

**PENNSYLVANIA SEA GRANT  
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**1. Cover Page**

- a. **Title:** Developing Quantitative Models for the Removal of Quaternary Ammonium Ions as Representative Cationic Emerging Contaminants by Cation Exchange Resins
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**2. Executive Summary**

Understanding the sorption mechanism of organic contaminants on cation exchange resins (CXR) will enable application of these resins for the removal of cationic organic compounds from contaminated water. In this study, sorption of a diverse set of 12 organic cations and 8 neutral aromatic solutes on two polystyrene CXRs, MN500 and Amberlite 200, was examined. MN500 showed higher sorption capacities due to its microporous structure. The sorption capacities followed the same trend of aromatic cations > aliphatic cations > neutral solutes for both resins. Generally, solute-solvent interactions, nonpolar moiety of the solutes, and resin matrix can affect selectivity of the cations. Sorption capacities of the neutral compounds were significantly less than those of the cations, indicating a combined effect of electrostatic and non-electrostatic interactions. By conducting multiple linear regression between Gibbs free energy of sorption and Abraham descriptors for all 20 compounds, polarity/polarizability (S), H-bond acidity (A), induced dipole (E), and electrostatic ( $J^+$ ) interactions were found to be involved in the sorption of the cations by the resins. After converting the aqueous sorption isotherms to sorption from the ideal gas-phase by water-wet resins, a more significant effect of  $J^+$  was observed. Predictive models were then developed based on the linear regressions and validated by accurately estimating the sorption of different test-set compounds with a root mean square error range of 0.91 to 1.1 and 0.76 to 0.85 for MN500 and Amberlite 200, respectively. The models also accurately predicted sorption behavior of aniline and imidazole between pH 3 and 10.

**3. Report**

**a. Introduction**

Many organic compounds are ionic in the aquatic environment. Aromatic amines such as substituted anilines, extensively used as pesticides, dyestuffs, and pharmaceuticals, can exist in aqueous solution as either cationic species under solution pH less than their pKa values or neutral species at pH greater than their pKa<sup>1-4</sup>. Other industrially significant compounds like quaternary ammoniums, commonly found in effluents from disinfectant, surfactant, fabric softener, antistatic agent, and wood preservation industries, exist in the cationic form in wastewater effluents<sup>5,6</sup>. The toxic effects of cationic organic contaminants (COCs) on human health and the environment require their efficient removal from contaminated water<sup>2,5-7</sup>. Although many treatment methods for water and wastewater effluents containing organic compounds have been developed, including photocatalytic oxidation<sup>8</sup>, electrolysis<sup>9</sup>, adsorption<sup>7</sup>, oxidation<sup>10</sup>, biodegradation<sup>11,12</sup>, and membrane<sup>13</sup>, there are only limited attempts for COCs removal from aqueous environments.

Ion exchange resins that consist of polymeric matrices and different functional groups can effectively remove ionic organic compounds (IOCs)<sup>14-16</sup> by exchanging with ionic solutes in solution. For cation exchange resins (CXR), the functional groups are mostly sulfonate or carboxylate groups<sup>17,18</sup>. Although activated carbon has been structurally modified for removing ionic compounds, it has shown lower selectivity and sorption capacity (about 100 times lower) than ion exchange resins in the removal of IOCs<sup>19</sup>. In addition, regeneration of the exhausted resin is attainable at ambient temperature with low

attrition rates as opposed to activated carbon whose thermal regeneration process is costly and energy intensive with high attrition rates<sup>20, 21</sup>.

