









شیمی کاربردی

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crosslinking reactions and high phase separation. Figure 2 show Influence of the UV irradiation time on the UV-blocking efficiency of the PU-TINUVIN, PU-P(S)-TINUVIN, and PU-P(S-DVB)-TINUVIN composite films. The rate of decreasing the UV-blocking efficiency with the time are as follows: $PU-PS-TINUVIN \geq PU-P(S-DVB)-TINUVIN > PU-TINUVIN > PU-P(MMA-EDGMA)-TINUVIN> PU-P(LMA-EDGMA)-TINUVIN> PU-anti UV nanofiber.$

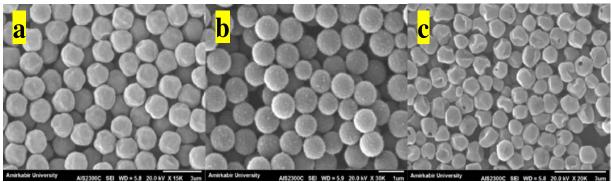


Figure 1. Scanning electron micrographs of a)PS-TIN25, b) PMMA-TIN25 and c) PLMA-TIN25 composite microspheres

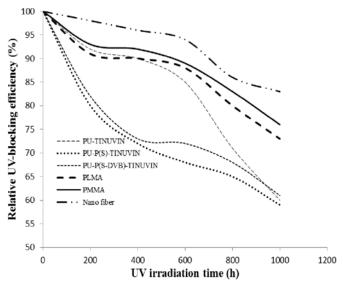


Figure 2. Influence of the UV irradiation time on the UV-blocking efficiency of the PU-TINUVIN, PU-P(S)-TINUVIN, and PU-P(S-DVB)-TINUVIN composite films.

Keywords: Non-spherical polymer particles, Dispersion polymerization, Anti UV property, Nanofibers, Organic anti UV.

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دانشگاه گیلان - مهرماه ۹۶







Corrosion Behavior of Environmentally Friendly Cerium-Based Conversion Coating on Al 2024-T3: A review

Mir Sajjad Mousavia*, Ali Asghar Sarabib, Seyyed Mohammad Mousavi khoiec

^aAmirkabir University of Technology, Corrosion Group, Bandar Abbas, Iran.

^bAmirkabir University of Technology, Faculty of Polymer Engineering & Color Technology, Tehran, Iran.

^cAmirkabir University of Technology, Faculty of Mining and Metallurgical Engineering, Tehran, Iran. Mirsajjadmousavi@aut.ac.ir

Abstract:

In the last few years non-toxic cerium conversion coating (CeCC) could be a proper option for replacing chromate conversion coating on Al 2024-T3 used in aircraft industry. This paper reviews the literature on conversion coating processes on Al 2024-T3, with particular emphasis on those based on cerium. It includes introduction to Al 2024-T3, preventing corrosion of Aluminium, introduction to CeCC, pretreatment of panels prior to coating, coating process and effects of solution parameters e.g. anion, pH, accelerator, time and temperature. It is concluded that several process areas are poorly understood, some of which are critical to further progress in the field. These include the development of industrially suitable pretreatments, technologies for coating non-aerospace alloys and seals to enhance corrosion performance and paint adhesion.

Keywords: Aluminium, Cerium, Conversion coating, Corrosion, Non-toxic, Rare earth.

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دانشگاه گیلان - مهرماه ۹۶







Synthesized and characterized of a novel unsymmetric rotaxane

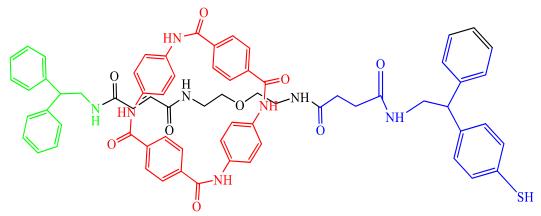
Atena Naeimia*, Emilio Perezb

^aFaculty of science, Department of Chemistry, University of Jiroft, Iran ^bIMDEA Nanoscience, Madrid, Spain a.naeimi@ujiroft.ac.ir

Abstract:

Pseudorotaxanes, characterized by a macrocyclic host component encircling a threaded guest axle, have been intensively studied and employed as fundamental building blocks in the preparation of advanced mechanically interlocked molecules, such as rotaxanes and catenanes. Rotaxanes have generated a lot of expectations due to their potential technological applications. They can be prepared by means of different intermolecular interactions such as hydrogen bonds, p-stacking, metal complexation. The applicability of these systems can be enhanced when using photo- and electroactive units like fullerenes. The field of rotaxanes is particularly active, mostly in relation to molecular machines 1 and new materials. The synthesis of these compounds is sometimes limited by the stoppering reaction, which has to be compatible with the other functions present in the precursor. Various organic or coordination chemistry reactions have been used but the yields are not always satisfactory particularly in the case of unstable rotaxane precursors¹⁻⁴.

