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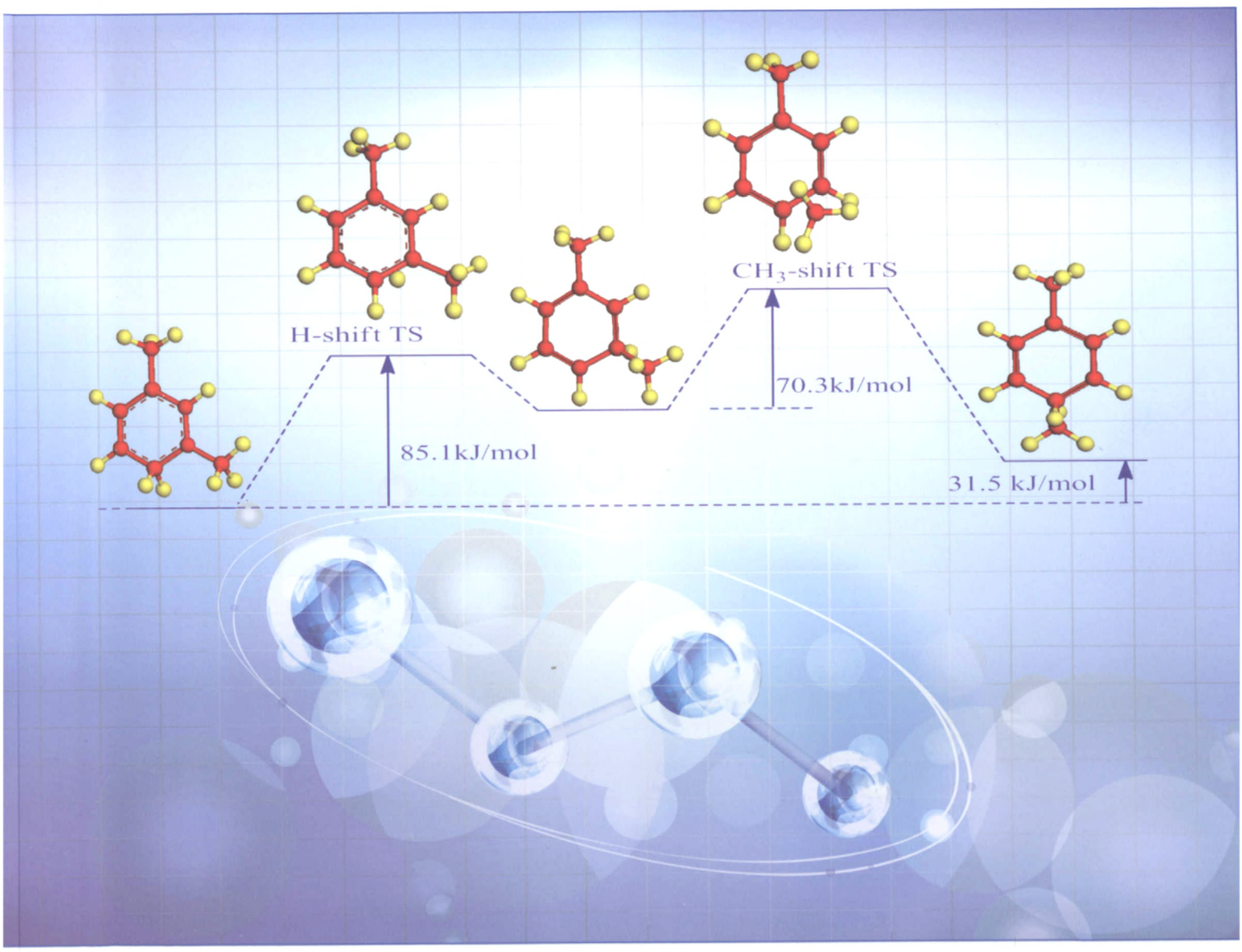
ACTA PETROLEI SINICA
(PETROLEUM PROCESSING SECTION)



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（石油加工）

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* 封面文章

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ACTA PETROLEI SINICA

(PETROLEUM PROCESSING SECTION)

Vol. 28 No. 4 Aug. 2012

CONTENTS

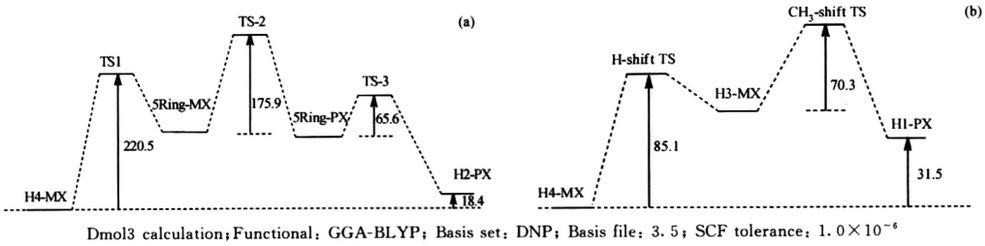
Research Articles

Acta Petrolei Sinica (Petroleum Processing Section), 2012, 28(4): 533-537 **doi**: 10.3969/j.issn.1001-8719.2012.04.001

Reaction Chemistry of Xylene Isomerization

KANG Chenglin LONG Jun ZHOU Zhenhuan WU Wei GU Haohui

The two different mechanisms of xylene intramolecular isomerization, 1,2-shift and 1,3-shift, was investigated, and the energy of intermediate and transition state was calculated and compared. The results showed that the 1,2-shift was the main mechanism path for xylene intramolecular isomerization.