Although sorption of IOCs by ion exchange resins is mainly a result of ion-exchange processes, it is also controlled by factors including hydrophobicity and types of functional groups of the solute, size and nature of the resin functional groups, dielectric constant of the solvent, and moisture content and matrix of the resin<sup>22-26</sup>. Several studies have shown that interactions between the nonpolar moieties (NPM) of an organic ion and those of the resin matrix determine the selectivity of the ion toward the resin<sup>23, 24, 27</sup>. For example, selectivity of polystyrene anion exchange resins for alkanesulfonic anions increased with increasing chain length of the anions<sup>23</sup>; higher selectivity was observed for larger aliphatic quaternary ammonium cations toward polystyrenesulfonic CXRs<sup>28, 29</sup>; and selectivity increased with increasing number of aromatic rings in the solutes due to the possibility of  $\pi$ - $\pi$  interactions between the aromatic compounds and the resin<sup>27</sup>. In addition, sorption reflects differences in interactions forces between solute-sorbent and solute-solvent, thus solvent-associated interactions (e.g. water-solute, water-sorbent, water-water interactions) have a profound effect on selectivity of sorption. For instance, sorption of ions with higher hydration energies or by resins with higher moisture contents is more difficult because expelling water molecules from the organic ions or from the resin matrix is more energy demanding<sup>24-26</sup>.

Poly-parameter linear free energy relationships (pp-LFERs) have been widely used for predicting partition behavior of neutral compounds from water to organic solvents<sup>30, 31</sup> or sorption of neutral compounds by various sorbents<sup>32, 33</sup> (eq 1). In the pp-LFERs method all possible interactions between a solute and a sorbent are considered in a general equation developed by Abraham<sup>34-37</sup>:

$$SP = eE + sS + aA + bB + vV + c \quad (1)$$

where SP represents a solvation property that is related to solute and solvent properties in a linear free energy relationship, and independent variables or descriptors E, S, A, B, and V account for the properties of the solute. E is the excess molar refraction accounting for nonspecific interactions due to London dispersive forces and Debye forces; V is McGown's characteristic molecular volume that accounts for cavitation energy and some additional nonspecific interactions; S is a combined dipolarity/polarizability descriptor; A and B are the overall solute hydrogen bond acidity and basicity; and c is a constant used to capture all other additional forces and might be entropy related<sup>30</sup>. The regression coefficients  $e$ ,  $s$ ,  $a$ ,  $b$ ,  $v$ , and  $c$  are determined by multiple linear regression analysis and reflect differences in the interaction forces between the solvent and the sorbent<sup>38</sup>.

Interactions that are responsible for sorption of organic ions by ion exchange should resins include the same nonspecific and specific (e.g. H-bonding,  $\pi$ - $\pi$ ) interactions for neutral solutes<sup>24, 39</sup>. In addition, electrostatic interactions is an important part of the specific interactions<sup>40, 41</sup>. To take into account any additional interactions in partition of an ion between two solvents, Abraham's group introduced new descriptors  $J^+$  and  $J^-$  for cationic and anionic solutes respectively, where  $J^-$  is zero for cations and  $J^+$  is zero for anions. Also, both descriptors are zero for neutral solutes<sup>42-44</sup>:

$$SP = eE + sS + aA + bB + vV + j^+ J^+ + j^- J^- + c \quad (2)$$

Like other regression coefficients in eq 1,  $j^+$  and  $j^-$  represent differences in the additional interaction forces between the two solvents.

Our recent work has successfully used the pp-LFERs approach to examine sorption of neutral organic solutes onto three non-ionic resins<sup>45</sup> or organic anions and neutral solutes onto three anion exchange resins<sup>46</sup>. Despite these, only a very limited number of studies have reported the uptake of organic cations by CXRs<sup>28, 39</sup> with little variation in the structures of the cations, understanding of molecular interactions remains phenomenological, and there is no *quantitative* model available to determine either sorption capacity or the level of electrostatic and non-electrostatic interactions between cations and CXRs. Toward this end, we investigated sorption mechanisms of 12 cationic and 8 neutral organic compounds over a

