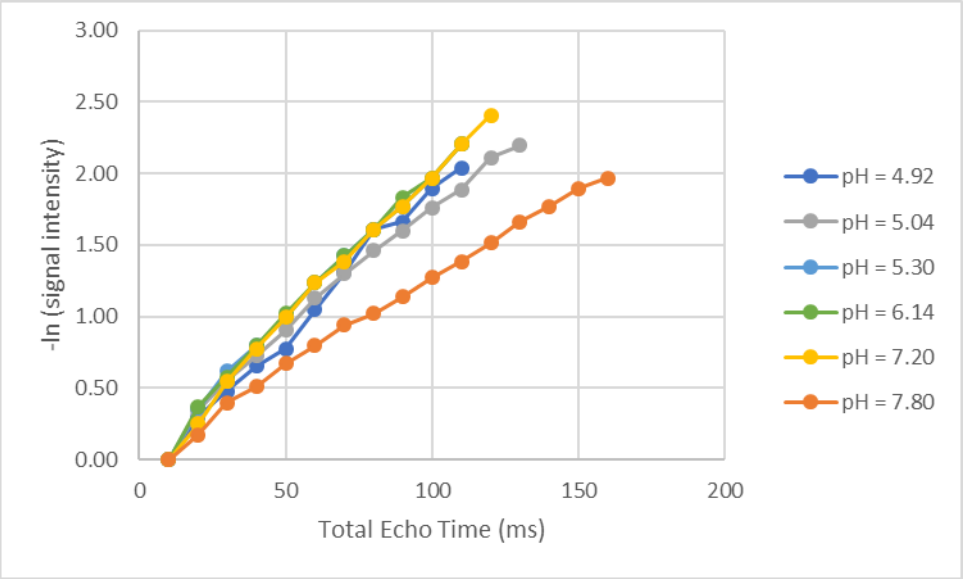

Figure 7: Relationship between pH and signal intensity for Fe_2O_3-Doped PDMS.

As seen in Figure 8, a small response in T_2 with pH was observed only for the sample acquired at a pH of 7.8. Here, changes in the observed signal decay arises from changes in the overall T_2 behavior of the materials, rather than in changes in conformational structure. For Fe_2O_3-doped PDMS, the observed changes in T_2 occurred in response to changes in the oxidation state of iron, which affects the magnetic properties of the sample. This result suggests that under the controlled conditions here, the Fe_2O_3 is only sensitive to pH for the pH 7.8 sample and thus there is no discernible influence on the measured T_2 in response to changes in pH.

Based on this behavior, it appears that PDMS sensors doped with Fe_2O_3 may only be sensitive to changes in pH above pH 7.8 and are insensitive to changes in pH at lower pH ranges. A sensor material constructed of Fe_2O_3-doped PDMS will therefore not be useful for measuring pH in most environmental applications, however this also means that Fe_2O_3 may be useful for measuring other parameters, such as DO or ORP, independent of variations in pH.

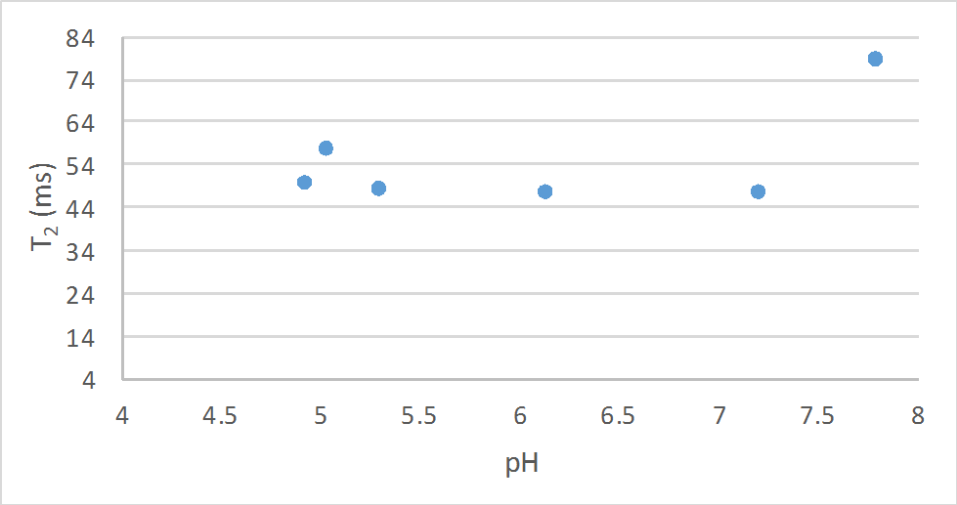

Figure 8: Change in T_2 with pH for Fe_2O_3 doped PDMS.

Uncontrolled Tests for pH

Natural water samples were collected from naturally aerobic and anaerobic environments (referred to as "natural" samples), To simulate the effects of remediation, the oxygen content was also changed from aerobic to anaerobic and vice versa on select samples through the amendment of ascorbic acid and/or bubbling of oxygen, respectively ("stimulated" samples). In total, four water samples were tested in the uncontrolled tests (aerobic "natural" and anaerobic "natural" waters, stimulated aerobic and stimulated anaerobic waters). Each water sample was placed in the NMR tube with a pH-sensitive polymer (medium-weight chitosan) and the T_2 response was monitored as the pH of each water sample was modified incrementally by adding small amounts of sodium dibasic phosphate and sodium monobasic phosphate.

Figure 9 illustrates the variable T_2 response for medium-weight chitosan sensor materials for natural waters under aerobic and anaerobic conditions (see Appendix C). As a comparison, the T_2 response for the controlled samples are also shown on the plot. As seen in Figure 9, the rate of T_2 decay is faster in the natural waters compared to the control samples (i.e., as decay increases, the slope of the NMR signal decay curve increases, and T_2,slow [=1/slope] decreases). This observation is most likely due to the presence of native paramagnetic species in the natural water samples that were not present in the controlled tests. Elevated concentrations of paramagnetic species will increase the overall rate of T_2 relaxation independent from the effects caused by variations in pH. The rate of T_2 decay also seems to increase with oxygen content in the water, likely due to the fact that dioxygen (O_2) is also weakly paramagnetic.

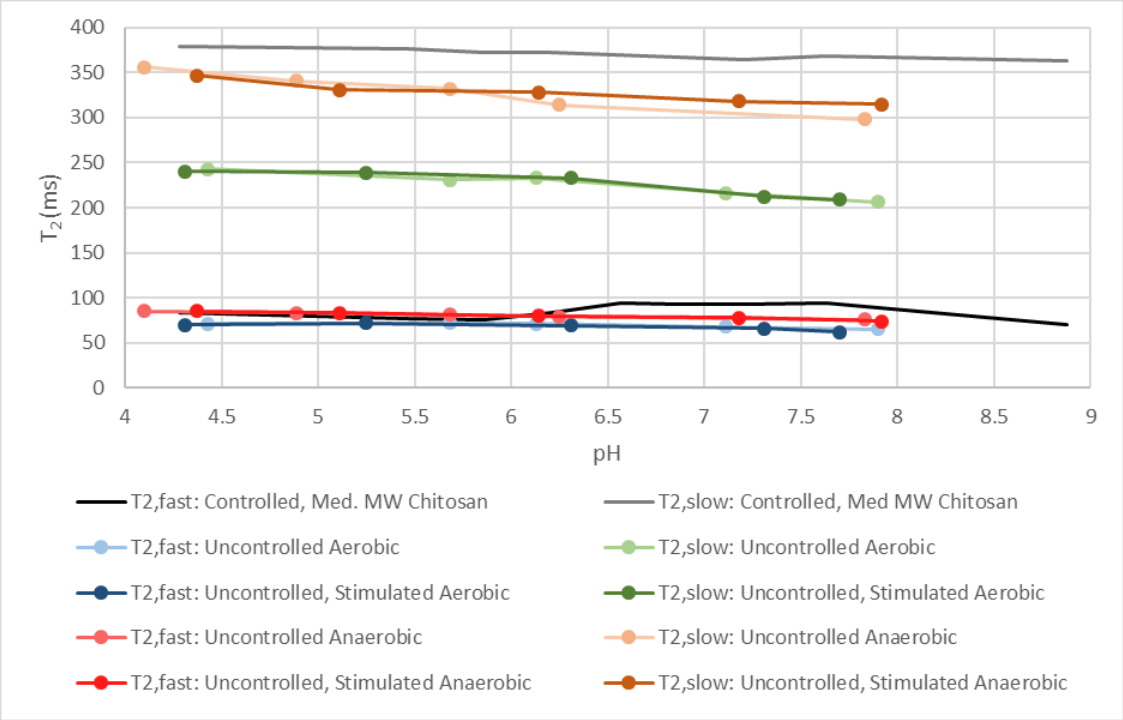

Figure 9: Variation in fast and slow-relaxing components of T_2 with pH for medium-weight chitosan for uncontrolled aerobic, anaerobic, and stimulated natural waters. The T_2 response for the controlled water sample with medium-weight chitosan sensor material is also shown as a reference.

As for the controlled tests with pH-sensitive polymers, the T_2 response in the uncontrolled tests was again non-linear and the ratio of fast-relaxing T_2 to slow-relaxing T_2 domain was evaluated as a means to monitor response to pH changes. Figure 10 and Table 2 compare the measured fraction of fast-relaxing T_2 domain of the medium-weight chitosan as a function of pH for the four uncontrolled water samples tested. The fraction of fast-relaxing T_2 to slow-relaxing T_2 is similar for all samples tested and also similar to the control samples, suggesting that for these polymer materials, the presence/absence of oxygen does not impact the ability to distinguish between pH changes when using the ratio of the fast-relaxing T_2 to slow-relaxing T_2 domain.

These findings further support the conclusion that pH sensors developed using these specific pH-sensitive polymer materials may be useful for monitoring pH changes within the neutral range and for identifying deviations from neutral (i.e., pH < 6 or pH > 7.5), but not for measuring specific pH values outside of the neutral range.

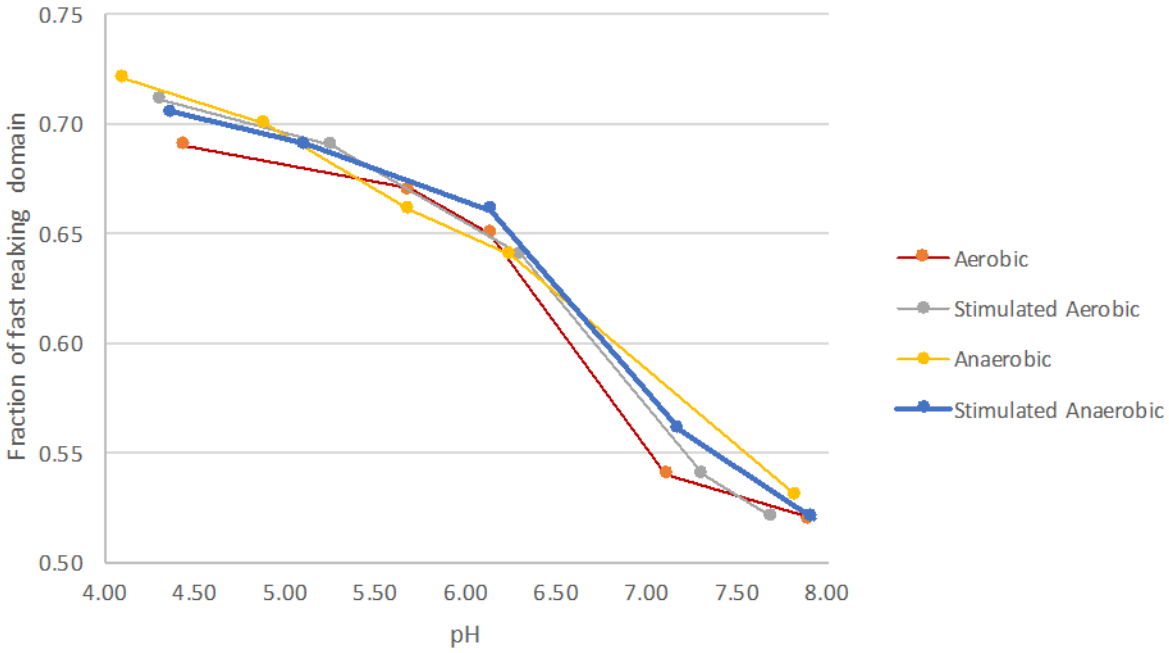

Figure 10: Fraction of fast-relaxing T_2 domain in medium weight chitosan as a function of pH for natural water samples.

Table 2: Decomposition of the T_2 behavior of medium-weight chitosan into fast ($fT_{2(fast)}$) and slow ($fT_{2(slow)}$) relaxing compartments for natural water samples.

Material	pH	$T_{2\,(fast)}$	$f\,T_{2(fast)}$	$T_{2\,(slow)}$	$f\,T_{2\,(slow)}$
Aerobic	**4.43**	71.0	0.69	243.0	0.31
	5.68	72.0	0.67	231.0	0.33
	6.13	71.0	0.65	233.0	0.35
	7.11	68.0	0.54	216.0	0.46
	7.90	65.0	0.52	206.0	0.48
Stimulated Aerobic	**4.31**	70.0	0.71	240.0	0.29
	5.25	72.0	0.69	239.0	0.31
	6.31	69.0	0.64	233.0	0.36
	7.31	66.0	0.54	212.0	0.46
	7.70	62.0	0.52	209.0	0.48
Anaerobic	**4.10**	85.0	0.72	356.0	0.28
	4.89	83.0	0.70	341.0	0.30
	5.68	81.0	0.66	332.0	0.34
	6.25	79.0	0.64	314.0	0.36
	7.83	76.0	0.53	298.0	0.47
Stimulated Anaerobic	**4.37**	85.0	0.71	347.0	0.30
	5.11	83.0	0.69	331.0	0.31
	6.14	80.0	0.66	328.0	0.34
	7.18	78.0	0.56	318.0	0.44
	7.92	74.0	0.52	315.0	0.48

Dissolved Oxygen

Dissolved oxygen tests were again conducted under both controlled and uncontrolled conditions. The results of each set of tests are described further below.

Controlled Tests

Water samples were prepared using deionized water amended with varied levels of dissolved oxygen by bubbling compressed air through the water to increase the amount of dissolved oxygen present, and by adding ascorbic acid[1] to decrease the amount of dissolved oxygen present. Tests

[1] Addition of ascorbic acid may reduce the pH; however, as discussed above, the T_2 response of the sensor material used for testing DO response (PDMS doped with Fe_2O_3) was relatively

of T_2 response to dissolved oxygen were conducted with the sensor material PDMS doped with Fe_2O_3 nanoparticles (see Appendix D).

Figure 11 and Table 3 compares the T_2 decay behavior of PDMS samples doped with different concentrations of Fe_2O_3 nanoparticles under ambient laboratory conditions (i.e. open to exchange with the lab air) with a DO concentration of ~4 mg/L (see Appendix E). The measured T_2 is found to correlate well to the concentration of Fe_2O_3 added into the polymer matrix, up to approximately 0.1 mg Fe_2O_3 per microliter (µL) of water. The sensitivity in T_2 response to Fe_2O_3 dose indicate that any observed changes in T_2 resulting from DO are likely the result of changes in the magnetic properties of the Fe_2O_3 particles due to changes in the oxidation/reduction environment, rather than with conformation changes in the structure of the polymeric matrix as was the case for the pH-sensitive polymers described above.

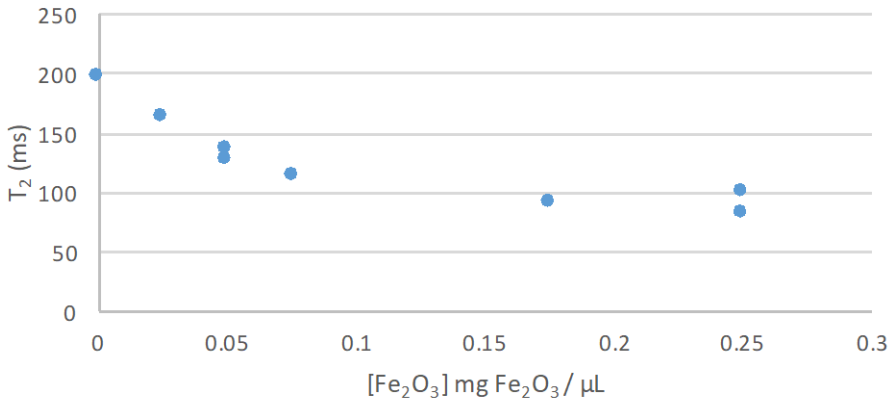

Figure 11: Relationship between T_2 and Fe_2O_3 doping concentration in the PDMS polymer.

Table 3: Relationship between Fe_2O_3 doping level and T_2 under ambient conditions.

Fe_2O_3 Concentration (mg Fe_2O_3 / µL)	T_2 (ms)	pH	DO (mg/L)
0	197	6.5	4.1
0.025	161	6.4	4.1
0.050	128	6.4	3.8
0.075	113	6.5	3.7
0.125	98	6.6	3.9
0.175	87	6.2	3.8
0.250	81	6.7	4.0

insensitive to pH changes below 7.8 (see Figure 6) and any changes observed between samples with different DO concentrations are likely to be due to DO, not pH.

As seen in Figure 12, the observed decay trends are linear, indicating a single major relaxation domain (i.e. water in the pore spaces without significant interactions at the polymer surfaces).

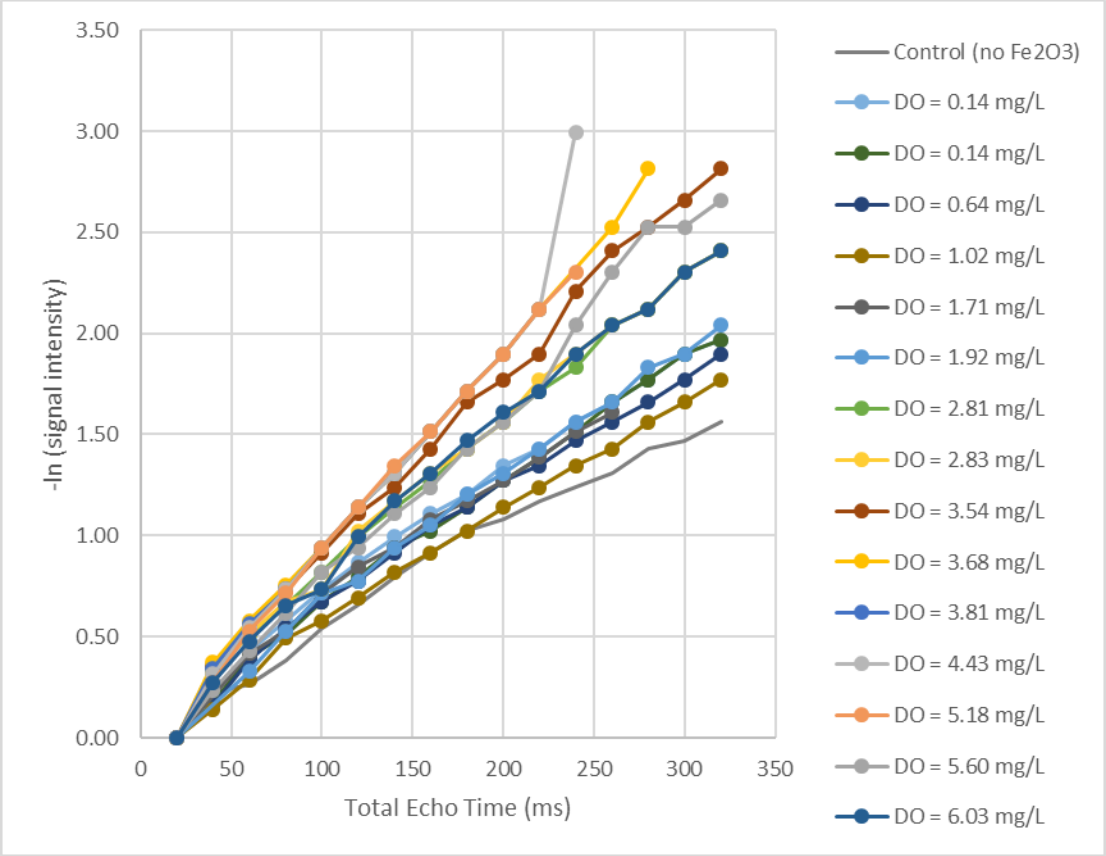

Figure 12: T_2 relaxation behavior for Fe_2O_3-doped PDMS sensors at a variety of DO concentrations under controlled conditions.

Figure 13 compares the variation of the observed T_2 in response to variations in the dissolved oxygen content in the water samples. The observed relationship is non-linear and non-unique. In general, the Fe_2O_3 particles are most sensitive to dissolved oxygen in mid to high concentrations (1 to 5 mg/L DO), and is not sensitive at all at low concentrations (<1 mg/L). At higher concentrations (5 to 6 mg/L DO), the trend reverses, resulting in a non-unique determination of DO. This observation is due to the relationship between the oxidation state of Fe, and thus the equilibrium between paramagnetic and diamagnetic species of iron, and the concentration of dissolved oxygen. Given the non-unique nature of the T_2 response of the Fe_2O_3-doped PDMS sensor material to DO, the material is not ideal for monitoring DO concentrations.

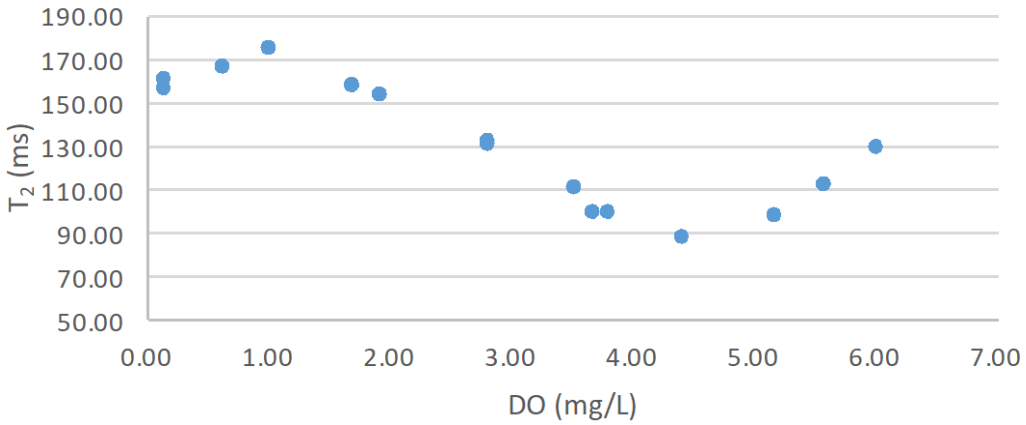

Figure 13: Relationship between T_2 and dissolved oxygen for PDMS doped with Fe_2O_3 in controlled water samples.

Uncontrolled Tests

Performance of the Fe_2O_3-doped PDMS sensor materials in monitoring DO in "natural" water samples was also evaluated for a range of dissolved oxygen concentrations. Naturally aerobic and anaerobic waters were tested as well as "stimulated" aerobic and anaerobic waters. In the "stimulated" tests, the DO of the "natural" waters was altered by bubbling oxygen through the water to increase DO or by amending the water sample with ascorbic acid to reduce DO.

Figure 14 compares the measured T_2 as a function of DO for the natural and stimulated water samples (see Appendix D). Trends similar to those found for the controlled samples are observed: the approach is poor at discriminating differences in DO levels under anaerobic conditions, but show some response at mid to high concentrations and is able to distinguish anaerobic from aerobic conditions.

The correlations between T_2 and DO observed in natural water samples are not the same as in the controlled tests. This observation is most likely due to the presence of native paramagnetic species in the natural water samples that were not present in the controlled tests. The differences between the controlled and the natural water tests suggest that this approach for measuring DO would need to be calibrated for the specific conditions of a given water, and would, consequently, be affected by even small variations in the concentrations of iron and manganese in the water over time.