Dmol3 calculation; Functional: GGA-BLYP; Basis set: DNP; Basis file: 3.5; SCF tolerance: 1.0×10^{-6}

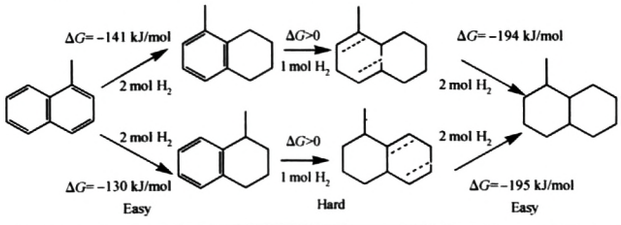
(a) 1,3-Shift; (b) 1,2-Shift

Acta Petrolei Sinica (Petroleum Processing Section), 2012, 28(4): 537-543 **doi**: 10.3969/j.issn.1001-8719.2012.04.002

Hydrogenation Saturation Discipline of 1-Methyl Naphthalene Over Ni-Mo Catalyst

JU Xueyan ZHANG Yuying HU Zhihai WANG Lixin LI Dadong

The reaction network of 1-methylthalene(1-MN) was deduced by experiments data and simulation calculation. The first aromatic ring of 1-MN was hydrogenated easily for lower ΔG while the second ring was rather difficult to be saturated, so 1-MN could be partial hydrogenation to tetralin with high selectivity, avoiding over-saturated to decalin.

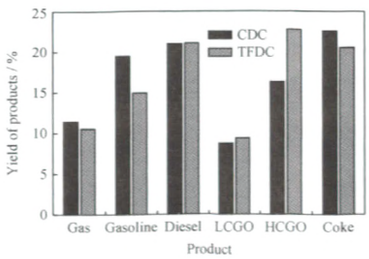


Acta Petrolei Sinica (Petroleum Processing Section), 2012, 28(4): 544-549 **doi**: 10.3969/j.issn.1001-8719.2012.04.003

A New Top Feeding Delayed Coking Process for Maximizing Liquid Yields

WANG Baoshi ZHU Jianhua WANG Longyan QIN Ruyi WANG Hongbin

A new top feeding delayed coking process (TFDC) characterized by top feeding and discharging reactors was developed. Compared to the conventional delayed coking process, the yield of liquid products obtained from TFDC process increased by 2.65 percent points, the yield of coke and gas decreased by 2.01 and 0.85 percent points, respectively.

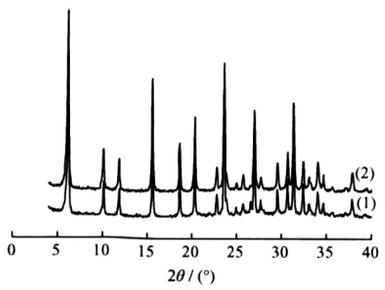


Acta Petrolei Sinica (*Petroleum Processing Section*), 2012, 28(4): 550-554 **doi**: 10.3969/j.issn.1001-8719.2012.04.004

Modification of Diatomite and the Preliminary Study on Synthesis of NaY Zeolite by Using Modified Diatomite

ZHENG Shuqin CHENG Yuankun QIAN Dong YAO Hua

The raw diatomite and alkali-modified diatomite were characterized by XRD, FT-IR and SEM. A preliminary study on the synthesis of NaY zeolite by in-situ crystallization with the modified diatomite as raw material was carried out. The results showed that the raw diatomite was transformed to cristobalite at 1100℃ and alkali-modified diatomite at 950℃.



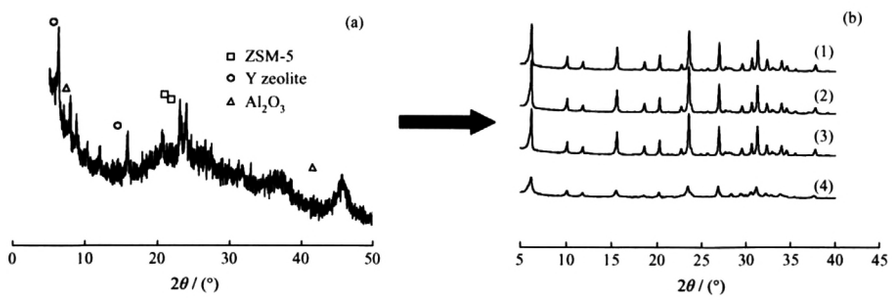
(1) Synthesized NaY; (2) Pure NaY

Acta Petrolei Sinica (*Petroleum Processing Section*), 2012, 28(4): 555-560 **doi**: 10.3969/j.issn.1001-8719.2012.04.005

Synthesis of Super-Fine Y Zeolite With FCC Spent Catalyst Fines

LIU Xinmei LI Liang YANG Tingting YAN Zifeng

The super-fine zeolite Y was successfully prepared by using FCC spent catalyst fines. The synthesized zeolite possessed large specific surface area, good hydrothermal stability and high cracking activity for heavy oil.



