

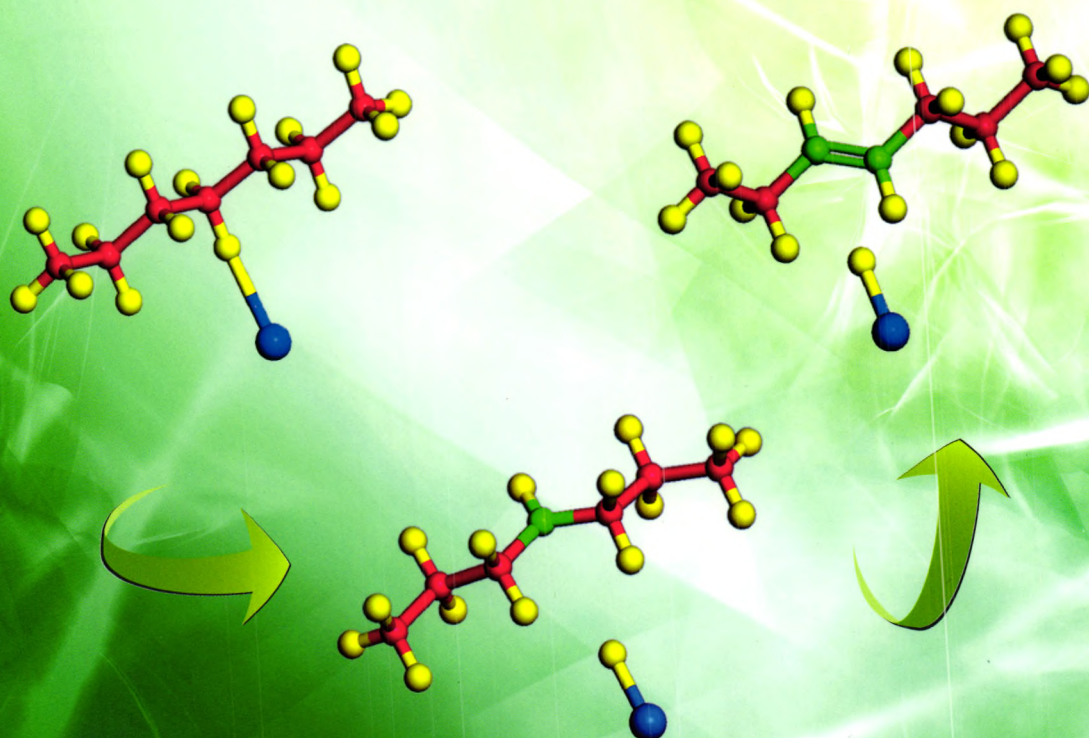


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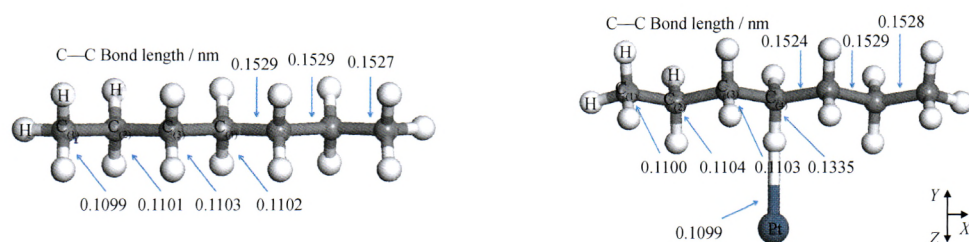
Research Articles

Acta Petrolei Sinica (Petroleum Processing Section), 2013, 29(2): 181-185 doi: 10.3969/j.issn.1001-8719.2013.02.001

Molecule Simulation of Dehydrogenation of *n*-Heptane to Produce Olefins

YU Ning LONG Jun ZHOU Han MA Aizeng DAI Zhenyu ZHAO Xiaoguang ZHAO Yi

Density functional theory (DFT) quantum chemical methods were used to study the process of dehydrogenation of *n*-heptane to produce olefins. The results showed that the main reaction products were 2-heptene, 3-heptene. In the presence of Pt catalyst, the reaction energy barrier was 99.63 kJ/mol.