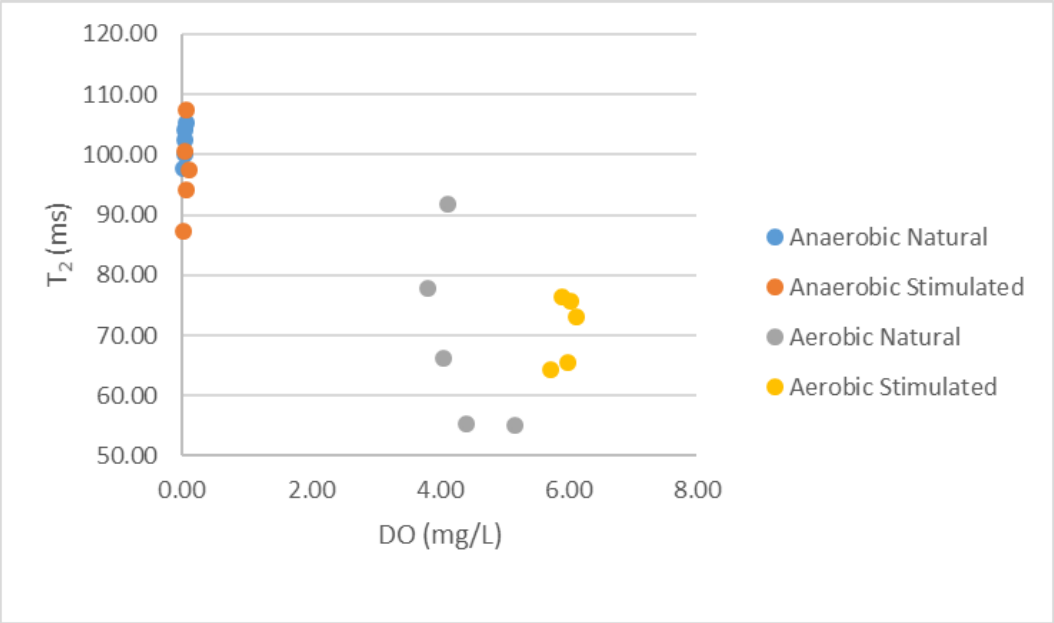

Figure 14: Relationship between T_2 and dissolved oxygen for PDMS doped with Fe_2O_3 in natural water samples.

Oxidation-Reduction Potential

Controlled tests for sensor response to ORP changes were completed using deionized water samples amended with small amounts of sodium persulfate to increase the ORP and sodium bisulphite to decrease the ORP value of the water. The sensor material tested was again PDMS doped with Fe_2O_3 nanoparticles.

The measured T_2 response to ORP changes for these sensor materials are shown in Figure 15 (see Appendix F). As seen in Figure 15, the measured T_2 response of these materials was found not to correlate with the oxidation-reduction potential in the controlled water samples.

The oxidation-reduction potential of water is controlled by several factors, including the amount of dissolved oxygen and the concentration and oxidation state of several metals, including iron and manganese. The presence of Fe_2O_3 in the sensor polymers negatively impact the ability of the sensor material to measure ORP because the sensor material itself strongly influences the ORP in the water being studied. This problem is exasperated by the relatively small volume of water being analyzed compared to the amount of sensor material (i.e. Fe_2O_3) present. It may be possible that a with much larger relative volume of water, as would be found in a real in situ application, the influence of the sensor material itself on the measurement of ORP may be negated. Such tests would require field-scale investigations and are outside the scope of the current study, which is limited to proof-of-concept lab-based tests based on the analysis of small volumes. Due to the poor response of these materials to ORP in controlled systems, their response to uncontrolled systems was not investigated.

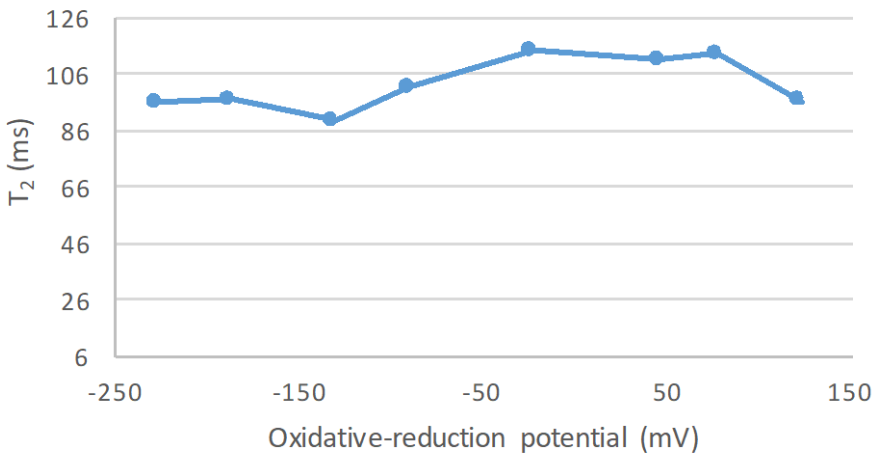

Figure 15: Relationship between ORP and T_2 for PDMS doped with Fe_2O_3.

Sensor Sensitivity to Chlorinated Ethenes

Two general approaches were used here to study the possible application of magnetic relaxation sensors to detect and quantify the presence of chlorinated ethenes: (i) the direct effect that the sorption of chlorinated ethenes has on the structural rigidity, and therefore the observed T_2, of polymer substrates; and (ii) the use of a polymer matrix doped with paramagnetic species that change their oxidation state, and thus paramagnetic parameters, upon exposure and reaction with chlorinated ethenes.

The Direct Effect of Exposure to Chlorinated Ethenes on the Observed T_2 Relaxation Properties of Polymeric Materials

Based on a review of available literature on polymer compatibility with chlorinated ethenes, a series of potential polymeric materials that may exhibit T_2 behavior that is sensitive to the presence of chlorinated ethenes was prepared. The potential suitability for these materials was based on the degree of compatibility of these materials with chlorinated ethenes. Materials that are known to be highly compatible with chlorinated ethenes are not expected to exhibit a change in the observed T_2 because the polymeric material and the chlorinated ethene do not interact. Conversely, materials that are known to be highly incompatible with chlorinated ethenes may exhibit a measurable change in the observed T_2 upon exposure, because the material and the chlorinated ethenes do interact in some manner. A list of potential materials is presented in Table 4.

Table 4: Materials tested for sensitivity to chlorinated ethenes.

Material	Form	Difference in T_2 between control and ethene exposure
Styrene Acrylonitrile (SAN)	Powder	Yes
Polyvinyl chloride (PVC)	Powder	Yes
Polypheylene Sulfide (PPS)	Powder	No
Polymethylpentene (PMP)	powder	No
Polyethylene terephthalate (PETP)	Pellet	No
Polysulfone (PSF)	Pellet	No
Low-Density Poly Ethylene (LDPE)	Powder	No
Polyethylene Oxide (PEO)	Powder	No

The sensitivity of these compounds to exposure to chlorinated ethenes was initially tested by exposing the material to high concentrations of aqueous-phase TCE, and measuring any variation in the observed T_2. In general, polymeric materials were tested in two forms: (i) small pellets, or, (ii) a fine powder. As shown in Table 4, none of the pelleted forms of the materials exhibited any variation in T_2 upon exposure to chlorinated ethenes, whereas a small number of the materials in fine powder form did exhibit a response (see Appendix G). It is important to recall here that the T_2 being measured is actually of the water that occupies the pore spaces between the polymeric walls. As such, the pelleted materials do not exhibit any change in observed T_2 because there is limited pore space for confined water to interact with polymeric surfaces. For powder forms, the porous structure has greater surface area that allows for more exposure of the polymer particles to chlorinated ethenes. This results in greater changes in the physical conformation of the surface of the polymer particles that in turn influences the confinement of water in the pore spaces. This results in small, but quantifiable, variations in the T_2 of the confined water originating from the interactions between the polymer surface and the chlorinated ethenes.

To test further the potential for the use of these types of measurements to assess the concentration of chlorinated ethenes, the material with the most significant response to exposure to chlorinated ethenes, polyvinylchloride (PVC), was examined further. Here, several tests were performed to examine the effect that different concentrations of PCE, TCE, 1,1 DCE, and ethene have on the observed T_2, and the effect that continued exposure to those same concentrations have over time.

Figure 16 compares the T_2 response of PVC alone (T_2 control) to solutions of TCE, PCE, 1,1 DCE, and ethene in contact with PVC (see Appendix H). As seen in Figure 16, only the exposure to TCE and 1,1 DCE exhibit a meaningful change in the T_2 from the control T_2. However, the mass of contaminant in contact with the PVC is very small in comparison to the PVC in the NMR tubes; this is not overly representative of a real-world situation where contaminant is continually being flushed past the sensor and being taken up (absorbed to) the PVC.

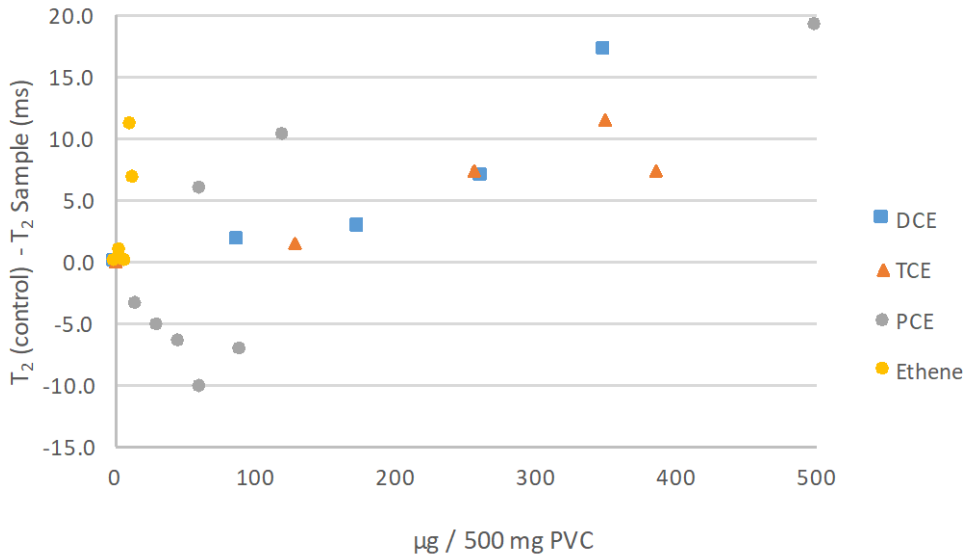

Figure 16: Changes in the measured T_2 of PVC upon exposure to dissolved PCE, TCE, 1,1 DCE, and ethene.

In Figure 17, the effect of the cumulative exposure to chlorinated ethenes was examined. Here, each sample was spiked with fresh TCE, PCE, and 1,1 DCE every couple of days to simulate the constant flushing of contaminant past the sensor that would occur in a field setting. Each sample was allowed to re-equilibrate after each dose and T_2 was re-measured. In general, the variation in the T_2 behavior from the control sample upon cumulative exposure to chlorinated ethenes is small, but follows a trend. After dosing, the T_2 is found to decrease in a manner that is correlated to the cumulative exposure to chlorinated ethenes. In general, as the exposure to the ethenes increases, the observed rate of T_2 relaxation decreases. This effect is observed to be linear for all compounds across the range studied until the cumulative exposure reaches a limit, after which the effect observed here becomes asymptotic, suggesting an upper sorptive limit for the PVC.

While there is a positive response of the sensor materials T_2 behavior with initial exposure to chlorinated ethenes, this response only becomes significant after cumulative exposure. As such, this approach is not well suited for instantaneous measurements of small concentration of these species, but may be useful to measure cumulative exposure over time. However, meaningful correlation of concentrations of chlorinated ethenes to T_2 response will require additional testing to define the asymptotic limits and the rate of absorption.

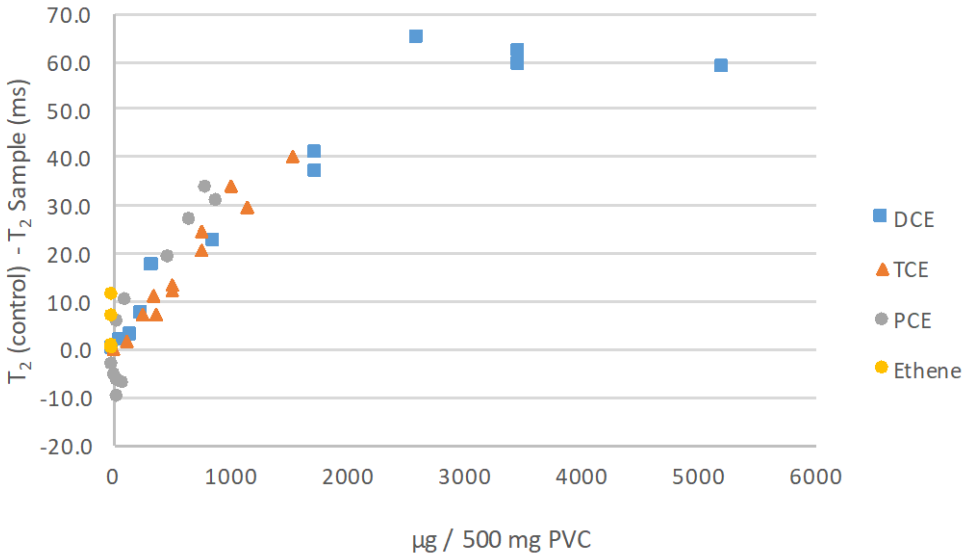

Figure 17: Changes in the measured T_2 of PVC upon cumulative exposure to PCE, TCE, 1,1 DCE, and ethene.

The Use of Paramagnetic Dopants as Relaxation Indicators of Chlorinated Ethene Concentration

The use of iron and manganese salts in a polymer matrix to detect the presence of chlorinated ethenes was tested. It has already been shown that T_2 is affected by the concentration of Fe_2O_3 alone, which contains iron in a paramagnetic oxidation state (see Figure 11). Figure 18 presents additional control tests without chlorinated ethenes to compare the sensitivity of observed T_2 on variations of the concentration of $FeSO_4$, Mn(III)acac, and $NaMnO_4$ in samples of PDMS (see Appendix I). As expected, the T_2 is affected by the concentration of Mn(III)acac, which is paramagnetic, but not by the concentration of $FeSO_4$ or $NaMnO_4$, which are not paramagnetic.

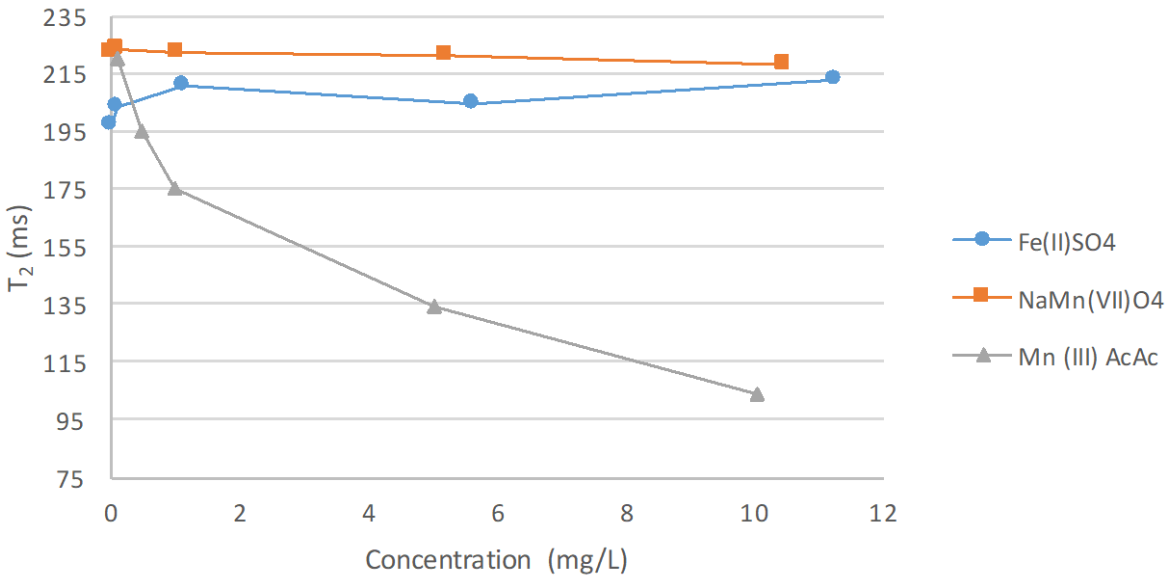

Figure 18: Changes in the measured T_2 of PDMS upon exposure to iron and manganese salts in control tests (no chlorinated ethenes).

The use of MnO_4^- as a proxy indicator for the presence of PCE and TCE was tested. Here, when MnO_4^- reacts with chlorinated ethenes, it is reduced to forms of manganese that are paramagnetic and that thus affect the measured T_2 of the sensor relative to their concentration. Samples of PDMS doped with the same mass of $NaMnO_4$ were prepared in 5mm NMR tubes and dosed with PCE and TCE. Figure 19 compares the observed T_2 to the amount of TCE or PCE added (see Appendix J). Here, the observed T_2 is linearly correlated to the concentration of chlorinated ethene, regardless of its identity. In general, the use of MnO_4^- dosed PDMS as a sensor material is sensitive to variations in chlorinated ethene concentrations and is able to show more significant responses to lower concentrations than from use of polymeric materials alone as the sensor (e.g., PVC). The sensitivity of this approach can be modified by adjusting the concentration of iron or manganese salts added.

While this approach is reasonably sensitive, in general it is unable to discriminate between different types of chlorinated ethenes. This is because the method for detection is based on the oxidation of the ethene structure through the reduction of Mn(VII) to lower oxidation states that are paramagnetic, and thus any species present in the sample that will react with MnO_4^- will produce the same response. Because the relaxation response is sensitive to changes in the concentration of paramagnetic species, any reactive compound that would change the concentration of such species, including iron and manganese would produce a response. In this way, variations in T_2 resulting from variations of paramagnetic ions could be used to monitor variations in the concentration of reactive substrates, including chlorinated ethenes. Additional testing would be needed to confirm whether mixtures of different solvents would act cumulatively on the T_2 and thus allow for quantification of total chlorinated ethenes.

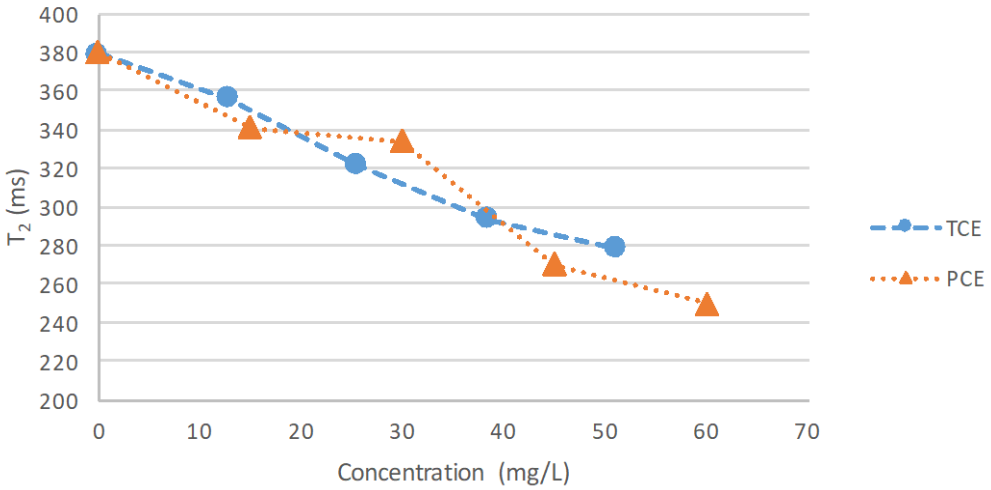

Figure 19: Changes in the measured T_2 of PDMS doped with $NaMnO_4$ upon exposure to PCE and TCE.

Conclusions and Implications for Future Research

This project focused on three key research questions:

1) Can NMR sensor designs previously developed to study changes in pH and DO in biological organisms be used to perform the same measurements in groundwater under environmental conditions?

2) Can polymer materials be identified that have potential to exhibit measurable changes in relaxation properties upon exposure to chlorinated ethenes?

3) Can relaxation contrast agents be activated by exposure to chlorinated ethenes and thus be used to induce observable changes in polymer sensor materials?

The proof-of-concept experiments conducted achieved partial success in meeting the key research objectives. For example, sensor materials were identified that produced a measurable response in the T_2 relaxation properties upon exposure to changes in pH and DO, and upon exposure to chlorinated ethenes. Similarly, polymer sensor materials embedded with relaxation contrast agents were found to be activated by exposure to chlorinated ethenes.

Identified limitations and considerations for future development of this approach included:

- For pH, the sensitivity of the sensor material appears to be controlled by the pKa of the surface functional groups present in the pH-sensitive polymer matrix. This response arises from changes in the protonation at the polymer surface that influences how water can bind to it. When a large amount of water can bind to the polymer surface due to H-bonding (i.e., under low pH conditions), the overall rate of T_2 relaxation is reduced because water bound to the polymer surface relaxes at a faster rate than water not bound to the polymer surface. For the sensor materials tested, the range over which changes in the rate of T_2 relaxation were discernible tended to range between pH of approximately 6 to 8, and pH changes above or below this range could not be accurately predicted. In theory, a pH sensor could be constructed of multiple polymers, each having a distinct pKa range that covers the spectrum of environmentally-significant values (e.g., 4 to 12), but additional research would be required to identify and test sensor materials with pKa values outside of the neutral pH range.

- The T_2 response for the tested sensor material (i.e., Fe_2O_3-doped PDMS) to DO was non-unique and thus could not be used to accurately predict concentrations in the water samples. The non-uniqueness arises due to dissolved oxygen reacting with the iron and modifying its oxidation state, which impacts the equilibrium between paramagnetic and diamagnetic species of iron (i.e., the T_2 response reflects the amount of paramagnetic species of iron in the sensor material). The T_2 response was also found to be sensitive to the presence of naturally occurring paramagnetic iron and manganese species in groundwater, which further increases the non-uniqueness of the T_2 response to specific DO concentrations.

- The sensor materials studied here were unable to produce meaningful predictions of the oxidation-reduction potential of water samples. The likely reason for this was that the sensor materials itself (Fe_2O_3) directly influenced the ORP of the samples being examined.

- For the chlorinated ethenes, although the T2 response for polymer materials was measurably different when exposed to different chlorinated ethene concentrations (due to changes induced in the structural rigidity of the polymer material), the effect is weak at typical concentrations observed in groundwater plumes and changes with cumulative exposure over time. The sensitivity increased with sensors constructed of non-reactive polymer embedded with paramagnetic materials (due to the changes in the paramagnetic species concentrations from reactions with the chlorinated ethenes); however, the T_2 response did not vary between the specific chlorinated ethenes for sensors constructed with either polymers or paramagnetic-embedded polymers, and therefore we cannot distinguish between individual concentrations of PCE, TCE, or 1,1-DCE. Similarly, any other species present that could be oxidized by the paramagnetic species would interfere with the measurement. This approach may be useful for monitoring total chlorinated ethenes, but more research is needed to confirm this.

- For most measurements with any sensor material, the presence of iron and manganese in native groundwater is likely to prevent a simple correlation between measurements made in controlled (laboratory) and uncontrolled (field) environments. Any magnetic relaxation sensor employed in the field would need to be calibrated against a water sample taken from the same source, and calibrations would have to somehow account for natural variability in the site groundwater. Due to their paramagnetic properties, which strongly influence the response of paramagnetic sensor materials, variations in iron and/or manganese concentrations over time would interfere with the reliability of any measurements of the targeted chemical parameters, including pH, DO, and the concentration of chlorinated ethenes.

