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Resin Longevity Studies

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Cover Photo: CG8 Resins Heated to 37, 53, and 70°C (Left to Right).

Executive Summary

This work is in support of the evaluation of the utility and safe disposal of ^{129}I containing organic waste resins. Portions of the work reported herein have been summarized in an interim report (Powell et al., 2002). All of the conclusions in the interim report are consistent with the additional data presented in this final report.

Waste specific K_d values measured previously (Kaplan et al., 2000; Kaplan and Serkiz, 1999) do not account for potential degradation of these types of resin wastes over an extended period of time. Some degradation due to the high organic composition of the resins would be expected over thousands of years and could lead to additional release of radionuclides. The objective of this study was to carry out laboratory experiments to simulate aging of organic resin wastes in order to determine the functional life span of CG8, GT73 and Dowex 21K resins under field (trench) conditions, and to determine the expected performance of these resins as they degrade. These studies were designed to simulate trench disposal because previous studies

demonstrated that waste specific K_d values were higher under acidic trench conditions than basic cementious disposal conditions (Kaplan et al., 2000; Kaplan and Serkiz, 1999).

In order to estimate the resin degradation rates under subsurface disposal conditions (~18 ° C), accelerated thermal-aging experiments were carried out with the three types of organic resins. In addition to these Arrhenius-type experiments, soil weathering tests designed to evaluate the microbial contribution to degradation were conducted. Relative rates of degradation were measured in terms of total carbon and iodine released from the resin.

An Arrhenius analysis of the total carbon data allowed for calculation of the first order rate constant (k) at subsurface temperature for the degradation of each of the three resins. First order rate constants were used to calculate the percentage of resin that would be released to an 18 ° C groundwater over 10,000 years, a duration of interest to Performance Assessment calculations. Less than 4 % of the resin was calculated to degrade over 10,000 years.

To evaluate the extent that the measured degradation rates (based on total carbon released from the resins) may influence waste disposal at this facility, the K_d values used by Collard (2001) in Special Analyses for the E-Area disposal site were recalculated to account for resin degradation. The resin-degradation-corrected-K_d values (Kd_{rdc}) differed negligibly (<0.0004%) from the original K_d values; well within the uncertainty of the original K_d values. Consequently, there is no need to conduct additional Special Analysis calculations to account for the small effect of resin degradation on enhanced ^{129}I release into the subsurface environment.

As a consequence of these results, Solid Waste has been released to dispose of 74 boxes of legacy resin wastes at SRS instead of repackaging and shipment to the Nevada Test Site (NTS). Onsite disposal in E-Area Low-Level Waste Facility trenches is less expensive than shipment to NTS.

1.0 Introduction

Radioactive resin waste has been generated at the Savannah River Site as a result of water treatment at F- and H-Areas. Key factors in the risk assessment of disposing of these materials in trenches include resin retention of ^{129}I, a long-lived isotope, and the degradation rate of the organic resin itself.

The E-Area Low-Level Waste (LLW) Facility is the site selected to dispose of the low-level radioactive waste generated at SRS during the next 20 years. This facility is located on 200 acres, of which only 100 acres have been developed. The remaining 100 acres will allow for expansion of low-level waste disposal capacity.

Based on recent performance assessment (PA) modeling, ^{129}I is a primary risk driver and constituent limiting the amount of ^{129}I-bearing waste that can be buried in the facility (McDowell-Boyer et al. 2000). Stated in regulatory terms, ^{129}I is a key radionuclide included in the Waste Acceptance Criteria (WAC) at this facility. The performance assessment modeling effort used the distribution coefficient (K_d value) construct to quantify aqueous ^{129}I chemical interactions with the waste and the geological materials. The K_d is defined as the radionuclide concentration in the solid phase divided by the concentration in the aqueous phase. Waste specific K_d values measured previously (Kaplan et al, 2000 and Kaplan and Serkiz, 1999) do not account for potential degradation of these types of resins over an extended period of time. Some degradation due to the high organic composition of the resins would be expected over thousands of years and could lead to additional release of radionuclides.

In order to estimate the degradation of resin wastes during underground burial, simulated aging studies were carried out with Dowex 21K, CG-8, and GT-73 ion exchange resins. These resins have a polystyrene-base but bear different functional groups. The specific resins considered in this study include anion (Dowex 21K), cation (CG8), and neutral (GT73) resins with, respectively, quaternary ammonium, sulfonate, and thiol functionalities.

1.1 Objectives

The objective of this study is to carry out laboratory experiments to simulate aging of organic resin wastes in order to:

1. determine the functional life span of CG8, GT73 and Dowex 21K resins under field (trench) conditions, and
2. determine the expected performance of these resins as they degrade.

1.2 General Approach

Two separate aging studies were designed to simulate trench disposal of the resins.

1. Soil weathering tests in SRS soil.

2. Thermal degradation of the resins in a representative SRS groundwater.

Resins used in both studies were prepared in the same manner by first saturating with a non-radioactive sodium iodide solution to provide a cold simulant of the actual resin wastes containing ^{129}I.

The first study was designed to provide qualitative information regarding the significance of any microbial degradation from microorganisms present in the soil. This microbial contribution to resin degradation was not accounted for in the design of the second more quantitative study. The thermal degradation studies will provide data for an Arrhenius analysis which will allow for calculation of the degradation rate of the resins under disposal conditions (~18 ° C). The two approaches together should provide a basis for evaluating the significance of both abiotic and biotic degradation.

1.2.1 Soil Weathering Tests

Of the two studies the soil weathering experiment most closely simulated actual burial because the resins were directly in contact with soil. Due of the nature of the experiment, it was necessarily a more qualitative experiment due to logistical problems of quantitatively recovering resins and their degradation products directly from soil.

The experiment was designed to enhance degradation of the resins by creating optimal conditions for microbial activity: by increasing the clay content of the soil, by providing a moist environment, and by providing an optimal temperature (30 ° C). Microbial activity is known to be related to the clay content of soil, and microorganisms are expected to thrive in a warm, moist environment.

1.2.2 Thermal-enhanced Degradation Studies

This study takes advantage of the Arrhenius relationship between temperature and rate constant to estimate the degradation of organic resins at subsurface SRS groundwater temperatures (~18 ° C). The rate of organic resin degradation is known to be extremely slow, and slow rates are generally difficult to measure accurately. An Arrhenius approach allows for the determination of the rate of a reaction at the temperature of interest based on measurement of the reaction rates in higher temperature regimes where that rate can be accurately measured. In the work reported herein, degradation of the organic resins in SRS surface water was carried out at a range of temperatures between 37- 87 ° C. Resin performance during degradation was measured as a function of the loss of carbon from the resin and also as a function of the loss of iodide. Results of these studies and Arrhenius treatment of the data are presented herein. A discussion of the Arrhenius equation is given below

1.2.2.1Arrhenius Approach

The rates of most reactions increase as the temperature is increased. The relationship between temperature and rate constant has been empirically observed, and numerous reactions have been shown to have rate constants that follow the Arrhenius equation:

$$\ln k = \ln A - \frac{E_a}{RT} \quad \text{eq 1}$$

where,

k = first order rate constant (1/s),
A = pre-exponential factor (1/mol),
E_a = activation energy (J),
R = gas constant (J/K· mol), and
T = temperature (K).

In reactions that follow the Arrhenius equation (eq 1), a plot of ln$k$ against 1/T gives a straight line (where �E_a/R is the slope and ln$A$ is the y-intercept). Therefore, the Arrhenius equation can be used to calculate the rate of the reaction at any given temperature. Because reactions at lower temperatures are slower, it is often impractical or impossible to measure their rates accurately. Measurement of the rates of the same reaction at a series of higher temperatures allows for the calculation of the activation energy (E_a) and the pre-exponential factor (A) that can be used to calculate the rate of the same reaction at the lower temperature.

2.0 Materials and Methods

Details of the experimental materials and methods for this set of experiments are found in Appendix A. The three resins used in this study, Dowex 21K, CG8, and GT73 were all obtained from the F- and H-areas Groundwater Treatment Facilities (GWTF) or the Effluent Treatment Facility (ETF) at SRS. These resins were "clean" resins not previously used for water treatment.

Uncontaminated resins were used in this study because safety and cost issues prohibited a practical experimental design with radioactive samples.

GT73 resin was filtered to remove excess water prior to use. The resins were treated with a 0.1 M aqueous solution of sodium iodide (50 % resin wt/vol). Resins were agitated on a shaker table for 5 hours and allowed to stand overnight before filtering and rinsing with copious (10 fold excess) amounts of deionized water.

2.1 Soil Weathering Experiment

Details of the experimental setup for this study can be found in Appendix A. Briefly, resins were buried in a surface soil from an SRS forest that had been enriched two-fold in clay. A portion of each resin was buried in a porous polymer mesh for ease of retrieval, and a second portion was in direct contact with the soil. The experiment was carried out in a growth chamber where temperature was maintained at 30 ° C. Rainwater was added to pots containing soil and resins every 4-5 days to maintain moisture. At the end of 8 months the resins were retrieved and analyzed by optical microscopy and elemental or trace microanalysis for iodide.

2.2 Thermal Degradation Experiment

1 L glass bottles were charged with 60 g of air-dried resin and approximately 900 mL of filtered surface water from Upper Three Runs Creek. A control reaction with surface water only was prepared for each temperature. The bottles were loosely capped and placed in ovens at 37, 53, 70 and 87 ° C (Figure 1). Oven temperatures were recorded, and bottles were capped and shaken by hand each working day. A 30 mL aliquot of the aqueous phase was collected for analysis after the first day. For the remaining samples, deionized water was added to replace water lost due to evaporation on the day prior to sampling. 25 mL aliquots were collected after 1, 3, 6, and 10 months. After collecting the final aqueous sample, the resins were filtered and air-dried.

Each aqueous sample was analyzed for total carbon (total inorganic (TIC) plus total organic (TOC) carbon), pH, and iodide by ion selective electrode (ISE). First and last samples were analyzed for major ions by ICP-AES. Iodide analyses by liquid chromatography (LC) and capillary electrophoresis (CE) methods were tested on the initial samples along with ISE. Both LC and CE demonstrated that iodate was not present in solution although both methods suffered from other interferences. Therefore, ISE was ultimately selected as the analytical technique for iodide in the remainder of samples in order to minimize the volume of sample removed.

Resins were analyzed by optical microscopy, thermal gravimetric analysis (TGA), FT-IR, and elemental and trace microanalyses (C, H, N, S, I, and Cl). The moisture content of each resin was measured by using reported methods (Sharma, 1970). CG8 was heated to 105 ° C for 48 hours. Dowex 21K and GT73 were dried in vacuo for 12 hours at 50 ° C.

Figure 1. Experimental Setup at 70° C with GT73, CG8, and Dowex21K Resins and a Control with Water Only.

Total carbon analyses were performed by the SRTC Analytical Development Section (ADS) or UGA Analytical Services. LC and ICP-AES were performed by ADS. Elemental and trace analyses of the resins were carried out by Huffman Laboratories, Golden, CO. All other analyses were performed in house by Waste Processing Technology (WPT).

3.0 Results and Discussion

3.1 Soil Weathering Studies

After about eight months of incubation under ideal microbial growing conditions, no degradation of the surface of the resins was observed by optical microscopy in this more qualitative type of approach. In the case of the Dowex 21K resin the initial resin appeared much darker when compared to the resin recovered from the soil (Figure 2). Presumably, this was due to loss of iodide from the resin. Weathered GT73 resins were indistinguishable from the unweathered (Figure 3). Broken resin beads were observed in both the weathered and unweathered CG8 resins used in this study (Figure 4). A different batch of CG8 resins (used in the thermal degradation studies) contained no broken beads before or after heating.

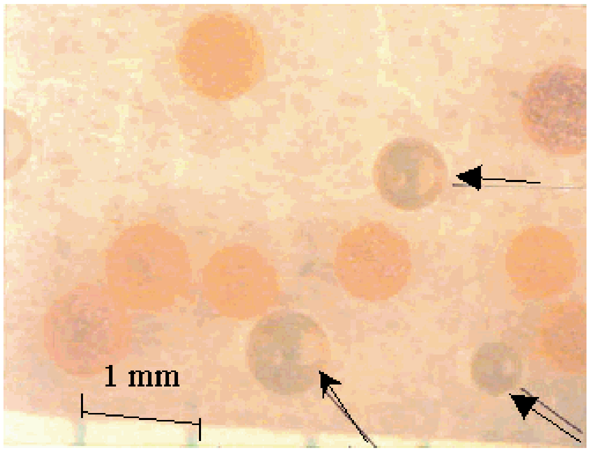


Figure 2. Dowex 21K Resin before (Arrows) and after Soil Weathering 8 Months in Soil at 30° C. Soil is Adhered to the Surface of the Weathered Resins.

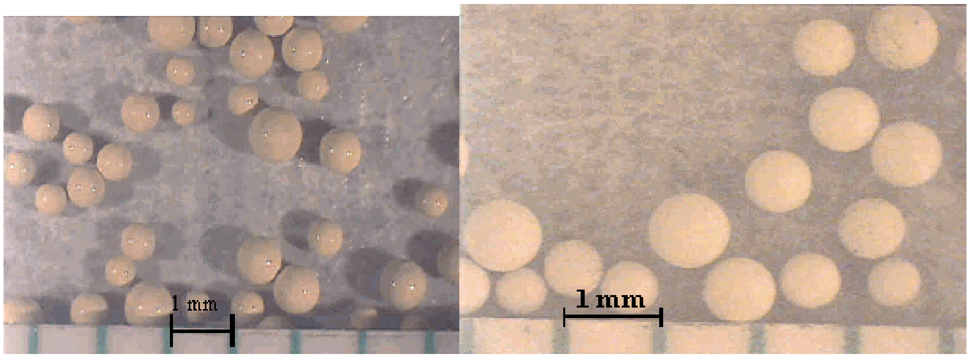


Figure 3. Unweathered (Left) and (Right) Weathered GT73 Resins

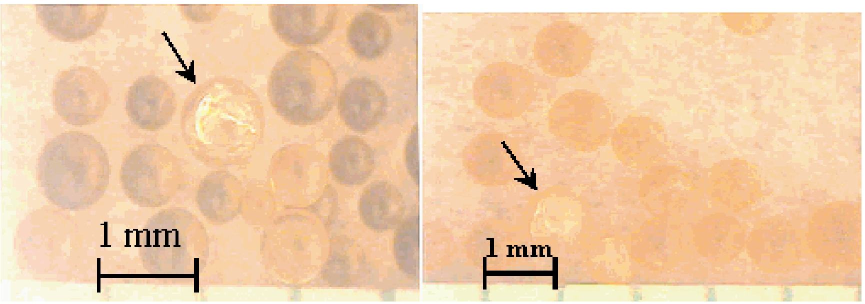
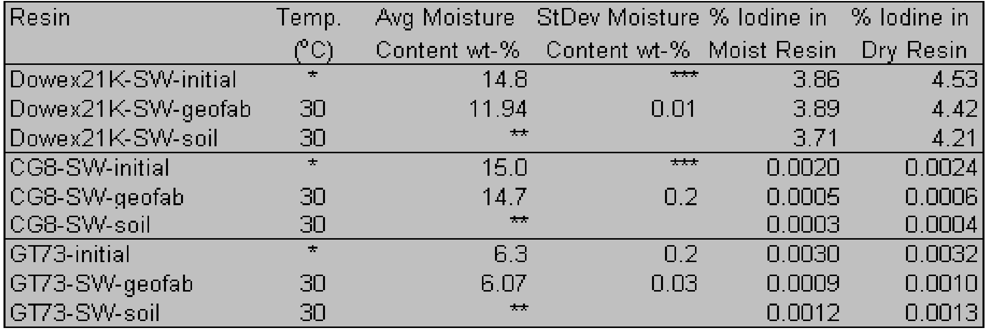


Figure 4. CG8 Resin before (Left) and after (Right) Weathering 8 Months in Soil at 30 ° C. Arrows Point to Broken Resin Spheres.