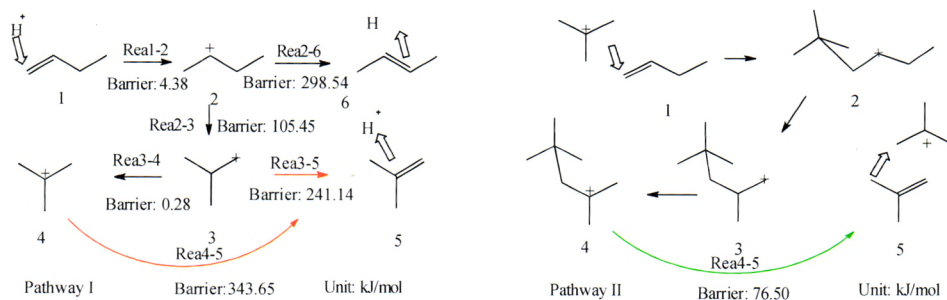


Acta Petrolei Sinica (Petroleum Processing Section), 2013, 29(2): 186-190 doi: 10.3969/j.issn.1001-8719.2013.02.002

A Density Functional Study of the Mechanism of Skeletal Isomerization of Butene-1

LI Jinzhi LONG Jun ZHAO Yi YU Zhongwei

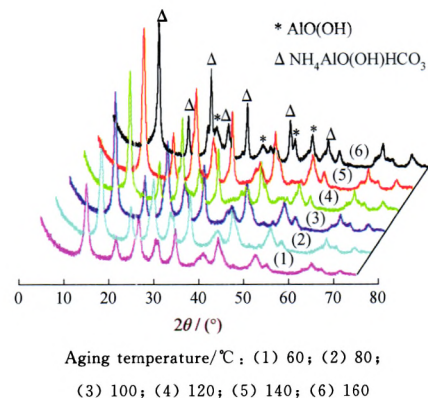
The results indicated that the processes of reaction 3 → 5 and reaction 4 → 5 in pathways of butane-1 skeletal isomerization were difficult to occur over the acidic sites of fresh zeolite, but the undesorbed primary carbenium ions can act as the new active sites to initiate the secondary reaction and cause higher selectivity of isobutene.



Synthesis of γ -Al₂O₃ by Solid-State Reaction and the Hydrodesulfurization Evaluation of Ni-Mo-P/ γ -Al₂O₃

HU Xiaofu ZHANG Min LI Guoliang YIN Changlong CUI Ruili
ZHAO Ruiyu LIU Chenguang

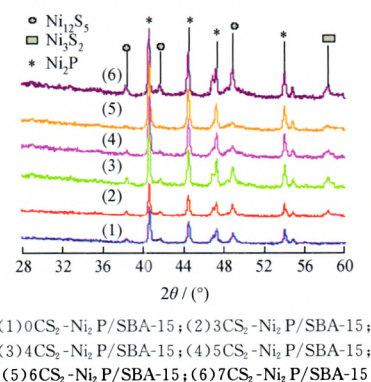
The crystallinity of ammonium aluminum carbonate hydroxide increased gradually with the increase of aging temperature. When the aging temperature was above 160°C, the pseudo-boehmite could also be obtained. It was recognized that the aging temperature was crucial condition in preparation of ammonium aluminum carbonate hydroxide hydrate. The highest aging temperature of ammonium aluminum carbonate hydroxide should not be more than 160°C.



Influence of Sulfurization Behavior on Structure and Hydrodesulfurization Performance of Ni₂P/SBA-15 Catalysts

GAO Lili WU Pingyi LAN Ling GUAN Yueming JI Shengfu

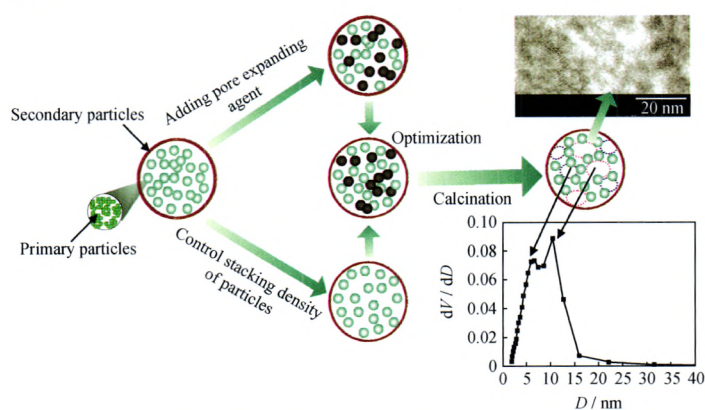
A series of x CS₂-Ni₂P/SBA-15 catalysts were prepared. The phases of Ni₂P, Ni₁₂P₅ and Ni₃S₂ existed in the catalysts. Ni existed in the Ni^{δ+} and Ni²⁺ species and P existed in the P^{δ-} and P⁵⁺ species on the catalyst surface. Ni₃S₂ phase played an important role on DBT conversion and direct desulfurization.