(a) FCC spent catalyst fines; (b) Y zeolite

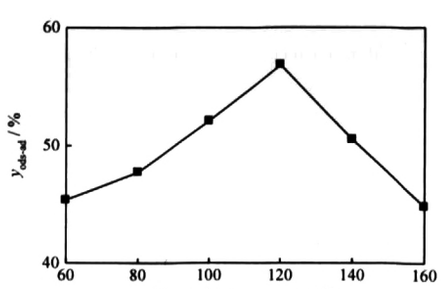
$n(NaCl)/n(Al_2O_3)$: (1) 0; (2) 0.5; (3) 1.0; (4) 1.5

Acta Petrolei Sinica (*Petroleum Processing Section*), 2012, 28(4): 561-565 **doi**: 10.3969/j.issn.1001-8719.2012.04.006

Oxidation-Adsorption Desulfurization of Gasoline by Mesoporous CuO/SiO_2

XU Kangwen FENG Lijuan WANG Jinggang LI Yuhui
LI Chunhu

Mesoporous CuO/SiO_2 was used in the oxidation-adsorption desulfurization process of gasoline. The results showed that the sulfur removal rate could reach 56.82% under the CuO/SiO_2 preparation conditions of calcination temperature 400℃, calcination time 2.0 h, CuO mass fraction 2%, and adsorption temperature of 120℃.



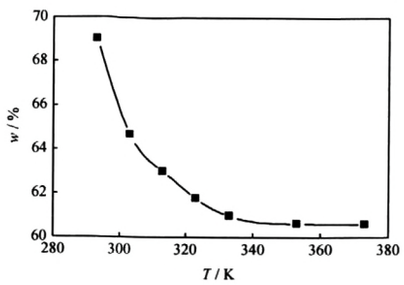
Calcination temperature of 400℃; $w(CuO)=2\%$;
Calcination time of 2.0 h; LHSV=6.0 h^{-1}

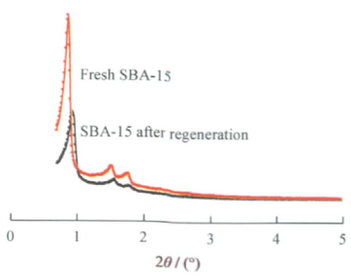
Acta Petrolei Sinica (*Petroleum Processing Section*), 2012, 28(4): 566-570 **doi**: 10.3969/j.issn.1001-8719.2012.04.007

Adsorption of Basic Nitrogen Compounds From Oil by SBA-15 Zeolite

ZHU Jinzhu SHEN Jian

SBA-15 mesoporous zeolite is one of ideal adsorbents because of its large specific surface area and thick pore wall. Experimental results showed that SBA-15 had better adsorptive ability to the basic nitrogen compounds and good reusability.



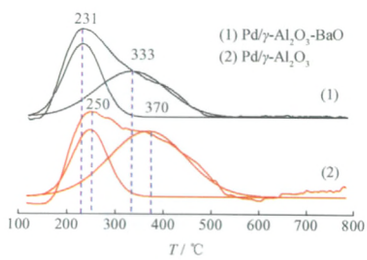


Acta Petrolei Sinica (*Petroleum Processing Section*), 2012, 28(4): 571-576 **doi**: 10.3969/j.issn.1001-8719.2012.04.008

The Deactivation and Modification of Pd/γ-Al_2O_3 Catalyst for Catalytic Amination of 2,6-Dimethylphenol

WANG Huabang MA Jianchao WU Zhiwei CHEN Ligong LI Yang

When Pd/γ-Al_2O_3 was doped BaO, the spinel $BaAl_2O_4$ was generated, then the acid capacity of Pd/γ-Al_2O_3 was significantly decreased, which accelerated the desorption of amino compounds from Pd/γ-Al_2O_3 and inhibited the formation of carbon deposition, therefore, the stability of Pd/γ-Al_2O_3-BaO was enhanced.