Elemental and trace microanalyses reveal that the iodine concentration in the Dowex 21K resin (4.53 %) was over a thousand times greater than the loading of the CG8 or GT73 resins (0.0024 % and 0.0032 %, respectively)(Table 1). This high loading is not unexpected in light of the fact that the Dowex 21K is an anionic resin included in the F- and H-Area Ground Water Treatment Unit for the express purpose of removing ^{129}I from the groundwater. The CG8 and the GT73 were included to remove various cations. During the eight month weathering period, the Dowex 21K retained iodide to a greater degree than either the CG8 resin or the GT73 resin, both of which retained less than half of the initial loading. The loss of iodide from the Dowex 21K resin was immeasurable by this technique, i.e., there was no significant difference in the iodide concentration at the start of the experiment and after eight months.

**Table 1. Iodine Concentration in Unweathered and Weathered Resins.
SW-Initial Denotes Unweathered Resins, SW-Geofab and SW-Soil Denote Weathered Resins
Collected from the Geo-Fabric and Directly from the Soil, Respectively.**



Resin	Temp. (°C)	Avg Moisture Content wt-%	StDev Moisture Content wt-%	% Iodine in Moist Resin	% Iodine in Dry Resin
Dowex21K-SW-initial	*	14.8	***	3.86	4.53
Dowex21K-SW-geofab	30	11.94	0.01	3.89	4.42
Dowex21K-SW-soil	30	**		3.71	4.21
CG8-SW-initial	*	15.0	***	0.0020	0.0024
CG8-SW-geofab	30	14.7	0.2	0.0005	0.0006
CG8-SW-soil	30	**		0.0003	0.0004
GT73-initial	*	6.3	0.2	0.0030	0.0032
GT73-SW-geofab	30	6.07	0.03	0.0009	0.0010
GT73-SW-soil	30	**		0.0012	0.0013

*initial air dried resin stored at ambient temperature without further treatment

**insufficient resin recovered for analysis; assumed moisture content equivalent to SW-geofab

***not measured in replicate

3.2 Thermal Degradation of Resins in Groundwater

Visual inspection of the color of the aqueous solution, resin appearance, and solution turbidity (see Figure 5) is indicative that the three resins are not likely exhibiting the same degradation behavior. The CG8 aqueous solution becomes more highly colored with time and increasing temperature than either the Dowex21K or GT73 resins. Note that discoloration of the 87 ° C vessels (far right in each picture) is due to fouling of the PVC safety coating on the outside of the glass and not to observable changes in the aqueous phase.

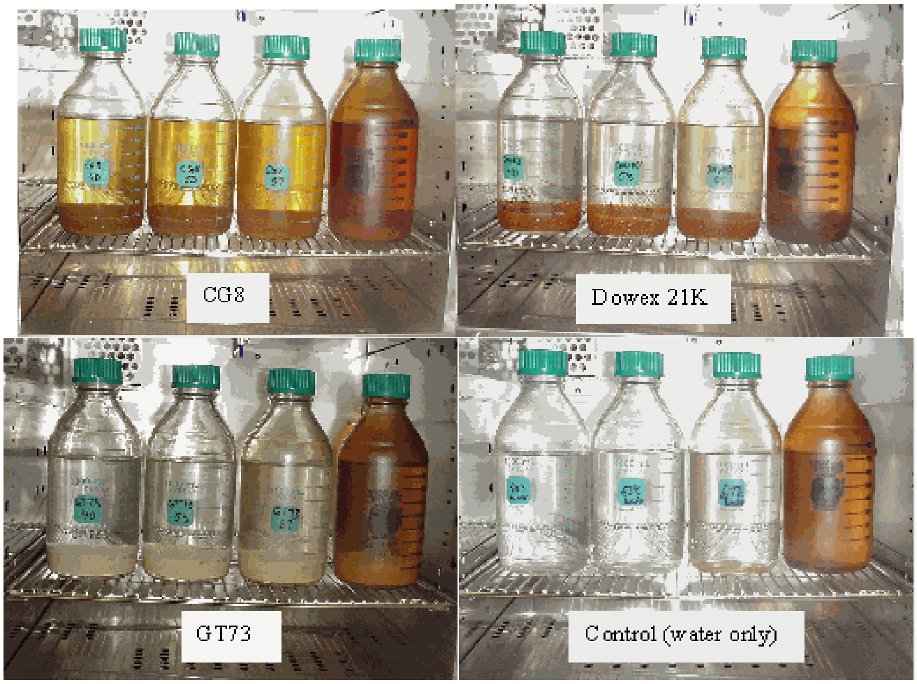


Figure 5. CG8, Dowex 21K, GT73, and Control Experiments (from Left to Right in Each Photo 37, 53, 70, and 87° C Temperatures Grouped Together for Comparison) after Heating for 10 Months.

3.2.1 Resin Degradation as a Function of Total Carbon Released

These visual observations were reflected by the aqueous total carbon data. As measured by total carbon released from the resins, the three resins degraded at measurably different rates as depicted in Figure 6 for the three resins equilibrated at 87 ° C. With the CG8 resin degrading faster than the Dowex21K or GT73 resins.

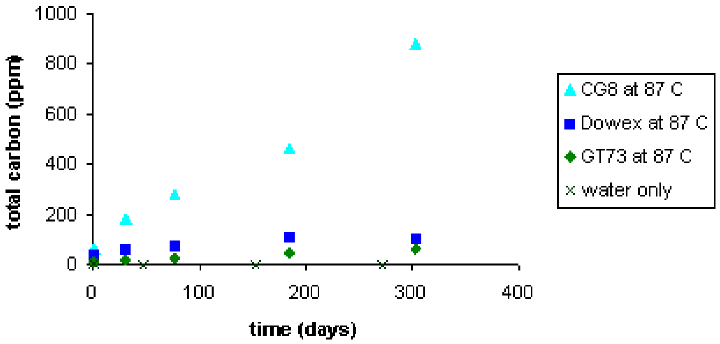


Figure 6. Total Organic Carbon Released from CG8, Dowex and GT 73 Resins into SRS Water at 87 ° C as a Function of Time.

Figure 7 shows total organic carbon released from the CG-8 resin as a function of time and temperature. Increasing slope with increasing temperature indicates a faster degradation rate. The degradation reaction for CG8 appears to follow first order behavior. A plot of $\ln(C/C_o)$ (where C is the resin (solid phase) concentration at a given time and C_o is the initial resin concentration) against time gives a straight line at all experimental temperatures (Figure 8). Rate constants for the degradation of GT73 and Dowex 21K resins were calculated similarly with the exception that for the Dowex 21K resin the first data point (t = 1 day) was not used. This data was omitted because there appeared to be an initial rate for the release of carbon that was at a different rate (faster) than the ultimate rate that was reached after one month and was constant for the duration of the study. One possible explanation for this initial large release of carbon may be that surface bound or carbon in the interstitial waters of the resins may have been initially flushed into the aqueous phase. This carbon likely did not enter the aqueous phase as a result of resin degradation as evidenced by its appearance after only one day and that it occurred at the lower, as well as the higher temperature treatments. Table 2 gives the rate constants for the degradation of each resin at each temperature studied.

According to the Arrhenius equation, a plot of ln *k* against 1/T gives a slope equal to �E_a/R with the intercept at 1/T = 0 equal to ln *A* (eq 1). See Figure 9 for the Arrhenius plot for the CG8 resin. Rate constants (k_{calc}) for the degradation of each resin were calculated using a subsurface temperature of 18.3 ° C (Table 2). The CG8 resin had the largest rate constant of the three.

Using the first order reaction rates calculated from the laboratory data for 18.3 ° C (Table 2), the amount of degradation can be calculated for various amounts of time using eq 2:

$$[A]_t = [A]_0 e^{-kt} \quad \text{eq 2}$$

where:

$[A]_t$ = carbon concentration at time = t,
$[A]_0$ = carbon concentration at time = 0,
k = first order rate constant (1/yr), and
t = time (yr).

For example, for the CG8 resin, the fraction of the resin remaining at t = 10,000 years is 96.13 % corresponding to 3.83 % loss from the resin (see Table 7). This will be discussed later in Sections 0 and 0 which deal with the implications of the findings of these experiments on waste disposal calculations.

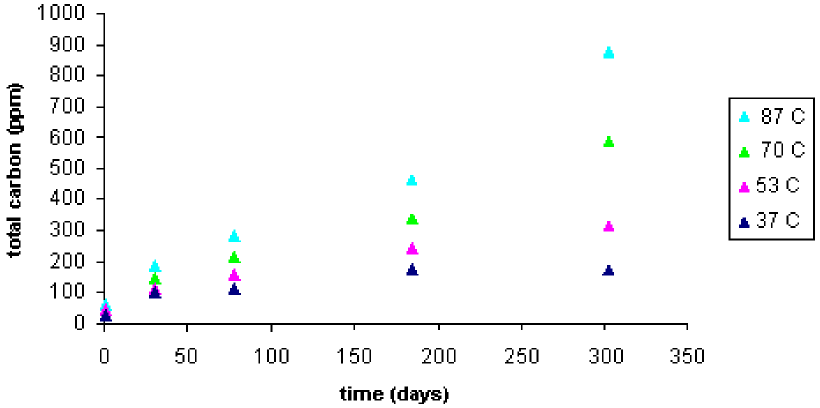


Figure 7. Total Organic Carbon Released into SRS Water from CG8 Resin as a Function of Time at 37, 53, 70, and 87° C Temperatures.

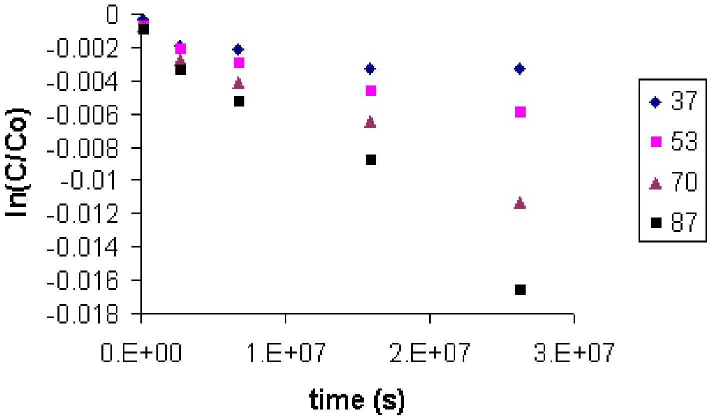


Figure 8. Plot of ln(C/Co) Against Time (s) for the Degradation of CG8 Resin. Slope of each Line Equals -*k* at that Temperature.

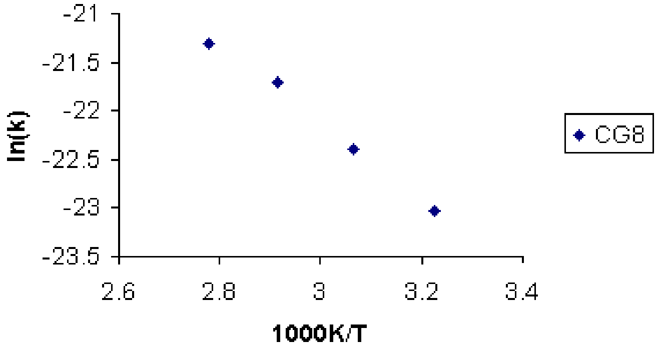
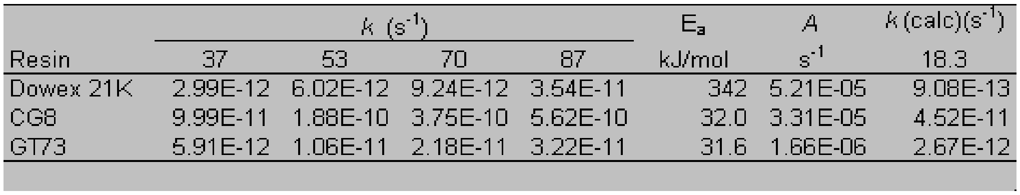


Figure 9. Arrhenius Plot of ln(k) Against 1/T(in Kelvin) for the CG8 Resin.

Table 2. Measured First-Order Rate Constants (*k*), and Calculated Arrhenius Constants: Calculated First-Order Rate

Constants ([*k*(calc)], Activation Energy (E_a), and Pre-Exponential Factor (*A*)).



	k (s^{-1})				E_a	A	k (calc)(s^{-1})
Resin	37	53	70	87	kJ/mol	s^{-1}	18.3
Dowex 21K	2.99E-12	6.02E-12	9.24E-12	3.54E-11	342	5.21E-05	9.08E-13
CG8	9.99E-11	1.88E-10	3.75E-10	5.62E-10	32.0	3.31E-05	4.52E-11
GT73	5.91E-12	1.06E-11	2.18E-11	3.22E-11	31.6	1.66E-06	2.67E-12

3.2.2 Iodide Released

Iodide released from the resin was measured as another indicator of resin performance. It is important to note that the magnitude of iodine release from these resins is *not* expected to be similar to that released from the actual waste resins because the conditions in which these resins were loaded with iodide were entirely different from those at the F- and H- Water Treatment Units. In particular, these resins were loaded to 100% holding capacity by adding high concentrations of NaI. A better measure of the release rate, or more specifically, the I-K_d value can be obtained from the Kd values measured using the actual waste (Kaplan et al. 1999 and Kaplan and Serkiz 2000). However, it was anticipated that the iodide data from these studies will permit some qualitative information about the changes in the ability of the resins to hold iodide as the resins degraded.

