Application of an easily water-compatible hypercrosslinked polymeric adsorbent for efficient removal of catechol and resorcinol in aqueous solution

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ABSTRACT

An easily water-compatible hypercrosslinked resin HJ-1 was developed for adsorbing catechol and resorcinol in aqueous solution in this study. Its adsorption performances for catechol and resorcinol were investigated in aqueous solution by using the commercial Amberlite XAD-4 as a reference. The adsorption dynamic curves were measured and the adsorption obeyed the pseudo-second-order rate equation of Boyer and Hsu. The adsorption isotherms were scaled and Freundlich isotherm model characterized the adsorption better. The adsorption thermodynamic parameters were calculated and the adsorption was an exothermic, favorable, and more ordered process. The fact that the adsorption capacity of catechol was larger than resorcinol and the adsorption enthalpy of catechol was more negative than resorcinol can be explained in terms of the solubility and the polarity of two adsorbates.

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1. Introduction

Phenol and substituted phenol are important organic intermediates for the products of industry and agriculture [1]. For example, catechol is widely used to produce food additive agents, hair dyes, and antioxidants [2]. Resorcinol is usually employed to produce dyes, plastics, and synthetic fibers [3]. As a result, catechol and resorcinol are extensively present in the effluents of their manufactures and hence introduced into water inevitably. However, these compounds are considered as the primary pollutants in the wastewater due to their high toxicity, high oxygen demand, and low biodegradability [4,5]. Consequently, removal of them from wastewater has attracted significant environmental concerns.

Many methods have been developed to deal with the wastewater containing phenolic compounds [6–10], and adsorption based on adsorbents is very effective [11]. Activated carbon is frequently used in the adsorption due to its large specific surface area and predominant proportion of micropores [12]. Nevertheless, its use is limited due to its high cost and inefficient regeneration. In contrast, synthetic polymeric adsorbents are more feasible because of its favorable regeneration and structural diversity [13].

Among the synthetic polymeric adsorbents, the Amberlite XAD-4 resin is considered to be one of the best adsorbents for removal of phenolic compounds from wastewater, especially for phenol [14]. Moreover, some other hypercrosslinked polymeric adsorbents are developed and they display large adsorption capacity towards some aromatic organic compounds with limited solubility in water [15–17], but they are helpless for the compounds exhibiting strong hydrophilic affinity to water due to their hydrophobic surface. Their adsorption selectivity is also very low as a result of absence from special functional groups on their matrix which can adsorb one solute or one family of solutes with similar chemical structure from a complex system. To obtain large adsorption capacity and high adsorption selectivity for a specific organic compound, development of the high selective adsorbents is requested [18–21]. These high selective adsorbents will only adsorb one single or a small number of solutes capable of interacting with the adsorbent through a certain mechanism [22,23].

The purpose of the present study was to develop an easily water-compatible hypercrosslinked resin HJ-1 with large capacity and strong affinity to catechol and resorcinol. This was achieved from chloromethylated poly(styrene-co-divinylbenzene) (PS) by using post-crosslinked reaction. The adsorption kinetics and equilibrium were thereafter tested in comparison with the XAD-4 resin in aqueous solution, and the adsorption thermodynamics were expounded in detail.
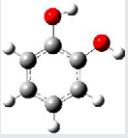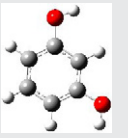
2. Materials and methods

2.1. Materials

Macroporous crosslinked chloromethylated PS was obtained from Langfang Chemical Co. Ltd. (Hebei province, China), its crosslinking degree was 6%, and the chlorine content was 17.3%. The

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Table 1
The main properties of catechol and resorcinol.

	Catechol	Resorcinol
Formula	$C_6H_4(OH)_2$	$C_6H_4(OH)_2$
Molecular structure[a]		
Molecular size[a]	0.55 nm × 0.55 nm	0.56 nm × 0.47 nm
Molecular weight (g/mol)	110.11	110.11
pK_a (at 298 K)[b]	9.4	9.4
Solubility (at 298 K, g/100 mL H_2O)[b]	45.1	123
λ_{max} in aqueous solution	273.2	275.2
Hydrogen bonding acidity (α)[c]	0.85	1.10
Hydrogen bonding basicity (β)[c]	0.52	0.58
The dipole moment (D)[d]	2.620	2.071

  [a] Taken from the results from Gaussian 03 software package [24].
  [b] Taken from Ref. [25].
  [c] Taken from Ref. [26].
  [d] Taken from Ref. [27].