wide range of aqueous concentrations on two CXRs (MN500 and Amberlite 200). Using the isotherm data and the pp-LFERs approach (eq 2), we interpreted the sorption mechanisms and developed predictive models to calculate sorption capacity and selectivity of a diverse range of organic compounds on the studied resins under changing pH. Solvent-associated interactions were then removed using ideal gas phase conversion to separate the effect of solvent-associated interactions from that of solute-sorbent interactions<sup>45</sup>. In this method, aqueous sorption was converted to sorption by a water-wet sorbent from the ideal gas phase where there are no intermolecular interactions<sup>45, 47, 48</sup>. The aqueous sorption isotherms were then reconstructed to analyze differences in the solute-sorbent interactions which were obscured in the original aqueous sorption.

## b. Methodology

**Materials.** Two strong CXRs, MN500 and Amberlite 200, and one weak CXR, Amberlite IRC-76, were provided by Purolite® and Dow® (U.S.) respectively (properties in Table S2 and analytical methods in Texts S6-8). Both strong CXRs are polystyrenic, MN500 is microporous while Amberlite 200 is porous; Amberlite IRC-76 is polyacrylic. Prior to use, the resins were sequentially washed by HCl, NaOH, NaCl and methanol (details in Text S4). Six aliphatic and three aromatic quaternary ammoniums, four substituted phenols, four substituted anilines, imidazole, and nitrobenzene (NB) were purchased from Fisher Scientific. Analytical grade chemicals were used as purchased to prepare solutions with nanopure deionized water. The properties of solutes and their abbreviations are listed in Table 1.

**Adsorption Experiments.** Batch experiments for adsorption isotherms were carried out in amber glass bottles with Teflon-lined screw caps at ambient temperature (22±1°C). For each isotherm at least 17 experimental data points were collected. The concentration of NaCl was 20 mM in all samples to keep ionic strength constant, and the aqueous concentration of all ionic solutes was between 0.003 and 4 mM. For neutral solutes, the equilibrium concentration range was selected based on the compound solubility. Trial experiments were conducted to determine solid to solution ratios to achieve 25%-75% removal of the solutes. The pH was adjusted using 0.2 M NaOH and HCl to keep the solutes in the desired charged form. The amber bottles containing resin and the target compound solution were shaken under 175 rpm for 48 hours. Preliminary kinetic experiments showed that all sorption reached equilibrium within a few hours and there was no significant removal after about 10 hours. After reaching equilibrium, NB, anilines, and phenols were analyzed using high-performance liquid chromatography (HPLC-Agilent) and the quaternary ammonium cations and imidazole were analyzed using a total organic carbon analyzer (TOC-Shimadzu) (details in Text S5). Sorption of the target compounds was determined from the differences between the initial and final concentrations.

**Table 1.** Physical-Chemical Properties of the Selected Organic Compounds.

Compound	logK <sub>GW</sub> <sup>a</sup>	Hydration Energy <sup>c</sup> (KJ/mol)	Solute Descriptors <sup>d</sup>					
			E	S	A	B	V <sup>§</sup>	J <sup>+</sup>
Aniline	-4.03	-5.09	0.96	0.96	0.26	0.41	0.82	0
4-Nitroaniline (4-NA)	-7.12	-22.72	1.24	1.83	0.51	0.34	0.99	0
2-Nitroaniline (2-NA)	-5.13	-11.36	1.18	1.37	0.30	0.36	0.99	0
4-Chloroaniline (4-CA)	-4.35	-6.91	0.91	1.36	0.36	0.25	0.96	0
Phenol	-4.59	-8.28	0.81	0.89	0.60	0.30	0.78	0
4-Nitrophenol (4-NP)	-7.66	-25.80	1.07	1.72	0.70	0.22	0.95	0
2-Nitrophenol (2-NP)	-3.1	0.22	1.02	1.05	0.05	0.37	0.95	0
4-Chlorophenol (4-CP)	-5.05	-10.91	0.92	1.24	0.55	0.22	0.90	0
2,6-Dichlorophenol (2,6-DCP)	-3.96	-4.96	0.90	0.90	0.38	0.24	1.02	0
4-Methylphenol (4-MP)	-4.15	-5.77	0.82	0.87	0.57	0.31	0.92	0
Nitrobenzene (NB)	-3.12	0.10	0.87	1.11	0.00	0.28	0.89	0
Protonated aniline (Aniline <sup>+</sup> )	-14.5 <sup>b</sup>	-64.82	0.81	1.62	1.93	0	0.84	0.62
Protonated N,N-dimethylaniline (DMA <sup>+</sup> )	-14.2 <sup>b</sup>	-63.11	0.81	1.85	1.84	0	1.12	0.81
Protonated Imidazole (Imidazole <sup>+</sup> )	-16.5 <sup>b</sup>	-76.23	0.56	2.5	1.61	0	0.56	1.05
Tetramethylammonium (NMe <sub>4</sub> <sup>+</sup> )	-9.76	-37.80	-0.20	1.48	0.82	0	0.81	1.24