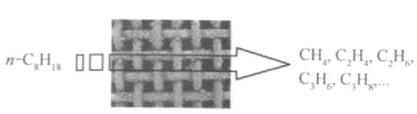


Acta Petrolei Sinica (*Petroleum Processing Section*), 2012, 28(4): 577-582 **doi**: 10.3969/j.issn.1001-8719.2012.04.009

Preparation and Catalytic Properties of ZSM-5 Zeolite Films on FeCrAl Alloy Grids

WU Huihui LI Gang

ZSM-5 film with ZSM-5 crystals on FeCrAl grids was prepared by using one-step growth method, which possessed higher catalytic activity for *n*-octane cracking. The conversion of *n*-octane at 400℃ was 24.2% over the ZSM-5 film, an order of magnitude higher than that over the bare FeCrAl grid (2.0%).

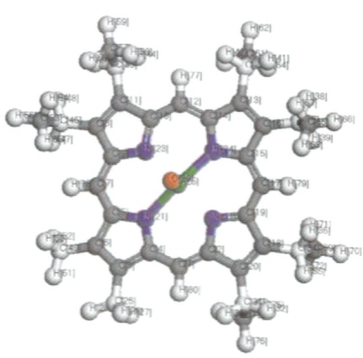


Acta Petrolei Sinica (*Petroleum Processing Section*), 2012, 28(4): 583-590 **doi**: 10.3969/j.issn.1001-8719.2012.04.010

Study of Metalloporphyrins in Yichang Tube-Transporting Oil Residua With Quantum Chemistry Calculation Based on DFT Method

GAO Yuanyuan SHEN Benxian LIU Jichang

Quantum chemistry calculation was used to study the metalloporphyrins. By molecular simulation and spatial structure optimization, the key parameters, dipole moments and characteristic absorption peak of Soret and Q absorption band in UV absorption spectrum were calculated. The stability order from strong to weak was C_{35}-(ETIO-Ni), C_{35}-(DPEP-Ni), C_{34}-(ETIO-VO) and C_{31}-(DPEP-VO).

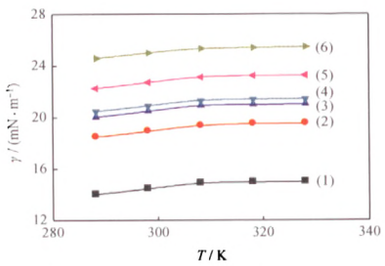


Acta Petrolei Sinica (*Petroleum Processing Section*), 2012, 28(4): 591-597 **doi**: 10.3969/j.issn.1001-8719.2012.04.011

Molecular Dynamics Simulation for Interface Behavior of Betaine Surfactants in Aqueous Solution

CHEN Yuping DING Wei YU Tao QU Guangmiao LIU Guoyu GAO Xiang

Series of betaine surfactants has good ability to reduce oil-water interfacial tension. The oil-water interfacial tension of octane + water + betaine surfactant system changed little with the increase of temperature, meaning that the system held good heat resistance.



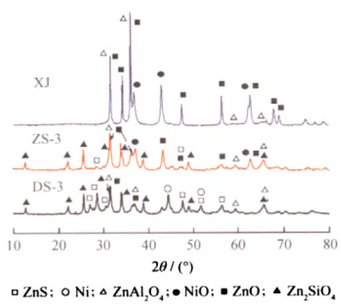
(1) ZSB9-1; (2) ZSB9-2; (3) ZSB9-3; (4) ZSB12-1; (5) ZSB12-2; (6) ZSB12-3

Acta Petrolei Sinica (*Petroleum Processing Section*), 2012, 28(4): 598-604 **doi**: 10.3969/j.issn.1001-8719.2012.04.012

Study of Rietveld Quantitative Phase Analysis of S Zorb Sorbent

ZOU Kang HUANG Nangui XU Guangtong

The deactivation of S Zorb sorbent was mainly attributed to the present of non-active zinc-type spinel. The Rietveld quantitative phase analysis (RPA) method was established for S Zorb fresh, spent and regenerated sorbents, respectively. The results obtained by XRD, XRF and ^{29}Si NMR were found to complement each other well. Obviously, the RPA method can be widely used in online monitoring of industrial equipment and S Zorb sorbent development.

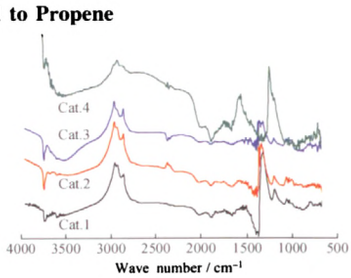


Acta Petrolei Sinica (*Petroleum Processing Section*), 2012, 28(4): 605-611 **doi**: 10.3969/j.issn.1001-8719.2012.04.013

Coking Process of Catalyst Based on In-Situ Diffuse FT-IR Spectroscopy in Reaction of Methanol to Propene

TANG Yueqi YU Xianbo WANG Jingdai YANG Yongrong

The change of pore structure, acidic sites and intensity of catalyst due to phosphorous modification and hydro-thermal treatment had significant influence on its coke composition and amount in the reaction of methanol to propene. Under the same reaction conditions, the coke composition on modified ZSM-5 catalysts was more complicated than that on ZSM-5. Moreover, coke amount increased with the acid intensity of catalyst.

