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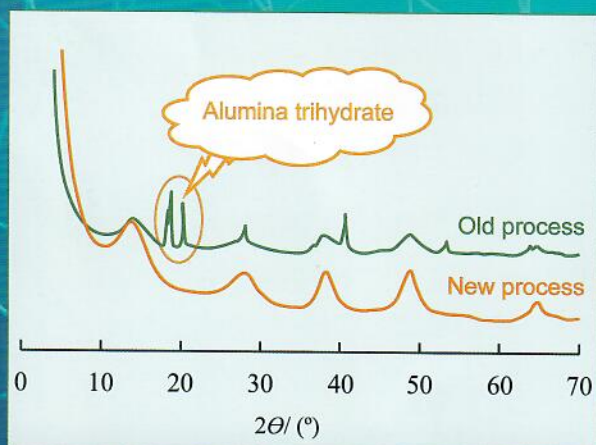
# 石油学报 (石油加工)

## ACTA PETROLEI SINICA (PETROLEUM PROCESSING SECTION)

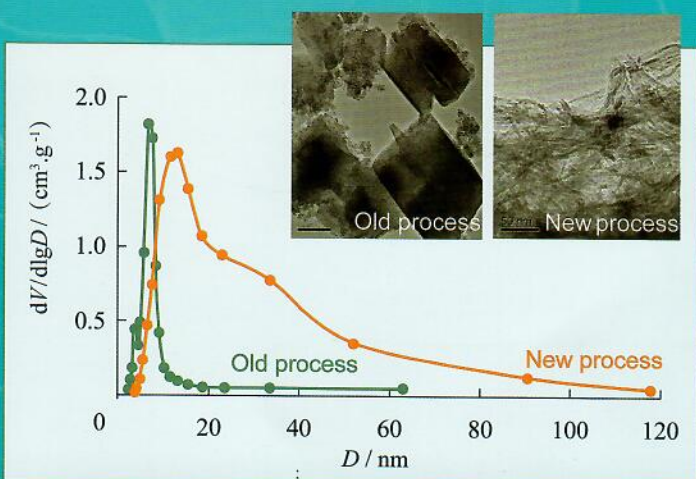
### Commercial application of new process



Pseudo-Boehmite



XRD patterns of pseudo-boehmite samples



Pore size distribution and TEM images of calcined samples

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中国石油学会主办  
石油化工科学研究院 承办

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# 石 油 学 报

## (石油加工)

第 37 卷 第 4 期 2021 年 7 月

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#### 信息

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#### \* 封面文章

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# ACTA PETROLEI SINICA

## ( PETROLEUM PROCESSING SECTION )

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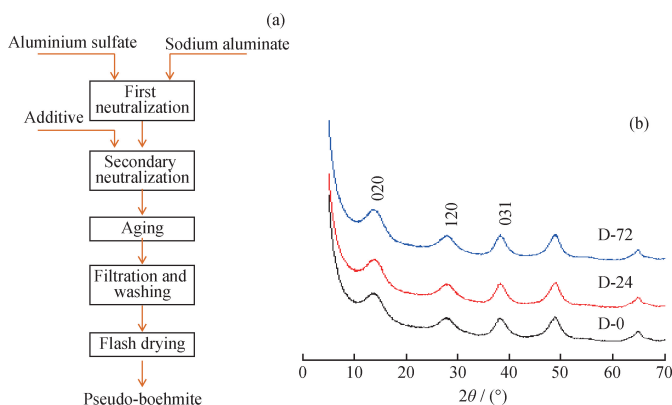
#### Research Articles

*Acta Petrolei Sinica (Petroleum Processing Section)*, 2021, 37(4): 0719-0727 doi: 10.3969/j.issn.1001-8719.2021.04.001

#### Minimizing Alumina Trihydrate Content in Pseudo-Boehmite Commercial Product

ZENG Shuangqin YANG Qinghe LIU Bin LIANG Weijun YU Bo LI Dadong NIE Hong

It is identified that local excess of  $\text{NaAlO}_2$  due to pH value fluctuation in local area is the reason for high content of alumina trihydrate in the product. A new stepwise continuous neutralization process can eliminate the possibility of alumina trihydrate formation. Commercial application shows that alumina trihydrate seed crystals formation cannot be found with using the new proposed process. Based on the new proposed process, the qualification ratio of alumina trihydrate content in the product can be 100%, and pore volume qualification ratio is 98.1%. In addition, product yield can increase 12.4 percentage, and annual output has increased 64.56%.