Tetraethylammonium (NEt <sub>4</sub> <sup>+</sup> )	-9.27	-35.00	-0.52	1.81	0.57	0	1.41	1.52
Tetrapropylammonium (NPr <sub>4</sub> <sup>+</sup> )	-8.67 <sup>b</sup>	-32.17	-0.07	1.72	0.49	0	1.92	1.64
Tetrabutylammonium (NBu <sub>4</sub> <sup>+</sup> )	-8.16 <sup>b</sup>	-29.36	-0.10	1.90	0.40	0	2.48	1.65
(2-Chloroethyl)trimethylammonium (CETM <sup>+</sup> )	-14.4 <sup>b</sup>	-64.25	0.11 <sup>e</sup>	1.83 <sup>f</sup>	0.85 <sup>f</sup>	0	1.06	1.80 <sup>f</sup>
(2-Bromoethyl)trimethylammonium (BETM <sup>+</sup> )	-15.4 <sup>b</sup>	-69.95	0.29 <sup>e</sup>	1.86 <sup>f</sup>	0.82 <sup>f</sup>	0	1.11	2.00 <sup>f</sup>
Phenyltrimethylammonium (PTM <sup>+</sup> )	-16.5 <sup>b</sup>	-76.23	0.67 <sup>e</sup>	2.07 <sup>f</sup>	0.82 <sup>f</sup>	0	1.26	2.00 <sup>f</sup>
Benzyltriethylammonium (BTM <sup>+</sup> )	-15.8 <sup>b</sup>	-72.23	0.53 <sup>e</sup>	2.40 <sup>f</sup>	0.57 <sup>f</sup>	0	1.82	2.20 <sup>f</sup>
Vinylbenzyl trimethylammonium (VBTM <sup>+</sup> )	-17.8 <sup>b</sup>	-83.64	0.89 <sup>e</sup>	2.17 <sup>f</sup>	0.87 <sup>f</sup>	0	1.64	2.15 <sup>f</sup>

<sup>a</sup>  $K_{GW}$  is the dimensionless Henry's law constant<sup>41</sup>; <sup>b</sup> estimated based on the modified bond contribution method<sup>44</sup>; <sup>c</sup> estimated based on  $\Delta G_{G,W,i} = -RT \ln K_{GW} + RT \ln V_W/V_G$  where  $V_W$  and  $V_G$  are the molar volume of water and the gas phase, respectively<sup>45</sup>; <sup>d</sup> Abraham descriptors<sup>31,42</sup>; <sup>e</sup> estimated from refractive index<sup>42</sup>; <sup>f</sup> estimated based on the group contribution method (Table S3)<sup>49</sup>; <sup>g</sup> McGowan's characteristic molecular volume<sup>49</sup>.