While the applications of relaxation-based sensors may not be well suited for the characterization of chlorinated ethenes in groundwater, other environmental contaminants may prove more fruitful. For example, the original development of these sensors was aimed at detecting trace concentrations of specific biomarkers of disease in biological samples; similar approaches could be developed to detect specific biomarkers of pathogens in water systems, or to detect contaminants such as heavy metals (i.e. Mercury) that are able to form unique and specific interactions with structural moieties bound to magnetic nanoparticles (e.g. mercury binding to sulfur) in ways that chlorinated ethenes can not.

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Appendix A: Relationship between T2 relaxation and pH in controlled tests using chitosan, polyacrylic acid, and polydimethylsiloxane.

Polymer		Chitosan Low MW - Controlled Conditions									
pH		4.26		5.89		6.57		7.4		8.21	
Delay	*Echo time (ms)*	*I*	*-ln(I/IO)*	*I*	*-ln(I/IO)*	*I*	*-ln(I/IO)*	*I*	*-ln(I/IO)*	*I*	*-ln(I/IO)*
1	20	0.63	0.00	0.68	0.00	0.67	0.00	0.73	0.00	0.76	0.00
2	40	0.42	0.41	0.48	0.35	0.46	0.38	0.55	0.28	0.59	0.25
3	60	0.30	0.74	0.35	0.66	0.33	0.71	0.43	0.53	0.47	0.48
4	80	0.23	1.01	0.26	0.96	0.25	0.99	0.34	0.76	0.38	0.68
5	100	0.19	1.20	0.20	1.22	0.20	1.21	0.28	0.96	0.32	0.86
6	120	0.16	1.37	0.17	1.39	0.16	1.43	0.24	1.11	0.27	1.01
7	140	0.14	1.50	0.14	1.58	0.13	1.64	0.20	1.29	0.24	1.15
8	160	0.12	1.66	0.12	1.73	0.12	1.72	0.18	1.40	0.21	1.27
9	180	0.11	1.75	0.10	1.92	0.10	1.90	0.16	1.52	0.19	1.38
10	200	0.10	1.84	0.09	2.02	0.09	2.01	0.14	1.65	0.17	1.48
11	220	0.09	1.95	0.08	2.14	0.08	2.13	0.13	1.73	0.16	1.57
12	240	0.09	1.95	0.07	2.27	0.07	2.26	0.12	1.81	0.14	1.66
13	260	0.08	2.06	0.07	2.27	0.07	2.26	0.11	1.89	0.13	1.75
14	280	0.07	2.20	0.06	2.43	0.06	2.41	0.10	1.99	0.12	1.82
15	300	0.07	2.20	0.06	2.43	0.06	2.41	0.09	2.09	0.11	1.90
16	320	0.06	2.35					0.08	2.21	0.11	1.97
17	340	0.06	2.35					0.08	2.28	0.10	2.05
18	360	0.05	2.53					0.07	2.34	0.09	2.13
19	380							0.06	2.50	0.08	2.20
20	400							0.06	2.50	0.08	2.27
21	420							0.05	2.68	0.07	2.35
22	440							0.05	2.68	0.07	2.42
23	460							0.05	2.68	0.06	2.50
24	480									0.06	2.57
25	500									0.05	2.64
26	520									0.05	2.72
27	540										
28	560										
29	580										
30	600										
31	620										
32	640										
		T2=	**157.21**	**T2=**	**118.84**	**T2=**	**121.43**	**T2=**	**175.08**	**T2=**	**204.51**

Polymer		Chitosan Medium MW -Controlled Conditions (1/3)							
pH		6.57		5.86		6.87		4.28	
Delay	*Echo time (ms)*	*I*	*-ln(I/IO)*	*I*	*-ln(I/IO)*	*I*	*-ln(I/IO)*	*I*	*-ln(I/IO)*
1	20	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.88	0.13	0.83	0.19	0.87	0.14	0.86	0.15
3	60	0.68	0.39	0.61	0.49	0.69	0.37	0.63	0.46
4	80	0.58	0.54	0.50	0.69	0.60	0.51	0.53	0.63
5	100	0.49	0.71	0.42	0.87	0.51	0.67	0.44	0.82
6	120	0.44	0.82	0.36	1.02	0.46	0.78	0.38	0.97
7	140	0.39	0.94	0.32	1.14	0.41	0.89	0.33	1.11
8	160	0.35	1.05	0.28	1.27	0.37	0.99	0.30	1.20
9	180	0.31	1.17	0.25	1.39	0.34	1.08	0.26	1.35
10	200	0.29	1.24	0.23	1.47	0.31	1.17	0.24	1.43
11	220	0.26	1.35	0.21	1.56	0.28	1.27	0.21	1.56
12	240	0.24	1.43	0.19	1.66	0.26	1.35	0.20	1.61
13	260	0.22	1.51	0.18	1.71	0.24	1.43	0.18	1.71
14	280	0.20	1.61	0.16	1.83	0.22	1.51	0.16	1.83
15	300	0.19	1.66	0.15	1.90	0.21	1.56	0.15	1.90
16	320	0.17	1.77	0.14	1.97	0.19	1.66	0.14	1.97
17	340	0.16	1.83	0.13	2.04	0.18	1.71	0.13	2.04
18	360	0.15	1.90	0.12	2.12	0.17	1.77	0.12	2.12
19	380	0.14	1.97	0.11	2.21	0.15	1.90	0.11	2.21
20	400	0.13	2.04	0.10	2.30	0.14	1.97	0.10	2.30
21	420	0.12	2.12	0.10	2.30	0.14	1.97	0.10	2.30
22	440	0.11	2.21	0.09	2.41	0.13	2.04	0.09	2.41
23	460	0.11	2.21	0.09	2.41	0.12	2.12	0.08	2.53
24	480	0.10	2.30	0.08	2.53	0.11	2.21	0.08	2.53
25	500	0.09	2.41	0.08	2.53	0.11	2.21	0.07	2.66
26	520	0.09	2.41	0.07	2.66	0.10	2.30	0.07	2.66
27	540	0.08	2.53	0.07	2.66	0.09	2.41	0.07	2.66
28	560	0.08	2.53	0.07	2.66	0.09	2.41	0.06	2.81
29	580	0.08	2.53	0.06	2.81	0.08	2.53	0.06	2.81
30	600	0.07	2.66	0.06	2.81	0.08	2.53	0.06	2.81
31	620	0.07	2.66	0.06	2.81	0.08	2.53	0.05	3.00
32	640	0.06	2.81	0.05	3.00	0.07	2.66	0.05	3.00
		T2=	**241.69**	**T2=**	**236.41**	**T2=**	**252.93**	**T2=**	**225.86**

Polymer		Chitosan Medium MW -Controlled Conditions (continued, 2/3)							
pH		8.88		5.47		6.21		7.21	
Delay	*Echo time (ms)*	*I*	*-ln(I/IO)*	*I*	*-ln(I/IO)*	*I*	*-ln(I/IO)*	*I*	*-ln(I/IO)*
1	20	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.72	0.33	0.69	0.37	0.71	0.34	0.76	0.27
3	60	0.63	0.46	0.58	0.54	0.61	0.49	0.67	0.40
4	80	0.55	0.60	0.49	0.71	0.53	0.63	0.59	0.53
5	100	0.49	0.71	0.43	0.84	0.46	0.78	0.53	0.63
6	120	0.44	0.82	0.37	0.99	0.40	0.92	0.48	0.73
7	140	0.40	0.92	0.33	1.11	0.36	1.02	0.43	0.84
8	160	0.36	1.02	0.29	1.24	0.32	1.14	0.39	0.94
9	180	0.33	1.11	0.26	1.35	0.29	1.24	0.35	1.05
10	200	0.31	1.17	0.23	1.47	0.26	1.35	0.32	1.14
11	220	0.28	1.27	0.21	1.56	0.23	1.47	0.30	1.20
12	240	0.26	1.35	0.19	1.66	0.21	1.56	0.27	1.31
13	260	0.25	1.39	0.18	1.71	0.20	1.61	0.25	1.39
14	280	0.23	1.47	0.17	1.77	0.18	1.71	0.24	1.43
15	300	0.22	1.51	0.15	1.90	0.17	1.77	0.22	1.51
16	320	0.20	1.61	0.14	1.97	0.16	1.83	0.20	1.61
17	340	0.19	1.66	0.13	2.04	0.15	1.90	0.19	1.66
18	360	0.18	1.71	0.13	2.04	0.14	1.97	0.18	1.71
19	380	0.17	1.77	0.12	2.12	0.13	2.04	0.17	1.77
20	400	0.16	1.83	0.11	2.21	0.12	2.12	0.16	1.83
21	420	0.15	1.90	0.10	2.30	0.11	2.21	0.15	1.90
22	440	0.14	1.97	0.10	2.30	0.11	2.21	0.14	1.97
23	460	0.14	1.97	0.09	2.41	0.10	2.30	0.13	2.04
24	480	0.13	2.04	0.09	2.41	0.10	2.30	0.12	2.12
25	500	0.12	2.12	0.08	2.53	0.09	2.41	0.12	2.12
26	520	0.11	2.21	0.08	2.53	0.09	2.41	0.11	2.21
27	540	0.11	2.21	0.07	2.66	0.08	2.53	0.10	2.30
28	560	0.10	2.30	0.07	2.66	0.07	2.66	0.10	2.30
29	580	0.10	2.30	0.07	2.66	0.07	2.66	0.09	2.41
30	600	0.09	2.41	0.06	2.81	0.07	2.66	0.09	2.41
31	620	0.09	2.41	0.06	2.81	0.06	2.81	0.08	2.53
32	640	0.08	2.53	0.06	2.81	0.06	2.81	0.08	2.53
		T2=	**283.58**	**T2=**	**247.31**	**T2=**	**247.37**	**T2=**	**266.81**

Polymer	Chitosan Medium MW - Controlled Conditions (continued, 3/3)		
pH	7.63		
Delay	*Echo time (ms)*	*I*	*-ln(I/IO)*
1	2	1.00	0.00
2	4	0.77	0.26
3	6	0.68	0.39
4	8	0.60	0.51
5	10	0.54	0.62
6	12	0.48	0.73
7	14	0.44	0.82
8	16	0.40	0.92
9	18	0.36	1.02
10	20	0.33	1.11
11	22	0.30	1.20
12	24	0.28	1.27
13	26	0.26	1.35
14	28	0.24	1.43
15	30	0.23	1.47
16	32	0.21	1.56
17	34	0.20	1.61
18	36	0.18	1.71
19	38	0.17	1.77
20	40	0.16	1.83
21	42	0.15	1.90
22	44	0.14	1.97
23	46	0.14	1.97
24	48	0.13	2.04
25	50	0.12	2.12
26	52	0.11	2.21
27	54	0.11	2.21
28	56	0.10	2.30
29	58	0.10	2.30
30	60	0.09	2.41
31	62	0.09	2.41
32	64	0.08	2.53
		T2=	**27.09**

Polymer		Chitosan High MW - Controlled Conditions									
pH		4.29		5.88		6.58		6.89		8.89	
Delay	*Echo time (ms)*	*I*	*-ln(I/IO)*	*I*	*-ln(I/IO)*	*I*	*-ln(I/IO)*	*I*	*-ln(I/IO)*	*I*	*-ln(I/IO)*
1	20	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.72	0.33	0.74	0.30	0.76	0.27	0.78	0.25	0.79	0.23
3	60	0.62	0.48	0.65	0.44	0.67	0.40	0.69	0.37	0.71	0.34
4	80	0.54	0.62	0.56	0.57	0.59	0.52	0.62	0.48	0.64	0.45
5	100	0.47	0.76	0.50	0.70	0.53	0.64	0.56	0.59	0.58	0.54
6	120	0.41	0.88	0.44	0.82	0.48	0.74	0.50	0.69	0.53	0.64
7	140	0.37	1.00	0.39	0.93	0.43	0.85	0.46	0.78	0.42	0.86
8	160	0.33	1.11	0.35	1.04	0.39	0.94	0.42	0.87	0.45	0.81
9	180	0.30	1.22	0.32	1.15	0.36	1.04	0.38	0.97	0.41	0.89
10	200	0.27	1.31	0.29	1.24	0.33	1.12	0.35	1.04	0.38	0.97
11	220	0.25	1.40	0.26	1.34	0.30	1.21	0.33	1.12	0.35	1.04
12	240	0.23	1.49	0.24	1.42	0.28	1.28	0.30	1.19	0.33	1.11
13	260	0.21	1.57	0.22	1.51	0.26	1.36	0.28	1.27	0.31	1.18
14	280	0.19	1.64	0.21	1.58	0.24	1.43	0.26	1.33	0.29	1.24
15	300	0.18	1.71	0.19	1.66	0.22	1.50	0.25	1.40	0.27	1.31
16	320	0.17	1.78	0.18	1.73	0.21	1.57	0.23	1.46	0.25	1.37
17	340	0.16	1.84	0.17	1.79	0.20	1.63	0.22	1.52	0.24	1.43
18	360	0.15	1.90	0.16	1.86	0.19	1.69	0.21	1.58	0.23	1.49
19	380	0.14	1.96	0.15	1.92	0.17	1.75	0.19	1.64	0.21	1.55
20	400	0.13	2.02	0.14	1.98	0.16	1.81	0.18	1.70	0.20	1.60
21	420	0.13	2.07	0.13	2.04	0.16	1.86	0.17	1.75	0.19	1.66
22	440	0.12	2.13	0.12	2.10	0.15	1.92	0.16	1.81	0.18	1.71
23	460	0.11	2.18	0.12	2.15	0.14	1.97	0.16	1.86	0.17	1.76
24	480	0.11	2.23	0.11	2.21	0.13	2.02	0.15	1.92	0.16	1.83
25	500	0.10	2.28	0.10	2.26	0.13	2.08	0.14	1.97	0.15	1.87
26	520	0.10	2.33	0.10	2.31	0.12	2.13	0.13	2.02	0.15	1.92
27	540	0.09	2.38	0.09	2.36	0.11	2.18	0.13	2.07	0.13	2.01
28	560	0.09	2.43	0.09	2.42	0.11	2.23	0.12	2.12	0.13	2.02
29	580	0.08	2.48	0.09	2.47	0.10	2.28	0.11	2.17	0.13	2.07
30	600	0.08	2.53	0.08	2.51	0.10	2.33	0.11	2.23	0.12	2.12
31	620	0.08	2.58	0.08	2.56	0.09	2.38	0.10	2.27	0.11	2.17
32	640	0.07	2.62	0.07	2.62	0.09	2.43	0.10	2.32	0.11	2.21
		T2=	**267.40**	**T2=**	**262.04**	**T2=**	**281.84**	**T2=**	**293.01**	**T2=**	**306.64**

	Polymer	Poly Acrylic Acid - Controlled Conditions											
	pH	4.24		5.23		5.86		6.53		6.80		8.76	
Delay	Echo time (ms)	I	-ln(I/IO)	I	-ln(I/IO)	I	-ln(I/IO)	I	-ln(I/IO)	I	-ln(I/IO)	I	-ln(I/IO)
1	20	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.70	0.36	0.72	0.33	0.75	0.29	0.76	0.27	0.77	0.26	0.78	0.24
3	60	0.59	0.53	0.62	0.48	0.65	0.43	0.67	0.40	0.69	0.38	0.62	0.47
4	80	0.50	0.69	0.53	0.63	0.57	0.56	0.59	0.52	0.61	0.50	0.56	0.58
5	100	0.43	0.85	0.46	0.77	0.50	0.69	0.53	0.64	0.54	0.61	0.51	0.68
6	120	0.37	0.99	0.40	0.91	0.44	0.81	0.47	0.76	0.49	0.72	0.46	0.79
7	140	0.32	1.13	0.35	1.04	0.40	0.93	0.42	0.87	0.44	0.83	0.41	0.88
8	160	0.28	1.27	0.31	1.17	0.35	1.04	0.38	0.97	0.40	0.93	0.38	0.98
9	180	0.25	1.39	0.28	1.29	0.32	1.15	0.34	1.07	0.36	1.02	0.34	1.07
10	200	0.22	1.51	0.25	1.40	0.29	1.24	0.31	1.17	0.33	1.12	0.31	1.16
11	220	0.20	1.62	0.22	1.51	0.26	1.34	0.28	1.27	0.30	1.21	0.29	1.24
12	240	0.18	1.73	0.20	1.61	0.24	1.44	0.26	1.35	0.27	1.30	0.27	1.33
13	260	0.16	1.83	0.18	1.71	0.22	1.53	0.24	1.44	0.25	1.39	0.24	1.41
14	280	0.15	1.92	0.65	0.43	0.20	1.61	0.22	1.53	0.23	1.47	0.23	1.49
15	300	0.13	2.01	0.15	1.90	0.18	1.69	0.20	1.61	0.21	1.56	0.21	1.57
16	320	0.12	2.10	0.14	1.98	0.17	1.78	0.18	1.69	0.20	1.63	0.19	1.65
17	340	0.11	2.17	0.13	2.06	0.16	1.85	0.17	1.77	0.18	1.71	0.18	1.72
18	360	0.11	2.25	0.12	2.15	0.15	1.93	0.16	1.85	0.17	1.79	0.17	1.80
19	380	0.10	2.33	0.11	2.23	0.14	2.00	0.15	1.92	0.16	1.86	0.15	1.87
20	400	0.09	2.41	0.10	2.30	0.13	2.08	0.14	2.00	0.14	1.94	0.14	1.94
21	420	0.08	2.48	0.93	0.07	0.12	2.15	0.13	2.06	0.13	2.01	0.13	2.01
22	440	0.08	2.55	0.09	2.45	0.11	2.22	0.12	2.14	0.13	2.08	0.13	2.08
23	460	0.07	2.62	0.08	2.51	0.10	2.28	0.11	2.21	0.12	2.15	0.12	2.15
24	480	0.07	2.69	0.08	2.59	0.10	2.35	0.10	2.27	0.11	2.23	0.11	2.23
25	500	0.06	2.75	0.07	2.66	0.09	2.42	0.10	2.34	0.10	2.29	0.10	2.29
26	520	0.06	2.81	0.07	2.72	0.08	2.49	0.09	2.41	0.10	2.35	0.10	2.35
27	540	0.06	2.88	0.06	2.80	0.08	2.55	0.08	2.48	0.09	2.43	0.09	2.42
28	560	0.05	2.94	0.06	2.86	0.07	2.62	0.08	2.54	0.08	2.49	0.08	2.49
29	580	0.05	3.02	0.05	2.92	0.07	2.69	0.07	2.60	0.08	2.56	0.08	2.55
30	600	0.05	3.08	0.05	2.98	0.06	2.75	0.07	2.67	0.07	2.63	0.07	2.62
31	620					0.06	2.81	0.07	2.73	0.07	2.69	0.07	2.69
32	640					0.06	2.88	0.06	2.80	0.06	2.76		
		T2=	207.60	T2=	221.77	T2=	234.03	T2=	238.31	T2=	240.30	T2=	244.93

	Polymer	Polydimethyl Siloxane - Controlled Conditions									
	pH	4.23		5.86		6.54		6.88		8.92	
Delay	Echo time (ms)	I	-ln(I/IO)	I	-ln(I/IO)	I	-ln(I/IO)	I	-ln(I/IO)	I	-ln(I/IO)
1	20	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.83	0.18	0.84	0.18	0.84	0.17	0.84	0.17	0.84	0.18
3	60	0.76	0.27	0.76	0.27	0.76	0.27	0.77	0.26	0.77	0.27
4	80	0.70	0.36	0.70	0.36	0.70	0.36	0.71	0.35	0.70	0.36
5	100	0.64	0.45	0.64	0.45	0.64	0.45	0.65	0.44	0.64	0.44
6	120	0.58	0.54	0.58	0.54	0.58	0.54	0.59	0.52	0.59	0.53
7	140	0.53	0.63	0.53	0.63	0.53	0.63	0.54	0.61	0.54	0.62
8	160	0.49	0.72	0.49	0.72	0.49	0.72	0.50	0.70	0.49	0.71
9	180	0.44	0.81	0.45	0.81	0.45	0.81	0.46	0.79	0.45	0.80
10	200	0.41	0.90	0.41	0.90	0.41	0.90	0.42	0.87	0.41	0.89
11	220	0.37	0.99	0.37	0.99	0.37	0.99	0.38	0.96	0.38	0.98
12	240	0.34	1.08	0.34	1.08	0.34	1.08	0.35	1.05	0.34	1.07
13	260	0.31	1.18	0.31	1.16	0.31	1.17	0.32	1.14	0.32	1.16
14	280	0.28	1.27	0.29	1.26	0.28	1.26	0.29	1.22	0.29	1.24
15	300	0.26	1.36	0.26	1.35	0.26	1.35	0.27	1.31	0.26	1.33
16	320	0.24	1.45	0.24	1.44	0.24	1.44	0.25	1.40	0.24	1.42
17	340	0.22	1.54	0.22	1.52	0.22	1.53	0.23	1.48	0.22	1.51
18	360	0.20	1.63	0.20	1.61	0.20	1.62	0.21	1.57	0.20	1.60
19	380	0.17	1.78	0.18	1.70	0.18	1.74	0.19	1.66	0.19	1.69
20	400	0.16	1.81	0.17	1.80	0.17	1.80	0.17	1.75	0.17	1.78
21	420	0.15	1.90	0.15	1.88	0.15	1.89	0.16	1.83	0.16	1.86
22	440	0.14	1.99	0.14	1.97	0.14	1.98	0.15	1.92	0.14	1.96
23	460	0.13	2.08	0.13	2.06	0.13	2.07	0.13	2.01	0.13	2.05
24	480	0.11	2.17	0.12	2.15	0.12	2.16	0.12	2.10	0.12	2.14
25	500	0.10	2.26	0.11	2.24	0.11	2.25	0.11	2.18	0.11	2.23
26	520	0.10	2.35	0.10	2.33	0.10	2.34	0.10	2.27	0.10	2.31
27	540	0.09	2.44	0.09	2.42	0.09	2.43	0.10	2.35	0.09	2.40
28	560	0.08	2.54	0.08	2.51	0.08	2.53	0.09	2.44	0.08	2.49
29	580	0.07	2.63	0.07	2.60	0.07	2.62	0.08	2.54	0.08	2.58
30	600	0.07	2.72	0.07	2.69	0.07	2.70	0.07	2.62	0.07	2.67
31	620	0.06	2.81	0.06	2.78	0.06	2.80	0.07	2.70	0.06	2.75
32	640	0.06	2.90	0.06	2.86	0.06	2.88	0.06	2.80	0.06	2.85
		T2=	**219.34**	**T2=**	**221.73**	**T2=**	**220.42**	**T2=**	**227.75**	**T2=**	**223.64**

Appendix B: Relationship between T_2 and pH in Fe_2O_3-doped PDMS.

		DO (mg/L) 0.14		***DO (mg/L) 0.02***		***DO (mg/L) 0***		***DO (mg/L) 0.08***		***DO (mg/L) 0***		***DO (mg/L) 0.77***	
		pH 7.8		pH 5.3		pH 5.04		pH 7.2		pH 4.92		pH 6.14	
Echo	**Total Echo Time (ms)**	**I**	**-LN(I/Io)**	**I**	**-LN(I/Io)**	**I**	**-LN(I/Io)**	**I**	**-LN(I/Io)**	**I**	**-LN(I/Io)**	**I**	**-LN(I/Io)**
1	10	1.00	0.00	1.00	0.00	0.99	0.00	1.00	0.00	1.00	0.00	1.00	0.00
2	20	0.84	0.17	0.70	0.36	0.70	0.35	0.78	0.25	0.74	0.30	0.69	0.37
3	30	0.67	0.40	0.54	0.62	0.57	0.55	0.58	0.54	0.62	0.48	0.56	0.58
4	40	0.60	0.51	0.45	0.80	0.48	0.72	0.46	0.78	0.52	0.65	0.45	0.80
5	50	0.51	0.67	0.37	0.99	0.40	0.91	0.37	0.99	0.46	0.78	0.36	1.02
6	60	0.45	0.80	0.29	1.24	0.32	1.13	0.29	1.24	0.35	1.05	0.29	1.24
7	70	0.39	0.94	0.24	1.43	0.27	1.30	0.25	1.39	0.27	1.31	0.24	1.43
8	80	0.36	1.02	0.20	1.61	0.23	1.46	0.20	1.61	0.20	1.61	0.20	1.61
9	90	0.32	1.14	0.17	1.77	0.20	1.60	0.17	1.77	0.19	1.66	0.16	1.83
10	100	0.28	1.27	0.14	1.97	0.17	1.76	0.14	1.97	0.15	1.90	0.14	1.97
11	110	0.25	1.39	0.11	2.21	0.15	1.89	0.11	2.21	0.13	2.04	0.11	2.21
12	120	0.22	1.51			0.12	2.11	0.09	2.41				
13	130	0.19	1.66			0.11	2.20						
14	140	0.17	1.77										
15	150	0.15	1.90										
16	160	0.14	1.97										
		T2=	**77.93**	**T2=**	**47.83**	**T2=**	**56.57**	**T2=**	**46.86**	**T2=**	**48.72**	**T2=**	**47.41**

Appendix C: Relationship between T_2 relaxation and pH for medium-weight chitosan in tests using natural waters.