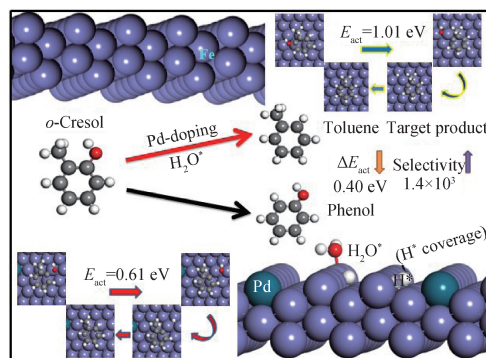
(a) Flow chart of pseudo-boehmite new production process; (b) XRD patterns of samples from the new pseudo-boehmite production process

*Acta Petrolei Sinica (Petroleum Processing Section)*, 2021, 37(4): 0728-0743 doi: 10.3969/j.issn.1001-8719.2021.04.002

#### Theoretical Study on Hydrodeoxygenation of *o*-Cresol Over Pd-Doped Fe Catalyst

ZHANG Zeshi NIE Xiaowa SONG Chunshan GUO Xinwen

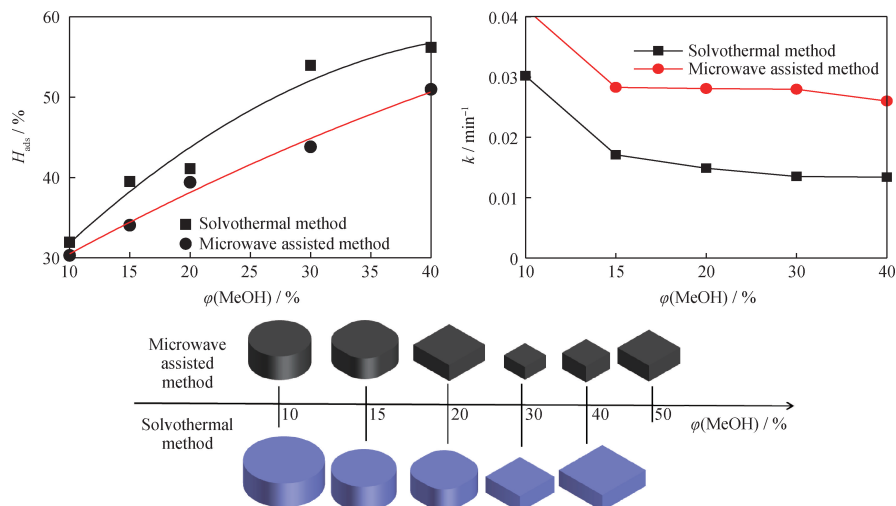
Reaction mechanism, effect of Pd doping and the important role of water in the hydrodeoxygenation of phenolic compounds over Fe-based catalysts are studied with density functional theory calculations. Pd-doped Fe catalyst exhibits good activity and selectivity for toluene production from hydrodeoxygenation of *o*-cresol.  $\text{H}_2\text{O}^*$  participation in the H-transfer process further decreases hydrodeoxygenation barriers.



## Effects of Solvent and Microwave Assistance on Synthesis of NH<sub>2</sub>-MIL-125-Ti and Its Photocatalytic Performance

TAN Yujian LIU Min GUO Xinwen HU Shen

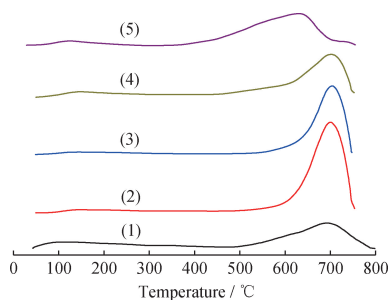
For synthesis of NH<sub>2</sub>-MIL-125-Ti, with increasing volume fraction of methanol in DMF-methanol mixed solvent from 10% to 50%, the morphology of NH<sub>2</sub>-MIL-125-Ti changed from circular flake to square flake. With methanol volume fraction increase in the mixed solvent, crystal size decreased in the beginning but became larger later, and the equilibrium adsorption capacity of RhB increased but the photocatalytic degradation rate decreased. When changing solvothermal method to microwave assisted method, photocatalytic degradation rate of RhB can be improved but equilibrium adsorption capacity became less.