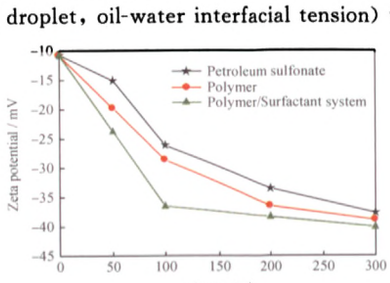


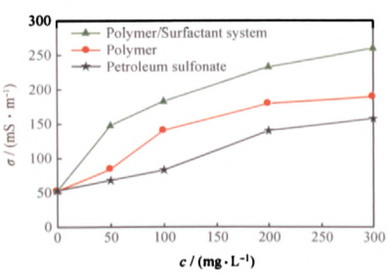
Acta Petrolei Sinica (*Petroleum Processing Section*), 2012, 28(4): 612-616 **doi**: 10.3969/j.issn.1001-8719.2012.04.014

Relevance Between Characterization Indices of the Stability of Chemical Flooding Produced Fluid

LI Meirong ZHAO Nana FANG Hongbo ZONG Hua MAO Leiting LI Ranran

The influence of different oil displacement agents on the properties of chemical flooding produced fluids was studied, and the relevance between the stability of emulsion (dehydration, SV value) and characterization indices(Zeta potential, conductivity, the middle size of oil droplet, oil-water interfacial tension) was researched for the first time.



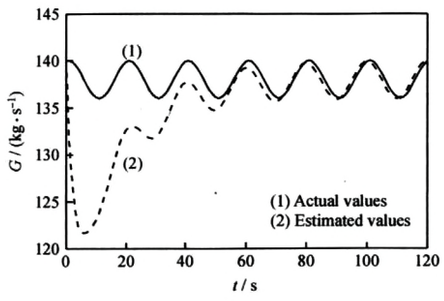


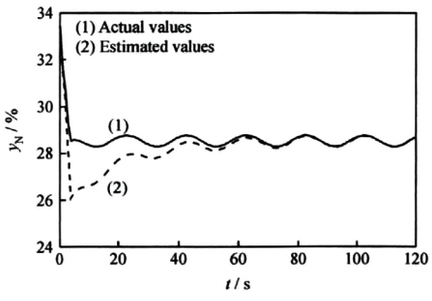
Acta Petrolei Sinica (*Petroleum Processing Section*), 2012, 28(4): 617-624 **doi**: 10.3969/j.issn.1001-8719.2012.04.015

On-Line Observation of FCCU Catalyst Circulation Rate

XU Feng LUO Xionglin

Based on the nonlinear differential-algebraic dynamic model of FCCU riser, the state observer could be used to estimate catalyst circulation rate and oil yields on-line with good performance when catalyst circulation rate and uncertain model parameters were augmented as state variables and appropriate temperature sensors were added to FCCU riser.



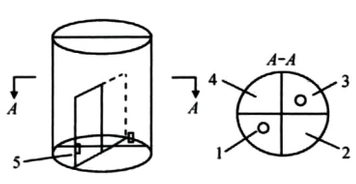


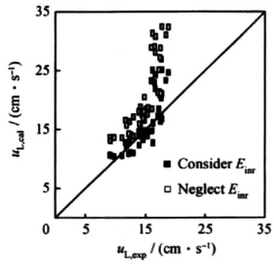
Acta Petrolei Sinica (*Petroleum Processing Section*), 2012, 28(4): 625-630 **doi**: 10.3969/j.issn.1001-8719.2012.04.016

Hydrodynamic Characteristics in Three-Phase MALR

ZHANG Wenfei LIU Yongmin WANG Lipeng

A hydrodynamic model was established on the basis of energy balance principle and drift-flux model in three phase multi-compartment airlift loop reactor. Interaction coefficient was proposed for describing energy dissipation due to the interaction between solid particles. The results showed that a good agreement between calculated value and experimental data was obtained.



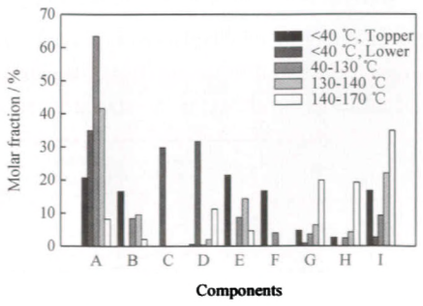


Acta Petrolei Sinica (*Petroleum Processing Section*), 2012, 28(4): 631-635 **doi**: 10.3969/j.issn.1001-8719.2012.04.017

Analysis of Chemical Compositions and Fuel Characteristics of Tars From Cornstalk Carbonization

SONG Feifei WU Shiyong WU Youqing GAO Jinsheng

Group compositions of four distillations from the reduced pressure distillation of cornstalk carbonization tar were analyzed. The distillation at 40 — 130℃ could be used as a promising liquid fuel due to its comparatively excellent fuel characteristics.