Ion selective electrode (ISE) for iodide provided a measurement of aqueous iodide concentration while elemental or trace microanalyses were used to analyze for iodine in all of the Dowex21K resins and the initial CG8 and GT73 resins used in the thermal degradation studies. Figure 10, Figure 11, and Figure 12 present iodide concentration in the resin as a function of time at 37, 53, 70, and 87 ° C. Loss of iodide from the Dowex 21K resin follows first order behavior. Rate constants for this reaction are given in Table 3 along with activation energy, E_a, and the pre-exponential factor, *A,* that follow from an Arrhenius analysis of the rate constants (eq 1). The rate constant, *k,* calculated at 18.3 ° C corresponds to a loss of 7.79 % of the iodine loaded onto the resin after 10,000 years. Comparison with the loss of organic carbon (0.08 % in 10,000 years; Table 7), suggests that a separate or additional mechanisms are present that are controlling the loss of iodine from the resins as compared to the loss of carbon from the resins. This is to be expected based on the anion exchange properties of the Dowex 21K resin.

The CG8 and GT73 resins did not follow first order behavior. For both resins after an initial release of iodide, iodide loss from the resin ceased, and iodide appeared to be reabsorbed by the resin. Clearly, a second mechanism was operable after the initial release. Thus, Arrhenius treatment of these data is not appropriate.

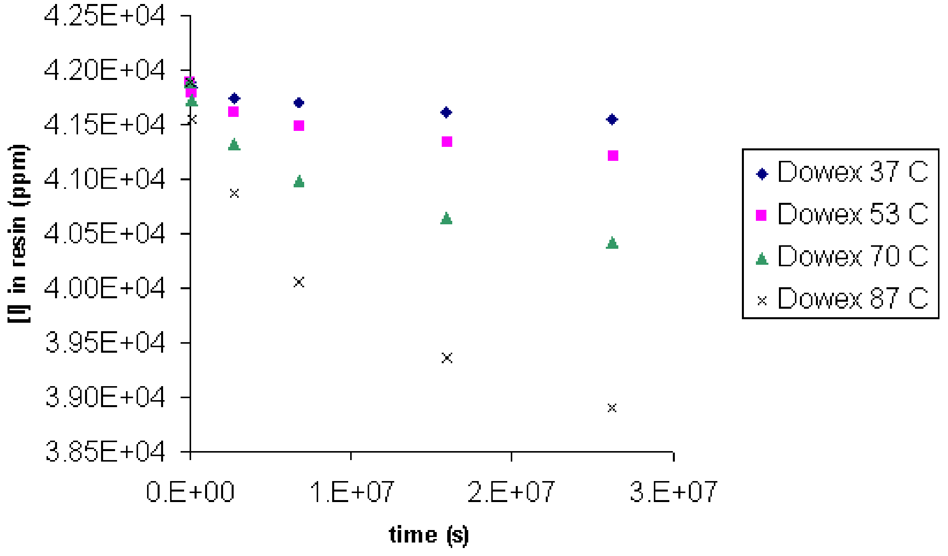


Figure 10. Concentration of Iodide in Dowex 21K as a Function of Time

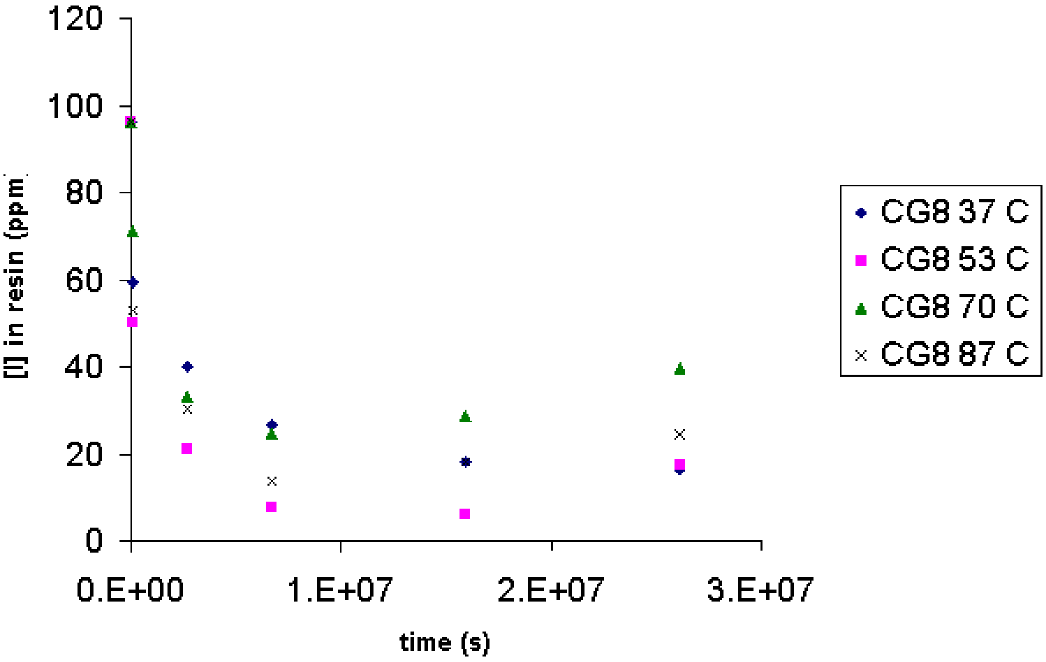


Figure 11. Concentration of Iodide in CG8 as a Function of Time.

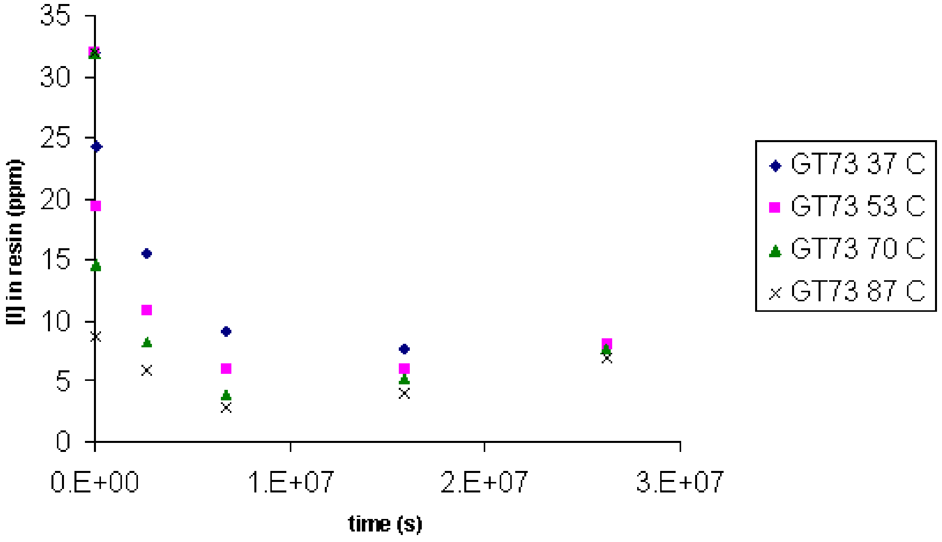


Figure 12. Concentration of Iodide in GT73 as a Function of Time.

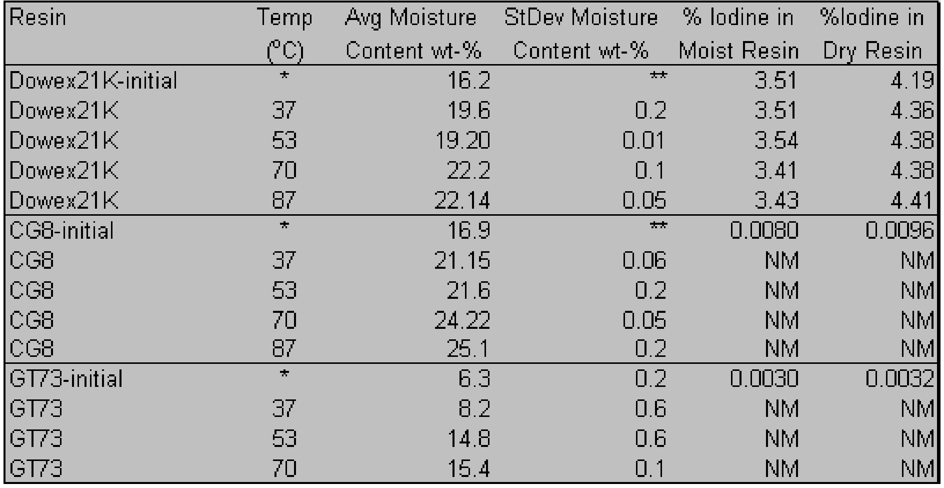
Table 3. Measured First-Order Rate Constants (k) Based on Loss of Iodide from Dowex 21K Resin, and Calculated Arrhenius Constants: Calculated First-Order Rate Constant ([k(calc)], Activation Energy (E_a), and Pre-Exponential Factor (A)..

	k (s^{-1})				E_a	A	k(calc)(s^{-1})
Resin	37	53	70	87	kJ/mol	s^{-1}	18.3
Dowex 21K	2.79E-10	-5.6E-10	-1.3E-09	-2.7E-09	41	3.30E-03	9.39E-11

Elemental and trace microanalyses were used to determine the initial concentration of iodide in all resins prior to thermal degradation. Elemental microanalyses were also carried out on the Dowex 21K resins after heating for 10 months (Table 4). As with the soil weathering experiments, the loss of iodide from the Dowex 21K resin was immeasurable by this technique, i.e., there was no significant difference in the iodide concentration at the start of the experiment and after ten months of heating in groundwater.

In summary, only one of the three resins, Dowex 21K, permitted Arrhenius treatment of the data. Solutions in contact with the other two resins, GT-73 and CG-8, had appreciably lower aqueous iodide concentrations, approaching detection limits. This is not surprising in light of the fact that these are not anion resins and therefore little iodide would be exchanged onto their surfaces. Consequently, spurious iodide concentration data were obtained that did not follow well-known trends in chemistry (such as increased iodide concentrations with lower temperature). Based on the Dowex 21K, about 8% of the initial iodide would be released as a result of resin degradation and anion exchange after 10,000 years. Again, quantitative iodide data for special analysis calculations should be based on actual waste, rather than the prepared materials used in this study.

Table 4. Iodine Concentration in Resins Before and After Thermal Degradation in Groundwater. (NM = Not Measured)



Resin	Temp (°C)	Avg Moisture Content wt-%	StDev Moisture Content wt-%	% Iodine in Moist Resin	%Iodine in Dry Resin
Dowex21K-initial	*	16.2	**	3.51	4.19
Dowex21K	37	19.6	0.2	3.51	4.36
Dowex21K	53	19.20	0.01	3.54	4.38
Dowex21K	70	22.2	0.1	3.41	4.38
Dowex21K	87	22.14	0.05	3.43	4.41
CG8-initial	*	16.9	**	0.0080	0.0096
CG8	37	21.15	0.06	NM	NM
CG8	53	21.6	0.2	NM	NM
CG8	70	24.22	0.05	NM	NM
CG8	87	25.1	0.2	NM	NM
GT73-initial	*	6.3	0.2	0.0030	0.0032
GT73	37	8.2	0.6	NM	NM
GT73	53	14.8	0.6	NM	NM
GT73	70	15.4	0.1	NM	NM

*initial air dried resin stored at ambient temperature without further treatment
**not measured in replicate

3.2.3 Other Analyses

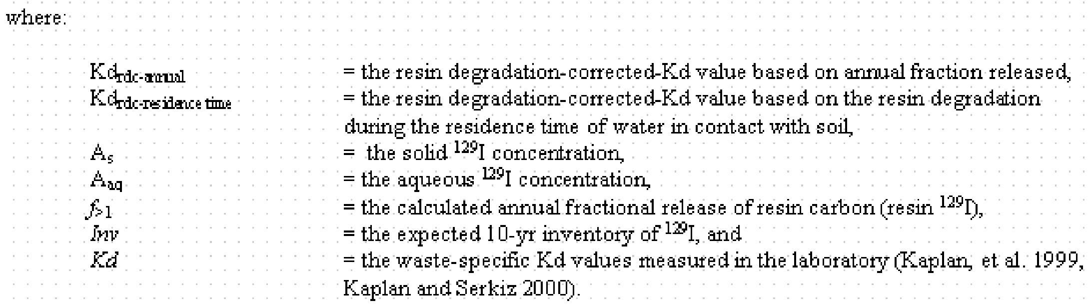
Thermal Gravimetric Analyses and FT-IR Spectra for the Dowex 21K resin did not result in quantifiable data. These measurements are included in Appendix D.

3.2.4 Implications to E-Area Disposal

Collard (2001) reported a strong correlation between waste-form K_d values and the inventory limits that can be disposed in the slit trenches at the E-Area Low-Level Waste Facility ($R^2 = 0.9995$). To evaluate the extent that the measured degradation rates (based on total carbon released from the resins) may influence waste disposal at this facility, the K_d values used by Collard (2001) were recalculated to account for resin degradation (Table 5). The resin-degradation-corrected-K_d values (Kd_{rdc}) were calculated by two equations (eq 3 and eq 4):

$$Kd_{rdc-annual} = \frac{A_s - (f_{>1} \times Inv)}{A_{aq} + (f_{>1} \times Inv)} \quad \text{eq 3}$$

$$Kd_{rdc-residencetime} = \frac{Kd - (0.0156 \times f_{>1})}{1 + (0.0156 \times f_{>1})} \quad \text{eq 4}$$



where:

$Kd_{rdc\text{-}annual}$ = the resin degradation-corrected-Kd value based on annual fraction released,
$Kd_{rdc\text{-}residence\ time}$ = the resin degradation-corrected-Kd value based on the resin degradation during the residence time of water in contact with soil,
A_s = the solid ^{129}I concentration,
A_{aq} = the aqueous ^{129}I concentration,
$f_{>1}$ = the calculated annual fractional release of resin carbon (resin ^{129}I),
Inv = the expected 10-yr inventory of ^{129}I, and
Kd = the waste-specific Kd values measured in the laboratory (Kaplan, et al. 1999, Kaplan and Serkiz 2000).