In this work, the new unsymmetric rotaxane was synthesized (Scheme 1) by down to top procedure. All the steps were checked and followed by ¹H NMR, ¹³C NMR, and Mass spectroscopy. Their host–guest complexation to form pseudorotaxanes was studied



Scheme 1. The structure of synthesized rotaxane

Keyword: Rotaxane, Unsymmetric, NMR, Mass spectroscopy

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دانشگاه گیلان - مهرماه ۹۶







Synthesis and characterization of $Mn_{0.5}Zn_{0.5}Fe_2O_4$ nanoparticles and investigation of their photocatalytic properties under visible light irradiation

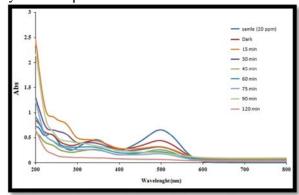
Razieh Nejat*

Faculty of science, Department of Chemistry, Kosar University of Bojnourd, Iran. organochem_nejat@yahoo.com

Abstract:

In recent years, worldwide attention to environmental problems has been increasing. Unfortunately, use of synthetic dyes (such as azo dyes), especially in the textile industries, in one hand and the discharge of wastes, containing these compounds with intensive color and toxicity, into the aquatic systems, in the other hand are considered as environmental threats among the researchers in this field. Azo dyes, consisting of azo bonds (-N=N-) as chromophores, are a well-known class of dyes, which are highly toxic and even carcinogenic to animals and humans, and are not readily degradable. Due to their complicated aromatic structures, diazo dyes (e.g., Congo red (CR) (sodium salt of benzidinediazobis-1-naphthylarnine-4-sulfonic acid)) are thermally and optically stable, and thus difficult to decompose. However, photocatalytic decomposition of such pollutants is a clean and repeatable way to decrease their harmful effects.

Adsorption process has become one of the most effective and comparable low-cost methods for the removal of dyes from aqueous solutions. In this study adsorption of different concentrations of Congo Red with $Mn_{0.5}Zn_{0.5}Fe_2O_4$ nanoparticles were investigated and high absorption of Congo Red dye from aqueous solution was showed.



Keywords: Mn_{0.5}Zn_{0.5}Fe₂O₄ nanoparticles, Adsorb, Congo Red.

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دانشگاه گیلان - مهرماه ۹۶







AFM and polarization studies to evaluate the inhibition effect of 1,4 -di[1'-methylene-3'-methylimidazulimbromide]-benzene on mild steel corrosion in 1M HCl solution

A. PourghasemiHanza^{a,*}, R. Naderi^b, E. Kowsari^c, M. Sayebani^d

^aAmirkabir University of Technology, Corrosion Group, Bandar Abbas, Iran.

^bAmirkabir University of Technology, Faculty of Polymer Engineering & Color Technology, Tehran,

Iran.

^cAmirkabir University of Technology, Department of Chemistry, Tehran, Iran. ^dAmirkabir University of Technology, Faculty of Marine Engineering, Tehran, Iran. a.pourghasemi@yahoo.com

Abstract:

Acid solutions are commonly used for removal of undesirable scale and rust in metal finishing processes, cleaning of boilers and heat exchangers. In these situations, hydrochloric acid is one of the most widely used agents. To prevent unexpected metal dissolution and excess acid consumption in the process of acid cleaning, inhibitors will be inevitably put into use. The use of organic molecules as corrosion inhibitor is one of the most practical methods for protecting metals against the corrosion and it is becoming increasingly popular. The existing data show that organic inhibitors act by adsorption and consequently film formation on the surface. Organic compounds bearing heteroatoms with high electron density such as phosphor, sulfur, nitrogen, oxygen or those containing multiple bonds that can act as adsorption centers, are effective corrosion inhibitors.^{2,3} In this study the inhibition action of an ionic liquid towards mild steel corrosion in 1.0 M HCl solution was investigated by polarization measurements. The effect of inhibitor concentration on the inhibition action was investigated. Polarization measurements showed that the 1,4-di[1'-methylene-3'-methylimidazulimbromide]-benzene acted as mixed inhibitor in 1.0M HCl solution. The surface morphology of the mild steel was studied using atomic force microscopy (AFM) in 1.0 M HCl solution with and without the inhibitor. Results obtained showed that the corrosion rate of the mild steel can be decrease form 143µA/cm² to 25 μA/cm² using 300 ppm of 1,4 -di[1'-methylene-3'-methylimidazulimbromide]-benzene in 1.0 M HCl solution.