**Estimating Abraham Descriptors.** Estimating descriptors for solutes that do not have reported descriptor values is important for using pp-LFERs. Descriptor V is the McGowan characteristic volume and was estimated based on the volumes of all atoms and the number of bonds in the molecular structure<sup>35,49</sup>. Descriptor E can be estimated from refractive index<sup>42</sup>. Cations typically have negligible H-bond basicity, so we fixed their B values at 0. Two methods were used for estimating descriptors A, S, and J<sup>+</sup> for quaternary ammoniums: the modified group contribution method<sup>49</sup>, and the method based on the reported pp-LFERs between compound's partition coefficients (lnP) and solute descriptors<sup>31</sup>. In the first method, the properties of each compound arise from the contributions of all functional groups in the structure. Thus, solute descriptors can be estimated as the sum of descriptor values of all functional groups. Tetramethylammonium (NMe<sub>4</sub><sup>+</sup>) was used as the basic structure and its reported descriptor values (Table 1) were modified based on the contributions of all additional functional groups in each solute structure. Detailed calculations are in Table S3.

In the pp-LFERs approach, the descriptors of a solute can be estimated based on the reported regression coefficients ( $c$ ,  $e$ ,  $s$ ,  $a$ ,  $b$ ,  $v$ , and  $j^+$ ) for multiple solvent-water systems and its respective experimental lnP values in these systems. First, the experimental lnP values were estimated based on the ion transfer energy ( $\Delta G_{tr}^o = -RT \ln P$ ) from SPARC (<http://www.archemcalc.com/sparc.html>), an online chemical properties calculator. Second, the lnP values of the solute in the solvent-water systems were calculated based on the known regression coefficients for each solvent using eq 2 and hypothetical descriptor values. Then, mathematical procedures such as Solver® in Microsoft Excel were used to calculate the unknown descriptors by minimizing differences (i.e. mean weighted square errors MWSE) between the experimental lnP values and the calculated ones<sup>35</sup>. Note that it is necessary to have solvents with different physical chemical properties, and the number of solvent-water systems should be greater than the number of unknown descriptors. The descriptors for DMA<sup>+</sup> and imidazole<sup>+</sup> were estimated based on the descriptors for the corresponding neutral solutes. Abraham and Acree<sup>31</sup> have developed a set of equations to predict descriptors for protonated amines based on the descriptors for neutral amines.

**Estimating Henry's Law Constants (logK<sub>GW</sub>) for Cationic Solutes.** Henry's law constants are required for the gas phase conversion analysis. Two approaches were examined for accuracy in estimating logK<sub>GW</sub> values. The first approach is based on  $\Delta G_{G-W} = -RT \ln K_{GW}$ , where  $\Delta G_{G-W}$  were calculated in SPARC or Gaussian in WebMO (<http://www.webmo.net/demo/index.html>), a web-based interface for computational chemistry programs. In comparison with the reported Henry's law constants, neither programs estimated  $\Delta G_{G-W}$  accurately (data now shown). The second approach is the modified bond contribution method<sup>50</sup> where logK<sub>GW</sub> can be estimated from logK<sub>GW</sub> of a structurally-related compound by adding or subtracting contributions of all additional bond values in the molecular structure (see one example in Table S4). The obtained logK<sub>GW</sub> values were then slightly adjusted ( $\pm < 0.55$  log units which is similar to the reported error for experimentally determined lnP<sup>31</sup>) to improve precision of the predictive model (root mean square error values or RMSE) after the gas-phase conversion.