$Kd_{rdc\text{-}annual}$ assumes that the Kd needs to be corrected for the amount of degradation that occurs in 1 year, the assumed length of time for steady state to be achieved (Table 5). In this calculation the fractional release rate of carbon from the resin is proportional to the fractional release rate of ^{129}I from the resin. This assumption is reasonable insofar that it assumes that the ^{129}I is evenly spread over the resin and that the carbon and ^{129}I released are proportional. A conservative assumption associated with eq 3 is that the amount of ^{129}I released in 1-yr from the resin is in equilibrium with the resin at a given time. Equation 4 drops this conservatism and assumes more realistically that the amount of ^{129}I released from the resin is based on the residence time of water in contact with a resin waste and that ^{129}I equilibrium can be achieved between the resins and the mobile aqueous phase during the time the water is in contact with the resin. Assuming a resin bulk density of 1.06 g/cm^3 (Using a resin bulk density of 1.65 g/cm^3 was less conservative, resulting in a residence time of 0.0156 yr. This difference resulted in essentially no real impact on calculated resin-degradation-corrected-Kd values).and a flow rate taken from the last performance assessment (McDowell-Boyer et al. 2000) of 40 cm/yr, the residence time was 0.024 yr (~9 days). Even though the carbon is not at equilibrium during the 9 day residence time, it is very likely that the aqueous ^{129}I concentrations, which are controlled by anion exchange, do come into equilibrium within a day (Sposito 1994). Calculations based on eq 4 are presented in Table 6. As expected these corrections for resin degradation ($Kd_{rdc\text{-}residence\ time}$) indicate an even smaller impact than those calculated using eq 3 ($Kd_{rdc\text{-}annual}$; Table 5).

Table 5. Calculation of $Kd_{rdc\text{-}annual}$ (eq 3).

	Original Kd Used in Special Analysis[a]	Annual fractional released at t>1 yr	$Kd_{rdc\text{-}annual}$	% decrease betw. Kd & $Kd_{rdc\text{-}annual}$	Kd decrease Kd - $Kd_{rdc\text{-}annual}$
	(mL/g)	(mol/mol-t)	(mL/g)	(%)	(mL/g)
CG-8/FGWTU	50	3.90E-06	49.9998	3.98E-04	0.00020
CG-8/HGWTU	380	3.90E-06	379.9985	3.91E-04	0.00149
Dowex 21K /FGWTU	6800	7.84E-08	6799.9995	7.84E-06	0.00053
Dowex 21K /HGWTU	15600	7.84E-08	15599.9988	7.84E-06	0.00122
GT-73/ETF	10000	2.30E-07	9999.9977	2.30E-05	0.00230
[a] Conservative waste-specific Kd values measured by Kaplan et al. (1999) and Kaplan and Serkiz (2000)					

Table 6. Calculation of $Kd_{rdc\text{-}residence\ time}$ (eq 4).

	Original Kd Used in Special Analysis[a]	Frational Release During 0.0236 yr	$Kd_{rdc\text{-}residence\ time}$	% decrease betw. Kd & $Kd_{rdc\text{-}residence\ time}$	Kd decrease Kd - $Kd_{rdc\text{-}residence\ time}$
	(mL/g)		(mL/g)	(%)	(mL/g)
CG-8/FGWTU	50	9.21E-08	50.00000	9.3917E-06	0.00000
CG-8/HGWTU	380	9.21E-08	379.99996	9.23178E-06	0.00004
Dowex 21K /FGWTU	6800	1.85E-09	6799.99999	1.85004E-07	0.00001
Dowex 21K /HGWTU	15600	1.85E-09	15599.99997	1.84988E-07	0.00003
GT-73/ETF	10000	5.43E-09	9999.99995	5.43215E-07	0.00005
[a] Conservative waste-specific Kd values measured by Kaplan et al. (1999) and Kaplan and Serkiz (2000)					

One time of interest for performance assessment calculations is 10,000 years. Based on eq 2 and the calculated first order rate constants at 18.3 ° C obtained from the carbon-released data (Table 2), the percent of resin estimated to be degraded over 10,000 years was negligible, <3.85 wt-% (Table 7). The resin-degradation corrected Kd value (eq 3; $Kd_{rdc\text{-}annual}$) is negligibly (<0.0004%) less than the original K_d values; well within the uncertainty of the original Kd values. Consequently, there is no need to conduct additional Performance Assessment or Waste Acceptance Criteria calculations to account for the small effect of resin degradation on enhanced ^{129}I release into the subsurface environment.

Table 7. Resin Degradation Correction of the K_d Values.

Resin	Waste Generating Facility	% Resin released after 10,000 yr	Original Kd Used in Special Analysis[(a)]	%-Δ Kd ($Kd-Kd_{rdc}/Kd$ *100)	Recommended Kd_{rdc}
		(%)	(mL/g)	(%)	(mL/g)
CG-8	F-GWTU	3.83	50	3.98E-04	50
CG-8	H-GWTU	3.83	380	3.91E-04	380
Dowex 21K	F-GWTU	0.08	6,800	7.84E-06	6,800
Dowex 21K	H-GWTU	0.08	15,600	7.84E-06	15,600
GT-73	ETF	0.23	10,000	2.30E-05	10,000

[(a)] Conservative waste-specific K_d values measured by Kaplan et al. (1999) and Kaplan and Serkiz (2000)

4.0 Conclusions

Collard (2001) reported a strong correlation between waste-form K_d values and the limiting inventory that can be disposed in the slit trenches at the E-Area Low-Level Waste Facility ($R^2 = 0.9995$). To evaluate the extent that the measured degradation rates (based on total carbon released from the resins) may influence waste disposal at this facility, the K_d values used by Collard (2001) were recalculated to account for resin degradation. The resin-degradation-corrected-K_d values (Kd_{rdc}) differed negligibly (<0.0004%) from the original K_d values; well within the uncertainty of the original Kd values. The tests also indicate that <4 % of the resin would be released into the groundwater after 10,000 years. Consequently, there is no need to conduct additional calculations to account for the small effect of resin degradation on enhanced ^{129}I release into the subsurface environment.

5.0 Acknowledgements

Bill Crooks and Beverly Wall from Actinide Technology initiated laboratory studies described in this report, and Cathy Coffey and Carl Black from Waste Processing Technology also assisted in the laboratory work. Anna Knox, of the Savannah River Ecology Laboratory, assisted in preparing and maintaining the soil weathering studies. Iodide analyses methods by Liquid Chromatography (LC) and Capillary Electrophoresis (CE) were tested by Robert Ray and Scott McWhorter, respectively, of the Analytical Development Section (ADS). Mike Summer of ADS provided assistance with optical microscopy.

6.0 References

1. Collard, L. B., 2001,"Special Analysis for Disposal of High-Concentration I-129 Waste in Slit Trenches at the E-Area Low-Level Waste Facility", WSRC-TR-2001-00021, Savannah River Site, Aiken, SC 29808.
2. Kaplan, D. I. and Serkiz, S. M. 2000,"I-129 Desorption from Resin, Activated Carbon, and Filtercake Waste Generated from the F- and H-Area Water Treatment Units", WSRC-TR-2000-00308, Savannah River Site, Aiken, SC 29808.
3. Kaplan, D. I., Serkiz, S. M. and Bell, N. C., 1999,"I-129 Desorption from SRS Water Treatment Media From the Effluent Treatment Facility and the F-Area Groundwater Treatment Facility (U)", WSRC-TR-99-00270, Savannah River Site, Aiken, SC 29808.
4. McDowell-Boyer, L., Yu, A. D., Cook, J. R., Kocher, D. C., Wilhite, E. L., Homes-Burns, H., Young, K. E. "Radiological Performance Assessment for the E-Area Low-Level Waste Facility". WSRC-RP-94-218 Rev. 1, Westinghouse Savannah River Company, Aiken, SC (2000).
5. Powell, K. R., Kaplan, D. I., 2002, "Resin Longevity Studies: Interim Report". WSRC-TR-2002-00037.
6. Sharma, H.D. and Subramanian, N. 1970, "Determination of Water in Ion-Exchange Resins: Anion Exchange Resins", *Analytical Chemistry*, 42:1287-1290.
7. Sposito, G. 1994, *Chemical Equilibria and Kinetics in Soils* The Oxford University Press, New York.

7.0 Appendix A: Detailed Description of Materials and Methods

Materials and Methods for Resin Longevity Studies

General Approach: The exchange sites of fresh resins will be saturated with stable I^-. Once the resins and I^- reached equilibrium, they will be rinsed with deionized water, and dried before recording the initial weight of the resin. The air dried iodine saturated resins will then be placed in a vessel containing groundwater which is covered but not sealed, and placed in an oven at various temperatures: approximately 40, 53, 67, and 80 ° C. Additionally, a growth-chamber experiment, conducted at 30 ° C with SRS soil will be carried out in order to test the resins' performance when exposed to soil microbes.

Materials:

4 ovens
16 1-L containers that can be placed in an oven
CG8 resin
Dowex 21K resin
GT-73 resin
5-L 0.1-M NaI
16-L SRS groundwater
geo-fabric: Spectra/mesh fluorocarbon filter (mesh opening 105 µm, 32% open area, thickness155 µm)
SRS soil: Surface Clayey Forest Sediment (collected from an uncontaminated area behind SREL)

Method:

For Thermal-enhance Degradation Studies:

1. Label 16 1-L containers as follows

Sample #	Description
1.	40°C CG8
2.	40°C Dowex 21K
3.	40°C GT-73
4	40°C groundwater only (no resin)
5.	53°C CG8
6.	53° Dowex 21K
7.	53°C GT-73
8.	53°C groundwater only (no resin)
9.	67°
10.	67°C Dowex 21K
11.	67°C GT-73
12.	67°C groundwater only (no resin)
13.	80°C CG8
14.	80°C Dowex 21K
15.	80°C GT-73

16.	80°C groundwater only (no resin)

2. Prepare 50% wt/vol mixture of resin with 0.1 M aqueous NaI solution.
3. Equilibrate overnight on a platform shaker.
4. Using tared filter paper and filtration apparatus, rinse resins with 10 fold excess d.i. water. Leave as little rinsate as possible on filter.
5. Air dry resin.
6. Weigh out 60 g of resin and place in 1-L glass container.
7. Add 900-mL groundwater to each container.
8. Record initial weight of container with resin and groundwater.
9. Place in appropriate oven set to 40, 53, 67, or 80°C.
10. Shake by hand once every working day.
11. Add deionized water if necessary to replace any water lost due to evaporation.
12. Remove 30-mL aliquots after 1 day and 1, 2, 3, 5, and 7 months. Reduce sampling volume after initial samples if possible.
13. Have ADS analyze aliquots for TIC/TOC, ICP-ES cations, and I^- (by either IC, CE, or ICP-MS).
14. Measure pH and I^- by ISE.
15. At end of experiment, characterize the resin using the following solid phase analytical techniques: FT-IR, TGA, DSC, environmental SEM, and observe under optical microscope.

For Soil Weathering Studies:

16. Prepare resins as described in steps 2-6.
17. Mix 1700 g sieved (2 mm, #10 seive) whole SRS soil with 60 g clay (<0.53 μ dry sieved fraction from the same soil). This effectively doubles the clay content of the soil used in this experiment).
18. Add 1/3 of soil mixture to a pot with holes on the bottom to permit water to drain freely.
19. Add filtered rainwater to saturate.
20. Place geofabric on soil.
21. Place 30 g resin on geofabric.
22. Fold geofabric over resin.
23. Place 1/3 of soil on top of geofabric.
24. Add filtered rainwater to saturate.
25. Add 30 g resin directly contacting soil.
26. Cover with remaining 1/3 of soil.
27. Add rainwater to saturate.
28. Place in growth chamber maintained at 30 ° C.
29. Apply rainwater as needed (every 4-5 days) to maintain soil moisture
30. Retrieve resins from the geo-fabric and the screen after 8 months and analyze as described in step 15.

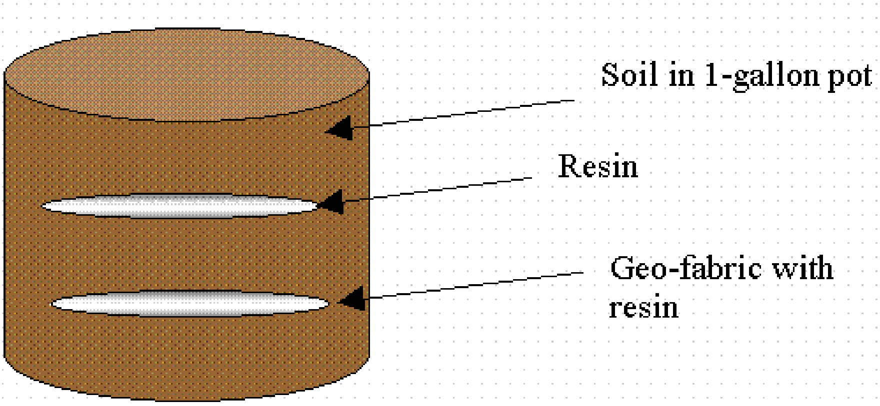
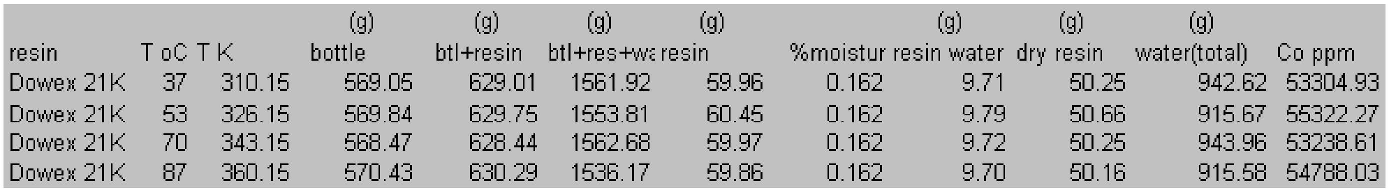
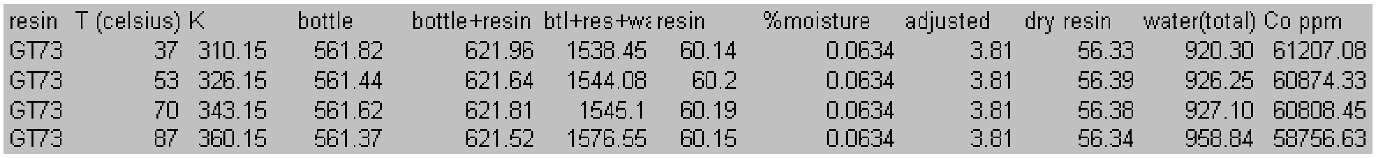


Figure A1. Growth-Chamber Set-Up.