Polymer		Medium Weight Chitosan - Aerobic Conditions									
pH		4.43		5.68		6.13		7.11		7.90	
Delay	*Echo time (ms)*	*I*	*-ln(I/IO)*	*I*	*-ln(I/IO)*	*I*	*-ln(I/IO)*	*I*	*-ln(I/IO)*	*I*	*-ln(I/IO)*
1	20	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.66	0.42	0.66	0.41	0.67	0.41	0.68	0.38	0.68	0.39
3	60	0.54	0.62	0.55	0.61	0.55	0.60	0.57	0.56	0.57	0.57
4	80	0.45	0.81	0.45	0.79	0.46	0.78	0.48	0.73	0.48	0.74
5	100	0.37	0.98	0.81	0.21	0.39	0.95	0.41	0.88	0.41	0.90
6	120	0.32	1.15	0.32	1.13	0.33	1.11	0.36	1.03	0.35	1.05
7	140	0.27	1.31	0.28	1.29	0.28	1.27	0.31	1.17	0.30	1.19
8	160	0.23	1.46	0.24	1.44	0.24	1.41	0.27	1.31	0.27	1.33
9	180	0.20	1.60	0.21	1.58	0.21	1.55	0.24	1.44	0.23	1.46
10	200	0.18	1.73	0.18	1.71	0.19	1.68	0.21	1.56	0.21	1.58
11	220	0.16	1.86	0.16	1.84	0.17	1.80	0.19	1.68	0.18	1.70
12	240	0.14	1.97	0.14	1.96	0.15	1.92	0.17	1.79	0.16	1.81
13	260	0.12	2.09	0.13	2.08	0.13	2.03	0.15	1.90	0.15	1.93
14	280	0.11	2.20	0.11	2.19	0.12	2.14	0.14	2.00	0.13	2.04
15	300	0.10	2.30	0.10	2.30	0.11	2.24	0.12	2.11	0.12	2.15
16	320	0.09	2.40	0.09	2.41	0.10	2.34	0.11	2.22	0.11	2.25
17	340	0.08	2.50	0.08	2.50	0.09	2.44	0.10	2.31	0.10	2.35
18	360	0.08	2.59	0.07	2.60	0.08	2.54	0.09	2.41	0.09	2.45
19	380	0.07	2.69	0.07	2.70	0.07	2.63	0.08	2.51	0.08	2.56
20	400	0.06	2.78	0.06	2.80	0.07	2.73	0.07	2.60	0.07	2.66
21	420	0.06	2.86	0.06	2.88	0.06	2.83	0.07	2.70	0.06	2.76
22	440	0.05	2.96	0.05	2.98	0.05	2.92	0.06	2.80	0.06	2.86
23	460			0.05	3.07	0.05	3.00	0.06	2.90	0.05	2.96
24	480					0.05	3.10	0.05	3.00	0.05	3.06
25	500										
26	520										
27	540										
28	560										
29	580										
30	600										
31	620										
32	640										
		T2=	**154.59**	**T2=**	**149.30**	**T2=**	**161.99**	**T2=**	**167.30**	**T2=**	**163.73**

Polymer		Medium Weight Chitosan - Stimulated Aerobic Conditions									
pH		4.31		5.25		6.31		7.31		7.70	
Delay	*Echo time (ms)*	*I*	*-ln(I/IO)*	*I*	*-ln(I/IO)*	*I*	*-ln(I/IO)*	*I*	*-ln(I/IO)*	*I*	*-ln(I/IO)*
1	20	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.65	0.44	0.66	0.42	0.66	0.41	0.68	0.39	0.67	0.40
3	60	0.53	0.64	0.54	0.61	0.55	0.60	0.64	0.45	0.56	0.58
4	80	0.43	0.83	0.45	0.80	0.46	0.79	0.48	0.74	0.47	0.76
5	100	0.36	1.02	0.38	0.98	0.39	0.95	0.41	0.90	0.40	0.91
6	120	0.30	1.19	0.32	1.15	0.33	1.11	0.35	1.05	0.35	1.06
7	140	0.26	1.35	0.27	1.31	0.28	1.27	0.30	1.20	0.30	1.20
8	160	0.22	1.51	0.23	1.46	0.24	1.41	0.26	1.33	0.26	1.34
9	180	0.19	1.66	0.20	1.59	0.21	1.55	0.23	1.46	0.23	1.47
10	200	0.17	1.79	0.18	1.73	0.19	1.67	0.21	1.58	0.21	1.58
11	220	0.15	1.92	0.16	1.86	0.17	1.80	0.18	1.70	0.18	1.70
12	240	0.13	2.04	0.14	1.98	0.15	1.91	0.16	1.81	0.16	1.83
13	260	0.12	2.16	0.12	2.10	0.13	2.02	0.15	1.93	0.15	1.92
14	280	0.10	2.27	0.11	2.21	0.12	2.13	0.13	2.03	0.13	2.03
15	300	0.09	2.38	0.10	2.31	0.11	2.23	0.12	2.15	0.12	2.14
16	320	0.08	2.48	0.09	2.42	0.10	2.33	0.11	2.24	0.11	2.23
17	340	0.08	2.58	0.08	2.51	0.09	2.43	0.10	2.34	0.10	2.33
18	360	0.07	2.67	0.07	2.62	0.08	2.53	0.09	2.44	0.09	2.44
19	380	0.06	2.76	0.07	2.70	0.07	2.62	0.08	2.55	0.08	2.54
20	400	0.06	2.86	0.06	2.80	0.07	2.70	0.07	2.65	0.07	2.63
21	420	0.05	2.96	0.06	2.90	0.06	2.80	0.04	3.22	0.07	2.73
22	440	0.05	3.04	0.05	2.98	0.06	2.88	0.08	2.53	0.06	2.83
23	460			0.05	3.08	0.05	2.98	0.05	2.94	0.05	2.94
24	480					0.05	3.08	0.48	0.73	0.05	3.02
25	500										
26	520										
27	540										
28	560										
29	580										
30	600										
31	620										
32	640										
		T2=	**150.31**	**T2=**	**155.55**	**T2=**	**164.09**	**T2=**	**200.22**	**T2=**	**166.86**

Polymer		Medium Weight Chitosan - Anaerobic Conditions									
pH		4.10		4.89		5.68		6.25		7.83	
Delay	*Echo time (ms)*	*I*	*-ln(I/IO)*	*I*	*-ln(I/IO)*	*I*	*-ln(I/IO)*	*I*	*-ln(I/IO)*	*I*	*-ln(I/IO)*
1	20	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.70	0.36	0.70	0.36	0.70	0.35	0.70	0.35	0.72	0.32
3	60	0.59	0.52	0.59	0.52	0.60	0.51	0.60	0.52	0.63	0.47
4	80	0.51	0.68	0.51	0.68	0.51	0.67	0.12	2.12	0.54	0.61
5	100	0.43	0.84	0.44	0.83	0.44	0.81	0.44	0.82	0.48	0.74
6	120	0.38	0.98	0.38	0.97	0.39	0.95	0.39	0.95	0.42	0.86
7	140	0.33	1.11	0.33	1.11	0.34	1.08	0.34	1.08	0.38	0.97
8	160	0.29	1.24	0.29	1.23	0.30	1.20	0.30	1.20	0.34	1.08
9	180	0.26	1.36	0.26	1.35	0.27	1.31	0.27	1.32	0.31	1.18
10	200	0.23	1.48	0.23	1.47	0.24	1.42	0.24	1.42	0.28	1.28
11	220	0.21	1.58	0.21	1.57	0.22	1.52	0.22	1.52	0.25	1.37
12	240	0.19	1.69	0.19	1.67	0.20	1.61	0.20	1.62	0.23	1.46
13	260	0.17	1.78	0.17	1.77	0.18	1.70	0.18	1.71	0.21	1.54
14	280	0.15	1.87	0.16	1.85	0.17	1.79	0.17	1.80	0.20	1.62
15	300	0.14	1.95	0.14	1.94	0.15	1.87	0.15	1.88	0.18	1.70
16	320	0.13	2.03	0.13	2.02	0.14	1.95	0.14	1.96	0.17	1.78
17	340	0.12	2.11	0.12	2.10	0.13	2.02	0.13	2.03	0.16	1.86
18	360	0.11	2.19	0.11	2.18	0.12	2.10	0.12	2.11	0.15	1.93
19	380	0.11	2.25	0.11	2.25	0.11	2.17	0.11	2.18	0.14	2.00
20	400	0.10	2.32	0.10	2.32	0.11	2.23	0.11	2.25	0.13	2.07
21	420	0.09	2.40	0.09	2.39	0.10	2.30	0.10	2.32	0.12	2.15
22	440	0.09	2.47	0.09	2.47	0.09	2.41	0.09	2.40	0.11	2.22
23	460	0.08	2.53	0.08	2.53	0.09	2.44	0.09	2.47	0.10	2.28
24	480	0.08	2.59	0.08	2.59	0.08	2.50	0.08	2.53	0.10	2.35
25	500	0.07	2.65	0.07	2.66	0.08	2.56	0.07	2.60	0.09	2.42
26	520	0.07	2.70	0.07	2.72	0.07	2.63	0.07	2.66	0.08	2.49
27	540	0.06	2.76	0.06	2.78	0.07	2.69	0.07	2.73	0.08	2.56
28	560	0.06	2.83	0.06	2.85	0.06	2.75	0.06	2.80	0.07	2.63
29	580	0.06	2.88	0.05	2.92	0.06	2.81	0.06	2.86	0.07	2.70
30	600	0.05	2.94	0.05	2.98	0.06	2.88	0.05	2.92	0.06	2.76
31	620	0.05	3.00	0.05	3.04	0.05	2.94	0.05	3.00	0.06	2.83
32	640	0.05	3.06	0.05	3.10	0.05	3.00	0.05	3.06	0.06	2.90
		T2=	**225.75**	**T2=**	**222.39**	**T2=**	**230.83**	**T2=**	**244.74**	**T2=**	**237.08**

Polymer		Medium Weight Chitosan - Stimulated Anaerobic Conditions									
pH		4.37		5.11		6.14		7.18		7.92	
Delay	*Echo time (ms)*	*I*	*-ln(I/IO)*	*I*	*-ln(I/IO)*	*I*	*-ln(I/IO)*	*I*	*-ln(I/IO)*	*I*	*-ln(I/IO)*
1	20	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.70	0.35	0.70	0.36	0.70	0.36	0.72	0.32	0.73	0.32
3	60	0.59	0.52	0.59	0.52	0.60	0.52	0.62	0.47	0.63	0.47
4	80	0.51	0.68	0.51	0.68	0.51	0.68	0.54	0.61	0.55	0.60
5	100	0.44	0.83	0.44	0.83	0.44	0.82	0.48	0.74	0.48	0.73
6	120	0.38	0.97	0.38	0.97	0.38	0.96	0.42	0.86	0.43	0.84
7	140	0.33	1.11	0.33	1.11	0.34	1.09	0.38	0.98	0.39	0.95
8	160	0.29	1.23	0.29	1.23	0.30	1.21	0.34	1.08	0.35	1.05
9	180	0.26	1.35	0.26	1.35	0.27	1.32	0.31	1.18	0.32	1.15
10	200	0.23	1.47	0.23	1.47	0.23	1.47	0.28	1.28	0.29	1.24
11	220	0.21	1.58	0.21	1.57	0.22	1.53	0.25	1.37	0.27	1.33
12	240	0.19	1.68	0.19	1.67	0.20	1.63	0.23	1.46	0.24	1.41
13	260	0.17	1.77	0.17	1.77	0.18	1.72	0.21	1.54	0.23	1.49
14	280	0.16	1.86	0.16	1.85	0.17	1.80	0.20	1.62	0.21	1.57
15	300	0.14	1.94	0.14	1.94	0.15	1.88	0.18	1.70	0.19	1.64
16	320	0.13	2.02	0.13	2.02	0.14	1.97	0.17	1.77	0.18	1.71
17	340	0.12	2.10	0.12	2.10	0.13	2.04	0.16	1.85	0.17	1.78
18	360	0.11	2.18	0.11	2.18	0.12	2.11	0.15	1.92	0.16	1.85
19	380	0.11	2.25	0.11	2.25	0.11	2.19	0.14	1.99	0.15	1.92
20	400	0.10	2.32	0.10	2.32	0.11	2.25	0.12	2.12	0.14	1.99
21	420	0.09	2.39	0.09	2.39	0.10	2.32	0.12	2.12	0.13	2.06
22	440	0.09	2.45	0.09	2.47	0.02	3.91	0.11	2.19	0.12	2.12
23	460	0.08	2.53	0.08	2.53	0.09	2.45	0.11	2.25	0.11	2.19
24	480	0.08	2.59	0.08	2.59	0.08	2.53	0.10	2.32	0.11	2.25
25	500	0.07	2.65	0.07	2.66	0.08	2.59	0.09	2.39	0.10	2.31
26	520	0.07	2.72	0.07	2.72	0.07	2.65	0.09	2.45	0.09	2.38
27	540	0.06	2.78	0.06	2.78	0.07	2.72	0.08	2.51	0.09	2.44
28	560	0.06	2.83	0.06	2.85	0.06	2.78	0.06	2.81	0.08	2.51
29	580	0.06	2.90	0.05	2.92	0.06	2.85	0.07	2.65	0.08	2.58
30	600	0.05	2.96	0.05	2.98	0.06	2.90	0.07	2.70	0.07	2.63
31	620	0.05	3.02	0.05	3.04	0.05	2.96	0.06	2.76	0.07	2.70
32	640	0.06	2.81	0.05	3.10	0.05	3.02	0.06	2.83		
		T2=	**227.73**	**T2=**	**222.35**	**T2=**	**221.69**	**T2=**	**240.65**	**T2=**	**248.13**

Appendix D: Relationship between T_2 and DO in Fe_2O_3-doped PDMS.

1) Control Samples

		Control		0.14 mg/L		0.14 mg/L		0.64 mg/L		1.02 mg/L	
Loops	Total Echo Time (ms)	I	-ln(I/Io)	I	ln(I/Io)	I	ln(I/Io)	I	ln(I/Io)	I	ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.80	0.22	0.80	0.22	0.84	0.17	0.85	0.16	0.87	0.14
3	60	0.77	0.26	0.65	0.43	0.67	0.40	0.68	0.39	0.75	0.29
4	80	0.68	0.39	0.56	0.58	0.60	0.51	0.58	0.54	0.61	0.49
5	100	0.58	0.54	0.48	0.73	0.51	0.67	0.51	0.67	0.56	0.58
6	120	0.52	0.65	0.42	0.87	0.45	0.80	0.46	0.78	0.50	0.69
7	140	0.45	0.80	0.37	0.99	0.39	0.94	0.40	0.92	0.44	0.82
8	160	0.40	0.92	0.33	1.11	0.36	1.02	0.35	1.05	0.40	0.92
9	180	0.36	1.02	0.30	1.20	0.32	1.14	0.32	1.14	0.36	1.02
10	200	0.34	1.08	0.26	1.35	0.28	1.27	0.28	1.27	0.32	1.14
11	220	0.31	1.17	0.24	1.43	0.25	1.39	0.26	1.35	0.29	1.24
12	240	0.29	1.24	0.21	1.56	0.22	1.51	0.23	1.47	0.26	1.35
13	260	0.27	1.31	0.19	1.66	0.19	1.66	0.21	1.56	0.24	1.43
14	280	0.24	1.43	0.17	1.77	0.17	1.77	0.19	1.66	0.21	1.56
15	300	0.23	1.47	0.15	1.90	0.15	1.90	0.17	1.77	0.19	1.66
16	320	0.21	1.56	0.14	1.97	0.14	1.97	0.15	1.90	0.17	1.77
		T2=	**196.72**	**T2 =**	**159.11**	**T2 =**	**155.86**	**T2 =**	**165.58**	**T2 =**	**174.56**

Loops	Total Echo Time (ms)	1.71 mg/L		1.92 mg/L		2.81 mg/L		2.83 mg/L		3.54 mg/L	
		I	ln(I/Io)	I	ln(I/Io)	I	ln(I/Io)	I	ln(I/Io)	I	ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00
2	40					0.72	0.33	0.73	0.31	0.70	0.36
3	60	0.66	0.42	0.72	0.33	0.60	0.51	0.60	0.51	0.58	0.54
4	80	0.59	0.53	0.59	0.53	0.52	0.65	0.51	0.67	0.48	0.73
5	100	0.49	0.71	0.49	0.71	0.44	0.82	0.48	0.73	0.40	0.92
6	120	0.43	0.84	0.46	0.78	0.37	0.99	0.36	1.02	0.33	1.11
7	140	0.39	0.94	0.39	0.94	0.32	1.14	0.31	1.17	0.29	1.24
8	160	0.34	1.08	0.35	1.05	0.28	1.27	0.27	1.31	0.24	1.43
9	180	0.31	1.17	0.30	1.20	0.24	1.43	0.24	1.43	0.19	1.66
10	200	0.28	1.27	0.27	1.31	0.21	1.56	0.21	1.56	0.17	1.77
11	220	0.25	1.39	0.24	1.43	0.18	1.71	0.17	1.77	0.15	1.90
12	240	0.22	1.51	0.21	1.56	0.16	1.83	0.15	1.90	0.11	2.21
13	260	0.20	1.61	0.19	1.66	0.13	2.04	0.13	2.04	0.09	2.41
14	280			0.16	1.83	0.12	2.12	0.12	2.12	0.08	2.53
15	300			0.15	1.90	0.10	2.30	0.10	2.30	0.07	2.66
16	320			0.13	2.04	0.09	2.41	0.09	2.41	0.06	2.81
		T2 =	**157.15**	**T2 =**	**152.26**	**T2 =**	**130.69**	**T2 =**	**129.34**	**T2 =**	**109.85**

Loops	Total Echo Time (ms)	3.68 mg/L		3.81 mg/L		4.43 mg/L		5.18 mg/L		5.60 mg/L	
		I	ln(I/Io)	I	ln(I/Io)	I	ln(I/Io)	I	ln(I/Io)	I	ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.69	0.37	0.71	0.34	0.73	0.31	0.76	0.27	0.79	0.24
3	60	0.56	0.58	0.57	0.56	0.58	0.54	0.59	0.53	0.65	0.43
4	80	0.47	0.76	0.48	0.73	0.48	0.73	0.49	0.71	0.54	0.62
5	100	0.39	0.94	0.39	0.94	0.39	0.94	0.39	0.94	0.44	0.82
6	120	0.32	1.14	0.32	1.14	0.32	1.14	0.32	1.14	0.39	0.94
7	140	0.27	1.31	0.27	1.31	0.27	1.31	0.26	1.35	0.33	1.11
8	160	0.22	1.51	0.22	1.51	0.22	1.51	0.22	1.51	0.29	1.24
9	180	0.18	1.71	0.18	1.71	0.18	1.71	0.18	1.71	0.24	1.43
10	200	0.15	1.90	0.15	1.90	0.15	1.90	0.15	1.90	0.21	1.56
11	220	0.12	2.12	0.12	2.12	0.12	2.12	0.12	2.12	0.18	1.71
12	240					0.05	3.00	0.10	2.30	0.13	2.04
13	260	0.08	2.53							0.10	2.30
14	280	0.06	2.81							0.08	2.53
15	300									0.08	2.53
16	320									0.07	2.66
		T2 =	**98.46**	**T2 =**	**99.07**	**T2 =**	**87.38**	**T2 =**	**97.85**	**T2 =**	**111.63**

		6.03 mg/L	
Loops	Total Echo Time (ms)	I	ln(I/Io)
1	20	1.00	0.00
2	40	0.76	0.27
3	60	0.62	0.48
4	80	0.52	0.65
5	100	0.48	0.73
6	120	0.37	0.99
7	140	0.31	1.17
8	160	0.27	1.31
9	180	0.23	1.47
10	200	0.20	1.61
11	220	0.18	1.71
12	240	0.15	1.90
13	260	0.13	2.04
14	280	0.12	2.12
15	300	0.10	2.30
16	320	0.09	2.41
		T2 =	**128.00**

2) Natural Waters

Anaerobic Natural Water

Loops	Total Echo Time (ms)	0.05 mg/L I	-ln(I/Io)	0.05 mg/L I	ln(I/Io)	0.03 mg/L I	ln(I/Io)	0.06 mg/L I	ln(I/Io)	0.05 mg/L I	ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.71	0.34	0.70	0.36	0.74	0.30	0.70	0.36	0.71	0.34
3	60	0.58	0.54	0.58	0.54	0.59	0.53	0.58	0.54	0.58	0.54
4	80	0.48	0.73	0.48	0.73	0.49	0.71	0.48	0.73	0.48	0.73
5	100	0.40	0.92	0.40	0.92	0.40	0.92	0.40	0.92	0.40	0.92
6	120	0.33	1.11	0.33	1.11	0.33	1.11	0.33	1.11	0.33	1.11
7	140	0.29	1.24	0.29	1.24	0.28	1.27	0.29	1.24	0.29	1.24
8	160	0.24	1.43	0.24	1.43	0.23	1.47	0.24	1.43	0.24	1.43
9	180	0.19	1.66	0.10	2.30	0.19	1.66	0.19	1.66	0.19	1.66
10	200	0.17	1.77	0.17	1.77	0.16	1.83	0.17	1.77	0.17	1.77
11	220	0.14	1.97	0.15	1.90	0.13	2.04	0.15	1.90	0.14	1.97
12	240	0.10	2.30	0.10	2.30	0.10	2.30	0.09	2.41	0.10	2.30
13	260	0.08	2.53	0.09	2.41	0.07	2.66	0.09	2.41	0.07	2.66
14	280			0.08	2.53			0.08	2.53		
15	300										
16	320										
		T2=	**102.36**	**T2=**	**104.11**	**T2=**	**97.79**	**T2=**	**105.28**	**T2=**	**100.10**

Anaerobic Stimulated

Loops	Total Echo Time (ms)	0.04 mg/L I	0.04 mg/L ln(I/Io)	0.07 mg/L I	0.07 mg/L ln(I/Io)	0.11 mg/L I	0.11 mg/L ln(I/Io)	0.06 mg/L I	0.06 mg/L ln(I/Io)	0.03 mg/L I	0.03 mg/L ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.74		0.70	0.36	0.72	0.33	0.75	0.29	0.73	0.31
3	60	0.59	0.53	0.58	0.54	0.58	0.54	0.59	0.53	0.58	0.54
4	80	0.49	0.71	0.48	0.73	0.48	0.73	0.49	0.71	0.48	0.73
5	100	0.40	0.92	0.40	0.92	0.40	0.92	0.39	0.94	0.39	0.94
6	120	0.33	1.11	0.33	1.11	0.33	1.11	0.32	1.14	0.32	1.14
7	140	0.28	1.27	0.29	1.24	0.28	1.27	0.27	1.31	0.27	1.31
8	160	0.23	1.47	0.24	1.43	0.23	1.47	0.22	1.51	0.22	1.51
9	180	0.19	1.66	0.15	1.90	0.19	1.66	0.18	1.71	0.18	1.71
10	200	0.16	1.83	0.17	1.77	0.16	1.83	0.15	1.90	0.15	1.90
11	220	0.13	2.04	0.15	1.90	0.13	2.04	0.12	2.12	0.12	2.12
12	240	0.10	2.30	0.10	2.30	0.08	2.53	0.08	2.53	0.05	3.00
13	260			0.09	2.41						
14	280			0.09	2.41						
15	300										
16	320										
		T2=	**100.63**	**T2=**	**107.48**	**T2=**	**97.51**	**T2=**	**94.14**	**T2=**	**87.38**