Amberlite XAD-4 resin was purchased from Rohm & Haas Company (USA). Catechol and resorcinol used as the adsorbates are analytical grades and their main properties are shown in Table 1 [24–27].

2.2. The polymeric adsorbent

80 g of chloromethylated PS beads were dried at 323 K in vacuum for 8 h and then swollen with 300 mL of nitrobenzene at 298 K overnight in a 500 mL of three-neck round-bottomed flask equipped with a thermometer, a reflux condenser, and a mechanical stirrer. 7.5 g of new-cauterized anhydrous zinc chloride was added into the reaction flask with the temperature at 323 K. Half an hour later, the reaction mixture was evenly heated to 388 K within 1 h, and HJ-1 beads were attained after 12 h. The polymeric beads were poured into water, and washed with 1% of hydrochloric acid (w/w) aqueous solution and ethanol until the solution is transparent. Finally, they were extracted with ethanol for 8 h.

2.3. Batch adsorption experiment

The HJ-1 resins are easily water-compatible and can be wetted easily by water, and hence they were accurately weighed (about 0.150 g) and introduced directly into a 25 mL of catechol or resorcinol aqueous solution with different initial concentrations, C_0 (mg/L), while the XAD-4 resin was wetted with 0.5 mL of methanol and rinsed with deionized water for three times before use. The initial concentration of catechol and resorcinol was set to be about 200, 400, 600, 800, 1000, and 1200 mg/L, respectively. Then the flasks were shaken in a thermostatic oscillator with identical rotational speed at a desired temperature until the adsorption equilibrium was reached. The equilibrium concentration, C_e (mg/L), was deter-

Table 2
The typical properties of HJ-1 resin in comparison with the Amberlite XAD-4 resin.

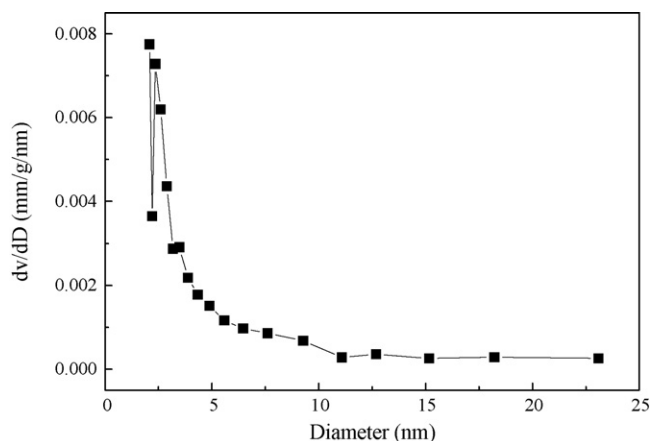| Properties	XAD-4	HJ-1 resin
Structure	Polystyrene	Polystyrene modified with a few formaldehyde carbonyl groups
Polarity	Non-polar	Moderate polar
Specific surface area (m^2/g)	750	727
Average pore diameter (nm)	5.8	3.25
Particle size (mm)	0.4–0.6	0.4–0.6
Porosity (mL/g)	1.0	0.59
Chlorine content (%)	–	3.66
Oxygen content (%)	0	5.65
Color	White	Brown

Fig. 1. The pore distribution of HJ-1 resin.

mined subsequently, and the equilibrium adsorption capacity, q_e (mg/g), was calculated by conducting a mass balance on the adsorbates before and after the test.

Adsorption kinetic studies for catechol and resorcinol were performed by analyzing the adsorption capacity with the different initial concentration of about 100, 300, and 500 mg/L at different time intervals at 293 K until the adsorption equilibrium was reached.

3. Results and discussion

3.1. The characterization of HJ-1 resin

Table 2 lists the typical properties of HJ-1 resin and XAD-4 resin, and it is displayed the chemical composition of the two resin is different. The pore distribution of HJ-1 resin is presented in Fig. 1, and the micro/mesopores play a predominant role in HJ-1 resin. One moderate vibrational band at 1704.8 cm^{-1} which can be assigned to formaldehyde carbonyl groups in the IR spectrum (not shown) of HJ-1 resin indicates that oxidation of the CH_2Cl groups has taken place [28].