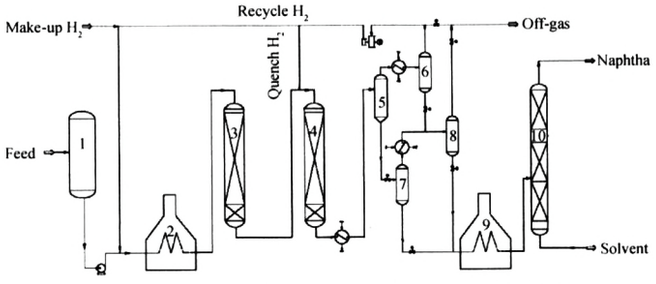
A—Phenols; B—Benzene and its derivatives (alkyl); C—Ketone; D—Pyridine and its derivatives; E—Naphthalene and its derivatives; F—Furan; G—Alkene; H—Alkane; I—Others

Acta Petrolei Sinica (*Petroleum Processing Section*), 2012, 28(4): 636-641 **doi**: 10.3969/j.issn.1001-8719.2012.04.018

Study on the Hydrotreatment of Fractions From Coal Tar Used as Coal Liquefaction Starting Solvent

GAO Shansong LI Kejian LI Yonglun JIANG Yuanbo

The mixture of wash oil and de-crystal anthracene oil (mass ratio 1:1) was used as the hydrotreatment feedstock to get coal liquefaction starting solvent. The research results showed that the hydrogenated solvent of mixture oil from coal tar was an excellent starting solvent for coal liquefaction.



1—Feed surge drum; 2—Feed heater; 3—Hydrogentreating 1st reactor; 4—Hydrogentreating 2nd reactor; 5—Hot high pressure separator; 6—Cold high pressure separator; 7—Hot low pressure separator; 8—Cold low pressure separator; 9—Fractionator feed heater; 10—Fractionator

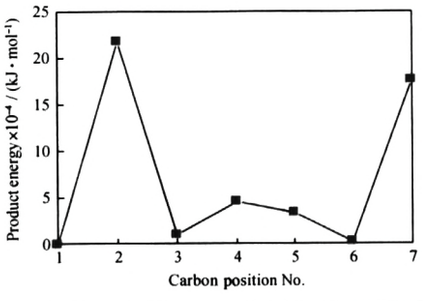
Research Notes

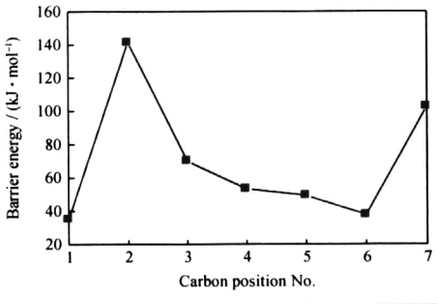
Acta Petrolei Sinica (*Petroleum Processing Section*), 2012, 28(4): 642-645 **doi**: 10.3969/j.issn.1001-8719.2012.04.019

Quantum Chemistry of the Initial Hydrogenation on Different C Positions in Phenanthrene Molecule

WANG Chunlu ZHOU Han WANG Zijun ZHAO Yi

Initial hydrogenation on different carbons in phenanthrene molecule was calculated by molecular modeling software Material Studio 5.5. The results showed that peripheral carbons in phenanthrene molecule were most likely to take preliminary hydrogenation, and the products were stable as well.



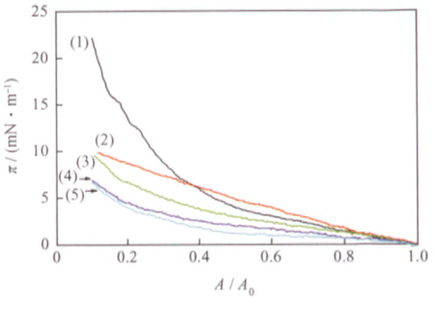


Acta Petrolei Sinica (*Petroleum Processing Section*), 2012, 28(4): 646-651 **doi**: 10.3969/j.issn.1001-8719.2012.04.020

Effect of Different Structure Demulsifiers on the Surface Film Properties of Crude Oil and Its Acidic-Basic Fractions

LIU Jinhe WANG Zongxian FANG Xiaowei YANG Pujiang

The different structure demulsifier had different effect on π-A/A_0 isothermal curve of crude oil. The decrease range of surface film pressure of crude oil was related to the structure and concentration of demulsifier. The branch chain demulsifier had stronger ability to reduce surface film pressure of Gudao crude oil then straight chain demulsifier.