Preparation of NiMoP Catalyst Supported on γ -Al₂O₃ of Bimodal Pore Distribution and Its Hydrogenation Performance for VGO + CGO

ZHANG Chengtao CHAI Yongming WANG Xiao LI Guoliang ZHANG Kongyuan ZHAO Ruiyu LIU Chenguang

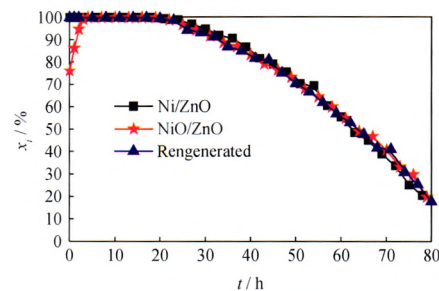
A γ -Al₂O₃ of bimodal porous distribution could be obtained by adding nano-carbon black and controlling water/pseudo-boehmite in extruding process of pseudo-boehmite. NiMoP/ γ -Al₂O₃ catalyst was synthesized by the wetness impregnation with the γ -Al₂O₃ of bimodal porous distribution. Compared to the catalyst of non-bimodal porous distribution, this catalyst showed higher activity in the hydrogenation for VGO+CGO.



Reactive Adsorption Desulfurization for Thiophene on Adsorbent of Ni-Zn Complex Oxides

WEI Yanyu LI Yonghong KONG Aihua

The adsorbents of Ni-Zn complex oxides were prepared by co-precipitation of corresponding nitrates with urea and sodium dodecyl sulfate. The results showed that Ni was the main active site of the adsorbent. Under the optimum conditions (673 K, 1.0 MPa), the sulfur capability of adsorbent was 360 mg/g. The adsorbent could be recovered by regeneration.

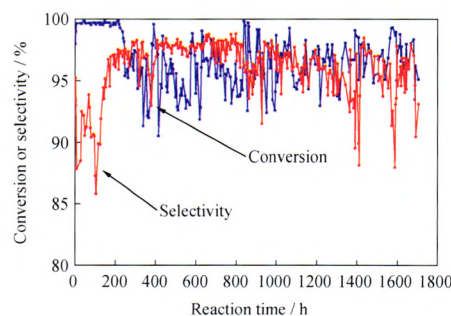


$T=573\text{ K}$; $p=1.0\text{ MPa}$; $LHSV=60\text{ h}^{-1}$;
 $V(\text{H}_2)/V(\text{Model oil})=200$ (volume of H_2 at standard state);
 $c_0=100\text{ mg/L}$

Study on Catalytic Material Used in HPPO Process

ZHU Bin

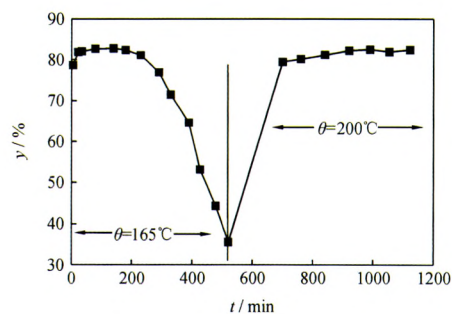
Based on the characteristic of propylene oxide preparation reaction from propylene with hydrogen peroxide as oxidant, catalytic material HTS was investigated thoroughly. The results in hydrogen peroxide-propylene oxide process (HPPO) pilot of titanium silicalite prepared under optimized condition were the conversion of H_2O_2 and the selectivity of propylene oxide both above 95%.



Catalytic Behavior of $\text{Pt}/\text{SO}_4^{2-}/\text{ZrO}_2\text{-Al}_2\text{O}_3$ in *n*-Hexane Isomerization

SONG Yueqin FENG Minchao TIAN Jing XIAO Hang ZHOU Xiaolong XU Longya ZHAO Shenghong HUANG Yi DU Changfei

The catalytic activity of $\text{Pt}/\text{SO}_4^{2-}/\text{ZrO}_2\text{-Al}_2\text{O}_3$ (PSZA) for *n*-hexane isomerization in the presence of H_2 decreased rapidly at low reaction temperature, but the stability of PSZA was greatly improved at relatively high temperature. Hydrogen spillover which was closely related with the temperature determined the catalytic behavior of PSZA in *n*-hexane isomerization at different reaction temperatures.