### c. Results

**pH effect on sorption capacities of resins.** The pH effect on the sorption of neutral aromatic and quaternary ammonium compounds was studied to examine the contribution of electrostatic versus non-electrostatic interaction to sorption capacity. The sorption capacity of quaternary ammoniums on two strong cation exchange resins, MN500 and Amberlite200, is pH-independent. The quaternary cations are permanently charged, indicating that electrostatic interactions are pH independent. Sorption of nitrobenzene (NB) on the cation exchange resins is also pH independent but is significantly lower than that of the cations, this is because neutral NB does not have any electrostatic interactions with the ion exchange resins. The pH effect was then investigated for aniline ( $pK_a = 4.67$ ) as a compound that undergoes proton transfer reaction under changing pH conditions. Aniline is protonated at  $pH < pK_a$  and neutral at  $pH > pK_a$ . Sorption of aniline is strongly pH-dependent which significantly decreased when the ratio of protonated aniline to neutral aniline decreased, showing that the protonated aniline had higher sorption capacity than neutral aniline. We attributed this to the fact that protonated aniline undergoes ion exchange reactions (electrostatic) in addition to hydrophobic (nonelectrostatic) interactions. Also, sorption of aniline slightly decreased when pH was lower than 3, due to competition with  $H^+$  for the sorption sites.

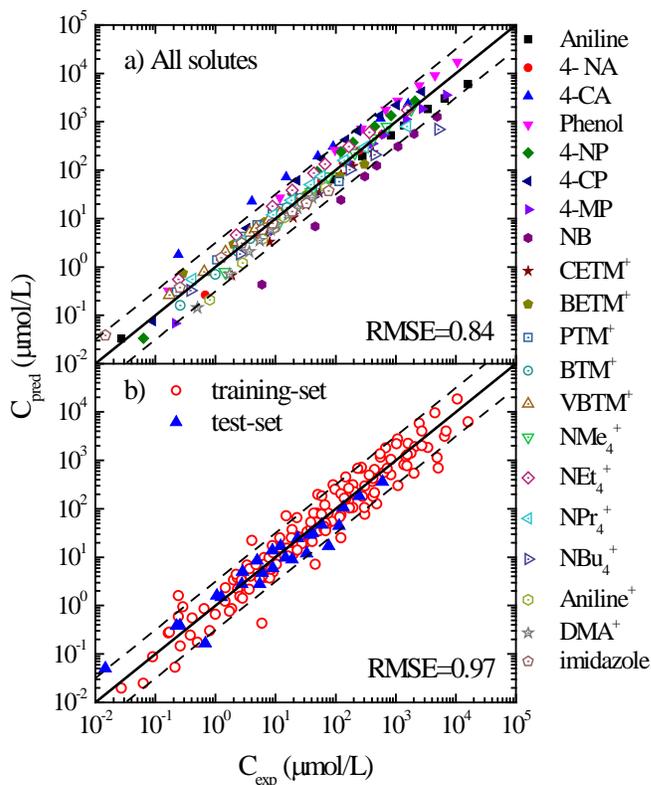
**Aqueous Sorption Isotherms.** In general, MN500 exhibits higher sorption capacity than Amberlite 200, because MN500 has a high proportion of micropores (more than 48% of pore volume) which enhanced sorption energy due to superposition of force fields of the opposite walls<sup>51</sup>. Although Amberlite 200 has a lower moisture content than MN500, it has a significantly lower surface area (42 versus 370  $m^2/g$ ), thus, there are less sites available for solute sorption. Sorption affinity of organic compounds on MN500 and Amberlite 200 follows the order of: aromatic cations > aliphatic cations > neutral aromatic solutes. The higher affinity of the cationic compounds indicates that the primary sorption process is ion exchange. The interactions between the nonpolar moieties of the ions and of the resins and solvent-associated interactions are two important factors that influence on the resin selectivity. The higher sorption affinities of the aromatic cations can be attributed to the strong non-electrostatic interactions resulting from  $\pi - \pi$  interactions between the aromatic rings of the resin matrix and the aromatic cations. While the neutral aromatic compounds have the ability of forming  $\pi - \pi$  interactions, the lack of electrostatic interactions resulted in their much lower removal by the cation exchange resins.