Aerobic Natural Water

Loops	Total Echo Time (ms)	4.13 mg/L I	4.13 mg/L -ln(I/Io)	3.81 mg/L I	3.81 mg/L ln(I/Io)	4.05 mg/L I	4.05 mg/L ln(I/Io)	4.41 mg/L I	4.41 mg/L ln(I/Io)	5.17 mg/L I	5.17 mg/L ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.72	0.33	0.72	0.33	0.68	0.39	0.61	0.49	0.62	0.48
3	60	0.57	0.56	0.56	0.58	0.52	0.65	0.46	0.78	0.45	0.80
4	80	0.47	0.76	0.45	0.80	0.40	0.92	0.31	1.17	0.32	1.14
5	100	0.38	0.97	0.35	1.05	0.31	1.17	0.20	1.61	0.22	1.51
6	120	0.31	1.17	0.29	1.24	0.25	1.39	0.16	1.83	0.17	1.77
7	140	0.26	1.35	0.23	1.47	0.19	1.66	0.10	2.30	0.11	2.21
8	160	0.21	1.56	0.19	1.66	0.15	1.90	0.08	2.53	0.07	2.66
9	180	0.17	1.77	0.14	1.97	0.09	2.41				
10	200	0.13	2.04	0.10	2.30	0.05	3.00				
11	220	0.10	2.30	0.06	2.81						
12	240										
13	260										
14	280										
15	300										
16	320										
		T2=	**91.74**	**T2=**	**77.83**	**T2=**	**66.29**	**T2=**	**55.39**	**T2=**	**54.98**

Stimulated Aerobic Conditions

Loops	Total Echo Time (ms)	5.91 mg/L I	5.91 mg/L -ln(I/Io)	5.72 mg/L I	5.72 mg/L ln(I/Io)	6.00 mg/L I	6.00 mg/L ln(I/Io)	6.03 mg/L I	6.03 mg/L ln(I/Io)	6.12 mg/L I	6.12 mg/L ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.70	0.36	0.68	0.39	0.65	0.43	0.69	0.37	0.69	0.37
3	60	0.54	0.62	0.52	0.65	0.49	0.71	0.54	0.62	0.53	0.63
4	80	0.43	0.84	0.40	0.92	0.36	1.02	0.42	0.87	0.42	0.87
5	100	0.33	1.11	0.30	1.20	0.27	1.31	0.33	1.11	0.32	1.14
6	120	0.27	1.31	0.24	1.43	0.21	1.56	0.27	1.31	0.26	1.35
7	140	0.21	1.56	0.18	1.71	0.15	1.90	0.21	1.56	0.20	1.61
8	160	0.17	1.77	0.14	1.97	0.11	2.21	0.17	1.77	0.16	1.83
9	180	0.12	2.12	0.06	2.81			0.11	2.21	0.09	2.41
10	200	0.08	2.53					0.08	2.53		
11	220										
12	240										
13	260										
14	280										
15	300										
16	320										
		T2=	**76.38**	**T2=**	**64.42**	**T2=**	**65.59**	**T2=**	**75.61**	**T2=**	**72.97**

Appendix E: Relationship between Fe_2O_3 concentration and T_2 in PDMS.

Stock [Fe_2O_3] = 30 µg/µL

		Control (no Fe_2O_3)		**5µL/ 600 µL**		**3.5 µL/ 600 µL**		**2.5µL/ 600 µL**		**2.5µL/ 600 µL (duplicate)**	
# Echos	Total Echo Time (ms)	I	-LN(I/Io)	I	-LN(I/Io)	I	-ln(I/Io)	I	-LN(I/Io)	I	-LN(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	-0.01	1.00	0.00	1.00	0.00
2	40	0.80	0.22	0.70	0.36	0.70	0.35	0.69	0.37	0.69	0.37
3	60	0.77	0.26	0.51	0.67	0.54	0.61	0.56	0.58	0.56	0.58
4	80	0.68	0.39	0.39	0.94	0.43	0.83	0.47	0.76	0.47	0.76
5	100	0.58	0.54	0.29	1.24	0.34	1.07	0.39	0.94	0.39	0.94
6	120	0.52	0.65	0.22	1.51	0.27	1.30	0.32	1.14	0.32	1.14
7	140	0.45	0.80	0.18	1.71	0.23	1.46	0.27	1.31	0.27	1.31
8	160	0.40	0.92	0.14	1.97	0.18	1.70	0.22	1.51	0.22	1.51
9	180	0.36	1.02	0.11	2.21	0.15	1.89	0.18	1.71	0.18	1.71
10	200	0.34	1.08	0.09	2.41	0.12	2.11	0.15	1.90	0.15	1.90
11	220	0.31	1.17	0.07	2.66	0.10	2.29	0.12	2.12	0.12	2.12
12	240	0.29	1.24	0.06	2.81						
13	260	0.27	1.31	0.05	3.00			0.08	2.53	0.08	2.53
14	280	0.24	1.43					0.06	2.81	0.06	2.81
15	300	0.23	1.47								
16	320	0.21	1.56								
		T2=	**196.72**	**T2=**	**80.90**	**T2 =**	**89.64**	**T2=**	**98.46**	**T2=**	**98.46**

		1.5 µL/ 600 µL		1µL/ 600 µL		1µL/ 600 µL (duplicate)		0.5 µL/ 600 µL	
# Echos	Total Echo Time (ms)	I	-ln(I/Io)	I	-LN(I/Io)	I	-ln(I/Io)	I	-ln(I/Io)
1	20	1.00	-0.01	1.00	0.00	0.99	0.00	1.00	-0.01
2	40	0.74	0.29	0.76	0.27	0.67	0.39	0.80	0.21
3	60	0.59	0.52	0.62	0.48	0.57	0.55	0.72	0.32
4	80	0.49	0.70	0.49	0.71	0.48	0.72	0.60	0.50
5	100	0.40	0.91	0.42	0.87	0.40	0.91	0.52	0.64
6	120	0.32	1.13	0.35	1.05	0.33	1.10	0.46	0.77
7	140	0.28	1.26	0.31	1.17	0.28	1.26	0.39	0.93
8	160	0.24	1.42	0.27	1.31	0.24	1.42	0.34	1.07
9	180	0.21	1.55	0.23	1.47	0.20	1.60	0.30	1.19
10	200	0.19	1.65	0.21	1.56	0.18	1.70	0.27	1.30
11	220	0.17	1.76	0.18	1.71	0.16	1.82	0.25	1.40
12	240	0.12	2.11	0.16	1.83	0.13	2.03	0.23	1.46
13	260	0.11	2.20	0.14	1.97	0.12	2.11	0.20	1.60
14	280	0.08	2.52	0.12	2.12	0.10	2.29	0.18	1.70
15	300	0.07	2.65	0.11	2.21	0.09	2.40	0.17	1.76
16	320			0.10	2.30	0.08	2.52	0.15	1.89
		T2 =	**112.26**	**T2 =**	**135.44**	**T2 =**	**125.40**	**T2 =**	**162.26**

Appendix F: Relationship between T_2 and ORP in Fe_2O_3-doped PDMS.

	ORP=	**-227 mv**		**-187 mV**		**-131 mV**		**-90 mV**		**-23 mv**	
Echo	Echo time (ms)	I	-ln(I/Io)	I	-ln(I/Io)	I	-ln(I/Io)	I	-ln(I/Io)	I	-ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.58	0.54	0.72	0.33	0.66	0.42	0.74	0.31	0.81	0.21
3	60	0.46	0.78	0.46	0.78	0.47	0.76	0.52	0.66	0.56	0.58
4	80	0.40	0.92	0.39	0.94	0.35	1.05	0.43	0.86	0.50	0.69
5	100	0.33	1.11	0.39	0.94	0.29	1.24	0.34	1.09	0.38	0.97
6	120	0.25	1.39	0.28	1.27	0.23	1.47	0.27	1.31	0.31	1.17
7	140	0.20	1.61	0.20	1.61	0.17	1.77	0.23	1.47	0.29	1.24
8	160	0.16	1.83	0.16	1.83	0.14	1.97	0.19	1.69	0.23	1.47
9	180	0.10	2.30	0.14	1.97	0.11	2.21	0.16	1.86	0.20	1.61
10	200	0.12	2.12	0.11	2.21	0.09	2.41	0.13	2.08	0.16	1.83
11	220	0.10	2.30	0.10	2.30	0.07	2.66	0.11	2.25	0.14	1.97
12	240	0.08	2.53	0.08	2.53	0.06	2.81	0.10	2.35	0.13	2.04
13	260	0.07	2.66	0.08	2.53	0.05	3.00	0.08	2.53	0.11	2.21
14	280	0.06	2.81	0.06	2.81	0.04	3.22	0.07	2.66	0.10	2.30
15	300	0.04	3.22	0.04	3.22	0.04	3.22	0.05	3.00	0.06	2.81
16	320	0.03	3.51	0.04	3.22	0.03	3.51	0.05	3.00	0.07	2.66
		T2=	**95.80**	**T2=**	**96.67**	**T2=**	**89.01**	**T2=**	**102.71**	**T2=**	**113.61**

	ORP=	56 mV		77 mv		123 mv	
Echo	Echo time (ms)	I	-ln(I/Io)	I	-ln(I/Io)	I	-ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.77	0.26	0.71	0.34	0.57	0.56
3	60	0.54	0.62	0.55	0.60	0.50	0.69
4	80	0.46	0.77	0.39	0.94	0.44	0.82
5	100	0.36	1.03	0.34	1.08	0.35	1.05
6	120	0.29	1.24	0.28	1.27	0.29	1.24
7	140	0.26	1.35	0.26	1.35	0.22	1.51
8	160	0.21	1.57	0.21	1.56	0.18	1.71
9	180	0.18	1.73	0.14	1.97	0.14	1.97
10	200	0.14	1.95	0.15	1.90	0.12	2.12
11	220	0.12	2.10	0.12	2.12	0.10	2.30
12	240	0.11	2.18	0.10	2.30	0.08	2.53
13	260	0.10	2.35	0.10	2.30	0.07	2.66
14	280	0.10	2.35	0.08	2.53	0.05	3.00
15	300	0.06	2.90	0.07	2.66	0.05	3.00
16	320	0.06	2.81	0.06	2.81	0.04	3.22
		T2=	**109.48**	**T2=**	**112.74**	**T2=**	**97.48**

Appendix G: Relaxation response to exposure to saturated TCE for selected polymer materials.

Polymer		Styrene Acrylonitrile (SAN)				Polyvinyl Chloride (PVC)			
		Clean Water		*Saturated TCE solution*		*Clean Water*		*Saturated TCE solution*	
Delay	Echo time (ms)	I	-LN(I/Io)	I	-LN(I/Io)	I	-LN(I/Io)	I	-LN(I/Io)
1	20	1	0.00	1.2	0.00	1.00	0.00	1.00	0.00
2	40	0.88	0.13	1.09	0.10	0.90	0.11	0.82	0.20
3	60	0.84	0.17	1.04	0.14	0.77	0.26	0.71	0.34
4	80	0.77	0.26	0.97	0.21	0.66	0.42	0.61	0.49
5	100	0.72	0.33	0.9	0.29	0.54	0.62	0.53	0.63
6	120	0.69	0.37	0.84	0.36	0.54	0.62	0.46	0.78
7	140	0.65	0.43	0.78	0.43	0.45	0.80	0.41	0.89
8	160	0.61	0.49	0.71	0.52	0.41	0.89	0.36	1.02
9	180	0.57	0.56	0.66	0.60	0.36	1.02	0.32	1.14
10	200	0.54	0.62	0.62	0.66	0.35	1.05	0.29	1.24
11	220	0.51	0.67	0.58	0.73	0.31	1.17	0.26	1.35
12	240	0.45	0.80	0.51	0.86	0.28	1.27	0.23	1.47
13	260	0.41	0.89	0.45	0.98	0.25	1.39	0.21	1.56
14	280	0.36	1.02	0.4	1.10	0.23	1.47	0.19	1.66
15	300	0.32	1.14	0.35	1.23	0.20	1.61		
16	320					0.19	1.66		
		T2=	**270.14**	**T2=**	**238.37**	**T2=**	**181.94**	**T2=**	**159.87**

Polymer		Polyphenylene Sulfide (PPS)				Polymethylpentene (PMP)			
		Clean Water		*Saturated TCE solution*		*Clean Water*		*Saturated TCE solution*	
Delay	Echo time (ms)	I	-LN(I/Io)	I	-LN(I/Io)	I	-LN(I/Io)	I	-LN(I/Io)
1	20	1	0.00	1	0.18	1	0.00	1	0.00
2	40	0.72	0.33	0.75	0.47	0.87	0.14	0.87	0.14
3	60	0.62	0.48	0.63	0.64	0.83	0.19	0.83	0.19
4	80	0.46	0.78	0.47	0.94	0.74	0.30	0.76	0.27
5	100	0.36	1.02	0.38	1.15	0.67	0.40	0.68	0.39
6	120	0.28	1.27	0.28	1.46	0.61	0.49	0.6	0.51
7	140	0.22	1.51	0.24	1.61	0.56	0.58	0.54	0.62
8	160	0.18	1.71	0.19	1.84	0.5	0.69	0.48	0.73
9	180	0.15	1.90	0.15	2.08	0.46	0.78	0.44	0.82
10	200	0.12	2.12	0.12	2.30	0.42	0.87	0.4	0.92
11	220	0.1	2.30	0.1	2.48	0.38	0.97	0.37	0.99
12	240	0.09	2.41	0.09	2.59	0.35	1.05	0.34	1.08
13	260								
14	280								
15	300								
16	320								
		T2=	**89.83**	**T2=**	**89.13**	**T2=**	**210.98**	**T2=**	**200.32**

Polymer		Polyethylene Terephthalate (PETP)				Polysulfone (PSF)			
		Clean Water		*Saturated TCE solution*		*Clean Water*		*Saturated TCE solution*	
Delay	Echo time (ms)	I	-LN(I/Io)	I	-LN(I/Io)	I	-LN(I/Io)	I	-LN(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.74	0.30	0.83	0.37	0.79	0.24	0.81	0.21
3	60	0.71	0.34	0.82	0.38	0.77	0.26	0.79	0.24
4	80	0.67	0.40	0.77	0.44	0.72	0.33	0.75	0.29
5	100	0.68	0.39	0.74	0.48	0.71	0.34	0.73	0.31
6	120	0.64	0.45	0.71	0.52	0.68	0.39	0.70	0.36
7	140	0.60	0.51	0.68	0.57	0.64	0.45	0.66	0.42
8	160	0.57	0.56	0.66	0.60	0.62	0.48	0.64	0.45
9	180	0.54	0.62	0.63	0.64	0.59	0.53	0.61	0.49
10	200	0.52	0.65	0.60	0.69	0.56	0.58	0.58	0.54
11	220	0.49	0.71	0.58	0.73	0.54	0.62	0.56	0.58
12	240	0.46	0.78	0.54	0.80	0.50	0.69	0.52	0.65
13	260	0.42	0.87	0.50	0.88	0.46	0.78	0.48	0.73
14	280	0.40	0.92	0.47	0.94	0.44	0.82	0.46	0.78
15	300	0.37	0.99	0.43	1.03	0.40	0.92	0.42	0.87
16	320	0.34	1.08	0.40	1.10	0.37	0.99	0.39	0.94
		T2=	**337.78**	**T2=**	**351.64**	**T2=**	**357.83**	**T2=**	**372.06**

Polymer		Low-Density Poly Ethylene (LDPE)				Polyethylene Oxide (PEO)			
		Clean Water		*Saturated TCE solution*		*Clean Water*		*Saturated TCE solution*	
Delay	Echo time (ms)	I	-LN(I/Io)	I	-LN(I/Io)	I	-LN(I/Io)	I	-LN(I/Io)
1	20	1	0.00	1	0.00	1	0.00	1	0.00
2	40	0.89	0.12	0.89	0.12	0.94	0.06	0.95	0.05
3	60	0.85	0.16	0.85	0.16	0.86	0.15	0.86	0.15
4	80	0.79	0.24	0.81	0.21	0.71	0.34	0.72	0.33
5	100	0.66	0.42	0.72	0.33	0.65	0.43	0.64	0.45
6	120	0.61	0.49	0.66	0.42	0.6	0.51	0.57	0.56
7	140	0.57	0.56	0.6	0.51	0.56	0.58	0.51	0.67
8	160	0.53	0.63	0.55	0.60	0.52	0.65	0.47	0.76
9	180	0.49	0.71	0.5	0.69	0.49	0.71	0.42	0.87
10	200	0.46	0.78	0.45	0.80	0.48	0.73	0.39	0.94
11	220	0.43	0.84	0.41	0.89	0.39	0.94	0.36	1.02
12	240	0.4	0.92	0.38	0.97	0.35	1.05	0.32	1.14
13	260					0.3	1.20	0.28	1.27
14	280					0.27	1.31	0.26	1.35
15	300					0.24	1.43	0.24	1.43
16	320					0.21	1.56	0.22	1.51
		T2=	**237.95**	**T2=**	**225.32**	**T2=**	**198.07**	**T2=**	**193.39**

Appendix H: Relationship between T_2 and ethene, 1,1 DCE, PCE and TCE concentration in PVC.

Relationship between T_2 relaxation and ethene concentration

Average T2 178.7 ms
DELTA T2 0 ms
Ethene = 0 µg/ 500 mg PVC

		Trial #1		Trial #2		Trial #3	
Delay	Total echo time (ms)	I	-ln(I/Io)	I	-ln(I/Io)	I	-ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.89	0.12	0.91	0.09	0.90	0.11
3	60	0.78	0.25	0.77	0.26	0.78	0.25
4	80	0.67	0.40	0.67	0.40	0.67	0.40
5	100	0.57	0.56	0.58	0.54	0.58	0.55
6	120	0.50	0.69	0.51	0.67	0.51	0.68
7	140	0.44	0.82	0.45	0.80	0.45	0.81
8	160	0.40	0.92	0.41	0.89	0.41	0.90
9	180	0.37	0.99	0.37	0.99	0.37	0.99
10	200	0.35	1.05	0.33	1.11	0.34	1.08
11	220	0.31	1.17	0.30	1.20	0.31	1.19
12	240	0.28	1.27	0.27	1.31	0.28	1.29
13	260	0.25	1.39	0.24	1.43	0.25	1.41
14	280	0.23	1.47	0.22	1.51	0.23	1.49
15	300	0.20	1.61	0.20	1.61	0.20	1.61
16	320	0.19	1.66	0.18	1.71	0.19	1.69
		T2=	**181.93**	**T2=**	**175.54**	**T2=**	**178.70**

Average T2 **178.9 ms**

DELTA T2 **0 ms**

Ethene = **7 µg/ 500 mg PVC**

		Trial #1		**Trial #2**		**Trial #3**	
Delay	Total echo time (ms)	I	-ln(I/Io)	I	-ln(I/Io)	I	-ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.77	0.26	0.85	0.16	0.82	0.20
3	60	0.68	0.39	0.77	0.26	0.74	0.30
4	80	0.59	0.53	0.67	0.40	0.66	0.42
5	100	0.51	0.67	0.58	0.54	0.58	0.54
6	120	0.44	0.82	0.52	0.65	0.52	0.65
7	140	0.39	0.94	0.46	0.78	0.47	0.76
8	160	0.34	1.08	0.42	0.87	0.42	0.87
9	180	0.31	1.17	0.38	0.97	0.38	0.97
10	200	0.27	1.31	0.34	1.08	0.35	1.05
11	220	0.24	1.43	0.31	1.17	0.32	1.14
12	240	0.22	1.51	0.28	1.27	0.29	1.24
13	260	0.19	1.66	0.25	1.39	0.26	1.35
14	280	0.17	1.77	0.23	1.47	0.24	1.43
15	300	0.16	1.83	0.21	1.56	0.22	1.51
16	320	0.14	1.97	0.19	1.66	0.20	1.61
		T2=	**159.11**	**T2=**	**183.93**	**T2=**	**193.51**

Average T2 **178.0 ms**

DELTA T2 **1 ms**

Ethene = **3.5 µg/ 500 mg PVC**

		Trial #1		**Trial #2**		**Trial #3**	
Delay	Total echo time (ms)	I	-ln(I/Io)	I	-ln(I/Io)	I	-ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.90	0.11	0.88	0.13	0.91	0.09
3	60	0.77	0.26	0.77	0.26	0.79	0.24
4	80	0.67	0.40	0.68	0.39	0.69	0.37
5	100	0.58	0.54	0.59	0.53	0.59	0.53
6	120	0.51	0.67	0.52	0.65	0.53	0.63
7	140	0.45	0.80	0.47	0.76	0.80	0.22
8	160	0.41	0.89	0.42	0.87	0.43	0.84
9	180	0.37	0.99	0.38	0.97	0.38	0.97
10	200	0.34	1.08	0.34	1.08	0.35	1.05
11	220	0.30	1.20	0.31	1.17	0.30	1.20
12	240	0.27	1.31	0.28	1.27	0.28	1.27
13	260	0.24	1.43	0.25	1.39	0.25	1.39
14	280	0.22	1.51	0.23	1.47	0.23	1.47
15	300	0.20	1.61	0.21	1.56	0.21	1.56
16	320	0.18	1.71	0.19	1.66	0.19	1.66
		T2=	**176.07**	**T2=**	**182.04**	**T2=**	**175.82**

Average T2 **167.6 ms**

DELTA T2 **11 ms**

Ethene = **10.5 µg/ 500 mg PVC**

Delay	Total echo time (ms)	Trial #1 I	Trial #1 -ln(I/Io)	Trial #2 I	Trial #2 -ln(I/Io)	Trial #3 I	Trial #3 -ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.82	0.20	0.77	0.26	0.80	0.23
3	60	0.71	0.34	0.67	0.40	0.69	0.37
4	80	0.63	0.46	0.58	0.54	0.61	0.50
5	100	0.56	0.58	0.50	0.69	0.53	0.63
6	120	0.49	0.71	0.44	0.82	0.47	0.77
7	140	0.44	0.82	0.39	0.94	0.42	0.88
8	160	0.40	0.92	0.34	1.08	0.37	0.99
9	180	0.36	1.02	0.30	1.20	0.33	1.11
10	200	0.33	1.11	0.27	1.31	0.30	1.20
11	220	0.30	1.20	0.24	1.43	0.27	1.31
12	240	0.27	1.31	0.22	1.51	0.25	1.41
13	260	0.24	1.43	0.20	1.61	0.22	1.51
14	280	0.22	1.51	0.18	1.71	0.20	1.61
15	300	0.20	1.61	0.16	1.83	0.10	2.30
16	320	0.18	1.71	0.14	1.97	0.16	1.83
		T2=	**183.37**	**T2=**	**161.98**	**T2=**	**157.46**