## Catalytic Performance of Fe-K Catalysts Supported on Alkaline Earth or Manganese-Containing Composite Oxides in Fischer-Tropsch Synthesis

LIU Zhenxin ZHAO Chenxi JIA Gaopeng TIAN Hongmei  
GAO Yuji XING Yu

Strong surface basicity of the basic sites favors high catalytic activity of the catalysts in Fischer-Tropsch reaction to olefins. The C-C coupling ability and hydrocarbon selectivity of light olefins are generally contrary to the basicity strength of Fe-K<sub>2</sub>O/MAl<sub>2</sub>O<sub>4</sub> catalysts.

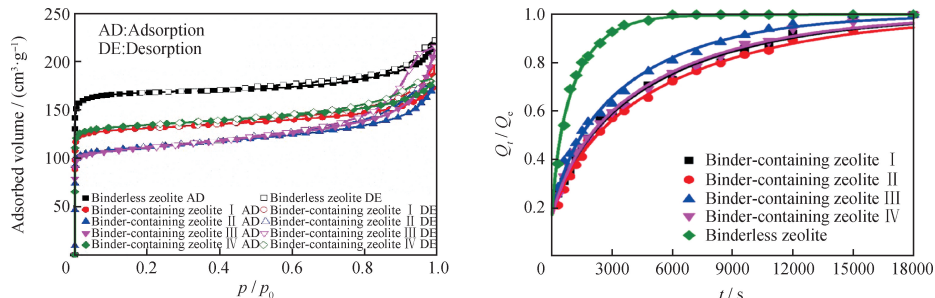


(1) Fe-K<sub>2</sub>O/MgAl<sub>2</sub>O<sub>4</sub>; (2) Fe-K<sub>2</sub>O/CaAl<sub>2</sub>O<sub>4</sub>; (3) Fe-K<sub>2</sub>O/SrAl<sub>2</sub>O<sub>4</sub>; (4) Fe-K<sub>2</sub>O/BaAl<sub>2</sub>O<sub>4</sub>; (5) Fe-K<sub>2</sub>O/MnAl<sub>2</sub>O<sub>4</sub>

### Adsorption Performance of 1-Hexene on Binderless Zeolite X Pellets

YAO Bin CHANG Xiaohu ZHAO Yi YE Fan XU Mengyao SUN Hui JIANG Hao SHEN Benxian

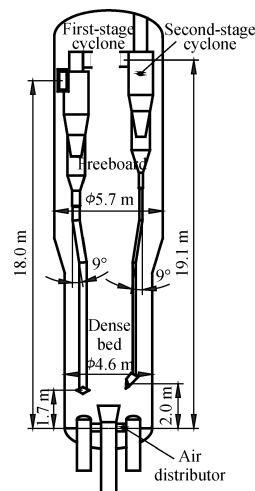
Synthesized binderless zeolite X has higher specific surface area and pore volume than those of commercial binder-containing samples. As for 1-hexene adsorption, the binderless sample shows 20%–50% higher adsorption capacity and 3.4–5.2 times larger apparent diffusion time constant than those of binder-containing samples.