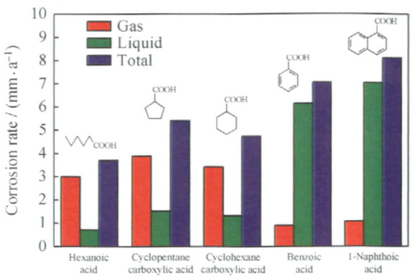


Acta Petrolei Sinica (*Petroleum Processing Section*), 2012, 28(4): 652-656 **doi**: 10.3969/j.issn.1001-8719.2012.04.021

Relationship Between Naphthenic Acid Structure and Its Corrosion Performance

ZHANG Qundan TIAN Songbai HUANG Shaokai WANG Jing

In order to investigate the corrosion ability of different naphthenic acid, the corrosion rates of 26 naphthenic acids were determined. The results showed that the corrosion ability of straight train fatty acid was decreased with the increase of its carbon number. The ring replacement in acid could increase the corrosion ability of the acid.

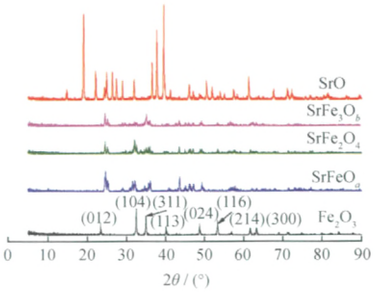


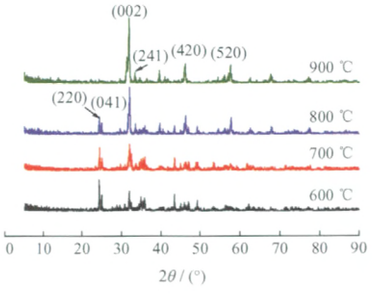
Acta Petrolei Sinica (*Petroleum Processing Section*), 2012, 28(4): 657-661 **doi**: 10.3969/j.issn.1001-8719.2012.04.022

Selective Catalytic Oxidation of Styrene to Benzaldehyde Over $SrFe_2O_4$ Catalysts

FENG Shihong YAN Shaofeng LIU Zili

Spinel type strontium ferrate was prepared through sol-gel method with styrene selective oxidation by H_2O_2 as probe reaction. The catalyst evaluation results showed that the optimum catalyst atomic ratio was $n(Fe) : n(Sr) = 2 : 1$ with high catalytic activity. The catalysts were detected by XRD. The optimum calcination temperature was 700℃.



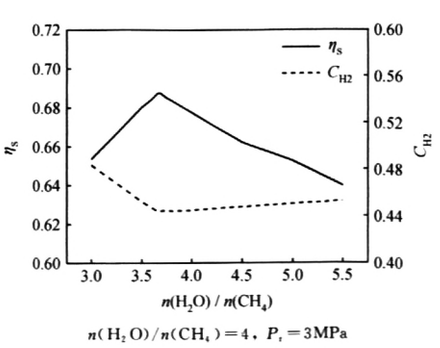


Acta Petrolei Sinica (*Petroleum Processing Section*), 2012, 28(4): 662-669 **doi**: 10.3969/j.issn.1001-8719.2012.04.023

Exergy Analysis of Hydrogen Production by Steam Reforming of Hydrocarbons and Its Carbon Emission Evaluation

CHEN Bo LIAO Zuwei WANG Jingdai YU Huanjun
YANG Yongrong

The influence of operation parameters and components of feedstock on system efficiency and carbon emission for unit H_2 production was identified by using exergy analysis for an industrial hydrogen production plant. An analytical expression for the relationship between efficiencies of system and its sub-units was given and used to investigate the process on sub-unit level.



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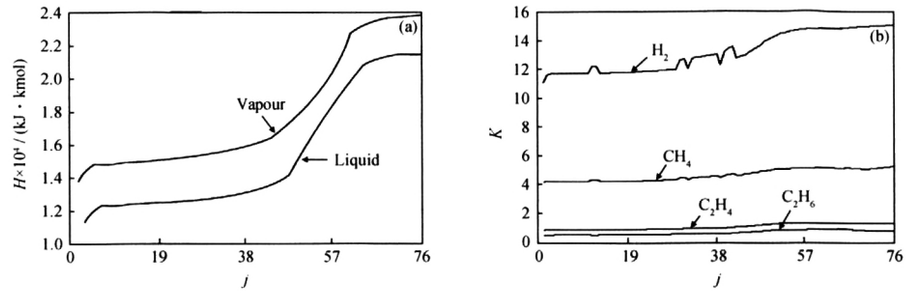
Complicated Mechanism Model Development of Ethylene Distillation Column for Online Analysis Application

HE Renchu

An ethylene rectifier was chosen as a representative model verification object. The rigorous steady mechanism model was built for a distillation column according to the standpoint of online analysis application. Results of model calculation were compared with results from lab data and calculation of Aspen Plus under an operating condition, which showed that the rigorous steady mechanism model developed for distillation column was of accurate