Keywords: Ionic liquid, Corrosion inhibition, Mild steel, Hydrochloric acid, Polarization methods

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دانشگاه گیلان - مهرماه ۹۶





2nd Iranian Student Chemistry Conference

University of Guilan, Rasht, 6-8 Oct. 2015



Dye-sensitized solar cells with quasi-solid state electrolyte prepared from solvent-free ionic liquids

Mahboobeh Rafieepoor Chirani*, Elaheh Kowsari

Department of Chemistry, Amirkabir University of Technology, Tehran, Iran m.chirani@aut.ac.ir

Abstract:

The effect of the addition of ionic liquid on the performance of dye-sensitized solar cells has been studied. Quasi-solid state electrolytes were prepared by the ionic liquid electrolytes containing N-methylidazolium iodide (NMBI) and 1-methyl-3-propylimidazolium iodide (MPII) and 2-(2-Thienyl)-1H-benzimidazole. The developments of the ionic conductivity and the diffusion coefficients of I_3 are witnessed in the ionic liquid mixture quasi-solid state electrolyte.

Ionic liquids have been an area of examination attentiveness due to their negligible vapor pressure, nonflammability, high ionic conductivity, wide electrochemical window and brilliant thermal and chemical stabilities, as well as their potential for DSSCs and other electrochemical devices. The maximum photovoltaic conversion efficiency described for DSSCs (>11%) has been attained by using electrolytes based on volatile organic solvents. Ionic liquid (ILs) based quasi solid-state electrolytes have developed as motivating alternative of unique advantage for fabrication of high efficiency DSSCs without evaporation and leakage of the electrolyte throughout the long-term operation.

The reliance of diverse photovoltaic performance parameters (V_{oc} , J_{sc} , ff, η) of DSSC upon different ionic liquids concentrations and ILs ratios in electrolytes has been studied by electrochemical impedance spectroscopy (EIS) and dark current measurements. A significant increase in the fill factor (FF) for optimum concentrations was related to the decrease in the series resistance (R_S) of the DSSCs. Moreover, short-circuit current density of the ILs based DSSC increase, as a result of the increasing transport of I_3^- in quasi-solid state electrolyte. The photon to electron conversion efficiency of the DSSCs containing ionic quasi-solid state electrolyte prepared from solvent-free ionic liquids was 4.38% under simulated sunlight (air mass 1.5) with a light intensity of 100 mW cm⁻². The long-term stability of DSSCs with ionic liquids based electrolyte, which is greater to that of an organic solvent-based electrolyte, was also studied.

This work has provided useful insight for further development of solvent-free electrolytes based on dye-sensitized solar cells.

Keywords: Ionic liquids, Dye-sensitized solar cells, Quasi-solid state electrolyte, Conductivity.

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2nd Iranian Student Chemistry Conference

University of Guilan, Rasht, 6-8 Oct. 2015



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دانشگاه گیلان - مهرماه ۹۶







Synthesis and characterization of silica coated Fe_3O_4 magnetic nanoparticles and anchore with a transition metal complex for Ion imprinted application

Farzaneh Sadeghi, Seyed Nezamoddin Mirsattari*

Department of chemistry, Shahreza Branch, Islamic Azad University, Shahreza, Iran Sadeghi_f10@yahoo.com
Mirsattari@iaush.ac.ir

Abstract:

Recently, magnetic nanoparticles (MNPs), especially Fe₃O₄, have attracted more and more attentions because of the outstanding properties such as easy separation and low toxicity. However, raw MNPs are susceptible to air oxidation and leaching under acidic conditions, and are easily aggregated in aqueous solutions because of anisotropic dipolar attraction, which reduces the sorption capacity and restricts the application range. To compensate for these shortages, surface modifications of MNPs based on covalent binding or physical coating have been widely explored.

In this research Fe_3O_4 magnetic nanoparticles synthesized from hydrothermal method and trisodium citrate ($Na_3CA.5H_2O$) was used as a surfactant. Hydrothermal method is an easy and one step route to prepare hydrophilic magnetite nanoparticles with different precursors. The trisodium citrate has been widely used as an important biological ligand because of the stable complexing bond between the carboxylic group (COO^-) in $Na_3CA.5H_2O$ and the metallic ions.