### Root Cause of Fine Catalyst Particle Loss in Methanol to Olefin Unit

JIN Haifeng ZHANG Yongmin LI Guofeng GUAN Fengzhong GAO Wengang WANG Yajun

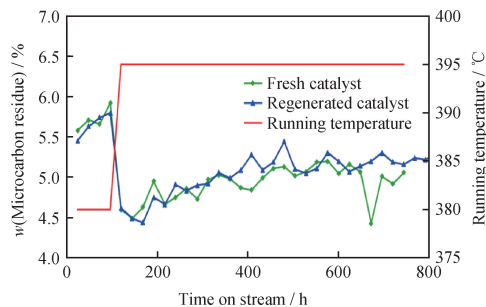
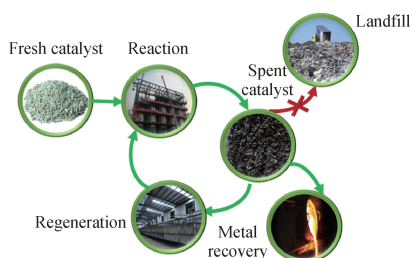
An industrial methanol to olefin (MTO) unit has a serious problem of catalyst fine particle loss. After systematic analysis and evaluation of multiple impact factors, it was found that the improper design of regenerator and its inside cyclones are the root cause of catalyst fine particle loss.



### Regeneration Conditions for Catalysts of Fixed Bed Residue Hydrodesulfurization and Microcarbon Residue Reduction

JIA Yanzi LIU Bin YANG Qinghe HU Dawei WANG Yifan DENG Zhonghuo ZHAO Xinqiang

Effects of regeneration conditions on the typical spent residue hydrodesulfurization catalysts unloaded from refineries were studied. Catalytic activity of the regenerated catalyst can be more than 85% of the fresh catalyst during long-term pilot plant test. This work can help both hazardous waste emission reduction and catalyst value maximization.

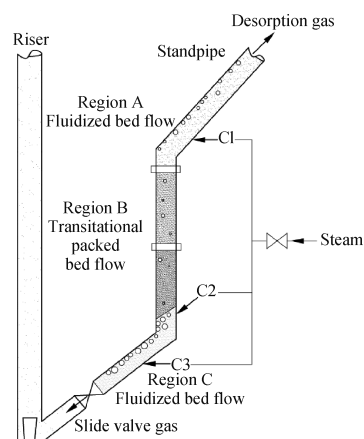


Reaction conditions:  $p = 14.0 \text{ MPa}$ ;  $\text{LHSV} = 0.5 \text{ h}^{-1}$ ;  $V(\text{H}_2)/V(\text{Oil}) = 600$

### Flow Patterns of Gas-Solid in FCC Standpipe and Their Effects on Reaction Temperature

PENG Wei LIU Junping ZHANG Junyi YU Liyong  
LIU Yansheng LIU Jianxin

Catalyst flow patterns in the regenerated standpipe was identified by pressure measurement on a 1.0 Mt/a FCC unit. There was no aeration nozzles installed in the middle of the standpipe, which resulted in the catalysts accumulating and the transitional packed bed flow forming. The big change of catalyst voidage caused by excessive aeration rate in the low part of inclined pipe is the main reason for reaction temperature fluctuation and catalyst density in the lower inclined pipe.

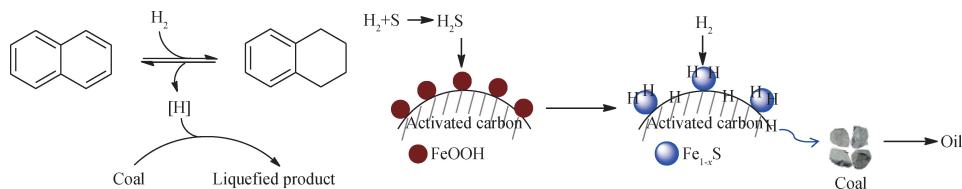


C1-C3—Cross sections of the regenerated standpipe

## Reaction Process and Hydrogen Transfer Mechanism in Coal-Oil Coprocessing

FAN Yingli CHANG Fangyuan JIANG Zhongshan SHI Xianying LI Dapeng LIU Zhongwen

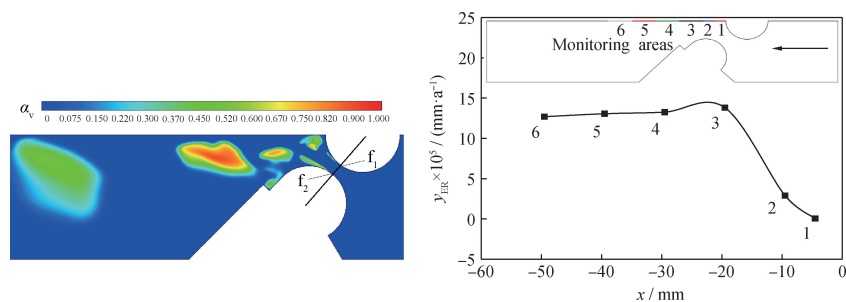
Coal-oil coprocessing experiments were performed with 1,2,3,4-tetrahydronaphthalene, *n*-eicosane, 9-phenylanthracene and 9-anthraldehyde as model compounds. Experimental results suggest that there are two main routes to transfer hydrogen into active hydrogen during coal liquefaction, i. e. , hydrogenation of aromatic compounds with hydrogen donation capability in heavy oils, and dissociation of the adsorbed hydrogen on catalyst surface. It was identified that the former is the dominant reaction.