Average T2 **172.1 ms**

DELTA T2 **7 ms**

Ethene = **14 µg/ 500 mg PVC**

Delay	Total echo time (ms)	Trial #1 I	Trial #1 -ln(I/Io)	Trial #2 I	Trial #2 -ln(I/Io)	Trial #3 I	Trial #3 -ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.78	0.25	0.76	0.27	0.82	0.20
3	60	0.68	0.39	0.66	0.42	0.73	0.31
4	80	0.59	0.53	0.58	0.55	0.65	0.43
5	100	0.52	0.66	0.51	0.68	0.57	0.56
6	120	0.45	0.80	0.45	0.80	0.51	0.67
7	140	0.40	0.92	0.40	0.92	0.46	0.78
8	160	0.36	1.04	0.36	1.04	0.41	0.89
9	180	0.32	1.16	0.32	1.14	0.37	0.99
10	200	0.29	1.26	0.29	1.24	0.34	1.08
11	220	0.26	1.37	0.26	1.35	0.31	1.17
12	240	0.23	1.46	0.23	1.46	0.28	1.27
13	260	0.21	1.56	0.21	1.56	0.25	1.39
14	280	0.19	1.66	0.19	1.66	0.23	1.47
15	300	0.13	2.04	0.14	2.00	0.21	1.56
16	320	0.15	1.90	0.17	1.77	0.19	1.66
		T2=	**160.75**	**T2=**	**167.71**	**T2=**	**187.85**

Relationship between T_2 relaxation and 1,1 DCE concentration

T2 178.6 ms
DELTA T2 0 ms
1,1DCE = 0 µg/ 500 mg PVC

Delay	Total echo time (ms)	Trial #1 I	Trial #1 -ln(I/Io)	Trial #2 I	Trial #2 -ln(I/Io)	Trial #3 I	Trial #3 -ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.90	0.11	0.91	0.09	0.91	0.09
3	60	0.77	0.26	0.77	0.26	0.78	0.25
4	80	0.66	0.42	0.67	0.40	0.67	0.40
5	100	0.54	0.62	0.58	0.54	0.56	0.58
6	120	0.54	0.62	0.51	0.67	0.51	0.68
7	140	0.45	0.80	0.46	0.78	0.45	0.81
8	160	0.41	0.89	0.41	0.89	0.41	0.90
9	180	0.36	1.02	0.37	0.99	0.37	0.99
10	200	0.35	1.05	0.34	1.08	0.34	1.08
11	220	0.31	1.17	0.30	1.20	0.31	1.19
12	240	0.28	1.27	0.27	1.31	0.28	1.29
13	260	0.25	1.39	0.23	1.47	0.24	1.43
14	280	0.23	1.47	0.22	1.51	0.23	1.49
15	300	0.20	1.61	0.20	1.61	0.20	1.61
16	320	0.19	1.66	0.19	1.66	0.18	1.71
		T2 =	**181.94**	**T2 =**	**176.56**	**T2 =**	**177.41**

T2 177.0 ms
DELTA T2 2 ms
1,1DCE = 87 µg/ 500 mg PVC

Delay	Total echo time (ms)	Trial #1 I	Trial #1 -ln(I/Io)	Trial #2 I	Trial #2 -ln(I/Io)	Trial #3 I	Trial #3 -ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.89	0.12	0.91	0.10	0.91	0.10
3	60	0.76	0.27	0.77	0.26	0.77	0.26
4	80	0.67	0.40	0.67	0.41	0.67	0.40
5	100	0.54	0.62	0.58	0.55	0.56	0.58
6	120	0.53	0.63	0.51	0.67	0.50	0.69
7	140	0.45	0.81	0.46	0.79	0.44	0.82
8	160	0.41	0.90	0.41	0.90	0.40	0.91
9	180	0.36	1.04	0.37	1.01	0.37	0.99
10	200	0.34	1.08	0.34	1.08	0.34	1.08
11	220	0.31	1.19	0.30	1.20	0.30	1.20
12	240	0.28	1.29	0.27	1.31	0.27	1.30
13	260	0.25	1.41	0.23	1.47	0.24	1.43
14	280	0.23	1.49	0.22	1.51	0.22	1.50
15	300	0.19	1.66	0.20	1.63	0.20	1.61
16	320	0.19	1.69	0.19	1.69	0.18	1.71
		T2 =	**178.35**	**T2 =**	**175.43**	**T2 =**	**177.24**

T2 **175.9 ms**

DELTA T2 **3 ms**

1,1DCE = **174 µg/ 500 mg PVC**

Delay	Total echo time (ms)	Trial #1 I	Trial #1 -ln(I/Io)	Trial #2 I	Trial #2 -ln(I/Io)	Trial #3 I	Trial #3 -ln(I/Io)
1	20	1	0	1.00	0	1.00	0
2	40	0.88	0.13	0.90	0.11	0.90	0.11
3	60	0.75	0.29	0.77	0.26	0.77	0.26
4	80	0.68	0.39	0.66	0.42	0.67	0.40
5	100	0.54	0.62	0.57	0.56	0.56	0.58
6	120	0.52	0.65	0.51	0.67	0.50	0.69
7	140	0.44	0.82	0.45	0.80	0.44	0.82
8	160	0.40	0.92	0.40	0.92	0.40	0.92
9	180	0.35	1.05	0.36	1.02	0.37	0.99
10	200	0.33	1.11	0.34	1.08	0.34	1.08
11	220	0.30	1.20	0.30	1.20	0.30	1.20
12	240	0.27	1.31	0.27	1.31	0.27	1.31
13	260	0.24	1.43	0.23	1.47	0.24	1.43
14	280	0.22	1.51	0.22	1.51	0.22	1.51
15	300	0.19	1.66	0.19	1.66	0.20	1.61
16	320	0.18	1.71	0.18	1.71	0.18	1.71
		T2 =	**176.37**	**T2 =**	**174.27**	**T2 =**	**177.07**

T2 **171.7 ms**

DELTA T2 **7 ms**

1,1DCE = **261 µg/ 500 mg PVC**

Delay	Total echo time (ms)	Trial #1 I	Trial #1 -ln(I/Io)	Trial #2 I	Trial #2 -ln(I/Io)	Trial #3 I	Trial #3 -ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.86	0.15	0.90	0.11	0.89	0.12
3	60	0.74	0.30	0.76	0.27	0.76	0.27
4	80	0.64	0.45	0.66	0.42	0.66	0.42
5	100	0.54	0.61	0.56	0.59	0.55	0.60
6	120	0.49	0.71	0.51	0.68	0.50	0.69
7	140	0.43	0.84	0.45	0.81	0.44	0.82
8	160	0.39	0.95	0.40	0.92	0.40	0.92
9	180	0.34	1.07	0.36	1.04	0.36	1.02
10	200	0.32	1.15	0.33	1.10	0.33	1.11
11	220	0.28	1.27	0.29	1.23	0.29	1.24
12	240	0.25	1.38	0.26	1.34	0.26	1.35
13	260	0.22	1.51	0.22	1.50	0.23	1.47
14	280	0.21	1.58	0.21	1.56	0.22	1.51
15	300	0.18	1.69	0.19	1.67	0.19	1.66
16	320	0.17	1.80	0.18	1.73	0.17	1.77
		T2 =	**170.43**	**T2 =**	**171.78**	**T2 =**	**172.78**

T2 **161.5 ms**

DELTA T2 **17 ms**

1,1DCE = **348 µg/ 500 mg PVC**

Delay	Total echo time (ms)	Trial #1 I	Trial #1 -ln(I/Io)	Trial #2 I	Trial #2 -ln(I/Io)	Trial #3 I	Trial #3 -ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.87	0.14	0.89	0.12	0.89	0.12
3	60	0.74	0.30	0.76	0.28	0.76	0.27
4	80	0.62	0.48	0.64	0.45	0.65	0.43
5	100	0.52	0.65	0.53	0.63	0.54	0.62
6	120	0.47	0.76	0.51	0.68	0.49	0.71
7	140	0.41	0.89	0.43	0.84	0.43	0.84
8	160	0.36	1.02	0.39	0.95	0.38	0.97
9	180	0.32	1.14	0.34	1.08	0.35	1.05
10	200	0.30	1.20	0.33	1.12	0.32	1.14
11	220	0.26	1.35	0.29	1.26	0.28	1.27
12	240	0.23	1.47	0.26	1.37	0.25	1.39
13	260	0.18	1.71	0.22	1.54	0.21	1.56
14	280	0.17	1.77	0.20	1.61	0.20	1.61
15	300	0.15	1.90	0.18	1.74	0.18	1.71
16	320	0.14	1.97	0.17	1.80	0.16	1.83
		T2 =	**152.16**	**T2 =**	**166.93**	**T2 =**	**165.29**

T2 **156.5 ms**

DELTA T2 **22 ms**

1,1DCE = **870 µg/ 500 mg PVC**

Delay	Total echo time (ms)	Trial #1 I	Trial #1 -ln(I/Io)	Trial #2 I	Trial #2 -ln(I/Io)	Trial #3 I	Trial #3 -ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.79	0.24	0.74	0.30	0.80	0.22
3	60	0.70	0.36	0.66	0.42	0.71	0.34
4	80	0.60	0.51	0.57	0.56	0.62	0.48
5	100	0.51	0.67	0.48	0.73	0.53	0.63
6	120	0.45	0.80	0.42	0.87	0.46	0.78
7	140	0.39	0.94	0.37	0.99	0.40	0.92
8	160	0.35	1.05	0.33	1.11	0.35	1.05
9	180	0.31	1.17	0.29	1.24	0.31	1.17
10	200	0.28	1.27	0.26	1.35	0.28	1.27
11	220	0.25	1.39	0.23	1.47	0.25	1.39
12	240	0.22	1.51	0.21	1.56	0.22	1.51
13	260	0.20	1.61	0.19	1.66	0.20	1.61
14	280	0.18	1.71	0.17	1.77	0.17	1.77
15	300	0.16	1.83	0.14	1.97	0.15	1.90
16	320	0.13	2.04	0.13	2.04	0.14	1.97
		T2 =	**157.90**	**T2 =**	**156.25**	**T2 =**	**155.33**

T2 **137.7 ms**

DELTA T2 **41 ms**

1,1DCE = **1740 µg/ 500 mg PVC**

Delay	Total echo time (ms)	Trial #1 I	Trial #1 -ln(I/Io)	Trial #2 I	Trial #2 -ln(I/Io)	Trial #3 I	Trial #3 -ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.79	0.24	0.79	0.24	0.78	0.25
3	60	0.69	0.37	0.69	0.37	0.68	0.39
4	80	0.59	0.52	0.59	0.53	0.58	0.54
5	100	0.50	0.69	0.50	0.70	0.49	0.71
6	120	0.44	0.83	0.44	0.83	0.42	0.87
7	140	0.38	0.98	0.37	0.99	0.36	1.02
8	160	0.33	1.10	0.33	1.11	0.33	1.11
9	180	0.29	1.23	0.29	1.24	0.27	1.31
10	200	0.26	1.35	0.26	1.36	0.24	1.43
11	220	0.23	1.48	0.22	1.50	0.21	1.58
12	240	0.20	1.63	0.19	1.66	0.17	1.77
13	260	0.17	1.75	0.17	1.78	0.15	1.91
14	280	0.15	1.88	0.15	1.92	0.12	2.09
15	300	0.13	2.04	0.12	2.09		
16	320						
		T2 =	**143.14**	**T2 =**	**140.06**	**T2 =**	**129.87**

DUPLICATE

T2 **141.8 ms**

DELTA T2 **37 ms**

1,1DCE = **1740 µg/ 500 mg PVC**

Delay	Total echo time (ms)	Trial #1 I	Trial #1 -ln(I/Io)	Trial #2 I	Trial #2 -ln(I/Io)	Trial #3 I	Trial #3 -ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.79	0.24	0.79	0.24	0.79	0.24
3	60	0.69	0.37	0.69	0.37	0.69	0.37
4	80	0.59	0.52	0.59	0.53	0.59	0.53
5	100	0.50	0.69	0.50	0.70	0.50	0.69
6	120	0.44	0.83	0.44	0.83	0.44	0.82
7	140	0.38	0.98	0.37	0.99	0.37	0.99
8	160	0.33	1.10	0.33	1.11	0.33	1.11
9	180	0.29	1.23	0.29	1.24	0.29	1.24
10	200	0.26	1.35	0.26	1.36	0.26	1.35
11	220	0.23	1.48	0.22	1.50	0.23	1.47
12	240	0.20	1.63	0.19	1.66	0.19	1.66
13	260	0.17	1.75	0.17	1.78	0.17	1.77
14	280	0.15	1.88	0.15	1.92	0.15	1.90
15	300	0.13	2.04	0.12	2.09	0.13	2.04
16	320						
		T2 =	**143.14**	**T2 =**	**140.06**	**T2 =**	**142.09**

T2 **113.7 ms**

DELTA T2 **65 ms**

1,1DCE = **2610 µg/ 500 mg PVC**

Delay	Total echo time (ms)	Trial #1 I	Trial #1 -ln(I/Io)	Trial #2 I	Trial #2 -ln(I/Io)	Trial #3 I	Trial #3 -ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.77	0.26	0.80	0.22	0.78	0.25
3	60	0.66	0.42	0.66	0.42	0.67	0.40
4	80	0.53	0.63	0.53	0.63	0.55	0.60
5	100	0.43	0.84	0.43	0.84	0.45	0.80
6	120	0.36	1.02	0.37	0.99	0.39	0.94
7	140	0.31	1.17	0.31	1.17	0.33	1.11
8	160	0.27	1.31	0.27	1.31	0.29	1.24
9	180	0.23	1.47	0.23	1.47	0.25	1.39
10	200	0.20	1.61	0.20	1.61	0.22	1.51
11	220	0.17	1.77	0.18	1.71	0.19	1.66
12	240	0.15	1.90	0.15	1.90	0.16	1.83
13	260	0.08	2.53	0.09	2.41	0.11	2.21
14	280						
15	300						
16	320						
		T2 =	**109.57**	**T2 =**	**111.98**	**T2 =**	**119.63**

T2 **116.4 ms**

DELTA T2 **62 ms**

1,1DCE = **3480 µg/ 500 mg PVC**

Delay	Total echo time (ms)	Trial #1 I	Trial #1 -ln(I/Io)	Trial #2 I	Trial #2 -ln(I/Io)	Trial #3 I	Trial #3 -ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.78	0.25	0.79	0.24	0.79	0.24
3	60	0.68	0.39	0.68	0.39	0.67	0.40
4	80	0.56	0.58	0.56	0.58	0.54	0.62
5	100	0.47	0.76	0.46	0.78	0.44	0.82
6	120	0.40	0.92	0.40	0.92	0.38	0.97
7	140	0.34	1.08	0.34	1.08	0.32	1.14
8	160	0.20	1.61	0.30	1.20	0.28	1.27
9	180	0.26	1.35	0.26	1.35	0.24	1.43
10	200	0.23	1.47	0.23	1.47	0.21	1.56
11	220	0.20	1.61	0.20	1.61	0.19	1.66
12	240	0.17	1.77	0.17	1.77	0.16	1.83
13	260	0.13	2.04	0.13	2.04	0.10	2.30
14	280	0.08	2.53	0.07	2.66		
15	300						
16	320						
		T2 =	**117.23**	**T2 =**	**115.21**	**T2 =**	**116.70**

DUPLICATE **T2** **119.5 ms**

DELTA T2 **59 ms**

1,1DCE = **3480 µg/ 500 mg PVC**

Delay	Total echo time (ms)	Trial #1 I	Trial #1 -ln(I/Io)	Trial #2 I	Trial #2 -ln(I/Io)	Trial #3 I	Trial #3 -ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.89	0.12	0.87	0.14	0.79	0.24
3	60	0.72	0.33	0.70	0.36	0.68	0.39
4	80	0.61	0.49	0.58	0.54	0.55	0.60
5	100	0.50	0.69	0.47	0.76	0.45	0.80
6	120	0.42	0.87	0.40	0.92	0.39	0.94
7	140	0.36	1.02	0.34	1.08	0.33	1.11
8	160	0.31	1.17	0.29	1.24	0.29	1.24
9	180	0.62	0.48	0.25	1.39	0.25	1.39
10	200	0.23	1.47	0.22	1.51	0.22	1.51
11	220	0.20	1.61	0.20	1.61	0.20	1.61
12	240	0.18	1.71	0.17	1.77	0.17	1.77
13	260	0.13	2.04	0.12	2.12	0.12	2.12
14	280	0.07	2.66				
15	300						
16	320						
		T2 =	**115.37**	**T2 =**	**119.78**	**T2 =**	**123.31**

T2 **120.2 ms**

DELTA T2 **58 ms**

1,1DCE = **5220 µg/ 500 mg PVC**

Delay	Total echo time (ms)	Trial #1 I	Trial #1 -ln(I/Io)	Trial #2 I	Trial #2 -ln(I/Io)	Trial #3 I	Trial #3 -ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.84	0.17	0.84	0.17	0.78	0.25
3	60	0.70	0.36	0.68	0.39	0.68	0.39
4	80	0.59	0.53	0.57	0.56	0.56	0.58
5	100	0.48	0.73	0.46	0.78	0.46	0.78
6	120	0.41	0.89	0.41	0.89	0.40	0.92
7	140	0.35	1.05	0.35	1.05	0.34	1.08
8	160	0.31	1.17	0.29	1.24	0.25	1.39
9	180	0.44	0.82	0.25	1.39	0.26	1.35
10	200	0.23	1.47	0.22	1.51	0.23	1.47
11	220	0.20	1.61	0.20	1.61	0.20	1.61
12	240	0.18	1.71	0.17	1.77	0.17	1.77
13	260	0.13	2.04	0.12	2.12	0.12	2.12
14	280	0.07	2.66				
15	300						
16	320						
		T2 =	**115.96**	**T2 =**	**121.23**	**T2 =**	**123.33**

Relationship between T_2 relaxation and TCE concentration

T2 178.6 ms
DELTA T2 0 ms
TCE 0 µg/ 500 mg PVC

Delay	Total echo time (ms)	Trial #1 I	Trial #1 -ln(I/Io)	Trial #2 I	Trial #2 -ln(I/Io)	Trial #3 I	Trial #3 -ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.90	0.11	0.91	0.09	0.91	0.09
3	60	0.77	0.26	0.77	0.26	0.78	0.25
4	80	0.66	0.42	0.67	0.40	0.67	0.40
5	100	0.54	0.62	0.58	0.54	0.56	0.58
6	120	0.54	0.62	0.51	0.67	0.51	0.68
7	140	0.45	0.80	0.46	0.78	0.45	0.81
8	160	0.41	0.89	0.41	0.89	0.41	0.90
9	180	0.36	1.02	0.37	0.99	0.37	0.99
10	200	0.35	1.05	0.34	1.08	0.34	1.08
11	220	0.31	1.17	0.30	1.20	0.31	1.19
12	240	0.28	1.27	0.27	1.31	0.28	1.29
13	260	0.25	1.39	0.23	1.47	0.24	1.43
14	280	0.23	1.47	0.22	1.51	0.23	1.49
15	300	0.20	1.61	0.20	1.61	0.20	1.61
16	320	0.19	1.66	0.19	1.66	0.18	1.71
		T2 =	**181.94**	**T2 =**	**176.56**	**T2 =**	**177.41**

T2 177.2 ms
DELTA T2 1 ms
TCE 128 µg/ 500 mg PVC

Delay	Total echo time (ms)	Trial #1 I	Trial #1 -ln(I/Io)	Trial #2 I	Trial #2 -ln(I/Io)	Trial #3 I	Trial #3 -ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.91	0.09	0.91	0.09	0.94	0.06
3	60	0.77	0.26	0.77	0.26	0.82	0.20
4	80	0.67	0.40	0.67	0.40	0.72	0.33
5	100	0.57	0.56	0.58	0.54	0.60	0.51
6	120	0.51	0.67	0.51	0.67	0.54	0.62
7	140	0.45	0.80	0.46	0.78	0.47	0.76
8	160	0.41	0.89	0.41	0.89	0.42	0.87
9	180	0.37	0.99	0.37	0.99	0.38	0.97
10	200	0.34	1.08	0.34	1.08	0.35	1.05
11	220	0.30	1.20	0.30	1.20	0.32	1.14
12	240	0.27	1.31	0.27	1.31	0.28	1.27
13	260	0.24	1.43	0.23	1.47	0.25	1.39
14	280	0.22	1.51	0.22	1.51	0.23	1.47
15	300	0.20	1.61	0.20	1.61	0.21	1.56
16	320	0.19	1.66	0.19	1.66	0.19	1.66
		T2 =	**177.88**	**T2 =**	**176.56**	**T2 =**	**177.00**

T2 **171.3 ms**

DELTA T2 **7 ms**

TCE **256 µg/ 500 mg PVC**

Delay	Total echo time (ms)	Trial #1 I	Trial #1 -ln(I/Io)	Trial #2 I	Trial #2 -ln(I/Io)	Trial #3 I	Trial #3 -ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.90	0.11	0.88	0.13	0.89	0.12
3	60	0.78	0.25	0.75	0.29	0.76	0.27
4	80	0.68	0.39	0.65	0.43	0.65	0.43
5	100	0.57	0.56	0.55	0.60	0.54	0.62
6	120	0.52	0.65	0.50	0.69	0.49	0.71
7	140	0.45	0.80	0.44	0.82	0.43	0.84
8	160	0.40	0.92	0.39	0.94	0.38	0.97
9	180	0.36	1.02	0.35	1.05	0.35	1.05
10	200	0.33	1.11	0.32	1.14	0.32	1.14
11	220	0.30	1.20	0.29	1.24	0.28	1.27
12	240	0.27	1.31	0.26	1.35	0.25	1.39
13	260	0.24	1.43	0.23	1.47	0.22	1.51
14	280	0.22	1.51	0.21	1.56	0.20	1.61
15	300	0.20	1.61	0.19	1.66	0.18	1.71
16	320	0.18	1.71	0.17	1.77	0.16	1.83
		T2 =	**175.29**	**T2 =**	**172.39**	**T2 =**	**166.14**

T2 **171.3 ms**

DELTA T2 **7 ms**

TCE **384 µg/ 500 mg PVC**

Delay	Total echo time (ms)	Trial #1 I	Trial #1 -ln(I/Io)	Trial #2 I	Trial #2 -ln(I/Io)	Trial #3 I	Trial #3 -ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.89	0.12	0.89	0.12	0.90	0.11
3	60	0.77	0.26	0.77	0.26	0.76	0.27
4	80	0.67	0.40	0.66	0.42	0.66	0.42
5	100	0.56	0.58	0.55	0.60	0.55	0.60
6	120	0.51	0.67	0.50	0.69	0.50	0.69
7	140	0.45	0.80	0.44	0.82	0.44	0.82
8	160	0.40	0.92	0.39	0.94	0.39	0.94
9	180	0.36	1.02	0.35	1.05	0.35	1.05
10	200	0.33	1.11	0.32	1.14	0.32	1.14
11	220	0.30	1.20	0.29	1.24	0.29	1.24
12	240	0.27	1.31	0.26	1.35	0.26	1.35
13	260	0.24	1.43	0.23	1.47	0.24	1.45
14	280	0.22	1.51	0.21	1.56	0.21	1.56
15	300	0.20	1.61	0.19	1.66	0.18	1.71
16	320	0.18	1.71	0.17	1.77	0.15	1.90
		T2 =	**176.75**	**T2 =**	**171.14**	**T2 =**	**166.15**

DUPLICATE **T2** **167.2 ms**
DELTA T2 **11 ms** 11

TCE **348 µg/ 500 mg PVC**

Delay	Total echo time (ms)	Trial #1 I	Trial #1 -ln(I/Io)	Trial #2 I	Trial #2 -ln(I/Io)	Trial #3 I	Trial #3 -ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.89	0.12	0.85	0.16	0.83	0.19
3	60	0.77	0.26	0.68	0.39	0.71	0.34
4	80	0.67	0.40	0.59	0.53	0.57	0.56
5	100	0.56	0.58	0.51	0.67	0.48	0.73
6	120	0.51	0.67	0.44	0.82	0.42	0.87
7	140	0.45	0.80	0.39	0.94	0.36	1.02
8	160	0.40	0.92	0.34	1.08	0.32	1.14
9	180	0.36	1.02	0.31	1.17	0.31	1.17
10	200	0.33	1.11	0.27	1.31	0.28	1.27
11	220	0.30	1.20	0.24	1.43	0.25	1.39
12	240	0.27	1.31	0.22	1.51	0.22	1.51
13	260	0.24	1.43	0.19	1.66	0.20	1.61
14	280	0.22	1.51	0.17	1.77	0.19	1.66
15	300	0.20	1.61	0.16	1.83	0.17	1.77
16	320	0.18	1.71	0.14	1.97	0.16	1.83
		T2 =	**176.75**	**T2 =**	**156.75**	**T2 =**	**168.17**