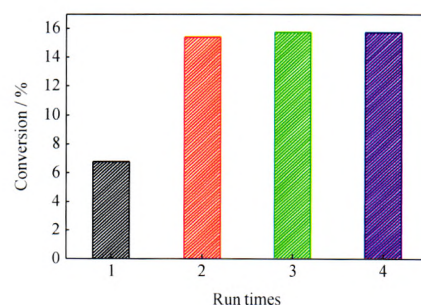


$p=2.0\text{ MPa}$; $MHSV=1\text{ h}^{-1}$; $n(\text{H}_2)/n(\text{C}_6)=4$

Catalytic Performance of MIL-101(Cr) in Oxidation of Cyclohexane With H_2O_2

ZHANG Jiangong HE Min FAN Binbin LI Ruifeng

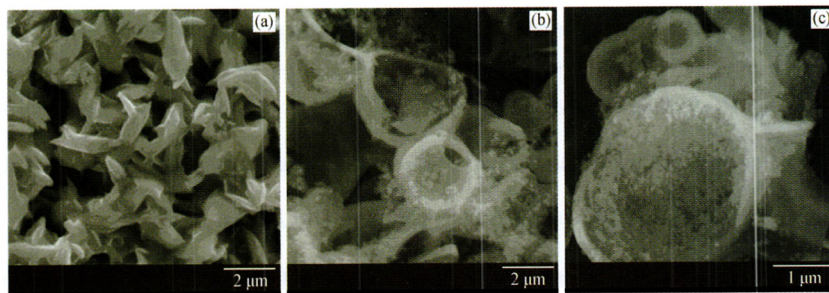
The crystalline structure of MIL-101(Cr) was not stable in oxidation of cyclohexane with H_2O_2 . The formed amorphous material exhibited much higher catalytic activity than the fresh MIL-101(Cr), and could be reused several times without significant change in its catalytic efficiency.



Preparation and Characterization of $H_6P_2W_{18}O_{62}/MCM-48$ and Its Application in Catalytic Synthesis of Adipic Acid

CAO Xiaohua REN Jie XU Changlong XIE Baohua YAN Ping

A novel type of supported catalyst $H_6P_2W_{18}O_{62}/MCM-48$ was successfully prepared by impregnation method and characterized by FT-IR, XRD, SEM and EDS. The catalysts acted as an efficient stable catalyst for the synthesis of adipic acid with cyclohexanone and 30% (mass fraction) H_2O_2 under microwave irradiation, and exhibited good reusability.

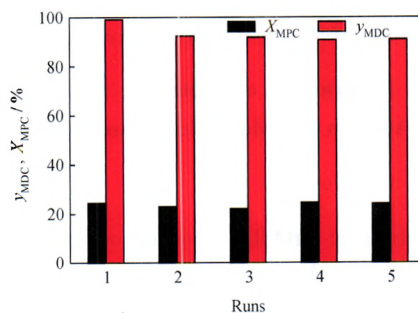


(a) P_2W_{18} ; (b) MCM-48; (c) 40% $P_2W_{18}/MCM-48$

Synthesis of Methylene Diphenyl Dimethylcarbamate Catalyzed by Brønsted-Lewis Acidic Ionic Liquid

KANG Lijuan ZHAO Xinqiang AN Hualiang WANG Yanji

$[HO_3S-(CH_2)_4-mim]Cl-0.7ZnCl_2$ showed high catalytic performance for the synthesis of methylene diphenyl dimethylcarbamate (MDC) from methyl *N*-phenyl carbamate (MPC) and formaldehyde (HCHO). Under the suitable reaction conditions, the yield of MDC was 99.1%. Moreover, the ILs could be easily recovered and used more than five times without significant loss in its catalytic performance.

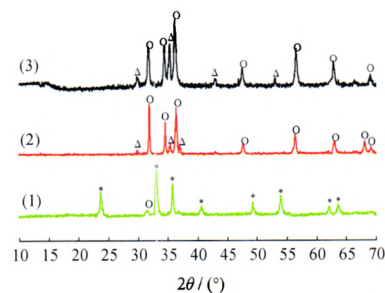


Results of reuse of $[HO_3S-(CH_2)_4-mim]Cl-0.7ZnCl_2$
Reaction conditions: $n(MPC)/n(HCHO)=10$; Reaction time 1 h; Reaction temperature 70°C; $m(ILs)/m(MPC)=2$

Preparation of Zn-Fe Mixed Oxides for the Synthesis of Dimethyl Carbonate From Methyl Carbamate and Methanol

WANG Dengfeng ZHANG Xuelan BAI Dong CAO Nan WEI Wei SUN Yuhan

The structure of Zn-Fe mixed oxide catalysts for the synthesis of dimethyl carbonate (DMC) from methyl carbamate and methanol was greatly influenced by preparation method and calcination temperature, which could further affect their catalytic performances. Zn-Fe mixed oxide possessed good reusability as a catalyst in DMC synthesis.