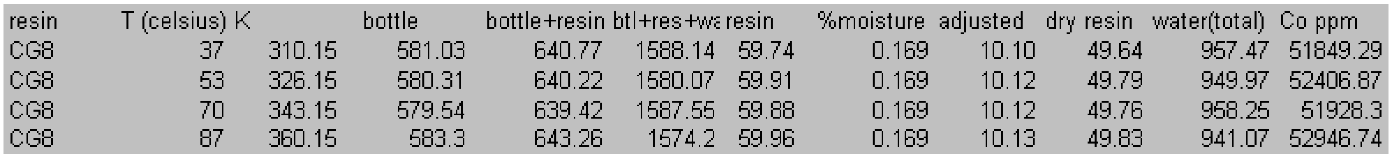
8.0 Appendix B: Total Carbon Data



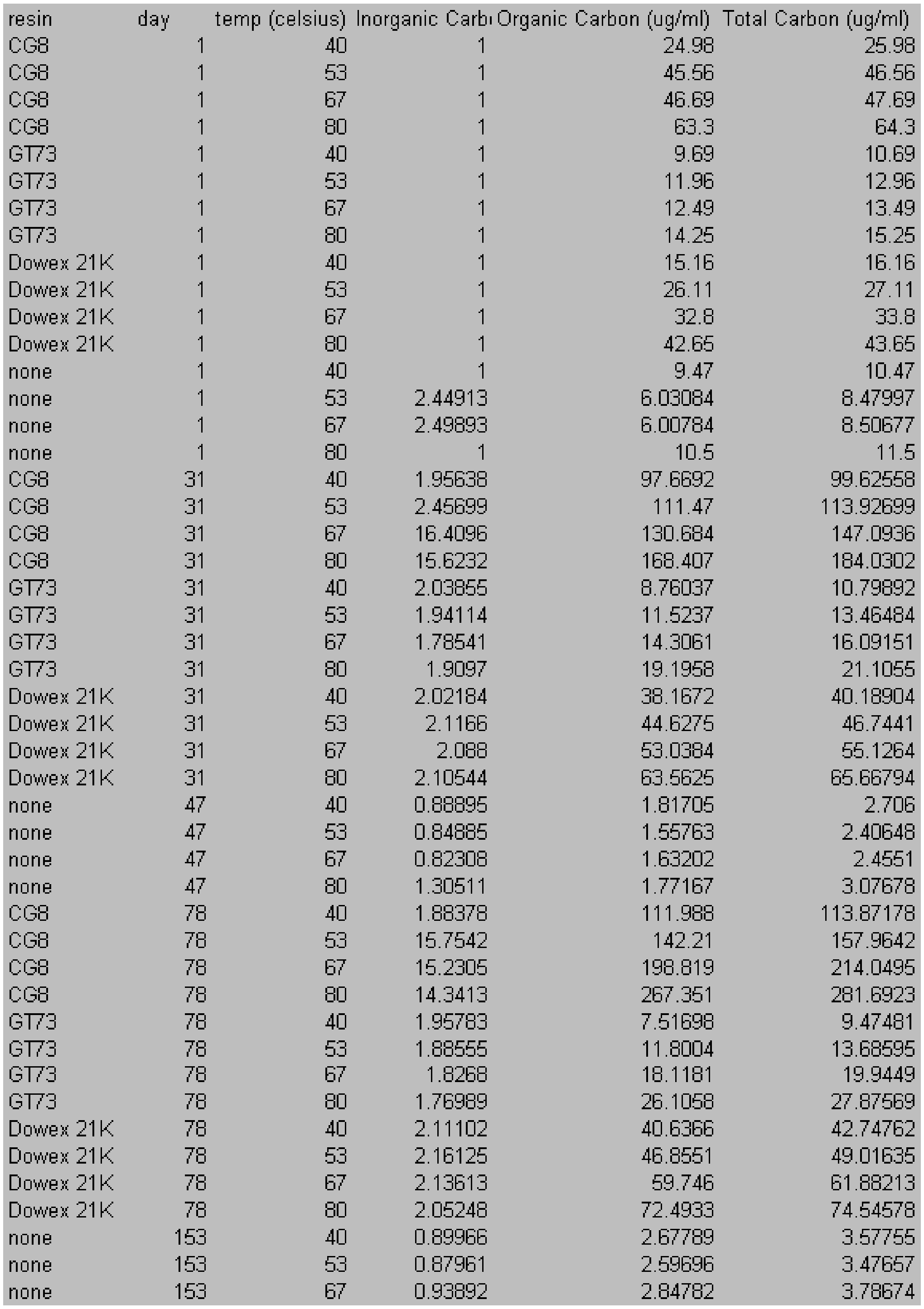
			(g)	(g)	(g)	(g)		(g)	(g)	(g)	
resin	T oC	T K	bottle	btl+resin	btl+res+wa	resin	%moistur	resin water	dry resin	water(total)	Co ppm
Dowex 21K	37	310.15	569.05	629.01	1561.92	59.96	0.162	9.71	50.25	942.62	53304.93
Dowex 21K	53	326.15	569.84	629.75	1553.81	60.45	0.162	9.79	50.66	915.67	55322.27
Dowex 21K	70	343.15	568.47	628.44	1562.68	59.97	0.162	9.72	50.25	943.96	53238.61
Dowex 21K	87	360.15	570.43	630.29	1536.17	59.86	0.162	9.70	50.16	915.58	54788.03



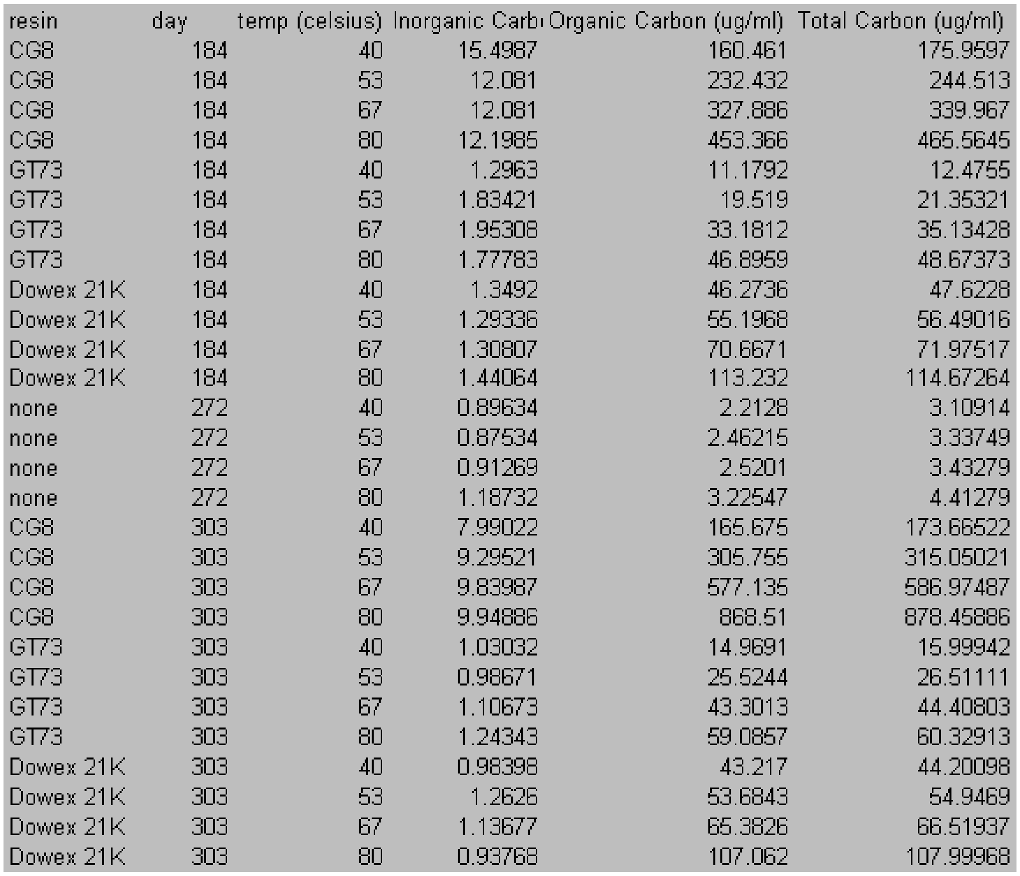
resin	T (celsius)	K	bottle	bottle+resin	btl+res+wa	resin	%moisture	adjusted	dry resin	water(total)	Co ppm
GT73	37	310.15	561.82	621.96	1538.45	60.14	0.0634	3.81	56.33	920.30	61207.08
GT73	53	326.15	561.44	621.64	1544.08	60.2	0.0634	3.81	56.39	926.25	60874.33
GT73	70	343.15	561.62	621.81	1545.1	60.19	0.0634	3.81	56.38	927.10	60808.45
GT73	87	360.15	561.37	621.52	1576.55	60.15	0.0634	3.81	56.34	958.84	58756.63



resin	T (celsius)	K	bottle	bottle+resin	btl+res+wa	resin	%moisture	adjusted	dry resin	water(total)	Co ppm
CG8	37	310.15	581.03	640.77	1588.14	59.74	0.169	10.10	49.64	957.47	51849.29
CG8	53	326.15	580.31	640.22	1580.07	59.91	0.169	10.12	49.79	949.97	52406.87
CG8	70	343.15	579.54	639.42	1587.55	59.88	0.169	10.12	49.76	958.25	51928.3
CG8	87	360.15	583.3	643.26	1574.2	59.96	0.169	10.13	49.83	941.07	52946.74

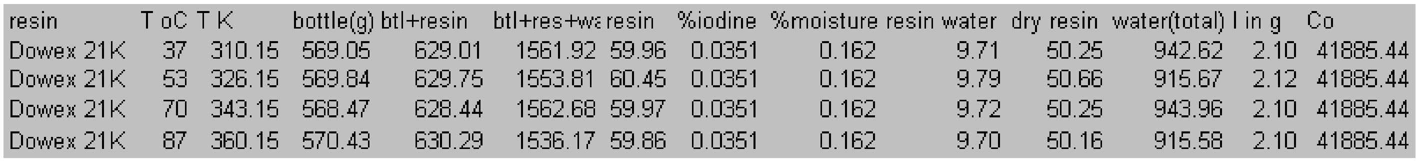


resin	day	temp (celsius)	Inorganic Carb	Organic Carbon (ug/ml)	Total Carbon (ug/ml)
CG8	1	40	1	24.98	25.98
CG8	1	53	1	45.56	46.56
CG8	1	67	1	46.69	47.69
CG8	1	80	1	63.3	64.3
GT73	1	40	1	9.69	10.69
GT73	1	53	1	11.96	12.96
GT73	1	67	1	12.49	13.49
GT73	1	80	1	14.25	15.25
Dowex 21K	1	40	1	15.16	16.16
Dowex 21K	1	53	1	26.11	27.11
Dowex 21K	1	67	1	32.8	33.8
Dowex 21K	1	80	1	42.65	43.65
none	1	40	1	9.47	10.47
none	1	53	2.44913	6.03084	8.47997
none	1	67	2.49893	6.00784	8.50677
none	1	80	1	10.5	11.5
CG8	31	40	1.95638	97.6692	99.62558
CG8	31	53	2.45699	111.47	113.92699
CG8	31	67	16.4096	130.684	147.0936
CG8	31	80	15.6232	168.407	184.0302
GT73	31	40	2.03855	8.76037	10.79892
GT73	31	53	1.94114	11.5237	13.46484
GT73	31	67	1.78541	14.3061	16.09151
GT73	31	80	1.9097	19.1958	21.1055
Dowex 21K	31	40	2.02184	38.1672	40.18904
Dowex 21K	31	53	2.1166	44.6275	46.7441
Dowex 21K	31	67	2.088	53.0384	55.1264
Dowex 21K	31	80	2.10544	63.5625	65.66794
none	47	40	0.88895	1.81705	2.706
none	47	53	0.84885	1.55763	2.40648
none	47	67	0.82308	1.63202	2.4551
none	47	80	1.30511	1.77167	3.07678
CG8	78	40	1.88378	111.988	113.87178
CG8	78	53	15.7542	142.21	157.9642
CG8	78	67	15.2305	198.819	214.0495
CG8	78	80	14.3413	267.351	281.6923
GT73	78	40	1.95783	7.51698	9.47481
GT73	78	53	1.88555	11.8004	13.68595
GT73	78	67	1.8268	18.1181	19.9449
GT73	78	80	1.76989	26.1058	27.87569
Dowex 21K	78	40	2.11102	40.6366	42.74762
Dowex 21K	78	53	2.16125	46.8551	49.01635
Dowex 21K	78	67	2.13613	59.746	61.88213
Dowex 21K	78	80	2.05248	72.4933	74.54578
none	153	40	0.89966	2.67789	3.57755
none	153	53	0.87961	2.59696	3.47657
none	153	67	0.93892	2.84782	3.78674

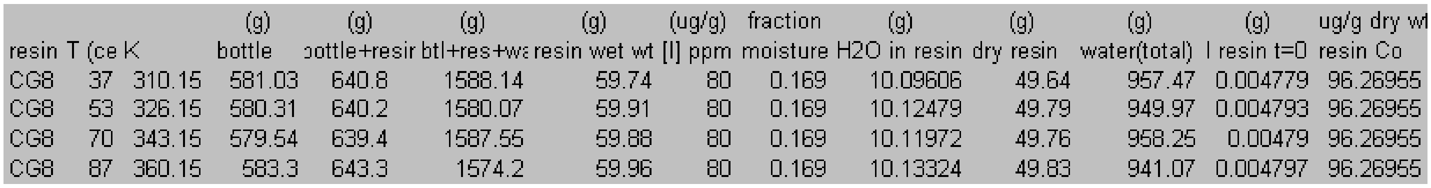


resin	day	temp (celsius)	Inorganic Carb	Organic Carbon (ug/ml)	Total Carbon (ug/ml)
CG8	184	40	15.4987	160.461	175.9597
CG8	184	53	12.081	232.432	244.513
CG8	184	67	12.081	327.886	339.967
CG8	184	80	12.1985	453.366	465.5645
GT73	184	40	1.2963	11.1792	12.4755
GT73	184	53	1.83421	19.519	21.35321
GT73	184	67	1.95308	33.1812	35.13428
GT73	184	80	1.77783	46.8959	48.67373
Dowex 21K	184	40	1.3492	46.2736	47.6228
Dowex 21K	184	53	1.29336	55.1968	56.49016
Dowex 21K	184	67	1.30807	70.6671	71.97517
Dowex 21K	184	80	1.44064	113.232	114.67264
none	272	40	0.89634	2.2128	3.10914
none	272	53	0.87534	2.46215	3.33749
none	272	67	0.91269	2.5201	3.43279
none	272	80	1.18732	3.22547	4.41279
CG8	303	40	7.99022	165.675	173.66522
CG8	303	53	9.29521	305.755	315.05021
CG8	303	67	9.83987	577.135	586.97487
CG8	303	80	9.94886	868.51	878.45886
GT73	303	40	1.03032	14.9691	15.99942
GT73	303	53	0.98671	25.5244	26.51111
GT73	303	67	1.10673	43.3013	44.40803
GT73	303	80	1.24343	59.0857	60.32913
Dowex 21K	303	40	0.98398	43.217	44.20098
Dowex 21K	303	53	1.2626	53.6843	54.9469
Dowex 21K	303	67	1.13677	65.3826	66.51937
Dowex 21K	303	80	0.93768	107.062	107.99968