3.2. Adsorption dynamics

Fig. 2 lists the adsorption kinetics of catechol and resorcinol with the temperature at 293 K. It is shown that the initial adsorbate concentration poses a profound effect on the required time for the adsorption process from the beginning to the equilibrium, and more time is required to reach the equilibrium for higher initial concentrations. In addition, the required time for the adsorption of resorcinol is shorter than catechol, coincident with the results of Sun et al. [21,29].

The second-order reversible interaction model proposed by Boyer and Hsu is employed in this study to elucidate the rate constants [30]. In this model, the adsorbent is assumed to interact with the adsorbates by a monovalent interaction that has a characteristic binding energy [31].

$$A' + A \underset{k_r}{\overset{k_f}{\rightleftharpoons}} A' \cdot A \tag{1}$$

where A' is the adsorbate in solution, A is the adsorption site of the adsorbent, and $A' \cdot A$ the adsorbate–adsorbent complex. The parameters k_f and k_r are forward and backward adsorption–desorption rate constants, respectively, and the rate of the adsorption for this
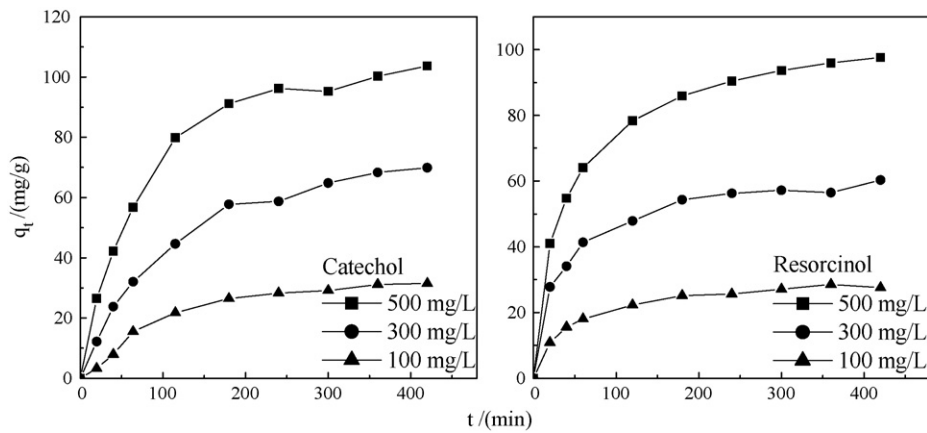
Fig. 2. The adsorption dynamic curves of catechol and resorcinol adsorbed onto HJ-1 resin with the initial concentration at 100, 300, and 500 mg/L, respectively.

type of interaction can be given by:

$$\frac{dq}{dt} = k_f c(q_m - q) - k_r q \qquad (2)$$

where c and q are the adsorbate concentrations in the liquid and on the adsorbent, respectively, and q_m represents the maximum adsorption capacity of the adsorbent.

The k_f and k_r predicted by the software MATLAB 7.0 are presented in Table 3, and it is found that the rate constants tend to decrease with increasing of the adsorbate concentration, and this drop probably reflects the differences in binding affinity in the adsorption process. In addition, it is seen that the rate constants of catechol is lower than the corresponding one of resorcinol at the same initial concentration, which are in consistent with the required time to the equilibrium for catechol and resorcinol.

3.3. Comparison of adsorption of catechol and resorcinol onto HJ-1 and XAD-4 in aqueous solution

The XAD-4 resin is usually used to treat the wastewater containing phenolic compounds, and we have compared the adsorption of catechol and resorcinol onto HJ-1 with the XAD-4 resin at 293 K in this study. As can be seen in Fig. 3, the adsorption capacities of catechol and resorcinol onto HJ-1 resin are much larger than the corresponding ones onto XAD-4 resin at the same equilibrium concentrations. The micro/mesopores dominate the pore distribution for HJ-1, which favors the adsorbate–adsorbate interaction via pore filling mechanism [32]. In addition, formaldehyde carbonyl groups are uploaded on the matrix of HJ-1, which can interact with the hydrogen atoms of the phenolic hydroxyl groups of catechol and resorcinol through hydrogen bonding [33–35]. The cumulative effects enhance the adsorption onto HJ-1.