## Cavitation Shedding Characteristics and Cavitation Damage Analysis in Sudden Change Channel

WANG Jiangyun WANG Zhuang HOU Linqian WANG Juan XIE Kai

Cavitation is a quasi-periodic unsteady process. The evolution of vacuoles includes primary, developmental, abscission, fusion and regeneration or direct collapse. The collapse of cavitation group causes the change of wall shear stress, and the damage degree increases along the flow direction, and then decreases gradually after reaching the peak value.



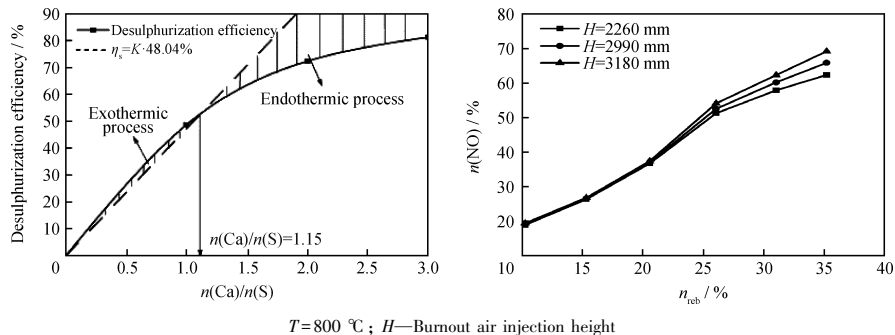
$f_1$ —Upper attachment point;  $f_2$ —Lower attachment point;

$\alpha_v$ —Vaporization volume fraction in the cavitation chamber

### Pollutant Emission and Control Characteristics of Oil Shale Retorting Residue Combustion in Fluidized Bed

YANG Yu CHEN Ye DENG Yuchuan JI Xuanyu LU Xiaofeng

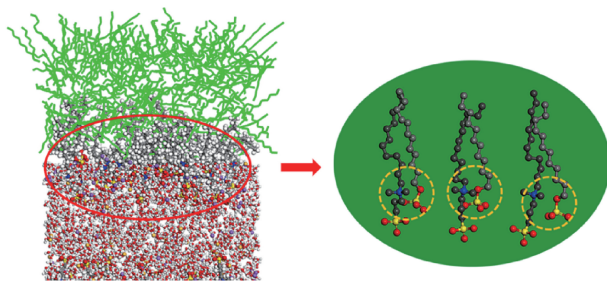
For oil shale retorting residue mono-combustion at 800 °C, the limestone in-furnace desulfurization reaction is exothermic when Ca/S molar ratio is less than 1.15. The application of natural gas reburning technique is beneficial for NO reduction, and NO removal efficiency increases with larger reburning ratios, higher reaction temperature and longer residence time.



### Molecular Dynamics Simulations of the Molecular Behavior and Synergistic Effect of Anionic/Zwitterionic Surfactants at Oil-Water Interface

WU Xu XIA Yu YUAN Lianhua YUAN Run HE Xuwen

Molecular dynamics simulations were used to study the aggregation behavior of the SDS/SB12-3 surface composite system at the oil-water interface. It is found that the electrostatic interactions between  $\text{—N}^+$  of SB12-3 and  $\text{—OSO}_3^-$  of SDS result in a thicker interface thickness and a more stable composite system.