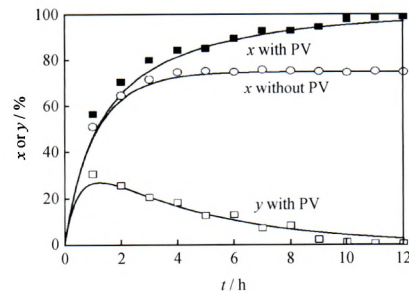


(1) Impregnation method; (2) Co-precipitation method; (3) Sol-gel method
* — Fe_2O_3 (JCPDS 13-0534); o — ZnO (JCPDS 36-1451);
Δ — $ZnFe_2O_4$ (JCPDS 22-1022)

Preparation of High-Flux Mordenite Membranes and the Application to Esterification of Acetic Acid

ZHOU Rongfei ZHANG Peng AN Shunyong ZHANG Youjun NIE Jing
CHEN Xiangshu

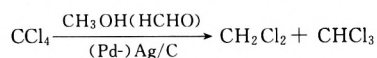
The convention of acetic acid esterified in mordenite membrane reactor arrived at almost 100% after 12 h by removing water from the reaction. The kinetic model for the esterification of acetic acid was in a good agreement with the experimental data.



Effect of Pd and Formaldehyde on In-Situ Liquid Phase Catalytic Hydrodechlorination of CCl₄ Over Ag/C Catalysts

ZHOU Xiulian LU Mohong ZHU Jie LI Mingshi SHAN Yuhua ZHU Jianjun

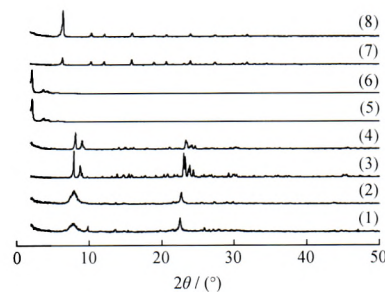
The effects of Pd and formaldehyde on the in-situ catalytic hydrodechlorination of CCl₄ in liquid phase over Ag/C catalyst were investigated. Pd-Ag/C catalyst with Pd/Ag molar ratio of 0.03 exhibited high activity in the reaction. Formaldehyde played an important role in promoting the transformation of surface Ag-Cl species to active Ag.



Catalytic Performance of Molecular Sieve Supported ZrOCl₂ Catalyst for Michael Addition of 2-Methyl Indole and Cyclohexenone-2

LIU Jie QIU Jun

The catalysts of ZrOCl₂ supporting on molecular sieves were prepared by impregnation method and characterized by XRD, SEM and BET. The catalytic performances of the catalysts for synthesis of 3-(2-methyl-1H-indol-3-yl) cyclohexanone were examined from the catalytic Michael addition with 2-methylindole and cyclohex-2-enone under solvent free condition. The results indicated that the specific surface area of molecular sieve greatly influenced the catalyst activity, and the catalytic synergistic effect of acidity of molecular sieve was not obvious.

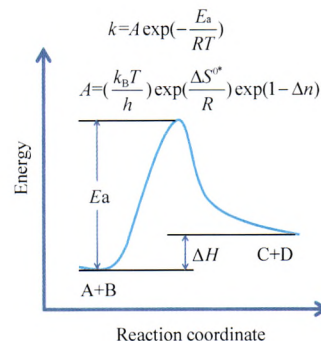


(1) H-BEA; (2) 10% ZrOCl₂/H-BEA; (3) H-ZSM-5; (4) 10% ZrOCl₂/H-ZSM-5; (5) H-MCM-41; (6) 10% ZrOCl₂/H-MCM-41; (7) H-USY; (8) 10% ZrOCl₂/H-USY

Kinetic Modeling of Catalytic Cracking of Monocyclic Cycloparaffins—Calculation of Pre-Exponential Factors

ZHANG Xu GUO Jinbiao ZHOU Xiang WANG Xinlei YU Bo GE Caixia

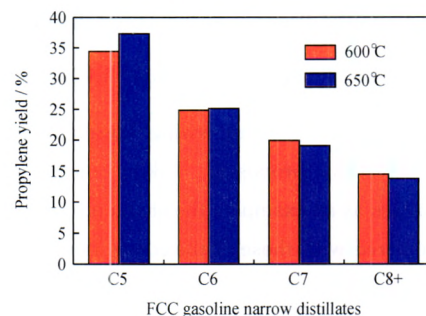
The pre-exponential factor calculation was mainly adopted the transition state theory combining the statistical thermodynamics. In the course of hypothesis and introduced correction factor, gas phase molecular translation entropy approximate was used instead of unavailable reaction activation state entropy and reactant entropy difference, which greatly reduced the workload and simplified the complex degree, the data accuracy was improved at the same time.