To compare the adsorption affinity of HJ-1 with XAD-4, the adsorption data in Fig. 3 is further dealt with the distribution ratio K_d (L/g) by the following equation [36]:

$$K_d = \frac{\text{mg of the solutes/1 g of dry adsorbent}}{\text{mg of the solutes/1 L of the solution}} \qquad (5)$$

Table 3
The correlated parameters for the adsorption dynamic curves for catechol and resorcinol adsorption onto HJ-1 resin with the temperature at 293 K according to the second-order reversible interaction model proposed by Boyer and Hsu.

	Catechol			Resorcinol		
	100	300	500	100	300	500
k_f (mL/(mg min))	0.1331	0.0269	0.0097	0.2833	0.0930	0.0472
k_r (/min)	0.0033	0.0068	0.0023	0.0249	0.0072	0.0078

The K_d value provides a measure of the adsorption affinity of the adsorbent. It is seen that (not shown) the adsorption affinity of HJ-1 decreases sharply with increase of the adsorbate uploading fraction (θ), where $\theta = q_e/q_m$ and q_m is the maximum adsorption capacity (mg/g). The K_d values on HJ-1 are much larger than those on XAD-4, especially at low adsorbate fractional loading.

3.4. Adsorption behaviors

The adsorption performance of catechol and resorcinol was studied in aqueous solution with three different temperatures: 293, 303, and 313 K, respectively, and the results are displayed in Fig. 4. It is clear that the adsorption capacity decreases with increase of the temperature. Compared to the present results with the other researchers' [21,29], it is evident that the adsorption of catechol and resorcinol onto HJ-1 resin is strengthened than NDA-100, and comparable with AH-1, AH-2, and AH-3 resins, which may be from the different uploaded functional groups on the matrix. Moreover, the adsorption capacity of catechol is a little larger than resorcinol, revealing the stronger interaction between the adsorbent and catechol [21]. Langmuir and Freundlich isotherms are adopted to describe the data [22,27], and the corresponding parameters are summarized in Table 4. The Freundlich model is more suitable for characterizing the adsorption than the Langmuir model, indicating that the adsorption may be a multilayer process and the adsorbent possesses a heterogeneous nature [23].
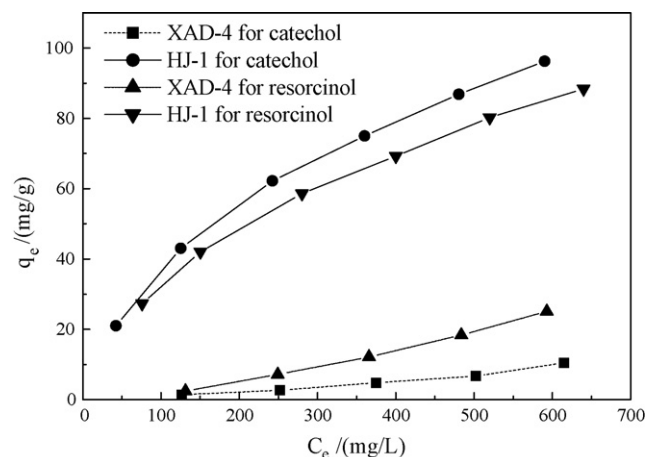