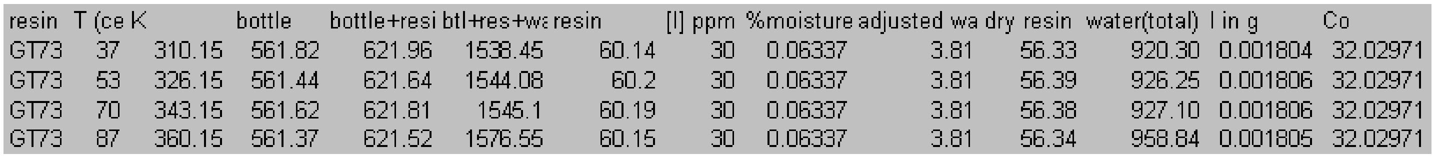
9.0 Appendix C: Iodide Data



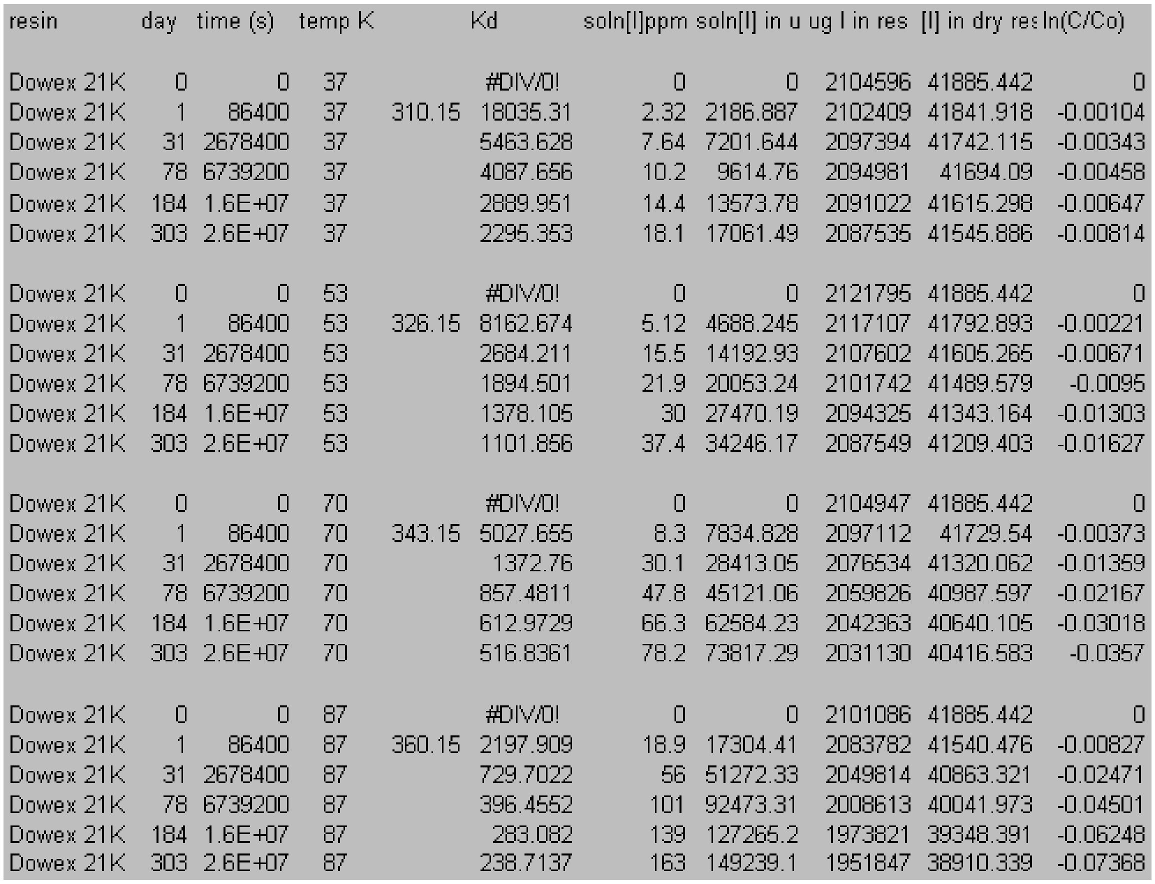
resin	T oC	T K	bottle(g)	btl+resin	btl+res+wa	resin	%iodine	%moisture	resin water	dry resin	water(total)	I in g	Co
Dowex 21K	37	310.15	569.05	629.01	1561.92	59.96	0.0351	0.162	9.71	50.25	942.62	2.10	41885.44
Dowex 21K	53	326.15	569.84	629.75	1553.81	60.45	0.0351	0.162	9.79	50.66	915.67	2.12	41885.44
Dowex 21K	70	343.15	568.47	628.44	1562.68	59.97	0.0351	0.162	9.72	50.25	943.96	2.10	41885.44
Dowex 21K	87	360.15	570.43	630.29	1536.17	59.86	0.0351	0.162	9.70	50.16	915.58	2.10	41885.44



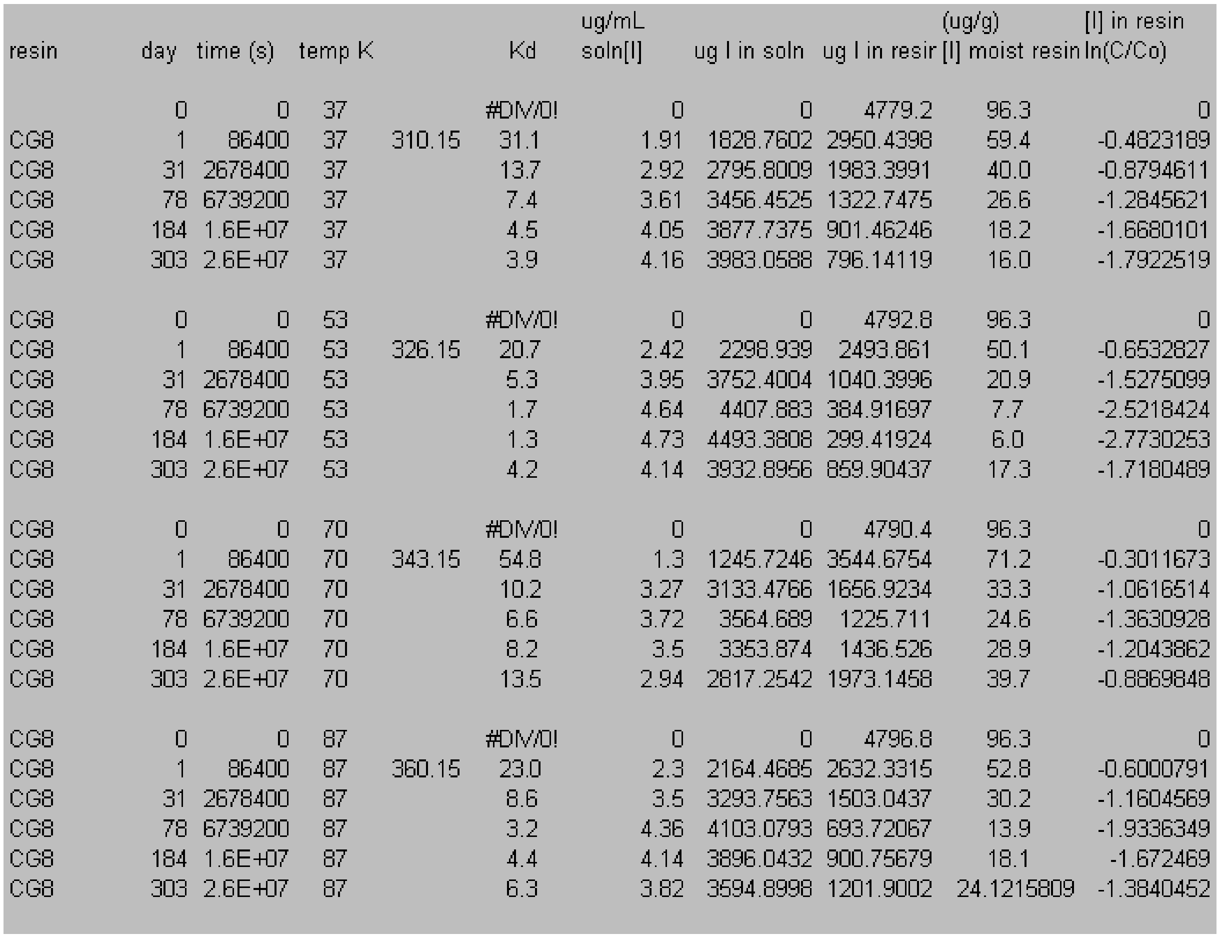
resin	T (ce	K	(g) bottle	(g) ottle+resir	(g) btl+res+wa	(g) resin wet wt	(ug/g) [I] ppm	fraction moisture	(g) H2O in resin	(g) dry resin	(g) water(total)	(g) I resin t=0	ug/g dry w resin Co
CG8	37	310.15	581.03	640.8	1588.14	59.74	80	0.169	10.09606	49.64	957.47	0.004779	96.26955
CG8	53	326.15	580.31	640.2	1580.07	59.91	80	0.169	10.12479	49.79	949.97	0.004793	96.26955
CG8	70	343.15	579.54	639.4	1587.55	59.88	80	0.169	10.11972	49.76	958.25	0.00479	96.26955
CG8	87	360.15	583.3	643.3	1574.2	59.96	80	0.169	10.13324	49.83	941.07	0.004797	96.26955



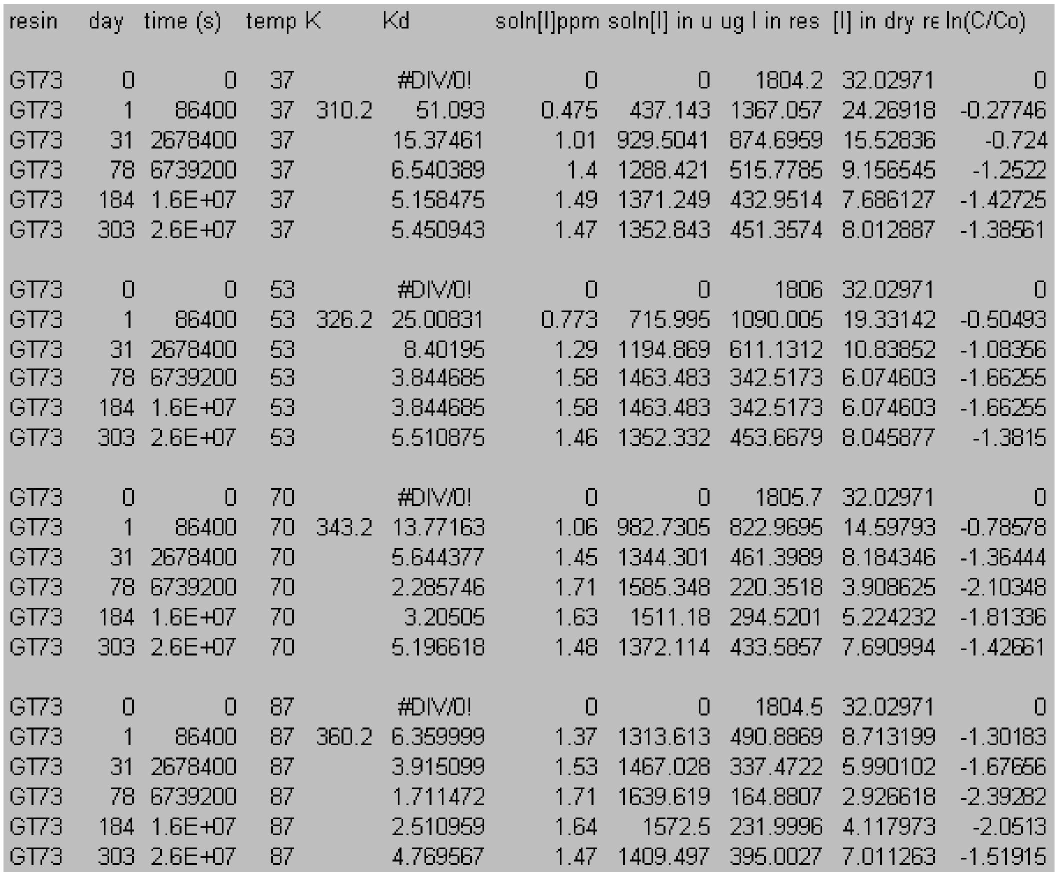
resin	T (ce	K	bottle	bottle+resi	btl+res+wa	resin	[I] ppm	%moisture	adjusted wa	dry resin	water(total)	I in g	Co
GT73	37	310.15	561.82	621.96	1538.45	60.14	30	0.06337	3.81	56.33	920.30	0.001804	32.02971
GT73	53	326.15	561.44	621.64	1544.08	60.2	30	0.06337	3.81	56.39	926.25	0.001806	32.02971
GT73	70	343.15	561.62	621.81	1545.1	60.19	30	0.06337	3.81	56.38	927.10	0.001806	32.02971
GT73	87	360.15	561.37	621.52	1576.55	60.15	30	0.06337	3.81	56.34	958.84	0.001805	32.02971