A Kinetic Model of Gasoline Catalytic Cracking to Propylene I. Model Establishment

HE Jinlong LI Bo LI Zheng HOU Shuandi

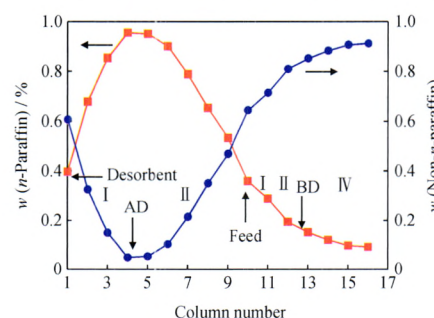
The kinetic reaction performances of narrow distillations, which were separated by carbon number in gasoline cut, were studied by using fixed bed. The experimental results showed that the propylene yield was determined by the rate of hydrocarbon cracking reaction and the second conversion reaction of propylene. And then a kinetic model was derived. The said model can not only predict the product yields, but also simulate the chemical composition of the products.



Optimization of Liquid-Phase Simulated Moving Bed Technology for Naphtha Separation by 5A Molecular Sieve Based on Molecular Management

CAO Jun SHEN Benxian LIU Jichang CAO Xin LIU Juntao

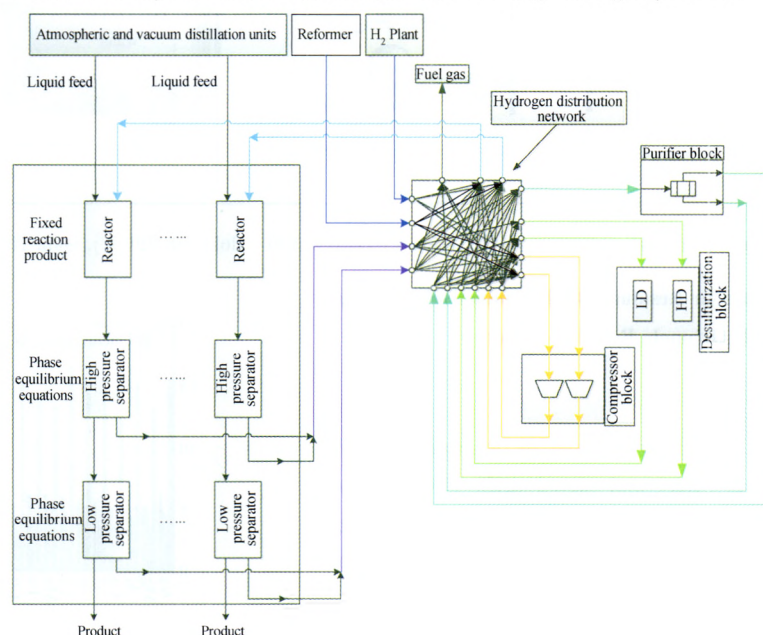
Optimal utilization of simulated moving bed technology on naphtha resource was studied. The concentration distribution of normal paraffins and non-normal paraffins in the bed was investigated and shown in this figure.



Multi-Contaminant H₂ Network Optimization Considering H₂S Remove

ZHOU Li LIAO Zuwei TOKOS Hella WANG Jingdai YANG Yongrong

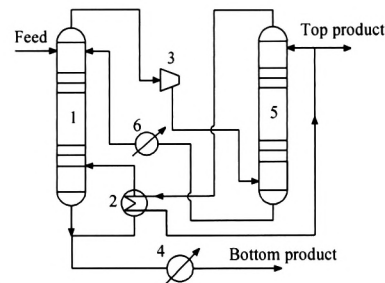
A mixed integer nonlinear programming model for the design of hydrogen networks was proposed. By introducing a desulfurization block into the state-space superstructure, the H₂S removal unit was incorporated with the H₂ removal unit, such as pressure swing adsorption and membrane. The superstructure was reduced based on engineering experience.



An Improved Pressure Swing Thermally Coupled Distillation

ZHANG Lühong LIU Jianbin LI Xingang JIANG Bin LI Hong

An improved pressure swing thermally coupled distillation (PSTCD) process was proposed. Taking methyl-cyclopentane/benzene binary mixture as an example, the characteristics of the improved PSTCD were compared with those of the conventional. Meanwhile, a general PSTCD process was proposed to describe the process systematically. The improved PSTCD had an energy saving efficiency of 3.50%, and had better performance than conventional PSTCD in energy saving.