Fig. 3. The adsorption isotherms of catechol and resorcinol adsorbed onto HJ-1 resin as well as those onto XAD-4 in aqueous solution with the temperature at 293 K.
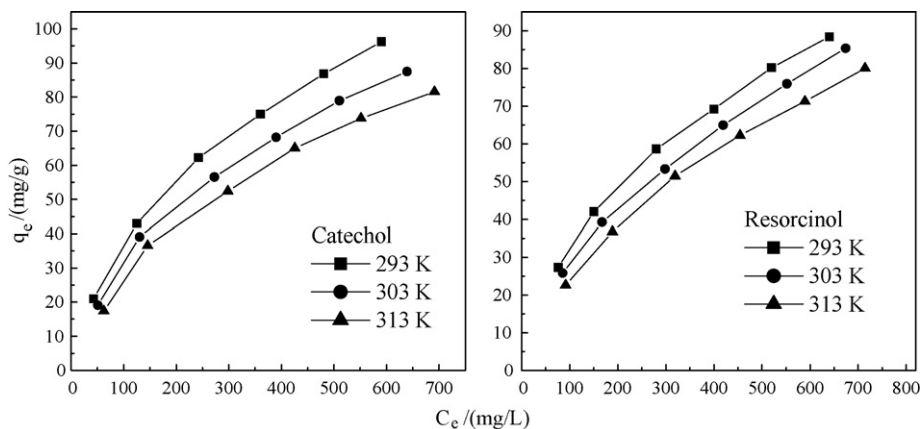
Fig. 4. The adsorption isotherms of catechol and resorcinol adsorbed onto HJ-1 resin in aqueous solution at 293, 303, and 313 K, respectively.
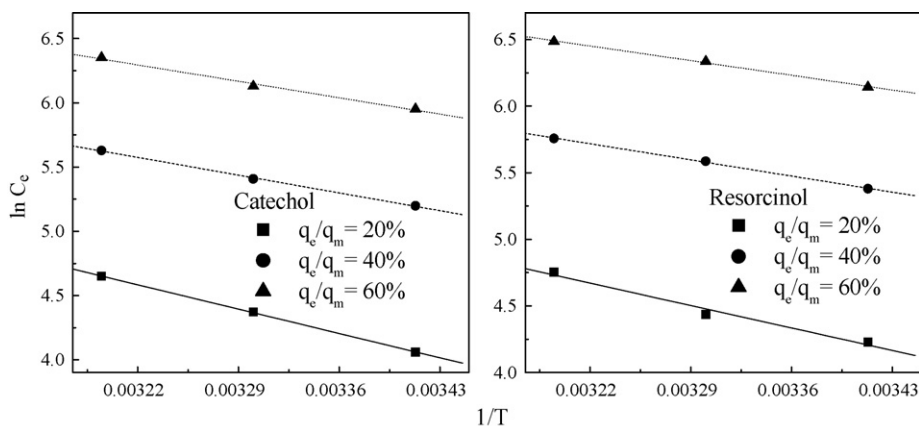

Fig. 5. The adsorption isosters of $\ln C_e$ versus $1/T$ corresponding to different occupancy percentage of the adsorbent surface for the adsorption of catechol and resorcinol onto HJ-1 resin in aqueous solution.

3.5. Adsorption thermodynamics

Following the derivative Clausius–Clapeyron equation [21]:

$$\ln C_e = \Delta H/(RT) + \ln K \tag{6}$$

here ΔH is the adsorption enthalpy (kJ/mol), T the absolute temperature (K), R the ideal gas constant, and K a constant. From Eq. (6), the adsorption enthalpy can be figured out from the isosters, plot of $\ln C_e$ versus $1/T$ (Fig. 5).

At low solute concentration, the adsorption free energy ΔG (kJ/mol) can be determined as [20]:

$$\Delta G = -RT \int_0^x q \frac{dx}{x} \tag{7}$$

where x is the mole fraction of the adsorbate in the solution. When the adsorption capacity q follows the Freundlich isotherm, incorporating the Freundlich isotherm into Eq. (7) will yield:

$$\Delta G = -nRT \tag{8}$$

here n is the characteristic constant in the Freundlich isotherm.

Adsorption entropy ΔS (J/(mol K)) can be calculated by Gibbs–Helmholtz equation:

$$\Delta S = (\Delta H - \Delta G)/T \tag{9}$$

The adsorption enthalpies corresponding to different occupancy percentage of the adsorbent surface, adsorption free energies, and adsorption entropies are presented in Table 5. The negative adsorption enthalpies indicate an exothermic process. The adsorption

Table 4
The correlated parameters for the adsorption isotherms of catechol and resorcinol onto HJ-1 resin according to Langmuir and Freundlich isotherm models.

	Langmuir isotherm model			Freundlich isotherm model		
	K_L (L/mg)	q_m (mg/g)	R^2	K_F [(mg/g)((L/mg)$^{1/n}$)]	n	R^2
Catechol						
293	0.0039	133.33	0.9876	2.5486	1.7413	0.9952
303	0.0033	126.58	0.9892	2.0059	1.6926	0.9902
313	0.0026	125.00	0.9924	1.4025	1.5860	0.9835
Resorcinol						
293	0.0033	128.21	0.9884	2.6357	1.8305	0.9974
303	0.0026	129.87	0.9777	2.0356	1.7434	0.9994
313	0.0022	128.21	0.9902	1.4441	1.6292	0.9974

Table 5
Adsorption thermodynamic parameters of catechol and resorcinol adsorbed onto HJ-1 resin in aqueous solution.