T2 **165.5 ms**
DELTA T2 **13 ms**

TCE **512 µg/ 500 mg PVC**

Delay	Total echo time (ms)	Trial #1 I	Trial #1 -ln(I/Io)	Trial #2 I	Trial #2 -ln(I/Io)	Trial #3 I	Trial #3 -ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.91	0.09	0.77	0.26	0.77	0.26
3	60	0.77	0.26	0.67	0.40	0.68	0.39
4	80	0.67	0.40	0.58	0.54	0.59	0.53
5	100	0.58	0.54	0.50	0.69	0.51	0.67
6	120	0.51	0.67	0.44	0.82	0.44	0.82
7	140	0.45	0.80	0.39	0.94	0.39	0.94
8	160	0.41	0.89	0.34	1.08	0.34	1.08
9	180	0.37	0.99	0.30	1.20	0.31	1.17
10	200	0.33	1.11	0.27	1.31	0.27	1.31
11	220	0.30	1.20	0.24	1.43	0.24	1.43
12	240	0.27	1.31	0.22	1.51	0.22	1.51
13	260	0.24	1.43	0.20	1.61	0.19	1.66
14	280	0.22	1.51	0.18	1.71	0.17	1.77
15	300	0.20	1.61	0.16	1.83	0.16	1.83
16	320	0.18	1.71	0.14	1.97	0.14	1.97
		T2 =	**175.54**	**T2 =**	**161.98**	**T2 =**	**159.11**

DUPLICATE **T2** **166.2 ms**

DELTA T2 **12 ms**

TCE **512 µg/ 500 mg PVC**

Delay	Total echo time (ms)	Trial #1 I	Trial #1 -ln(I/Io)	Trial #2 I	Trial #2 -ln(I/Io)	Trial #3 I	Trial #3 -ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.81	0.21	0.84	0.17	0.81	0.21
3	60	0.70	0.36	0.73	0.31	0.71	0.34
4	80	0.60	0.51	0.63	0.46	0.62	0.48
5	100	0.52	0.65	0.55	0.60	0.53	0.63
6	120	0.46	0.78	0.48	0.73	0.46	0.78
7	140	0.41	0.89	0.42	0.87	0.41	0.89
8	160	0.36	1.02	0.38	0.97	0.36	1.02
9	180	0.32	1.14	0.34	1.08	0.33	1.11
10	200	0.29	1.24	0.30	1.20	0.29	1.24
11	220	0.26	1.35	0.27	1.31	0.26	1.35
12	240	0.23	1.47	0.25	1.39	0.24	1.43
13	260	0.21	1.56	0.22	1.51	0.21	1.56
14	280	0.19	1.66	0.20	1.61	0.19	1.66
15	300	0.17	1.77	0.18	1.71	0.17	1.77
16	320	0.15	1.90	0.16	1.83	0.15	1.90
		T2 =	**165.32**	**T2 =**	**168.44**	**T2 =**	**164.81**

T2 **154.1 ms**

DELTA T2 **25 ms**

TCE **768 µg/ 500 mg PVC**

Delay	Total echo time (ms)	Trial #1 I	Trial #1 -ln(I/Io)	Trial #2 I	Trial #2 -ln(I/Io)	Trial #3 I	Trial #3 -ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.80	0.22	0.83	0.19	0.81	0.21
3	60	0.70	0.36	0.72	0.33	0.71	0.34
4	80	0.60	0.51	0.62	0.48	0.61	0.49
5	100	0.52	0.65	0.54	0.62	0.52	0.65
6	120	0.45	0.80	0.47	0.76	0.46	0.78
7	140	0.40	0.92	0.41	0.89	0.40	0.92
8	160	0.35	1.05	0.37	0.99	0.35	1.05
9	180	0.31	1.17	0.33	1.11	0.32	1.14
10	200	0.28	1.27	0.29	1.24	0.28	1.27
11	220	0.25	1.39	0.26	1.35	0.25	1.39
12	240	0.22	1.51	0.24	1.43	0.23	1.47
13	260	0.20	1.61	0.21	1.56	0.20	1.61
14	280	0.18	1.71	0.19	1.66	0.18	1.71
15	300	0.16	1.83	0.17	1.77	0.16	1.83
16	320	0.11	2.21	0.12	2.12	0.11	2.21
		T2 =	**152.79**	**T2 =**	**157.03**	**T2 =**	**152.39**

DUPLICATE **T2** **157.8 ms**

DELTA T2 **21 ms**

TCE **768 µg/ 500 mg PVC**

		Trial #1		**Trial #2**		**Trial #3**	
Delay	Total echo time (ms)	I	-ln(I/Io)	I	-ln(I/Io)	I	-ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.82	0.20	0.82	0.20	0.79	0.24
3	60	0.71	0.34	0.72	0.33	0.70	0.36
4	80	0.61	0.49	0.62	0.48	0.60	0.51
5	100	0.53	0.63	0.53	0.63	0.52	0.65
6	120	0.46	0.78	0.47	0.76	0.45	0.80
7	140	0.41	0.89	0.41	0.89	0.40	0.92
8	160	0.36	1.02	0.36	1.02	0.35	1.05
9	180	0.32	1.14	0.33	1.11	0.32	1.14
10	200	0.29	1.24	0.29	1.24	0.28	1.27
11	220	0.26	1.35	0.26	1.35	0.25	1.39
12	240	0.23	1.47	0.24	1.43	0.23	1.47
13	260	0.21	1.56	0.21	1.56	0.20	1.61
14	280	0.19	1.66	0.19	1.66	0.18	1.71
15	300	0.17	1.77	0.17	1.77	0.16	1.83
16	320	0.12	2.12	0.12	2.12	0.13	2.04
		T2 =	**157.75**	**T2 =**	**157.61**	**T2 =**	**158.14**

T2 **144.4 ms**

DELTA T2 **34 ms**

TCE **1024 µg/ 500 mg PVC**

		Trial #1		**Trial #2**		**Trial #3**	
Delay	Total echo time (ms)	I	-ln(I/Io)	I	-ln(I/Io)	I	-ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.81	0.21	0.81	0.21	0.79	0.24
3	60	0.70	0.36	0.71	0.34	0.69	0.37
4	80	0.59	0.53	0.60	0.51	0.59	0.53
5	100	0.51	0.67	0.51	0.67	0.50	0.69
6	120	0.44	0.82	0.45	0.80	0.43	0.84
7	140	0.39	0.94	0.39	0.94	0.38	0.97
8	160	0.31	1.17	0.34	1.08	0.33	1.11
9	180	0.30	1.20	0.31	1.17	0.30	1.20
10	200	0.27	1.31	0.27	1.31	0.26	1.35
11	220	0.24	1.43	0.24	1.43	0.23	1.47
12	240	0.21	1.56	0.22	1.51	0.21	1.56
13	260	0.18	1.71	0.18	1.71	0.18	1.71
14	280	0.15	1.90	0.15	1.90	0.14	1.97
15	300						
16	320						
		T2 =	**144.68**	**T2 =**	**145.36**	**T2 =**	**143.04**

T2 **138.5 ms**

DELTA T2 **40 ms**

TCE **1536 µg/ 500 mg PVC**

Delay	Total echo time (ms)	Trial #1 I	Trial #1 -ln(I/Io)	Trial #2 I	Trial #2 -ln(I/Io)	Trial #3 I	Trial #3 -ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.82	0.20	0.82	0.20	0.79	0.24
3	60	0.71	0.34	0.72	0.33	0.70	0.36
4	80	0.60	0.51	0.61	0.49	0.60	0.51
5	100	0.52	0.65	0.52	0.65	0.51	0.67
6	120	0.45	0.80	0.46	0.78	0.44	0.82
7	140	0.40	0.92	0.40	0.92	0.39	0.94
8	160	0.34	1.08	0.35	1.05	0.34	1.08
9	180	0.31	1.17	0.32	1.14	0.31	1.17
10	200	0.28	1.27	0.28	1.27	0.27	1.31
11	220	0.25	1.39	0.25	1.39	0.24	1.43
12	240	0.22	1.51	0.23	1.47	0.22	1.51
13	260	0.20	1.61	0.20	1.61	0.19	1.66
14	280	0.17	1.77	0.17	1.77	0.16	1.83
15	300	0.09	2.41	0.09	2.41	0.08	2.53
16	320						
		T2 =	**139.84**	**T2 =**	**139.94**	**T2 =**	**135.72**

T2 **149.0 ms**

DELTA T2 **30 ms**

TCE **1152 µg/ 500 mg PVC**

Delay	Total echo time (ms)	Trial #1 I	Trial #1 -ln(I/Io)	Trial #2 I	Trial #2 -ln(I/Io)	Trial #3 I	Trial #3 -ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.82	0.20	0.82	0.20	0.79	0.24
3	60	0.71	0.34	0.72	0.33	0.70	0.36
4	80	0.60	0.51	0.61	0.49	0.60	0.51
5	100	0.52	0.65	0.52	0.65	0.51	0.67
6	120	0.45	0.80	0.46	0.78	0.44	0.82
7	140	0.40	0.92	0.40	0.92	0.39	0.94
8	160	0.33	1.11	0.35	1.05	0.34	1.08
9	180	0.31	1.17	0.32	1.14	0.31	1.17
10	200	0.28	1.27	0.28	1.27	0.27	1.31
11	220	0.25	1.39	0.25	1.39	0.24	1.43
12	240	0.22	1.51	0.23	1.47	0.22	1.51
13	260	0.19	1.66	0.19	1.66	0.19	1.66
14	280	0.16	1.83	0.16	1.83	0.15	1.90
15	300						
16	320						
		T2 =	**149.21**	**T2 =**	**149.82**	**T2 =**	**147.88**

Relationship between T_2 relaxation and PCE concentration

T2 178.6 ms
DELTA T2 0 ms
PCE 0 µg/ 500 mg PVC

Delay	Total echo time (ms)	Trial #1 I	Trial #1 -ln(I/Io)	Trial #2 I	Trial #2 -ln(I/Io)	Trial #3 I	Trial #3 -ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.90	0.11	0.91	0.09	0.91	0.09
3	60	0.77	0.26	0.77	0.26	0.78	0.25
4	80	0.66	0.42	0.67	0.40	0.67	0.40
5	100	0.54	0.62	0.58	0.54	0.56	0.58
6	120	0.54	0.62	0.51	0.67	0.51	0.68
7	140	0.45	0.80	0.46	0.78	0.45	0.81
8	160	0.41	0.89	0.41	0.89	0.41	0.90
9	180	0.36	1.02	0.37	0.99	0.37	0.99
10	200	0.35	1.05	0.34	1.08	0.34	1.08
11	220	0.31	1.17	0.30	1.20	0.31	1.19
12	240	0.28	1.27	0.27	1.31	0.28	1.29
13	260	0.25	1.39	0.23	1.47	0.24	1.43
14	280	0.23	1.47	0.22	1.51	0.23	1.49
15	300	0.20	1.61	0.20	1.61	0.20	1.61
16	320	0.19	1.66	0.19	1.66	0.18	1.71
		T2 =	**181.94**	**T2 =**	**176.56**	**T2 =**	**177.41**

T2 182.3 ms
DELTA T2 -4 ms
PCE 15 µg/ 500 mg PVC

Delay	Total echo time (ms)	Trial #1 I	Trial #1 -ln(I/Io)	Trial #2 I	Trial #2 -ln(I/Io)	Trial #3 I	Trial #3 -ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.67	0.40	0.89	0.12	0.71	0.34
3	60	0.63	0.46	0.74	0.30	0.65	0.43
4	80	0.56	0.58	0.65	0.43	0.57	0.56
5	100	0.49	0.71	0.56	0.58	0.49	0.71
6	120	0.43	0.84	0.49	0.71	0.43	0.84
7	140	0.39	0.94	0.43	0.84	0.39	0.94
8	160	0.36	1.02	0.39	0.94	0.35	1.05
9	180	0.33	1.11	0.35	1.05	0.31	1.17
10	200	0.30	1.20	0.32	1.14	0.28	1.27
11	220	0.28	1.27	0.28	1.27	0.25	1.39
12	240	0.25	1.39	0.26	1.35	0.23	1.47
13	260	0.23	1.47	0.23	1.47	0.21	1.56
14	280	0.22	1.51	0.21	1.56	0.19	1.66
15	300	0.20	1.61	0.19	1.66	0.17	1.77
16	320	0.18	1.71	0.18	1.71	0.16	1.83
		T2 =	**197.82**	**T2 =**	**173.99**	**T2 =**	**175.01**

T2 **184.0 ms**

DELTA T2 **-5 ms**

PCE **30 µg/ 500 mg PVC**

Delay	Total echo time (ms)	Trial #1 I	Trial #1 -ln(I/Io)	Trial #2 I	Trial #2 -ln(I/Io)	Trial #3 I	Trial #3 -ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.93	0.07	0.75	0.29	0.74	0.30
3	60	0.81	0.21	0.67	0.40	0.67	0.40
4	80	0.70	0.36	0.58	0.54	0.59	0.53
5	100	0.61	0.49	0.51	0.67	0.50	0.69
6	120	0.54	0.62	0.46	0.78	0.44	0.82
7	140	0.48	0.73	0.41	0.89	0.39	0.94
8	160	0.44	0.82	0.37	0.99	0.36	1.02
9	180	0.39	0.94	0.33	1.11	0.32	1.14
10	200	0.36	1.02	0.30	1.20	0.29	1.24
11	220	0.33	1.11	0.27	1.31	0.26	1.35
12	240	0.29	1.24	0.25	1.39	0.24	1.43
13	260	0.27	1.31	0.23	1.47	0.22	1.51
14	280	0.25	1.39	0.21	1.56	0.20	1.61
15	300	0.23	1.47	0.19	1.66	0.18	1.71
16	320	0.21	1.56	0.17	1.77	0.17	1.77
		T2 =	**189.60**	**T2 =**	**183.24**	**T2 =**	**179.16**

T2 **185.2 ms**

DELTA T2 **-7 ms**

PCE **45 µg/ 500 mg PVC**

Delay	Total echo time (ms)	Trial #1 I	Trial #1 -ln(I/Io)	Trial #2 I	Trial #2 -ln(I/Io)	Trial #3 I	Trial #3 -ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.74	0.30	0.84	0.17	0.71	0.34
3	60	0.71	0.34	0.77	0.26	0.65	0.43
4	80	0.63	0.46	0.68	0.39	0.57	0.56
5	100	0.55	0.60	0.58	0.54	0.49	0.71
6	120	0.48	0.73	0.52	0.65	0.43	0.84
7	140	0.42	0.87	0.47	0.76	0.38	0.97
8	160	0.38	0.97	0.42	0.87	0.35	1.05
9	180	0.34	1.08	0.38	0.97	0.31	1.17
10	200	0.31	1.17	0.35	1.05	0.28	1.27
11	220	0.28	1.27	0.32	1.14	0.25	1.39
12	240	0.26	1.35	0.29	1.24	0.23	1.47
13	260	0.24	1.43	0.26	1.35	0.21	1.56
14	280	0.22	1.51	0.24	1.43	0.19	1.66
15	300	0.20	1.61	0.22	1.51	0.17	1.77
16	320	0.19	1.66	0.21	1.56	0.16	1.83
		T2 =	**187.70**	**T2 =**	**192.73**	**T2 =**	**175.19**

T2 **188.9 ms**

DELTA T2 **-10 ms**

PCE **60 µg/ 500 mg PVC**

Delay	Total echo time (ms)	Trial #1 I	Trial #1 -ln(I/Io)	Trial #2 I	Trial #2 -ln(I/Io)	Trial #3 I	Trial #3 -ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.74	0.30	0.73	0.31	0.71	0.34
3	60	0.65	0.43	0.69	0.37	0.65	0.43
4	80	0.58	0.54	0.61	0.49	0.57	0.56
5	100	0.51	0.67	0.52	0.65	0.48	0.73
6	120	0.45	0.80	0.46	0.78	0.43	0.84
7	140	0.42	0.87	0.42	0.87	0.38	0.97
8	160	0.39	0.94	0.38	0.97	0.34	1.08
9	180	0.36	1.02	0.34	1.08	0.31	1.17
10	200	0.33	1.11	0.31	1.17	0.28	1.27
11	220	0.30	1.20	0.28	1.27	0.25	1.39
12	240	0.28	1.27	0.25	1.39	0.23	1.47
13	260	0.26	1.35	0.23	1.47	0.21	1.56
14	280	0.24	1.43	0.21	1.56	0.19	1.66
15	300	0.22	1.51	0.19	1.66	0.17	1.77
16	320	0.20	1.61	0.18	1.71	0.15	1.90
		T2 =	**208.85**	**T2 =**	**184.49**	**T2 =**	**173.41**

DUPLICATE

T2 **172.9 ms**

DELTA T2 **6 ms**

PCE **60 µg/ 500 mg PVC**

Delay	Total echo time (ms)	Trial #1 I	Trial #1 -ln(I/Io)	Trial #2 I	Trial #2 -ln(I/Io)	Trial #3 I	Trial #3 -ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.93	0.07	0.93	0.07	0.77	0.26
3	60	0.77	0.26	0.77	0.26	0.68	0.39
4	80	0.67	0.40	0.67	0.40	0.59	0.53
5	100	0.58	0.54	0.58	0.54	0.51	0.67
6	120	0.52	0.65	0.52	0.65	0.44	0.82
7	140	0.46	0.78	0.46	0.78	0.39	0.94
8	160	0.42	0.87	0.42	0.87	0.34	1.08
9	180	0.38	0.97	0.38	0.97	0.31	1.17
10	200	0.35	1.05	0.35	1.05	0.27	1.31
11	220	0.31	1.17	0.31	1.17	0.24	1.43
12	240	0.28	1.27	0.28	1.27	0.22	1.51
13	260	0.26	1.35	0.26	1.35	0.19	1.66
14	280	0.24	1.43	0.24	1.43	0.17	1.77
15	300	0.20	1.61	0.20	1.61	0.16	1.83
16	320	0.18	1.71	0.18	1.71	0.14	1.97
		T2 =	**179.78**	**T2 =**	**179.78**	**T2 =**	**159.11**

T2 **185.9 ms**

DELTA T2 **-7 ms**

PCE **90 µg/ 500 mg PVC**

		Trial #1		**Trial #2**		**Trial #3**	
Delay	Total echo time (ms)	I	-ln(I/Io)	I	-ln(I/Io)	I	-ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.84	0.17	0.80	0.22	0.73	0.31
3	60	0.76	0.27	0.72	0.33	0.66	0.42
4	80	0.67	0.40	0.63	0.46	0.58	0.54
5	100	0.58	0.54	0.55	0.60	0.50	0.69
6	120	0.51	0.67	0.49	0.71	0.44	0.82
7	140	0.45	0.80	0.44	0.82	0.39	0.94
8	160	0.41	0.89	0.40	0.92	0.36	1.02
9	180	0.37	0.99	0.36	1.02	0.32	1.14
10	200	0.34	1.08	0.33	1.11	0.20	1.61
11	220	0.31	1.17	0.30	1.20	0.26	1.35
12	240	0.28	1.27	0.27	1.31	0.23	1.47
13	260	0.26	1.35	0.25	1.39	0.22	1.51
14	280	0.24	1.43	0.23	1.47	0.20	1.61
15	300	0.22	1.51	0.21	1.56	0.18	1.71
16	320	0.20	1.61	0.19	1.66	0.17	1.77
		T2 =	**190.78**	**T2 =**	**190.02**	**T2 =**	**177.02**

T2 **168.5 ms**

DELTA T2 **10 ms**

PCE **120 µg/ 500 mg PVC**

		Trial #1		**Trial #2**		**Trial #3**	
Delay	Total echo time (ms)	I	-ln(I/Io)	I	-ln(I/Io)	I	-ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.82	0.20	0.82	0.20	0.77	0.26
3	60	0.73	0.31	0.72	0.33	0.90	0.11
4	80	0.64	0.45	0.63	0.46	0.60	0.51
5	100	0.55	0.60	0.55	0.60	0.51	0.67
6	120	0.48	0.73	0.48	0.73	0.45	0.80
7	140	0.43	0.84	0.43	0.84	0.40	0.92
8	160	0.38	0.97	0.39	0.94	0.36	1.02
9	180	0.34	1.08	0.35	1.05	0.32	1.14
10	200	0.31	1.17	0.31	1.17	0.24	1.43
11	220	0.28	1.27	0.28	1.27	0.26	1.35
12	240	0.25	1.39	0.26	1.35	0.23	1.47
13	260	0.23	1.47	0.23	1.47	0.21	1.56
14	280	0.21	1.56	0.21	1.56	0.19	1.66
15	300	0.19	1.66	0.19	1.66	0.17	1.77
16	320	0.16	1.83	0.16	1.83	0.14	1.97
		T2 =	**172.76**	**T2 =**	**174.02**	**T2 =**	**158.78**

T2 **159.5 ms**

DELTA T2 **19 ms**

PCE **500 µg/ 500 mg PVC**

		Trial #1		**Trial #2**		**Trial #3**	
Delay	Total echo time (ms)	I	-ln(I/Io)	I	-ln(I/Io)	I	-ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.82	0.20	0.82	0.20	0.81	0.21
3	60	0.72	0.33	0.72	0.33	0.71	0.34
4	80	0.62	0.48	0.62	0.48	0.62	0.48
5	100	0.54	0.62	0.54	0.62	0.54	0.62
6	120	0.47	0.76	0.47	0.76	0.47	0.76
7	140	0.42	0.87	0.42	0.87	0.42	0.87
8	160	0.37	0.99	0.38	0.97	0.38	0.97
9	180	0.34	1.08	0.34	1.08	0.34	1.08
10	200	0.30	1.20	0.30	1.20	0.30	1.20
11	220	0.27	1.31	0.27	1.31	0.27	1.31
12	240	0.25	1.39	0.25	1.39	0.25	1.39
13	260	0.22	1.51	0.22	1.51	0.22	1.51
14	280	0.20	1.61	0.20	1.61	0.20	1.61
15	300	0.15	1.90	0.15	1.90	0.15	1.90
16	320	0.13	2.04	0.13	2.04	0.13	2.04
		T2 =	**159.33**	**T2 =**	**159.28**	**T2 =**	**159.87**

T2 **151.9 ms**

DELTA T2 **27 ms**

PCE **680 µg/ 500 mg PVC**

		Trial #1		**Trial #2**		**Trial #3**	
Delay	Total echo time (ms)	I	-ln(I/Io)	I	-ln(I/Io)	I	-ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.82	0.20	0.82	0.20	0.80	0.22
3	60	0.72	0.33	0.72	0.33	0.71	0.34
4	80	0.61	0.49	0.62	0.48	0.61	0.49
5	100	0.53	0.63	0.53	0.63	0.53	0.63
6	120	0.46	0.78	0.47	0.76	0.46	0.78
7	140	0.41	0.89	0.41	0.89	0.41	0.89
8	160	0.36	1.02	0.37	0.99	0.36	1.02
9	180	0.33	1.11	0.33	1.11	0.33	1.11
10	200	0.29	1.24	0.29	1.24	0.29	1.24
11	220	0.26	1.35	0.26	1.35	0.26	1.35
12	240	0.24	1.43	0.24	1.43	0.24	1.43
13	260	0.21	1.56	0.21	1.56	0.21	1.56
14	280	0.19	1.66	0.19	1.66	0.18	1.71
15	300	0.12	2.12	0.12	2.12	0.12	2.12
16	320						
		T2 =	**152.24**	**T2 =**	**151.79**	**T2 =**	**151.80**

T2 **145.3 ms**

DELTA T2 **33 ms**

PCE **800 µg/ 500 mg PVC**

		Trial #1		**Trial #2**		**Trial #3**	
Delay	Total echo time (ms)	I	-ln(I/Io)	I	-ln(I/Io)	I	-ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.82	0.20	0.82	0.20	0.80	0.22
3	60	0.72	0.33	0.72	0.33	0.71	0.34
4	80	0.61	0.49	0.62	0.48	0.61	0.49
5	100	0.53	0.63	0.53	0.63	0.52	0.65
6	120	0.46	0.78	0.47	0.76	0.45	0.80
7	140	0.41	0.89	0.41	0.89	0.40	0.92
8	160	0.35	1.05	0.36	1.02	0.35	1.05
9	180	0.32	1.14	0.33	1.11	0.32	1.14
10	200	0.29	1.24	0.29	1.24	0.28	1.27
11	220	0.26	1.35	0.26	1.35	0.25	1.39
12	240	0.23	1.47	0.24	1.43	0.23	1.47
13	260	0.20	1.61	0.20	1.61	0.20	1.61
14	280	0.18	1.71	0.18	1.71	0.17	1.77
15	300			0.09	2.41	0.08	2.53
16	320						
		T2 =	**156.05**	**T2 =**	**141.87**	**T2 =**	**138.00**

T2 **148.1 ms**

DELTA T2 **30 ms**

PCE **900 µg/ 500 mg PVC**

		Trial #1		**Trial #2**		**Trial #3**	
Delay	Total echo time (ms)	I	-ln(I/Io)	I	-ln(I/Io)	I	-ln(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.81	0.21	0.82	0.20	0.80	0.22
3	60	0.72	0.33	0.72	0.33	0.71	0.34
4	80	0.62	0.48	0.62	0.48	0.61	0.49
5	100	0.53	0.63	0.53	0.63	0.53	0.63
6	120	0.46	0.78	0.47	0.76	0.45	0.80
7	140	0.41	0.89	0.41	0.89	0.40	0.92
8	160	0.36	1.02	0.36	1.02	0.35	1.05
9	180	0.33	1.11	0.33	1.11	0.32	1.14
10	200	0.29	1.24	0.29	1.24	0.28	1.27
11	220	0.26	1.35	0.26	1.35	0.25	1.39
12	240	0.24	1.43	0.24	1.43	0.23	1.47
13	260	0.20	1.61	0.20	1.61	0.20	1.61
14	280	0.18	1.71	0.18	1.71	0.17	1.77
15	300	0.09	2.41	0.13	2.04	0.13	2.04
16	320						
		T2 =	**142.29**	**T2 =**	**151.76**	**T2 =**	**150.39**

Appendix I: Relationship between T_2 and $FeSO_4$, Mn(III) acac, and $NaMnO_4$.