The sorption behavior of two neutral compounds (phenol and NB) on ionic and nonionic resins was studied in order to investigate the effect of resin structure. The neutral resins showed much higher sorption capacities (at least 5 times higher) than the ionic resins with sorption capacity following the order of: MN200 > XAD-4 > XAD-7 > MN500 > IRA-96 > IRA-910. This behavior can be mainly contributed to the higher surface areas of the neutral resins and the highly hydrophilic nature of the ionic resins (due to the presence of functional groups). Sorption of the neutral compounds on MN200 exhibits the highest sorption capacity among the neutral resins due to its high surface area and microporous structure with high sorption potential<sup>45</sup>. Comparing with XAD-7, XAD-4 has a larger pore volume (1.25 versus 1.12  $cm^3/g$ ) and a higher proportion of micropores (12.4% > 2.3%). Moreover, XAD-7 has the highest moisture content (67%) due to its polar acrylic structure, while the moisture content of XAD-4 and MN200 is 56% and 58%. Lower sorption affinity of IRA-96 and IRA-910, two anion exchange resins, can be related to their higher moisture contents than the cation exchange resin MN500. IRA-910 and IRA-96 have higher ion exchange capacities (5.33 and 6.19 meq/g-dry respectively) than MN500 and Amberlite200 (1.07 and 2.43 meq/g-dry respectively), which can result in more hydrophilic structures.

Multiple linear correlations between the natural logarithm of selectivity and Abraham's solute descriptors was conducted at different sorbed concentrations to examine the contribution of different

interactions to the overall selectivity of the cations. We found that selectivity was mainly promoted by dipolar/polarizability effects; induced dipole (E), electrostatic ( $J^+$ ), and H-accepting interactions (A) had some positive effects on the selectivity. H-bond basicity (B) had a large positive effect which applies to the neutral compounds only since B is almost zero for all cations. After the gas phase conversion, the contribution of solvent-associated interactions to the Gibbs free energy change has been eliminated, and consequently the contribution of solute-sorbent interactions can be obtained. Unlike the aqueous phase, electrostatic interaction has the most dominant effect on the sorption of the cationic compounds from the gas phase.

**Development of Predictive Model.** A predictive model was developed based on the above obtained regression coefficients at various sorbed concentrations and was then used to estimate aqueous equilibrium concentration at any given  $Q_e$ . Details of the model development are included in our recently accepted paper in Environmental Science & Technology.<sup>52</sup> **Figures 1** illustrates the correlation of the estimated equilibrium concentrations using the predictive model with the experimental values. The good correlation results indicate that the predictive model is able to accurately predict the sorption behavior of a diverse range of cationic and neutral solutes. Overall these findings will provide guidance to resin selection processes in a given treatment scenario, and will also help polymer industry synthesizing resins with desired physical-chemical properties.



**Figure 1.** Aqueous equilibrium concentrations calculated based on the predictive model versus the experimental values for a) a training-sets including 12 cations and 8 neutral aromatic solutes with 169 data points and b) a training-set of 17 solutes with 153 data points and 3 test set solutes (4-NA, PTM+, and imidazole) with 27 data points for MN500. The solid lines show a perfect prediction, where the predicted value for  $C_e$  exactly equals the experimental value; the dashed lines are 0.5 log units above or below the solid lines.

#### d. Conclusions

Overall, our results show that CXRs can be effective in the removal of COCs from contaminated water. Understanding the sorption mechanism is fundamental for selecting and synthesizing appropriate resin for a given contaminant. The sorption of organic solutes by CXRs is mainly affected by resin properties like moisture content, resin matrix, and surface area as well as solute structure. The selective removal of ionic organic contaminants by CXRs through ion exchange processes is promoted by non-electrostatic interactions between the non-polar moieties of the solutes and the resin matrix. pp-LFERs enable us to identify the predominant molecular interactions between solute and resin and to develop predictive models for estimating the sorption capacity of a target contaminant on a given resin at any environmentally relevant pH. Further addition of compounds with diverse structures to the training set will expand the ability of the predictive models to handle a large number of solutes. The gas-phase conversion is a useful approach for eliminating solute-solvent effects which obscure solute-sorbent interactions in the aqueous phase.