resin	day	time (s)	temp K		Kd	soln[I]ppm	soln[I] in u	ug I in res	[I] in dry res	ln(C/Co)
Dowex 21K	0	0	37		#DIV/0!	0	0	2104596	41885.442	0
Dowex 21K	1	86400	37	310.15	18035.31	2.32	2186.887	2102409	41841.918	-0.00104
Dowex 21K	31	2678400	37		5463.628	7.64	7201.644	2097394	41742.115	-0.00343
Dowex 21K	78	6739200	37		4087.656	10.2	9614.76	2094981	41694.09	-0.00458
Dowex 21K	184	1.6E+07	37		2889.951	14.4	13573.78	2091022	41615.298	-0.00647
Dowex 21K	303	2.6E+07	37		2295.353	18.1	17061.49	2087535	41545.886	-0.00814
Dowex 21K	0	0	53		#DIV/0!	0	0	2121795	41885.442	0
Dowex 21K	1	86400	53	326.15	8162.674	5.12	4688.245	2117107	41792.893	-0.00221
Dowex 21K	31	2678400	53		2684.211	15.5	14192.93	2107602	41605.265	-0.00671
Dowex 21K	78	6739200	53		1894.501	21.9	20053.24	2101742	41489.579	-0.0095
Dowex 21K	184	1.6E+07	53		1378.105	30	27470.19	2094325	41343.164	-0.01303
Dowex 21K	303	2.6E+07	53		1101.856	37.4	34246.17	2087549	41209.403	-0.01627
Dowex 21K	0	0	70		#DIV/0!	0	0	2104947	41885.442	0
Dowex 21K	1	86400	70	343.15	5027.655	8.3	7834.828	2097112	41729.54	-0.00373
Dowex 21K	31	2678400	70		1372.76	30.1	28413.05	2076534	41320.062	-0.01359
Dowex 21K	78	6739200	70		857.4811	47.8	45121.06	2059826	40987.597	-0.02167
Dowex 21K	184	1.6E+07	70		612.9729	66.3	62584.23	2042363	40640.105	-0.03018
Dowex 21K	303	2.6E+07	70		516.8361	78.2	73817.29	2031130	40416.583	-0.0357
Dowex 21K	0	0	87		#DIV/0!	0	0	2101086	41885.442	0
Dowex 21K	1	86400	87	360.15	2197.909	18.9	17304.41	2083782	41540.476	-0.00827
Dowex 21K	31	2678400	87		729.7022	56	51272.33	2049814	40863.321	-0.02471
Dowex 21K	78	6739200	87		396.4552	101	92473.31	2008613	40041.973	-0.04501
Dowex 21K	184	1.6E+07	87		283.082	139	127265.2	1973821	39348.391	-0.06248
Dowex 21K	303	2.6E+07	87		238.7137	163	149239.1	1951847	38910.339	-0.07368



						ug/mL			(ug/g)	[I] in resin
resin	day	time (s)	temp K		Kd	soln[I]	ug I in soln	ug I in resi	[I] moist resin	ln(C/Co)
	0	0	37		#DIV/0!	0	0	4779.2	96.3	0
CG8	1	86400	37	310.15	31.1	1.91	1828.7602	2950.4398	59.4	-0.4823189
CG8	31	2678400	37		13.7	2.92	2795.8009	1983.3991	40.0	-0.8794611
CG8	78	6739200	37		7.4	3.61	3456.4525	1322.7475	26.6	-1.2845621
CG8	184	1.6E+07	37		4.5	4.05	3877.7375	901.46246	18.2	-1.6680101
CG8	303	2.6E+07	37		3.9	4.16	3983.0588	796.14119	16.0	-1.7922519
CG8	0	0	53		#DIV/0!	0	0	4792.8	96.3	0
CG8	1	86400	53	326.15	20.7	2.42	2298.939	2493.861	50.1	-0.6532827
CG8	31	2678400	53		5.3	3.95	3752.4004	1040.3996	20.9	-1.5275099
CG8	78	6739200	53		1.7	4.64	4407.883	384.91697	7.7	-2.5218424
CG8	184	1.6E+07	53		1.3	4.73	4493.3808	299.41924	6.0	-2.7730253
CG8	303	2.6E+07	53		4.2	4.14	3932.8956	859.90437	17.3	-1.7180489
CG8	0	0	70		#DIV/0!	0	0	4790.4	96.3	0
CG8	1	86400	70	343.15	54.8	1.3	1245.7246	3544.6754	71.2	-0.3011673
CG8	31	2678400	70		10.2	3.27	3133.4766	1656.9234	33.3	-1.0616514
CG8	78	6739200	70		6.6	3.72	3564.689	1225.711	24.6	-1.3630928
CG8	184	1.6E+07	70		8.2	3.5	3353.874	1436.526	28.9	-1.2043862
CG8	303	2.6E+07	70		13.5	2.94	2817.2542	1973.1458	39.7	-0.8869848
CG8	0	0	87		#DIV/0!	0	0	4796.8	96.3	0
CG8	1	86400	87	360.15	23.0	2.3	2164.4685	2632.3315	52.8	-0.6000791
CG8	31	2678400	87		8.6	3.5	3293.7563	1503.0437	30.2	-1.1604569
CG8	78	6739200	87		3.2	4.36	4103.0793	693.72067	13.9	-1.9336349
CG8	184	1.6E+07	87		4.4	4.14	3896.0432	900.75679	18.1	-1.672469
CG8	303	2.6E+07	87		6.3	3.82	3594.8998	1201.9002	24.1215809	-1.3840452



resin	day	time (s)	temp	K	Kd	soln[I]ppm	soln[I] in u	ug I in res	[I] in dry re	ln(C/Co)
GT73	0	0	37		#DIV/0!	0	0	1804.2	32.02971	0
GT73	1	86400	37	310.2	51.093	0.475	437.143	1367.057	24.26918	-0.27746
GT73	31	2678400	37		15.37461	1.01	929.5041	874.6959	15.52836	-0.724
GT73	78	6739200	37		6.540389	1.4	1288.421	515.7785	9.156545	-1.2522
GT73	184	1.6E+07	37		5.158475	1.49	1371.249	432.9514	7.686127	-1.42725
GT73	303	2.6E+07	37		5.450943	1.47	1352.843	451.3574	8.012887	-1.38561
GT73	0	0	53		#DIV/0!	0	0	1806	32.02971	0
GT73	1	86400	53	326.2	25.00831	0.773	715.995	1090.005	19.33142	-0.50493
GT73	31	2678400	53		8.40195	1.29	1194.869	611.1312	10.83852	-1.08356
GT73	78	6739200	53		3.844685	1.58	1463.483	342.5173	6.074603	-1.66255
GT73	184	1.6E+07	53		3.844685	1.58	1463.483	342.5173	6.074603	-1.66255
GT73	303	2.6E+07	53		5.510875	1.46	1352.332	453.6679	8.045877	-1.3815
GT73	0	0	70		#DIV/0!	0	0	1805.7	32.02971	0
GT73	1	86400	70	343.2	13.77163	1.06	982.7305	822.9695	14.59793	-0.78578
GT73	31	2678400	70		5.644377	1.45	1344.301	461.3989	8.184346	-1.36444
GT73	78	6739200	70		2.285746	1.71	1585.348	220.3518	3.908625	-2.10348
GT73	184	1.6E+07	70		3.20505	1.63	1511.18	294.5201	5.224232	-1.81336
GT73	303	2.6E+07	70		5.196618	1.48	1372.114	433.5857	7.690994	-1.42661
GT73	0	0	87		#DIV/0!	0	0	1804.5	32.02971	0
GT73	1	86400	87	360.2	6.359999	1.37	1313.613	490.8869	8.713199	-1.30183
GT73	31	2678400	87		3.915099	1.53	1467.028	337.4722	5.990102	-1.67656
GT73	78	6739200	87		1.711472	1.71	1639.619	164.8807	2.926618	-2.39282
GT73	184	1.6E+07	87		2.510959	1.64	1572.5	231.9996	4.117973	-2.0513
GT73	303	2.6E+07	87		4.769567	1.47	1409.497	395.0027	7.011263	-1.51915

10.0 Appendix D: TGA and FT-IR

10.1 Thermal Gravimetric Analyses

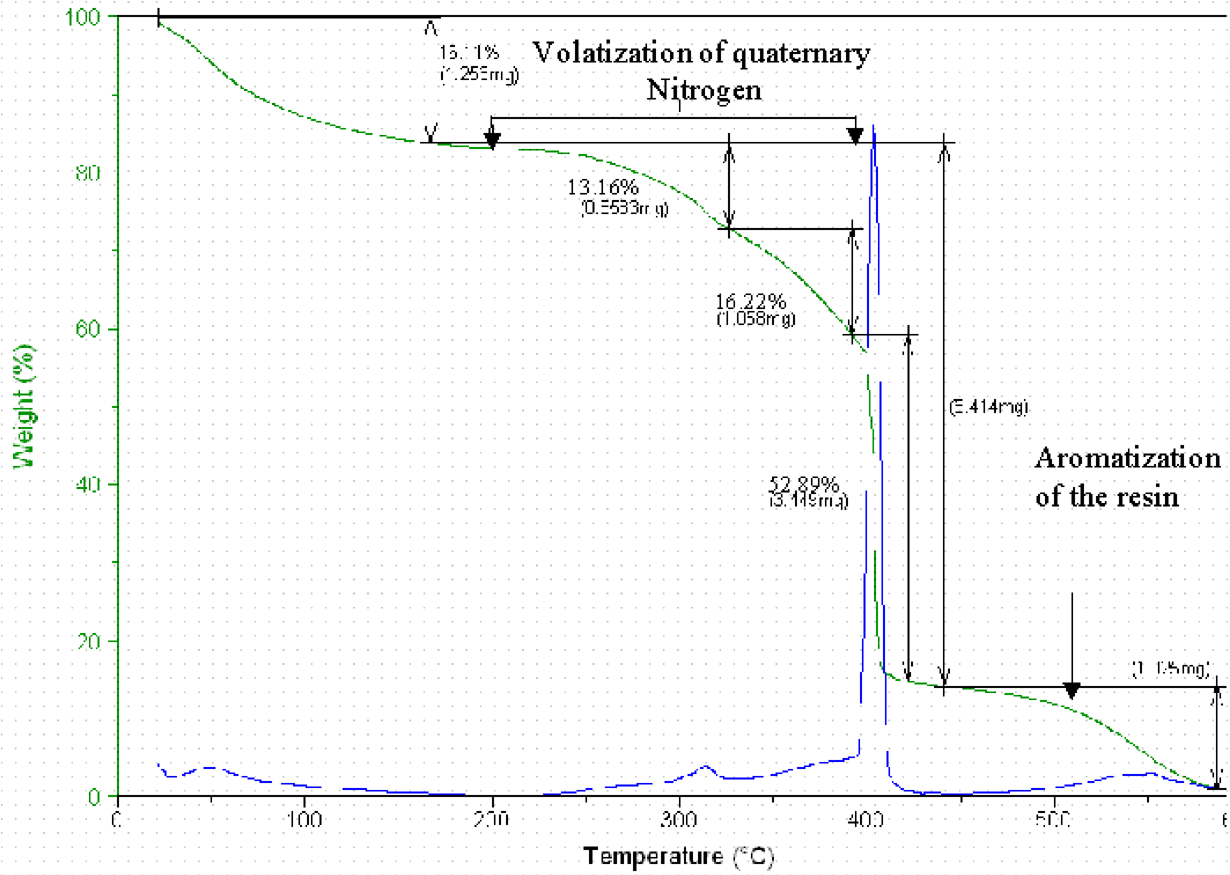


Figure D1. The Thermal Gravimetry Loss of the Dowex 21K-SW-Initial.

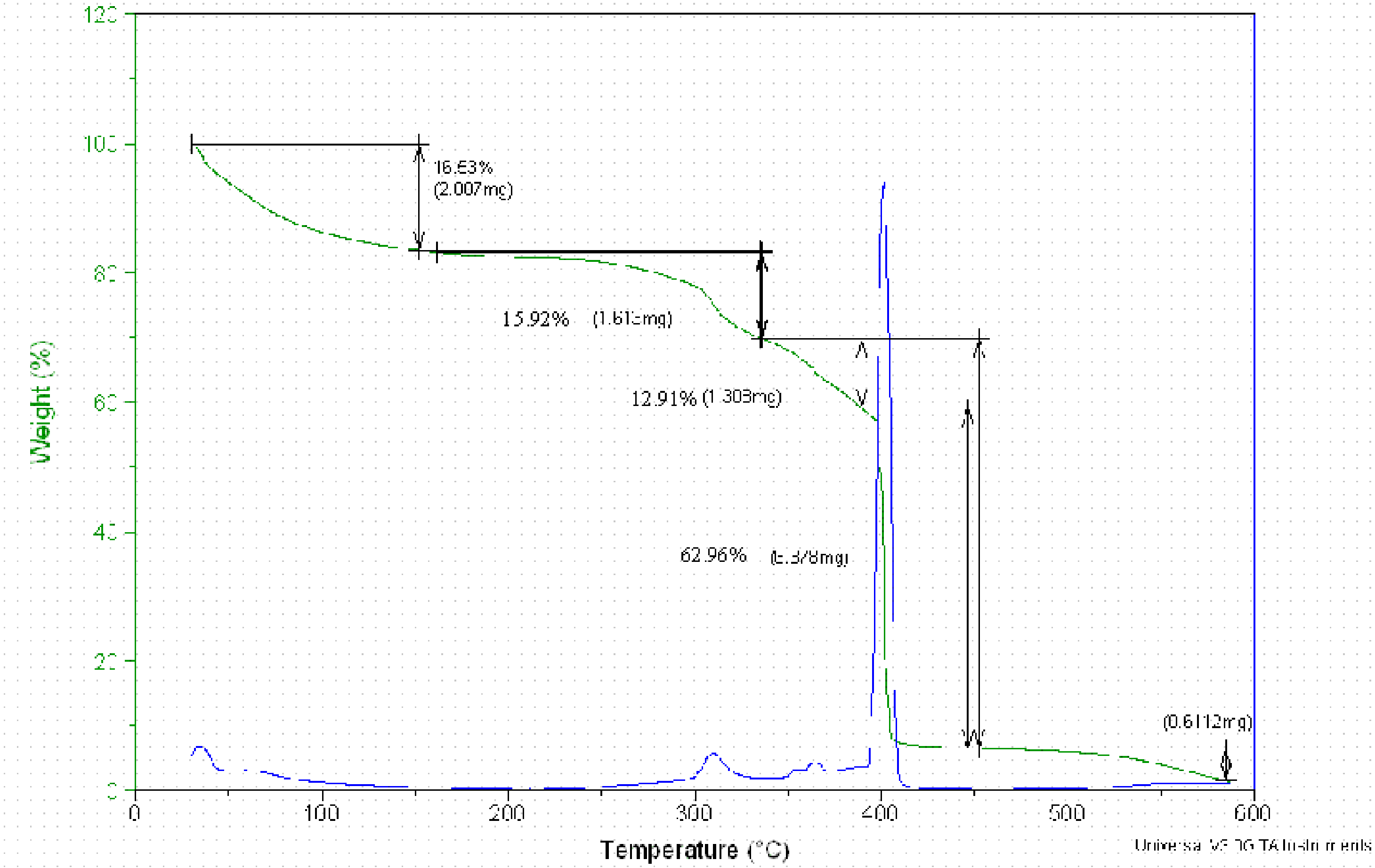


Figure D2. The Thermal Gravimetry Loss of the Dowex 21K Resin Treated at 37�C.