Mn(III) Acac

		10 mg/L		5 mg/L		1 mg/L		0.5 mg/L		0.1 mg/L	
Delay	Echo time (ms)	I	-LN(I/Io)	I	-LN(I/Io)	I	-LN(I/Io)	I	-LN(I/Io)	I	-LN(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.67	0.40	0.79	0.24	0.80	0.22	0.85	0.16	0.89	0.12
3	60	0.57	0.56	0.67	0.40	0.67	0.40	0.73	0.31	0.78	0.25
4	80	0.48	0.73	0.57	0.56	0.60	0.51	0.65	0.44	0.69	0.37
5	100	0.40	0.92	0.48	0.73	0.53	0.63	0.57	0.56	0.61	0.49
6	120	0.32	1.14	0.41	0.89	0.47	0.76	0.53	0.64	0.56	0.58
7	140	0.27	1.31	0.35	1.05	0.41	0.89	0.46	0.78	0.51	0.67
8	160	0.22	1.51	0.30	1.20	0.37	0.99	0.42	0.87	0.47	0.76
9	180	0.18	1.71	0.26	1.35	0.34	1.08	0.39	0.95	0.43	0.84
10	200	0.15	1.90	0.23	1.47	0.30	1.20	0.35	1.06	0.39	0.94
11	220	0.12	2.12	0.20	1.61	0.27	1.31	0.32	1.14	0.36	1.02
12	240	0.10	2.30	0.17	1.77	0.24	1.43	0.29	1.26	0.33	1.11
13	260	0.09	2.41	0.15	1.90	0.22	1.51	0.27	1.33	0.31	1.17
14	280	0.07	2.66	0.13	2.04	0.20	1.61	0.24	1.43	0.28	1.27
15	300	0.06	2.81	0.12	2.12	0.18	1.71	0.22	1.51	0.26	1.35
16	320	0.05	3.00	0.10	2.30	0.17	1.77	0.21	1.56	0.24	1.43
		T2=	**103.81**	**T2=**	**134.19**	**T2=**	**175.17**	**T2=**	**195.68**	**T2=**	**214.93**

Fe_2SO_4

Delay	Echo time (ms)	11.24 mg/L		5.62 mg/L		1.124 mg/L		0.1124 mg/L		0.01124 mg/L	
		I	-LN(I/Io)	I	-LN(I/Io)	I	-LN(I/Io)	I	-LN(I/Io)	I	-LN(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00	1.00	0.00
2	40	0.79	0.24			0.85	0.16	0.81	0.21	0.83	0.19
3	60	0.68	0.39	0.67	0.40	0.71	0.34	0.69	0.37	0.69	0.37
4	80	0.61	0.49	0.62	0.48	0.63	0.46	0.62	0.48	0.62	0.48
5	100	0.55	0.60	0.55	0.60	0.55	0.60	0.55	0.60	0.54	0.62
6	120	0.50	0.69	0.49	0.71	0.50	0.69	0.49	0.71	0.49	0.71
7	140	0.46	0.78	0.45	0.80	0.46	0.78	0.46	0.78	0.45	0.80
8	160	0.42	0.87	0.41	0.89	0.42	0.87	0.41	0.89	0.41	0.89
9	180	0.39	0.94	0.37	0.99	0.39	0.94	0.37	0.99	0.38	0.97
10	200	0.36	1.02	0.34	1.08	0.36	1.02	0.34	1.08	0.34	1.08
11	220	0.33	1.11	0.31	1.17	0.33	1.11	0.31	1.17	0.31	1.17
12	240	0.30	1.20	0.28	1.27	0.30	1.20	0.29	1.24	0.28	1.27
13	260	0.28	1.27	0.26	1.35	0.28	1.27	0.26	1.35	0.25	1.39
14	280	0.25	1.39	0.24	1.43	0.26	1.35	0.24	1.43	0.24	1.43
15	300	0.23	1.47	0.22	1.51	0.24	1.43	0.23	1.47	0.22	1.51
16	320	0.22	1.51	0.21	1.56	0.22	1.51	0.21	1.56	0.20	1.61
			212.84		**204.04**		**210.43**		**203.01**		**197.11**

MnO_4^-

Delay	Echo time (ms)	10.43 mg/L I	10.43 mg/L -LN(I/Io)	5.215 mg/L I	5.215 mg/L -LN(I/Io)	1.043 mg/L I	1.043 mg/L -LN(I/Io)	0.1043 mg/L I	0.1043 mg/L -LN(I/Io)	0.01043 mg/L I	0.01043 mg/L -LN(I/Io)
1	20	1.00	0.00	1.00	0.00	1.00	0.00	1.10	-0.10	0.78	0.25
2	40					0.87	0.14			0.82	0.20
3	60			0.73	0.31	0.73	0.31	0.69	0.37	0.68	0.39
4	80	0.61	0.49	0.65	0.43	0.64	0.45	0.62	0.48	0.59	0.53
5	100	0.55	0.60	0.57	0.56	0.58	0.54	0.56	0.58	0.53	0.63
6	120	0.50	0.69	0.51	0.67	0.52	0.65	0.50	0.69	0.48	0.73
7	140	0.45	0.80	0.47	0.76	0.48	0.73	0.46	0.78	0.44	0.82
8	160	0.42	0.87	0.44	0.82	0.44	0.82	0.48	0.73	0.41	0.89
9	180	0.38	0.97	0.40	0.92	0.42	0.87	0.40	0.92	0.38	0.97
10	200	0.35	1.05	0.37	0.99	0.38	0.97	0.37	0.99	0.35	1.05
11	220	0.33	1.11	0.34	1.08	0.35	1.05	0.35	1.05	0.32	1.14
12	240	0.30	1.20	0.31	1.17	0.33	1.11	0.32	1.14	0.29	1.24
13	260	0.28	1.27	0.29	1.24	0.30	1.20	0.29	1.24	0.27	1.31
14	280	0.25	1.39	0.27	1.31	0.28	1.27	0.27	1.31	0.25	1.39
15	300	0.24	1.43	0.25	1.39	0.26	1.35	0.26	1.35	0.23	1.47
16	320	0.23	1.47	0.24	1.43	0.24	1.43	0.24	1.43	0.21	1.56
			218.14		**220.91**		**222.43**		**223.38**		**222.00**

Appendix J: Relationship between T_2 and PCE and TCE concentration in MnO_4-doped PDMS.

PCE		**0 mg/L PCE**		**Average T2=**	**382 ms**		
		#1		#2		#3	
Delay	Echo time (ms)	I	-ln(I/IO)	I	-ln(I/IO)	I	-ln(I/IO)
1	2	1	0	1	0	1	0
5	10			0.87	0.139262067	0.97	0.03045921
15	30	0.86	0.15082289	0.87	0.139262067	0.92	0.08338161
30	60	0.74	0.30110509	0.74	0.301105093	0.72	0.32850407
45	90	0.68	0.38566248	0.67	0.400477567	0.7	0.35667494
60	120	0.61	0.49429632	0.59	0.527632742	0.61	0.49429632
80	160	0.53	0.63487827	0.52	0.653926467	0.55	0.597837
100	200	0.47	0.75502258	0.47	0.755022584	0.57	0.56211892
125	250	0.42	0.86750057	0.42	0.867500568	0.32	1.13943428
150	300	0.36	1.02165125	0.31	1.171182982	0.35	1.04982212
175	350	0.32	1.13943428	0.3	1.203972804	0.32	1.13943428
200	400	0.29	1.23787436	0.28	1.272965676	0.29	1.23787436
225	450	0.26	1.34707365	0.27	1.30933332	0.25	1.38629436
250	500	0.24	1.42711636	0.25	1.386294361	0.24	1.42711636
275	550	0.22	1.51412773	0.24	1.427116356	0.22	1.51412773
300	600	0.19	1.66073121	0.22	1.514127733	0.21	1.56064775
		T2=	**378.906453**	**T2=**	**397.0882386**	**T2=**	**370.37063**

PCE		**15 mg/L PCE**		**Average T2=**	**349 ms**		
		#1		#2		#3	
Delay	Echo time (ms)	I	-ln(I/IO)	I	-ln(I/IO)	I	-ln(I/IO)
1	2	1	0	1	0	1	0
5	10			0.78	0.248461359	0.92	0.08338161
15	30	0.87	0.13926207	0.74	0.301105093	0.85	0.16251893
30	60	0.78	0.24846136	0.61	0.494296322	0.76	0.27443685
45	90	0.71	0.34249031	0.54	0.616186139	0.71	0.34249031
60	120	0.65	0.43078292	0.5	0.693147181	0.66	0.41551544
80	160	0.58	0.54472718	0.46	0.776528789	0.61	0.49429632
100	200	0.52	0.65392647	0.49	0.713349888	0.56	0.5798185
125	250	0.44	0.82098055	0.42	0.867500568	0.52	0.65392647
150	300	0.4	0.91629073	0.31	1.171182982	0.44	0.82098055
175	350	0.36	1.02165125	0.25	1.386294361	0.38	0.96758403
200	400	0.31	1.17118298	0.25	1.386294361	0.35	1.04982212
225	450	0.26	1.34707365	0.27	1.30933332	0.29	1.23787436
250	500	0.22	1.51412773	0.2	1.609437912	0.24	1.42711636
275	550	0.2	1.60943791	0.15	1.897119985	0.19	1.66073121
300	600	0.17	1.77195684	0.13	2.040220829	0.15	1.89711998
		T2=	**351.529864**	**T2=**	**342.833374**	**T2=**	**353.092572**

PCE **30 mg/L PCE** **Average T2=** **335 ms**

		#1		#2		#3	
Delay	Echo time (ms)	I	-ln(I/IO)	I	-ln(I/IO)	I	-ln(I/IO)
1	2	1	0	1	0	1	0
5	10	0.95	0.05129329	0.99	0.010050336	0.95	0.05129329
15	30	0.9	0.10536052	0.98	0.020202707	0.9	0.10536052
30	60	0.79	0.23572233	0.86	0.15082289	0.79	0.23572233
45	90	0.67	0.40047757	0.71	0.342490309	0.67	0.40047757
60	120	0.57	0.56211892	0.605	0.502526821	0.57	0.56211892
80	160	0.52	0.65392647	0.55	0.597837001	0.52	0.65392647
100	200	0.49	0.71334989	0.53	0.634878272	0.49	0.71334989
125	250	0.46	0.77652879	0.505	0.68319685	0.46	0.77652879
150	300	0.38	0.96758403	0.41	0.891598119	0.38	0.96758403
175	350	0.33	1.10866262	0.36	1.021651248	0.33	1.10866262
200	400	0.3	1.2039728	0.33	1.108662625	0.3	1.2039728
225	450	0.26	1.34707365	0.3	1.203972804	0.26	1.34707365
250	500	0.22	1.51412773	0.255	1.366491734	0.22	1.51412773
275	550	0.17	1.77195684	0.19	1.660731207	0.17	1.77195684
300	600	0.14	1.96611286	0.15	1.897119985	0.14	1.96611286
		T2=	**330.387013**	**T2=**	**344.1295388**	**T2=**	**330.387013**

PCE **45 mg/L PCE** **Average T2=** **272 ms**

		#1		#2		#3	
Delay	Echo time (ms)	I	-ln(I/IO)	I	-ln(I/IO)	I	-ln(I/IO)
1	2	1	0	1	0	1	0
5	10	0.82	0.19845094	0.88	0.127833372	0.86	0.15082289
15	30	0.74	0.30110509	0.81	0.210721031	0.85	0.16251893
30	60	0.63	0.46203546	0.68	0.385662481	0.75	0.28768207
45	90	0.54	0.61618614	0.6	0.510825624	0.66	0.41551544
60	120	0.49	0.71334989	0.51	0.673344553	0.58	0.54472718
80	160	0.41	0.89159812	0.45	0.798507696	0.5	0.69314718
100	200	0.35	1.04982212	0.38	0.967584026	0.48	0.73396918
125	250	0.31	1.17118298	0.32	1.139434283	0.37	0.99425227
150	300	0.25	1.38629436	0.27	1.30933332	0.31	1.17118298
175	350	0.21	1.56064775	0.23	1.46967597	0.26	1.34707365
200	400	0.19	1.66073121	0.19	1.660731207	0.22	1.51412773
225	450	0.14	1.96611286	0.16	1.832581464	0.19	1.66073121
250	500	0.12	2.12026354	0.14	1.966112856	0.16	1.83258146
275	550	0.1	2.30258509	0.12	2.120263536	0.14	1.96611286
300	600	0.08	2.52572864	0.1	2.302585093	0.12	2.12026354
		T2=	**256.75872**	**T2=**	**270.3303201**	**T2=**	**287.460557**

PCE **60 mg/L PCE** **Average T2=** **241 ms**

		#1		#2		#3	
Delay	Echo time (ms)	I	-ln(I/IO)	I	-ln(I/IO)	I	-ln(I/IO)
1	2	1	0	1	0	1	0
5	10	0.84	0.17435339	0.93	0.072570693	0.82	0.19845094
15	30	0.75	0.28768207	0.82	0.198450939	0.74	0.30110509
30	60	0.65	0.43078292	0.72	0.328504067	0.63	0.46203546
45	90	0.54	0.61618614	0.64	0.446287103	0.54	0.61618614
60	120	0.48	0.73396918	0.56	0.579818495	0.49	0.71334989
80	160	0.31	1.17118298	0.47	0.755022584	0.41	0.89159812
100	200	0.25	1.38629436	0.42	0.867500568	0.35	1.04982212
125	250	0.26	1.34707365	0.32	1.139434283	0.31	1.17118298
150	300	0.19	1.66073121	0.26	1.347073648	0.25	1.38629436
175	350	0.17	1.77195684	0.21	1.560647748	0.21	1.56064775
200	400	0.18	1.71479843	0.16	1.832581464	0.19	1.66073121
225	450	0.12	2.12026354	0.13	2.040220829	0.14	1.96611286
250	500	0.11	2.20727491	0.1	2.302585093	0.12	2.12026354
275	550	0.09	2.40794561	0.08	2.525728644	0.1	2.30258509
300	600	0.09	2.40794561	0.05	2.995732274	0.08	2.52572864
		T2=	**251.525992**	**T2=**	**214.9403389**	**T2=**	**256.75872**

TCE **0 mg/L TCE** **Average T2=** **382 ms**

		#1		#2		#3	
Delay	Echo time (ms)	I	-ln(I/IO)	I	-ln(I/IO)	I	-ln(I/IO)
1	2	1.00	0.00	1.00	0.00	1.00	0.00
5	10	0.97	0.03	0.91	0.09	0.94	0.06
15	30	0.83	0.19	0.87	0.14	0.85	0.16
30	60	0.75	0.29	0.74	0.30	0.75	0.29
45	90	0.70	0.36	0.69	0.37	0.70	0.36
60	120	0.67	0.40	0.62	0.48	0.45	0.80
80	160	0.59	0.53	0.53	0.63	0.56	0.58
100	200	0.57	0.56	0.48	0.73	0.53	0.64
125	250	0.47	0.76	0.44	0.82	0.46	0.79
150	300	0.42	0.87	0.37	0.99	0.40	0.93
175	350	0.39	0.94	0.33	1.11	0.36	1.02
200	400	0.36	1.02	0.30	1.20	0.33	1.11
225	450	0.30	1.20	0.27	1.31	0.29	1.26
250	500	0.27	1.31	0.25	1.39	0.26	1.35
275	550	0.22	1.51	0.21	1.56	0.22	1.54
300	600	0.19	1.66	0.17	1.77	0.18	1.71
		T2=	**390.10**	**T2=**	**366.60**	**T2=**	**390.12**

TCE	12.8 mg/L TCE		Average T2=	359 ms			
		#1		#2		#3	
Delay	Echo	I	-ln(I/IO)	I	-ln(I/IO)	I	-ln(I/IO)
1	2	1.00	0.00	1.00	0.00	1.00	0.00
5	10	0.79	0.24	0.92	0.08	0.88	0.13
15	30	0.81	0.21	0.86	0.15	0.84	0.18
30	60	0.71	0.34	0.74	0.30	0.73	0.32
45	90	0.68	0.39	0.68	0.39	0.68	0.39
60	120	0.58	0.54	0.61	0.49	0.60	0.52
80	160	0.54	0.62	0.53	0.63	0.54	0.63
100	200	0.52	0.65	0.47	0.76	0.50	0.70
125	250	0.44	0.82	0.42	0.87	0.43	0.84
150	300	0.40	0.92	0.36	1.02	0.38	0.97
175	350	0.36	1.02	0.32	1.14	0.34	1.08
200	400	0.31	1.17	0.29	1.24	0.30	1.20
225	450	0.26	1.35	0.26	1.35	0.26	1.35
250	500	0.22	1.51	0.24	1.43	0.23	1.47
275	550	0.18	1.71	0.21	1.56	0.20	1.63
300	600	0.15	1.90	0.17	1.77	0.16	1.83
		T2=	**356.47**	**T2=**	**362.08**	**T2=**	**357.99**

TCE	25.6 mg/L TCE		Average T2=	324 ms			
		#1		#2		#3	
Delay	Echo (ms)	I	-ln(I/IO)	I	-ln(I/IO)	I	-ln(I/IO)
1	2	1.00	0.00	1.00	0.00	1.00	0.00
5	10	0.88	0.13	0.86	0.15	0.84	0.17
15	30	0.87	0.14	0.74	0.30	0.73	0.31
30	60	0.78	0.25	0.65	0.43	0.67	0.40
45	90	0.71	0.34	0.58	0.54	0.54	0.62
60	120	0.65	0.43	0.51	0.67	0.53	0.63
80	160	0.58	0.54	0.45	0.80	0.45	0.80
100	200	0.52	0.65	0.42	0.87	0.38	0.97
125	250	0.44	0.82	0.36	1.02	0.36	1.02
150	300	0.40	0.92	0.31	1.17	0.28	1.27
175	350	0.36	1.02	0.24	1.43	0.25	1.39
200	400	0.31	1.17	0.23	1.47	0.23	1.47
225	450	0.26	1.35	0.19	1.66	0.21	1.56
250	500	0.22	1.51	0.16	1.83	0.17	1.77
275	550	0.20	1.61	0.14	1.97	0.15	1.90
300	600	0.17	1.77	0.12	2.12	0.12	2.12
		T2=	**353.24**	**T2=**	**303.83**	**T2=**	**314.72**

TCE	38.4 mg/L TCE			Average T2=	296 ms		
		#1		#2		#3	
Delay	Echo	I	-ln(I/IO)	I	-ln(I/IO)	I	-ln(I/IO)
1	2	1.00	0.00	1.00	0.00	1.00	0.00
5	10	0.86	0.15	0.84	0.17	0.85	0.16
15	30	0.85	0.16	0.74	0.30	0.80	0.23
30	60	0.75	0.29	0.65	0.43	0.70	0.36
45	90	0.66	0.42	0.58	0.54	0.62	0.48
60	120	0.58	0.54	0.51	0.67	0.55	0.61
80	160	0.50	0.69	0.46	0.78	0.48	0.73
100	200	0.48	0.73	0.41	0.89	0.45	0.81
125	250	0.37	0.99	0.36	1.02	0.37	1.01
150	300	0.31	1.17	0.31	1.17	0.31	1.17
175	350	0.26	1.35	0.26	1.35	0.26	1.35
200	400	0.22	1.51	0.23	1.47	0.23	1.49
225	450	0.19	1.66	0.19	1.66	0.19	1.66
250	500	0.16	1.83	0.16	1.83	0.16	1.83
275	550	0.14	1.97	0.14	1.97	0.14	1.97
300	600	0.12	2.12	0.12	2.12	0.12	2.12
		T2=	**287.46**	**T2=**	**305.77**	**T2=**	**296.06**

TCE	51.2 mg/L TCE			Average T2=	276 ms		
		#1		#2		#3	
Delay	Echo	I	-ln(I/IO)	I	-ln(I/IO)	I	-ln(I/IO)
1	2	1.00	0.00	1.00	0.00	1.00	0.00
5	10	0.86	0.15	0.87	0.14	0.86	0.15
15	30	0.77	0.26	0.79	0.24	0.77	0.26
30	60	0.67	0.40	0.70	0.36	0.67	0.40
45	90	0.60	0.51	0.63	0.46	0.60	0.51
60	120	0.51	0.67	0.56	0.58	0.51	0.67
80	160	0.46	0.78	0.49	0.71	0.46	0.78
100	200	0.41	0.89	0.42	0.87	0.41	0.89
125	250	0.35	1.05	0.36	1.02	0.35	1.05
150	300	0.30	1.20	0.30	1.20	0.30	1.20
175	350	0.25	1.39	0.25	1.39	0.25	1.39
200	400	0.21	1.56	0.21	1.56	0.21	1.56
225	450	0.17	1.77	0.18	1.71	0.17	1.77
250	500	0.14	1.97	0.15	1.90	0.14	1.97
275	550	0.12	2.12	0.12	2.12	0.12	2.12
300	600	0.10	2.30	0.10	2.30	0.10	2.30
		T2=	**276.80**	**T2=**	**274.67**	**T2=**	**276.80**