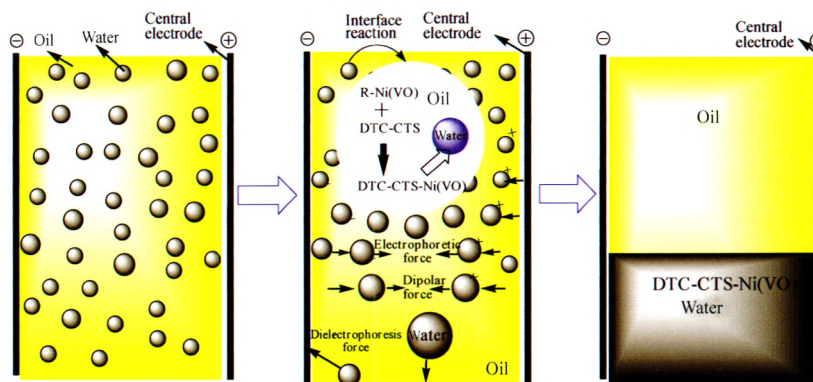


1—Low pressure section; 2—Main heat exchanger; 3—Compressor; 4—Bottom product cooler; 5—High pressure section; 6—Middle cooler

Removal of Ni and V From Tahe Crude Oil by Using DTC-CTS

LI Long HAN Linxin REN Mannian XIAO Tiancun CAO Fahai

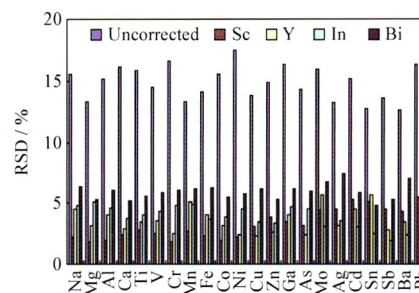
The demetallization agent (DTC-CTS) reacted with Ni and V on the interface between oil and water. The resultant chelates dissolved in water. Then the water drops coalesced in the alternating electric field. At last, bigger droplets settled down and the process of dehydration and demetallization finished.



Determination of Trace Elements in Residual Oil by Inductively Coupled Plasma Mass Spectroscopy With Octopole Reaction System

NIE Xidu XIE Hualin

In this method, Sc, Y, In and Bi were used as internal standard elements to compensate matrix effect and signal drift. Twenty two elements were determined for 6 times before and after the correction of internal standard elements, and the relative standard deviations (RSD) of the results were calculated and compared.



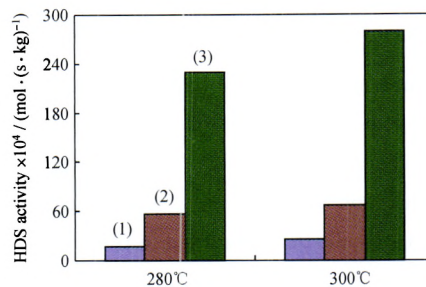
Acta Petrolei Sinica (Petroleum Processing Section), 2013, 29(2): 331-335

doi: 10.3969/j.issn.1001-8719.2013.02.023

Preparation, Characterization and Hydrodesulfurization Properties of NiWO₄ Nanoparticles

WANG Chaofeng

NiWO₄ nanoparticles were prepared by a hydrothermal approach and their hydrodesulfurization activity was evaluated on micro device. Compared with bulky NiWO₄ and commercial NiW/Al₂O₃, NiWO₄ nanoparticles had an extremely high hydrodesulfurization activity for 4,6-dimethyldibenzothiophene.



$p(\text{H}_2) = 4.2 \text{ MPa}$; H_2 flow rate of 400 mL/min;
Feed flow rate of 0.2 mL/min

(1) Bulky NiWO₄; (2) RN-10; (3) NiWO₄ nanoparticles

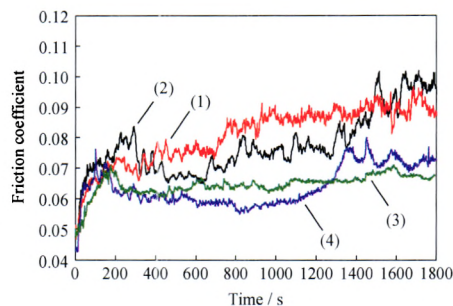
Acta Petrolei Sinica (Petroleum Processing Section), 2013, 29(2): 336-340

doi: 10.3969/j.issn.1001-8719.2013.02.024

Tribological Properties of Functionalized Ionic Liquid as an Additive in Rapeseed Oil

ZHU Liye CHEN Ligong LIU Hanchen XIONG Xiaolong

The tribological properties of synthesized functionalized ionic liquid, 1-ethoxycarbonylmethyl-3-methylimidazolium bis (trifluoromethylsulfonyl) imide (LF1-4), as an additive in rapeseed oil (RO) were evaluated. Results showed that LF1-4 additive possessed good friction-reducing and anti-wear ability in RO. The optimum addition amount of LF1-4 in RO was 1.0%, when the wear scar diameter could be decreased by 38%.