O (Red), N (Blue), C (Gray), H (White),  $\text{Na}^+$  (Purple),  $\text{Cl}^-$  (Orange), Oil (Green)

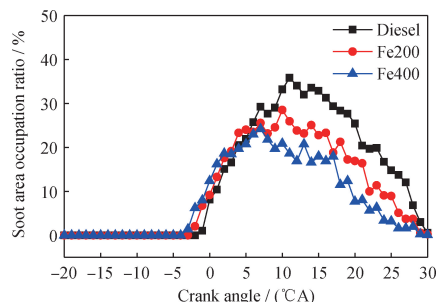
$n(\text{SDS})/n(\text{SB12-3})=1/1$



## Effects of Fe-Based Fuel Borne Catalyst on Soot Formation Characteristics of Diesel Engine

JI Qian ZHANG Qi DOU Zhancheng ZHAO Lian SUN Ping LIU Junheng

The effects of Fe-based fuel borne catalyst on soot formation characteristics of diesel engine have been studied. The results show that, at 100% load, the peak area of soot of Fe 200 and Fe 400 blended fuels decreased by 20.3% and 41.6% respectively as compared with pure diesel, and the distribution of soot decreases rapidly at the late burning period. At the same time, the smoke generated during the combustion process is continuously oxidized by Fe-FBC, resulting in the reduction of soot concentration.

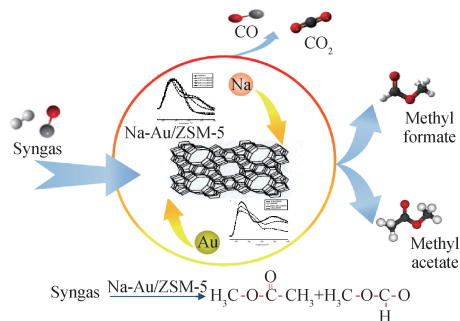


## Research Notes

## Preparation, Characterization and Catalytic Performance in Carbonylation of Syngas of Na Ion Modified Au/HZSM-5 Catalyst

FANG Yaping, Dilinur · Ali, GAO Xiran, BI Kunhao, MA Fengyun, Aisha · Nulahong

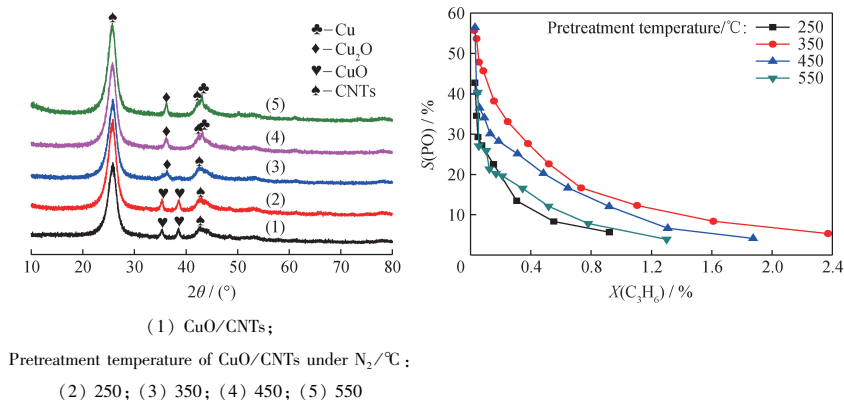
Supported Au/HZSM-5 catalyst was prepared by negative pressure deposition precipitation method, and modified by Na ions. With the increase of Na loading on Au/HZSM-5 catalyst, strong acid sites are changed into medium strong acid sites, which plays an important role in promoting carbonylation of syngas.