The next core/shell of Fe₃O₄/SiO₂ magnetic nanoparticles were synthesized. In the next synthesis process, 3-choloropropyltrimethoxysilane (CPTMS) was added to the mixture in which Fe₃O₄/SiO₂ was dispersed in anhydrous toluene to form Fe₃O₄/SiO₂/Si-(CH₂)₃-Cl and an choloro functionalized silica shell with magnetic core of Fe₃O₄ nanoparticle has been successfully synthesized. Following was synthesized of an aldehyde with anchoring OH groups. Then imine ligand synthesis of aldehyde was done in the previous step and synthesis of transition metal complex by imine ligand.

In the last step imine complex with anchor group OH contact to the functionalized nanoparticles with Cl. Finally study of application compound from method ion imprinted will be discussed. Figure 1 shows the Procedure of ion imprinted.

The nanoparticles were characterized by Fourier transform infrared spectroscopy (FT-IR), UV-Vis, Atomic absorbtion spectroscopy (AAS), Field emission scanning electron microscopy (FESEM), Energy-dispersive X-ray spectroscopy (EDX), Map analysis, Transmission electron microscopy (TEM), X-ray diffraction (XRD) and magnetic measurements(VSM).





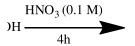


Figure 1. Procedure of ion imprinted

Keywords: Magnetic nanoparticles, Fe₃O₄, Solvothermal, Imine Complex, Ion imprinted, CPTMS.

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دانشگاه گیلان - مهرماه ۹۶







Preparation of silver nanoparticles by chemical reduction method

Maryam safaripoor, Bahram keyvani*, Akbar Ghaemi

Department of Chemistry, Faculty of Engineering, Islamic Azad University, Saveh Branch, Saveh, Iran maryam.safaripoor@gmail.com
bkeyvani@iau-ac-ir

Abstract:

Nowadays, nanomaterials have been improved as a result of truly important recent advances by applying "green" chemistry rules to nanotechnology and material science. Silver nanoparticles (Ag-NPs) have been widely used during the past few years in various applications, such as biomedicine, biosensor and catalysis. ¹

Many methods can be used to synthesize Ag-NPs. A number of methods, including microemulsion², reverse micelles³, microwaves method⁴, electrochemical deposition⁵ to name but a few have been applied to synthesize silver nanostructure. The chemical reduction method in the synthesis of colloidal metal particles is believed to provide convenient operation and ease of control. ⁶

The synthesis of silver nanoparticles *via* chemical reduction method described in this work. Well dispersed silver nanoparticles were synthesized by reducing silver nitrate (AgNO₃) with sucrose in the presence of protective agent polyvinyl pyrrolidone (PVP). Sodium hydroxide (NaOH) was used to enhance the reaction velocity. Upon aging step, a pale yellow solution indicating the formation of Ag nanoparticles was resulted. The X-ray diffraction (XRD) analysis (X'Pert PRO MPD made by USA) results confirm the successful formation of silver nanoparticles. Figure 1 depicts the Scanning Electron Microscope (SEM) image (Hitachi, s-4160 made by Japan) of silver nanoparticles. Based on the results from SEM images silver spherical nanoparticles with mean particle size of 78 nm are formed.

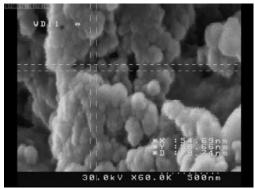


Figure 1. SEM images of the silver nanoparticles synthesized using sucrose as reducing agent.

Keywords: Silver, Nanoparticles, Polyvinyl pyrrolidone, Sucrose.

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دانشگاه گیلان - مهرماه ۹۶







A study on the effect of nanoemulsion on fish fillets

Shabnam Shadman^a, Seyed Ebrahim Hosseini^{a,*}, Hadi Ershad Langroudi^b, Shahrokh Shabani^a

^aDepartment of Food Science and Technology, Science and Research Branch, Islamic Azad University, Tehran, Iran.