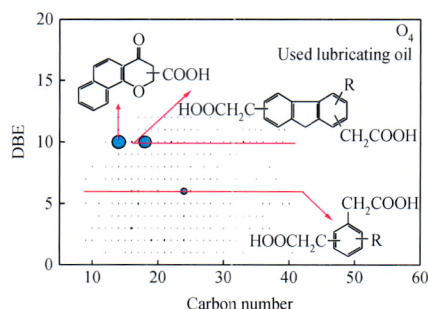
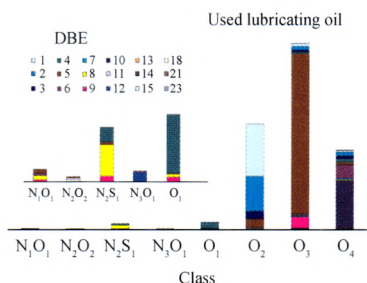
Acta Petrolei Sinica (Petroleum Processing Section), 2013, 29(2): 341-347

doi: 10.3969/j.issn.1001-8719.2013.02.025

Composition and Distribution of Acidic Components in Used Vehicle Lubricating Oil Identified by Negative Electrospray Ionization Fourier Transform Ion Cyclotron Resonance Mass Spectrometry

LI Xiaohui ZHU Jianhua WU Bencheng ZHOU Yong MAO Xinhua

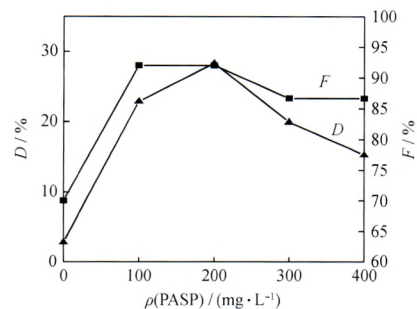
The difference of occurrence states of acidic compounds between fresh and used vehicle lubricating oil was mainly investigated for revealing the aging mechanism of fresh lubricating oil by negative-ion ESI FT-ICR MS. The remarkable point was that the considerable amount of O₄ class species was found in used vehicle lubricating oil, but it was not found in fresh vehicle lubricating oil.



Chelate Effect of Polyaspartic Acid and Iron Component in Crude Oil

LI Meirong LI Ranran PU Ming FANG Hongbo ZONG Hua WANG Yuhui

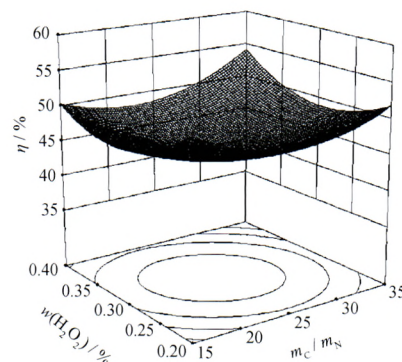
The iron in crude oil mainly existed as oil-soluble organacid salts and complex. For the aging crude oil emulsion with water mass fraction of 50%, under the conditions that the operating temperature was 60°C, the time was 20 min, demulsifier BSE-238 concentration was 100 mg/L and compound complexing agent concentration was 200 mg/L, the deferrization rate reached its highest value 29.26%.



Strengthening Bioremediation of Oil Contaminated Soil by Activation Agent and Optimization of Bioremediation Conditions

ZHANG Xiuxia TENG Zhi WU Jiadong BAI Xuejing

Four kinds of activation agents were added to oil contaminated soil for strengthening bioremediation. According to strengthening bioremediation effects, three significant factors most affecting oil degradation were chosen for the response surface optimization research, then the optimal conditions of strengthening bioremediation were obtained.



Special Review

Review on the Progress of Producing Bio-Jet Fuel

LI Yi ZHANG Zhemin QU Hongliang MENG Xiangkun

The processes of producing bio-jet fuel were reviewed. There are four routes to produce bio-jet fuel from vegetable oil, animal fat and biomass.