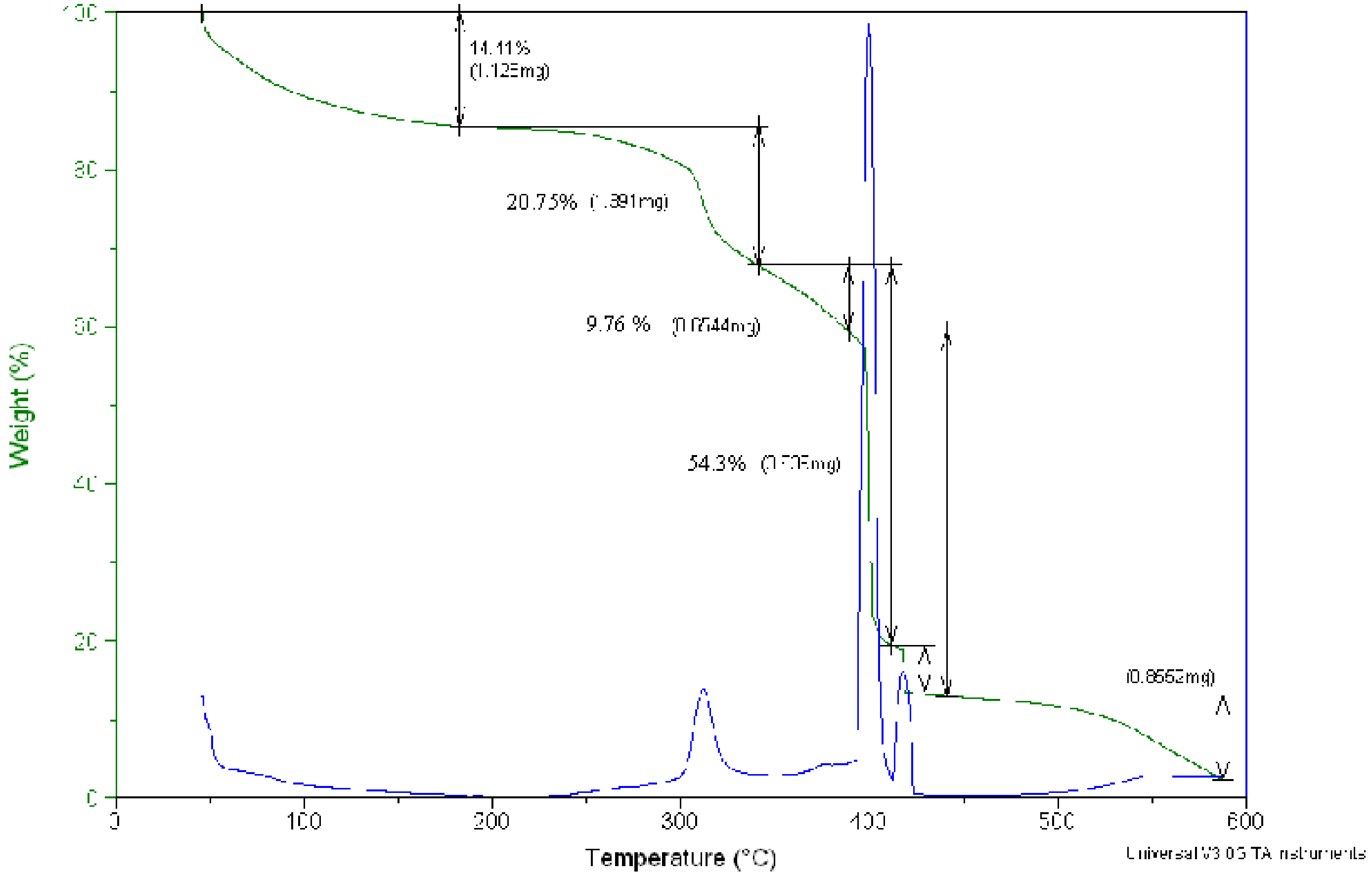


Figure D3. The Thermal Gravimetry Loss of the Dowex 21K Resin Treated at 53�C.

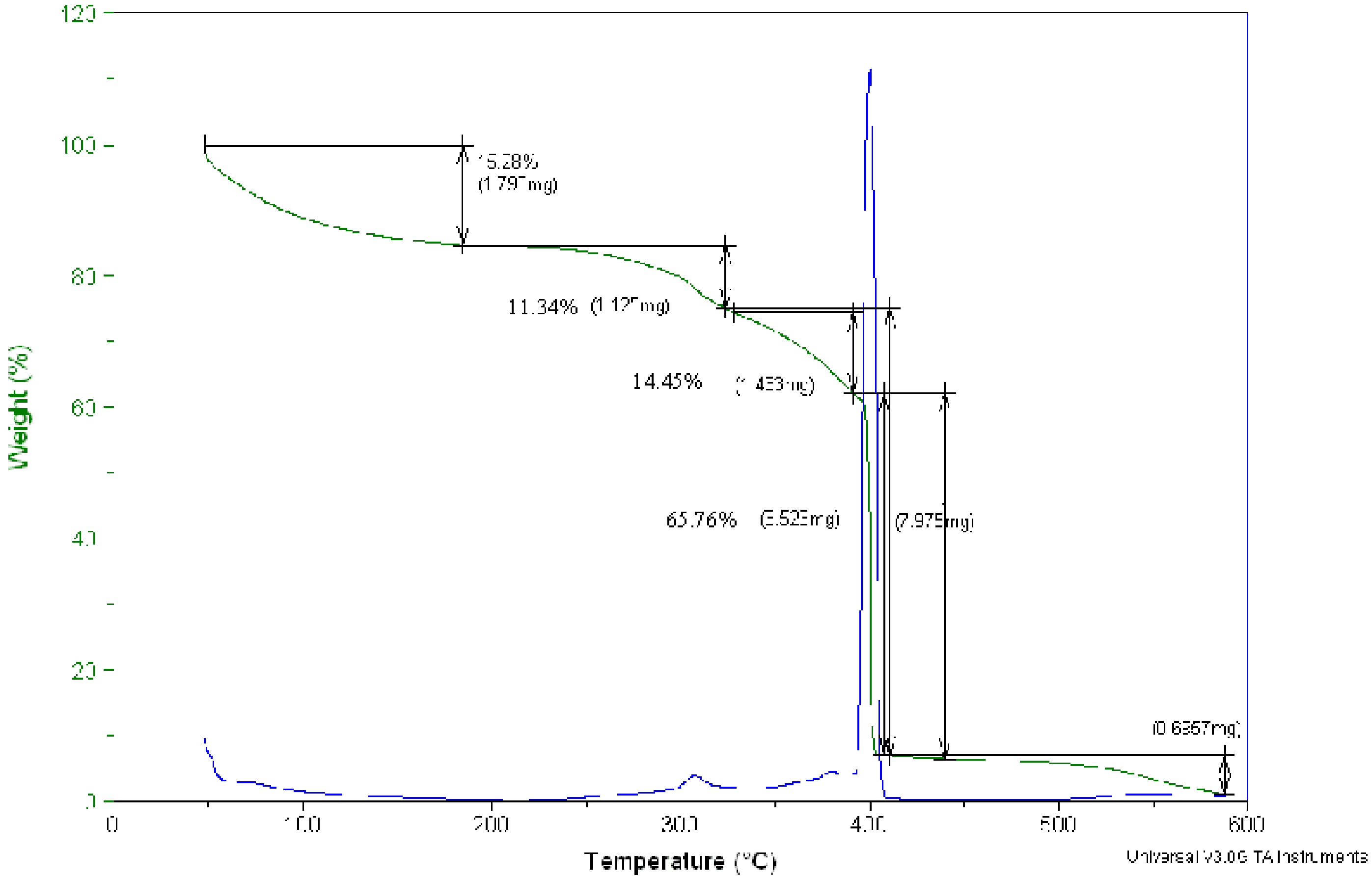


Figure D4. The Thermal Gravimetry Loss of the Dowex 21K Resin Treated at 70�C.

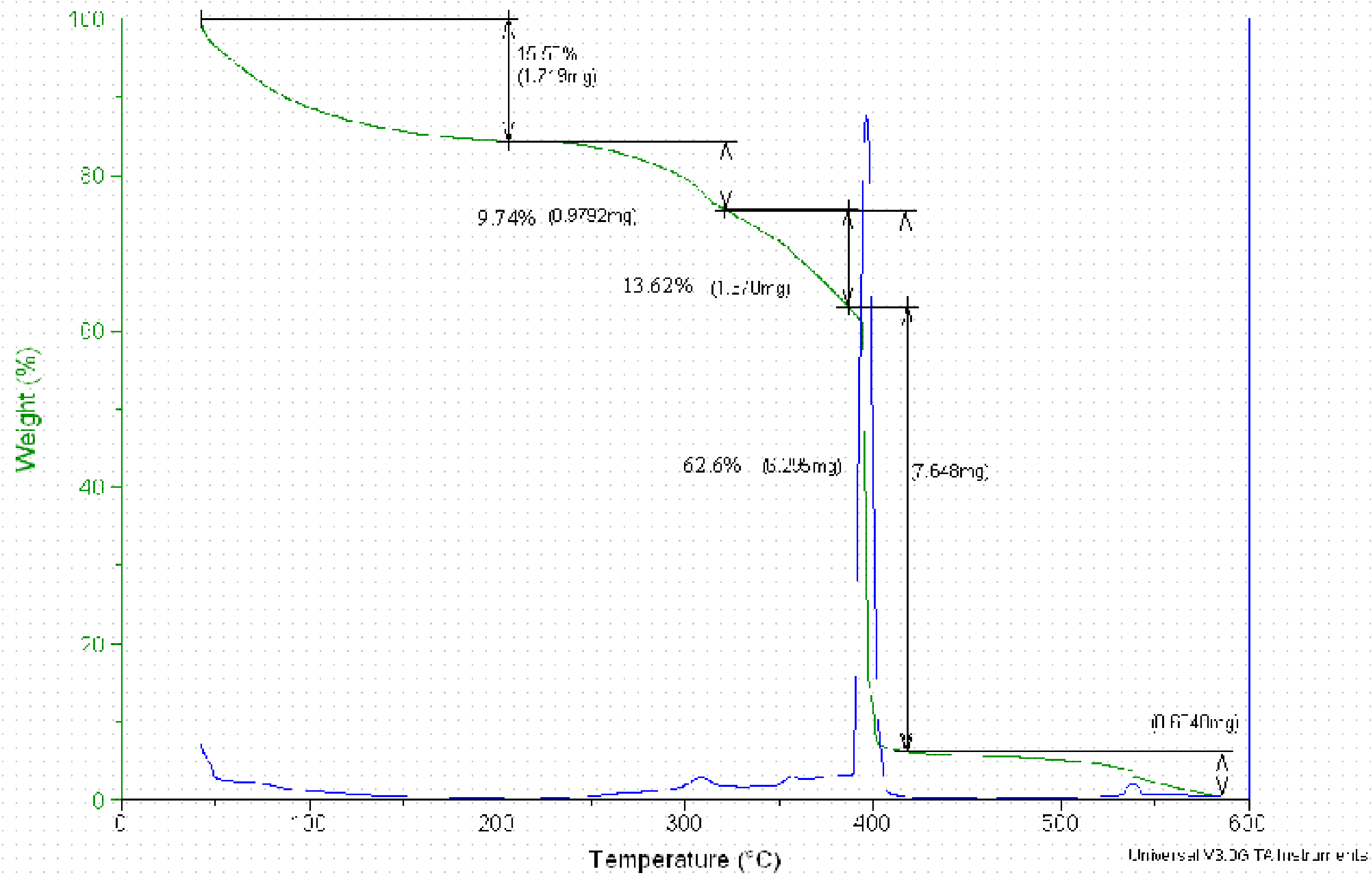


Figure D5. The Thermal Gravimetry Loss of the Dowex 21K Resin Treated at 87�C.

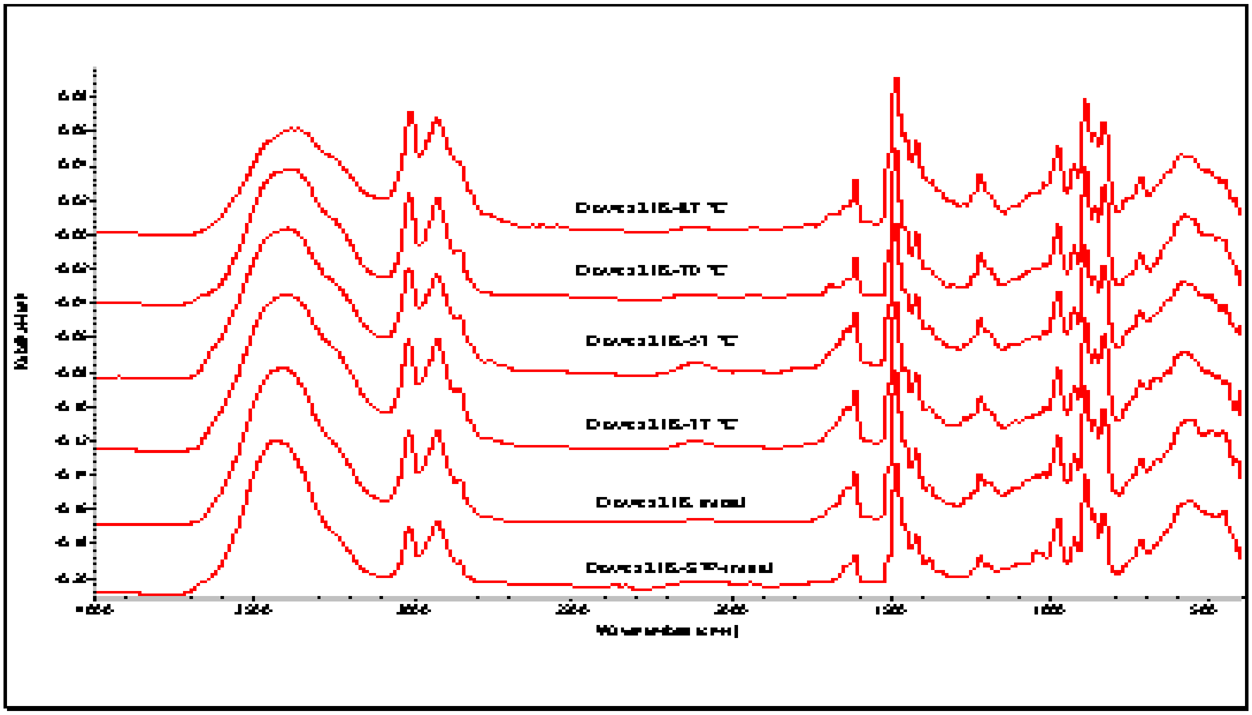


Figure D6. FT-IR Spectrum of the Dowex 21K Resins (2 mg of Resin to 250 mg of KBr). The Mixture was Placed in Diffuse Reflectance Accessory. The Accessory was Placed in NICOLET 210 Spectrometer. The Sample was Scanned 254 Times at a Resolution of 4 cm $^{�1}$.