$q_e/q_m \times 100\%$	$-\Delta H$ (kJ/mol)	$-\Delta G$ (kJ/mol)			$-\Delta S$ (J/(mol K))		
		293 K	303 K	313 K	293 K	303 K	313 K
Catechol							
20%	22.53	4.2418	4.2639	4.1272	62.42	60.28	58.89
40%	16.44	4.2418	4.2639	4.1272	41.63	40.19	39.34
60%	15.19	4.2418	4.2639	4.1272	37.37	36.06	35.34
Resorcinol							
20%	20.02	4.4591	4.3919	4.2396	53.11	51.58	50.42
40%	14.40	4.4591	4.3919	4.2396	33.93	33.03	32.46
60%	13.06	4.4591	4.3919	4.2396	29.35	28.61	28.18

enthalpy decreases with increase of the occupancy percentage of the adsorbent surface resulted from the energetic heterogeneity of the adsorbent surface [11]. The initial adsorption enthalpy of catechol is greater than resorcinol, displaying the interaction of the adsorbent with catechol is a little stronger [21]. The negative adsorption free energies imply a favorable and spontaneous process, and the adsorption free energy is independent on the occupancy percentage of the adsorbent surface. The negative adsorption entropies reveal that more ordered arrangement of the adsorbates is shaped on the adsorbent surface.

Fig. 5 shows that the adsorption capacity of catechol is a little larger than resorcinol at the same temperature and equilibrium concentration, and Table 5 indicates that the adsorption enthalpy of catechol is a little more negative than resorcinol at the same occupancy percentage of the adsorbent surface. This different adsorbability can be explained in terms of the solubility and the polarity of two adsorbates [21,29]. The solubility of resorcinol in water is larger than that of catechol (123 and 45.1 g/100 mL H_2O at 298 K for resorcinol and catechol, respectively), thus it shows stronger affinity towards water. This may be one of the reasons for its smaller adsorption capacity. That is, hydrophobic interaction may be one of the driving forces. In addition, the matching of the polarity between the adsorbent and the adsorbate is also an important factor affecting the adsorption. The formaldehyde carbonyl groups of HJ-1 have a large dipole moment, and the dipole moment of catechol is larger than that of resorcinol (2.620 and 2.071 D for catechol and resorcinol, respectively), therefore, the interaction between the adsorbent and catechol is expected to be stronger than resorcinol.

4. Conclusions

The hypercrosslinked polymeric adsorbent HJ-1 can be used without any wetting process and it can adsorb catechol and resorcinol in aqueous solution efficiently. The adsorption dynamic curves can be fitted by the pseudo-second-order rate equation and the adsorption isotherms can be corrected to the Freundlich isotherm model. The equilibrium adsorption capacity of catechol is a little larger than resorcinol at the same temperature and concentration and the adsorption enthalpy of catechol is a little more negative than resorcinol at the same occupancy percentage of the adsorbent surface.

In conclusion, HJ-1 resin can be synthesized easily and it shows excellent adsorption characteristics for catechol and resorcinol in aqueous solution. Therefore, it is possible that this resin may be feasible to treat the wastewater containing catechol and resorcinol.