**e. Additional Research Indicated**  
N/A

**f. Citations**

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#### 4. Appendix A

##### a. Staff

- i. Number of individuals: 1
- ii. Number of full-time employees (as part of the grant): 1  
Dr. Huichun (Judy) Zhang
- iii. Number of full-time employees (as part of match): 0

##### b. Students Supported

- i. Number of Undergraduate Students: 1  
Quiana M Waters, Civil & Environmental engineering, undergraduate student
- ii. Number of Graduate Students: 1
- iii. Number of Ph.D. Students: 1  
Ms. Nastaran Jadbabaei, Ph. D. Candidate
- iv. Degrees Awarded (please indicate level)  
Quiana M Waters, B. S. in Civil engineering (Environmental engineering concentration)  
Ms. Nastaran Jadbabaei has not graduated yet.

##### c. Outreach/Extension

- i. Number of meetings, workshops, or conferences, and number of attendees:  
3 professional meetings, the first one had about 40 attendees and the second one had about 30 attendees (details below), the third one (2014 Gordon Research Conferences: Environmental Sciences: Water) had about 170 attendees.
- ii. Number of public or professional presentations, and number of attendees:  
2 professional meetings, the first one had about 40 attendees and the second one had about 30 attendees.

Jadbabaei, N.; **Zhang, H.**; "Revisit sorption mechanisms of organic compounds on cation exchange resins", 246<sup>th</sup> ACS National Meeting, Division of Environmental Chemistry, Indianapolis, IN, USA, Sept. 8 – 12, 2013.

Jadbabaei, N.; **Zhang, H.**; “Revisit sorption mechanisms of organic compounds on cation exchange resins”, *American Water Resources Association*, Philadelphia Metropolitan Area Section (AWRA-PMAS) on “Constructed Wetlands for On-site Wastewater Treatment”, Philadelphia, PA, Feb 20, 2014.

## 5. Appendix B

**Impact Statement(s) (< 250 Words each)** Impact statements document the verifiable results of the research and how efforts have made a difference in the lives of coastal residents, communities, and environments. They should effectively describe the significant economic, societal, and/or environmental benefits of the research, outreach/extension, education, and communications work.

Impact Statement Format

(<http://seagrant.noaa.gov/NetworkResources/EvaluationandReporting/ImpactStatementGuidance.aspx>):

- **Relevance:** A fundamental understanding of the sorption mechanisms and development of predictive models will contribute to a major advance in the development, synthesis, and application of cation exchange resins as a new water treatment technology targeting cationic organic contaminants removal at the local, state, regional, national and even international scale.
- **Results:** Removal of cationic organic contaminants from drinking water will directly protect human health while cleaned wastewater will protect receiving waters from contamination and enable more wastewater to be recycled to alleviate increasing shortages of fresh water supplies.<sup>53</sup> Application of the developed models and approaches to other sorbents will also take the understanding of sorption processes in general to a new level that is not accessible using current approaches. In addition to being used in water treatment, resins have found numerous applications in separation and purification processes. For example, many bioproducts can be effectively recovered and purified from their fermentation broths using resins;<sup>54-58</sup> chemical intermediates and products can also be effectively separated from renewable resources (e.g. biomass-based feedstocks) by resins.<sup>59</sup> Therefore, results from this project will also facilitate the application of resins to other processes where separation and purification of materials are needed.
- **Response:** We have successfully developed predictive models for two cation exchange resins (MN500 and Amberlite 200) that can be used to accurately estimate sorbed concentrations of a number of cationic organic contaminants by these two resins at any given solution pH.
- **Project Partners:** PA-WRRC, Purolite® (Philadelphia, PA)