^bDepartment of Fisheries, Lahijan Branch, Islamic Azad University, Lahijan, Iran. sh.shadman2009@gmail.com ebhoseini@srbiau.ac.ir

Abstract:

Nanotechnology can be briefly defined as 'the engineering of very small systems and structures. The main feature of nanotechnology is defined by the size of the systems of work: the 'nanoscale'.¹

Nanoemulsions are known as self-preserving antimicrobials due to the fact that water present in them is effectively bound by its structure and access to the water by organisms is limited.²

The deterioration of fresh fish is due to bacterial and enzymatic action and during spoilage, fish undergo to colour, flavor and texture changes.³

This work aims at preparing a nanoemulsion to be used as a safe food preservative and for shelf life extension of fish fillets. Sunflower oil based nanoemulsion was prepared and subjected to ultrasound and droplet size was determined by dynamic light scattering (DLS) method.

The quality changes of farmed rainbow trout (*Oncorhynchus mykiss*) fillets treated with the nanoemulsion were studied on days 0, 5, 10 and 15 during storage in $(4^{\circ}C\pm 1)$ and evaluated by microbiological analyses. Total viable counts and psychrophilic bacteria were determined. Changes in total viable count during storage at 4 ± 1 °C are shown in Table 1.

Table1. Changes in total viable count during storage at 4 ± 1 °C

Storage time	Control	Nanoemulsion	
(days)	(T1)	(T2)	
0	2.31±0.014Aa*	2.05±0.07Aa	
5	2.45±0.21Aa	2.32±0.03Bb	
10	3.72±0.035Bb	3.51±0.01Cc	
15	4.62±0.028Cc	4.72±0.035Dd	

^{*}Values are means and \overline{S} .D. of triplicate; Means with the same small letter in a raw were not significantly different at P < 0.05 level in different treatment. Means with the same capital letter in a column were not significantly different at P < 0.05 level during storage at 4°C.

The results showed that the nanoemulsion had significant effect (P<0.05) on total viable counts. No growth of psychrophilic bacteria was found. Antibacterial effect of the Nanoemulsion was confirmed and microbiological results were acceptable until day 15 of storage. The nanoemulsion can be introduced as a new preservative for rainbow trout fillets.

Keyword: Nanoemulsion, Ultrasound, Shelf Life, Rainbow Trout (Oncorhynchus mykiss).





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دانشگاه گیلان - مهرماه ۹۶







Catalytic effect of acid-modified natural zeolite on the rate constants of the esterification reaction of Sebacic acid with methanol (and ethanol)

Delbar Sharafi, Farshid Salimi*

Department of Chemistry, Ardabil Branch, Islamic Azad University, Ardabil, Iran delbarsharafi@gmail.com sibsalimi@yahoo.com

Abstract:

Generally, esters are prepared in a reaction between a carboxylic acid and an alcohol in the presence of small amounts of strong acids. In such cases, there is no effective procedure for isolating of catalysts from obtained products which over time can lead to decomposition of the ester. There are still numerous global efforts to replace these environmentally harmful chemicals with more eco-friendly and suitable catalysts.

In a typical kinetic run, 0.4g (2 mmol) sebacic acid was mixed with 0.04 g H₃PO₄, H₂SO₄, HNO₃ and HCl-modified zeolite in 4.5 ml alcohol (as reactant and solvent) in a 50 ml flask and heated to boiling point of the mixture. The unconverted sebacic acid was determined by titration method (with 0.lN NaOH) at various time intervals. The pseudo-first-order reaction rate constants were calculated from the plot of unconverted sebacic acid versus time using [A] = $[A_0]$ exp(-KT) equation. In all cases, the values of the pseudo-first order reaction constants with methanol are greater than that of obtained with ethanol. Both HCl and H₂SO₄-modified zeolites have high catalytic effect. The SEM images of natural zeolite, sulfuric and hydrochloric acidmodified zeolite show that the size of the particles is about 1 to 20 µm and the shape of them is irregular form. The pseudo-first-order reaction rate constants of the esterification reaction of sebacic acid with methanol (and ethanol) were obtained at reflux condition in the presence of phosphoric, sulfuric, nitric and hydrochloric acid-modified natural zeolites as catalyst. With any catalyst used, methanol exhibited greater reaction rate constant than ethanol. This is probably because of small size of methanol, decreasing energy activation of esterification (ΔG^{\ddagger}). Among the above-mentioned catalysts, both H₂SO₄ and HCl-modified zeolites enhanced the reaction rate constants, significantly.

Keywords: Modified zeolite, Pseudo-first-order conditions, Sebacic acid, Methanol, Ethanol.