Acknowledgments

References

[1] B.K. Körbahti, A. Tanyolaç, Continuous electrochemical treatment of phenolic wastewater in a tubular reactor, Water Res. 37 (2003) 1505–1514.
[2] B. Dellinger, W.A. Pryor, R. Cueto, G.L. Squadrito, V. Hegde, W.A. Deutsch, Role of free radicals in the toxicity of airborne fine particulate matter, Chem. Res. Toxicol. 14 (2001) 1371–1377.
[3] M.D. Hays, P.M. Fine, C.D. Geron, M.J. Kleeman, B.K. Gullett, Open burning of agricultural biomass: physical and chemical properties of particle-phase emissions, Atmos. Environ. 39 (2005) 6747–6764.
[4] W. Phutdhawong, S. Chowwanapoonpohn, D. Buddhasukh, Electro coagulation and subsequent recovery of phenolic compounds, Anal. Sci. 16 (2000) 1083–1084.
[5] M.B.M. Van Duursen, J.T. Sanderson, P.C. de Jong, M. Kraaij, M. van den Berg, Phytochemicals inhibit catechol-o-methyltransferase activity in cytosolic fractions from healthy human mammary tissues: implications for catechol estrogen-induced DNA damage, Toxicol. Sci. 81 (2004) 316–324.
[6] M. Marini, B. Pourabbas, F. Pilati, P. Fabbri, Functionally modified core-shell silica nanoparticles by one-pot synthesis, Colloids Surf., A 317 (2008) 473–481.
[7] C.A. Kozlowski, W. Sliwa, The use of membranes with cyclodextrin units in separation processes: recent advances, Carbohydrate Polym. 74 (2008) 1–9.
[8] S. Hamoudi, K. Belkacemi, F. Larachi, Catalytic oxidation of aqueous phenolic solutions catalyst deactivation and kinetics, Chem. Eng. Sci. 54 (1999) 3569–3576.
[9] B. Pourabbas, B. Jamshidi, Preparation of MoS_2 nanoparticles by a modified hydrothermal method and the photo-catalytic activity of MoS_2/TiO_2 hybrids in photooxidation of phenol, Chem. Eng. J. 138 (2008) 55–62.
[10] B.K. Körbahti, N. Aktas, A. Tanyolaç, Optimization of electrochemical treatment of industrial paint wastewater with response surface methodology, J. Hazard. Mater. 148 (2007) 83–90.
[11] H.T. Li, M.C. Xu, Z.Q. Shi, B.L. He, Isotherm analysis of phenol adsorption on polymeric adsorbents from nonaqueous solution, J. Colloid Interface Sci. 271 (2004) 47–54.
[12] K. László, P. Podkościelny, A. Dąbrowski, Heterogeneity of activated carbons with different surface chemistry in adsorption of phenol from aqueous solutions, Appl. Surf. Sci. 252 (2006) 5752–5762.
[13] J.H. Huang, K.L. Huang, S.Q. Liu, Q. Luo, M.C. Xu, Adsorption properties of tea polyphenols onto three polymeric adsorbents with amide group, J. Colloid Interface Sci. 315 (2007) 407–414.
[14] Z.Y. Xu, Q.X. Zhang, C.L. Wu, L.S. Wang, Adsorption of naphthalene derivatives on different macroporous polymeric adsorbents, Chemosphere 35 (1997) 2269–2276.
[15] M.P. Tsyurupa, V.A. Davankov, Porous structure of hypercrosslinked polystyrene: state-of-the-art mini-review, React. Funct. Polym. 66 (2006) 768–779.
[16] V.A. Davankov, M.P. Tsyurupa, N.N. Alexienko, Selectivity in preparative separations of inorganic electrolytes by size-exclusion chromatography on hypercrosslinked polystyrene and microporous carbons, J. Chromatogr. A 1100 (2005) 32–39.
[17] V.A. Davankov, C.S. Sychov, M.M. Ilyin, K.O. Sochilina, Hypercrosslinked polystyrene as a novel type of high-performance liquid chromatography column packing material: mechanisms of retention, J. Chromatogr. A 987 (2003) 67–75.
[18] J.H. Huang, K.L. Huang, S.Q. Liu, Q. Luo, S.Y. Shi, Synthesis, characterization, and adsorption behavior of aniline modified polystyrene resin for phenol in hexane and in aqueous solution, J. Colloid Interface Sci. 317 (2008) 434–441.
[19] R. Saad, K. Belkacemi, S. Hamoudi, Adsorption of phosphate and nitrate anions on ammonium-functionalized MCM-48: effects of experimental conditions, J. Colloid Interface Sci. 311 (2007) 375–381.