(a) Gas-liquid phase enthalpy; (b) Phase equilibrium constant

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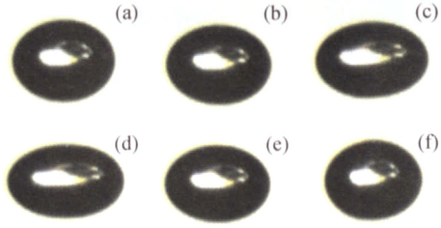
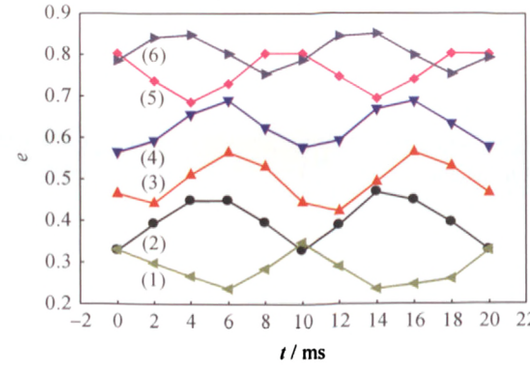
Experiment of the Oscillation Characteristics of Single Drop in High-Voltage AC Electric Field

YANG Donghai HE Limin YE Tuanjie LUO Xiaoming LÜ Yuling

Deformation of water droplet in oil was affected by electric field strength, diameter and interfacial tension of oil-water. Oscillation amplitude of the droplet was affected by electric filed frequency, oil viscosity and interfacial tension of oil-water. Higher frequency, higher oil viscosity and lower interfacial tension of oil-water led to smaller oscillation amplitude of water droplet in oil, while electric field strength and diameter had no obvious influence.



θ=15.0 ℃; D=866 μm; E=840 kV/m; f=50 Hz
t/ms: (a)0; (b)2; (c)4; (d)6; (e)8; (f)10



θ=15℃; f=50 Hz; D=866 μm
E/(kV·m^{-1}): (1)366; (2)488; (3)610; (4)732; (5)793; (6)841

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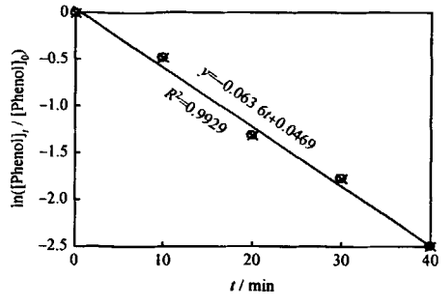
Degradation Efficiency and Kinetics of Ozonation of Phenol in Water

YANG Demin WANG Bing YUAN Jianmei

Under the conditions of this experiment, the degradation rate of phenol was 99.65%, and the degradation of the phenol followed the apparent pesudo-first-order kinetic model, and its correlation coefficient R^2 was 0.9991 and the rate constants k was $1.01 \times 10^{-3}\ s^{-1}$.



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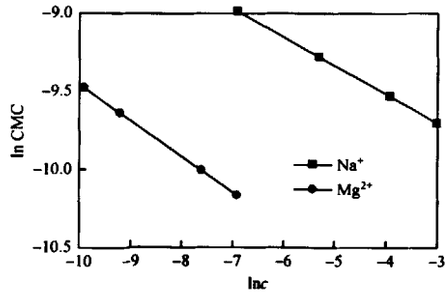
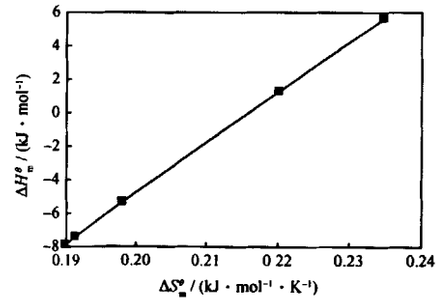
Effects of Additive on Micellization of 2,4-Dimethyl-5-(1'-Butyl)Decyl Benzene Sulfonate Sodium in Aqueous Solution

DING Wei ZHANG Zhiwei LI Zhong DONG Zhilong YU Tao QU Guangmiao YUAN Dandan LI Shujie

The thermodynamic properties of the micellization of alkyl aryl sulfonate were investigated by surface tension method. The results showed that micellization process of alkyl aryl sulfonate in aqueous solution was mainly from the entropy-driven and there was a phenomenon of enthalpy-entropy compensation, enthalpy-driven force increased with the increase of temperature.





Acta Petrolei Sinica (*Petroleum Processing Section*), 2012, 28(4): 696-704 **doi**: 10.3969/j.issn.1001-8719.2012.04.028

Primary Study on the Bio-remediation of Oil Contaminated Soil of Karamay Oilfield

ZHAO Dongfeng WU Weilin ZHANG Yunbo YANG Haibin ZHAO Chaocheng

The short chain *n*-alkanes ($C_{12} - C_{14}$) were first degraded by bacteria, which could not be detected after 70 d degradation. The GC peak shape of *n*-alkanes changed greatly, from symmetrical to "left slow, right steep", and the relative content of isoparaffin increased, the base line of GC was significantly elevated.