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دانشگاه گیلان - مهرماه ۹۶







Experimental investigation of enhanced oil recovery using nanosilica/hydrolyzed polyacrylamide

Hojjat Allah Yousefvand, Arezou Jafari*, Mahdi Abdollahi

Chemical Engineering Department, Tarbiat Modares University, Tehran, Iran ajafari@modares.ac.ir

Abstract:

The use of polymer flooding as one of the enhanced oil recovery (EOR) methods has recently increased. Also addition of nanoparticles in the polymer flooding process can enhance the oil recovery factor. But there exists few researches on the polymer performance in the presence of nanoparticles. In addition, there is no information about the effect of silica nanoparticles on the heavy oil recovery during the polymer flooding by anionic hydrolyzed polyacrylamide (HPAM). Therefore, in this study the performance of HPAM and also the modified HPAM in the presence of nanosilica (NS) and salt on the oil recovery factor has been investigated in a micromodel setup. The experimental system consists of two main parts, the injection and optical systems. In the injection fluid system highly accurate syringe pump is used for flow control in the micromodel and the optical system which is the most valuable section because the most data are gathered from this part. So a high resolution camera for taking digital photos at every two minutes was used and the image processing technique by Adobe Photoshop CS6 was applied to analyze the displacement mechanisms and also for calculation of the efficiency in each flooding test by counting the oil pixels at any time step.

For making the glass micromodel in accordance with a thin section from a real porous medium the pattern has been drawn by Corel Draw software. Then by the laser technique the model has been etched on a glass and finally it has been putted in the furnace. After that to investigate the effect of HPAM solutions and nanosuspensions on the oil recovery, the injected fluids were prepared: (1) two types of HPAM solutions: to prepare the polymer solutions, at first a certain amount of salt (30000 ppm) added to distilled water, then solid HAPM (800 ppm) was added to brine water and samples were slowly stirred by the mechanical stirrer in 100 rpm for 48 hr and (2) suspension of silica nanoparticles in HPAM solutions: firstly NS (0.5 wt%) stirred for 30 minutes in distilled water by the magnet stirrer (400 rpm) then, 1200 ppm sodium dodecyl sulfate (SDS) was added and stirred again for 30 minutes. After that the suspensions sonicated by ultrasonic probe (400W, 20k Hz) for 30 minutes and simultaneously solid HAPM (800 ppm) was added to water with 30000 ppm salinity and the samples were slowly stirred by the mechanical stirrer in 100 rpm for 48 hr. Then, the polymer solutions were added slowly by burette to the NS solutions. Then five flooding tests (water flood (WF) with 3000 ppm salinity, HPAM solution (PF1), the modified HPAM solution (PF2), nanosilica/HPAM (NPF1) and nanosilica/modified HPAM (NPF2) were performed in a strongly oil wet quarter five spot glass micromodel that oil wet condition was prepared with help of sodium hydroxide, distilled water, dilute solution of 2% tri chloro methyl silane (TCMS) and 98% dehydrate toluene and methanol.³

Results of stability tests showed severe deposition of nanosilica because of salt, but with applying SDS this problem redeemed and longer stable nanosuspensions was observed at least for a day. The samples viscosities in the same condition were measured by Brookfield





viscometer (Table 1). It is clear that an increase in the nanosuspensions viscosity with respect to polymer solutions was observed because nanoparticles make a network with polymer chains. Results of flooding tests (Figure 1 and Table 1) showed better efficiency of HPAM rather than the modified HPAM and also after one pore volume of the injected fluid an increase about 10% and 20% in the oil recovery respect to water flooding has been observed for HPAM (PF1) and nanosuspension (NPF1), respectively. In addition, an enhancement about 5% and 15% in the oil recovery factor respect to water flooding sequently for the modified HPAM (PF2) and the second nanosuspension (NPF2) has been observed.

Table 1. Results of flooding tests

Test	Breakthrough time (min)	Ultimate Recovery (%)	Viscosity of the injected fluid (cp)
WF	42	16.63	1
PF1	64	26.32	8
PF2	52	21.50	6
NPF1	84	35.00	35
NPF2	76	31.67	25

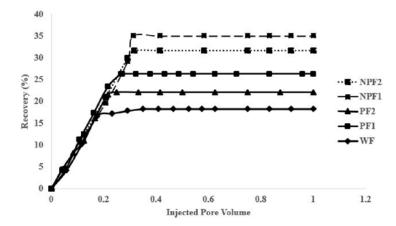


Figure 1. Results of the heavy oil recovery versus the pore volume of injected fluids

Keywords: Enhanced Oil Recovery, Polymer Flooding, Nanosilica, Polyacrylamide.

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