[20] B.K. Körbahti, A. Tanyolaç, Electrochemical treatment of simulated textile wastewater with industrial components and Levafix Blue CA reactive dye: optimization through response surface methodology, J. Hazard. Mater. 151 (2008) 422–431.
[21] Y. Sun, J.L. Chen, A.M. Li, F.Q. Liu, Q.X. Zhang, Adsorption of resorcinol and catechol from aqueous solution by aminated hypercrosslinked polymers, React. Funct. Polym. 64 (2005) 63–73.
[22] A.M. Li, Q.X. Zhang, G.C. Zhang, J.L. Chen, Z.H. Fei, F.Q. Liu, Adsorption of phenolic compounds from aqueous solutions by a water-compatible hypercrosslinked polymeric adsorbent, Chemosphere 47 (2002) 981–989.
[23] H.T. Li, Y.C. Jiao, M.C. Xu, Z.Q. Shi, B.L. He, Thermodynamics aspect of tannin sorption on polymeric adsorbents, Polymer 45 (2004) 181–188.
[24] M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, J.A. Montgomery Jr., T. Vreven, K.N. Kudin, J.C. Burant, J.M. Millam, S.S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G.A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J.E. Knox, H.P. Hratchian, J.B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R.E. Stratmann, O. Yazyev, A.J. Austin, R. Cammi, C. Pomelli, J.W. Ochterski, P.Y. Ayala, K. Morokuma, G.A. Voth, P. Salvador, J.J. Dannenberg, V.G. Zakrzewski, S. Dapprich, A.D. Daniels, M.C. Strain, O. Farkas, D.K. Malick, A.D. Rabuck, K. Raghavachari, J.B. Foresman, J.V. Ortiz, Q. Cui, A.G. Baboul, S. Clifford, J. Cioslowski, B.B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R.L. Martin, D.J. Fox, T. Keith, M.A. Al-Laham, C.Y. Peng, A. Nanayakkara, M. Challacombe, P.M.W. Gill, B. Johnson, W. Chen, M.W. Wong, C. Gonzalez, J.A. Pople, Gaussian 03, Revision B. 05, Gaussian Inc., Pittsburgh, PA, 2003.
[25] J.T. Wang, Q.M. Hu, B.S. Zhang, Y.M. Wang, Organic Chemistry, Nankai University Press, Tianjing, 1998.
[26] M.H. Abraham, Chem. Soc. Rev. 22 (1993) 73–83.
[27] G.R. Chen, Chemical Industry Encyclopedia, Chemical Industry Press, Beijing, China, 1990.
[28] G.H. Meng, A.M. Li, W.B. Yang, F.Q. Liu, X. Yang, Q.X. Zhang, Mechanism of oxidative reaction in the post crosslinking of hypercrosslinked polymers, Eur. Polym. J. 43 (2007) 2732–2737.
[29] Y. Sun, X.T. Li, C. Xu, J.L. Chen, A.M. Li, Q.X. Zhang, Adsorption of catechol from aqueous solution by aminated hypercrosslinked polymers, J. Environ. Sci. 17 (2005) 584–588.
[30] P.M. Boyer, J.T. Hsu, Effects of ligand concentration on protein adsorption in dye-ligand adsorbents, Chem. Eng. Sci. 47 (1992) 241–251.
[31] H.A. Chase, Prediction of the performance of preparative affinity chromatography, J. Chromatogr. 297 (1984) 179–202.

[32] M. Dutta, N.N. Dutta, K.G. Bhattacharya, Aqueous phase adsorption of certain betalactam antibiotics onto polymeric resins and activated carbon, Sep. Purif. Techol. 16 (1999) 213–224.

[33] J.H. Huang, K.L. Huang, S.Q. Liu, Q. Luo, M.C. Xu, Adsorption behavior, thermodynamics, and mechanism of phenol on polymeric adsorbents with amide group in cyclohexane, J. Colloid Interface Sci. 316 (2007) 10–18.

[34] J.S. Mattson, H.B. Mark, Surface chemistry of active carbon: specific adsorption of phenols, J. Colloid Interface Sci. 31 (1969) 116–130.

[35] M.C. Xu, Y. Zhou, J.H. Huang, Adsorption behaviors of three polymeric adsorbents with amide groups for phenol in aqueous solution, J. Colloid Interface Sci. 327 (2008) 9–14.

[36] C. Long, J.D. Lu, A.M. Li, D.B. Hu, F.Q. Liu, Q.X. Zhang, Adsorption of naphthalene onto the carbon adsorbent from waste ion exchange resin: equilibrium and kinetic characteristics, J. Hazard. Mater. 150 (2008) 656–661.