### Propylene Epoxidation by Oxygen Over CuO<sub>x</sub>/CNTs Catalysts

SU Weiguang KONG Lei ZHANG Ce SONG Xudong WANG Jiaofei YU Guangsuo YAO Min

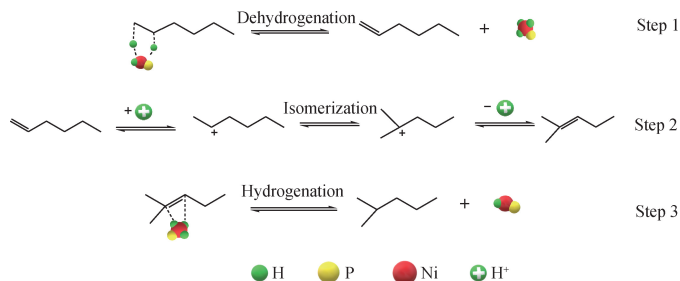
Propylene epoxidation activity is in good agreement with the content of Cu<sup>+</sup> species. High concentration of Cu<sup>+</sup> species favors the catalytic activities of CuO<sub>x</sub>/CNTs in propylene epoxidation. It is proposed that Cu<sup>+</sup> species are favorable to the formation of propylene oxide and Cu<sup>+</sup> species in CuO<sub>x</sub>/CNTs catalyst are the active sites for propylene epoxidation reaction by O<sub>2</sub>.



### Catalytic Performance and Mechanism of NiP/H $\beta$ Catalyst in *n*-Hexane Isomerization

ZHANG Mei LIU Xianshang DUAN Zunbin ZHU Lijun XIA Daohong

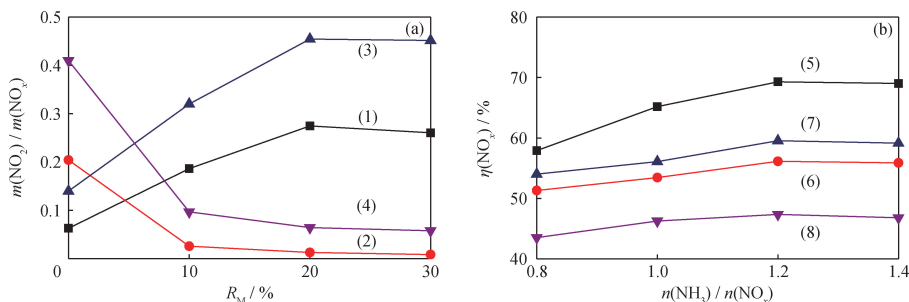
The optimum reaction condition and mechanism of *n*-hexane isomerization over NiP/H $\beta$  were investigated. It is proved that H-NiP is the active intermediates, providing good hydrogenation/dehydrogenation functions.



### Effects of DOC/SCR on the NO<sub>x</sub> Emission of Polyoxymethylene Dimethyl Ethers/Methanol Dual-Fuel Engine

ZHAO Lian SUN Ping LIU Junheng JI Qian YANG Jun

The study deals with the effect of diesel oxidation catalyst (DOC) and selective catalytic reduction (SCR) catalytic converter on the NO<sub>x</sub> emission characteristics of polyoxymethylene dimethyl ethers (PODE)/methanol dual-fuel engine. The results show that, after the purification of DOC,  $m(\text{NO}_2)/m(\text{NO}_x)$  of dual-fuel decreases, while pure PODE shows an opposite trend. With the increase of  $n(\text{NH}_3)/n(\text{NO}_x)$ , the conversion efficiency of NO<sub>x</sub> first rises and then falls, and the addition of methanol reduces the conversion efficiency of NO<sub>x</sub>.

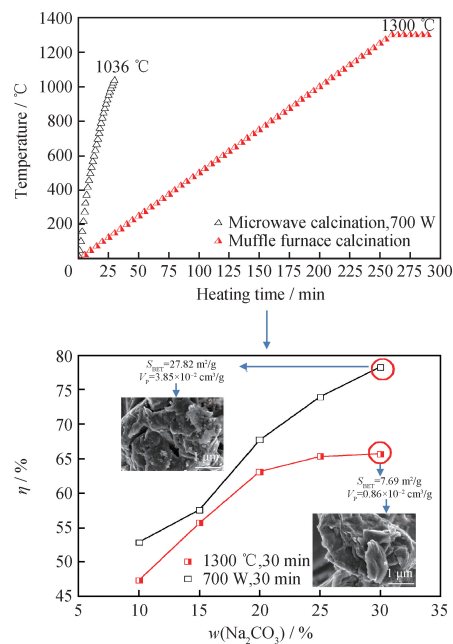


(1) BMEP=0.605 MPa, Before DOC; (2) BMEP=0.605 MPa, After DOC; (3) BMEP=0.242 MPa, Before DOC; (4) BMEP=0.242 MPa, After DOC;  
 (5) BMEP=0.605 MPa,  $R_M=0$ ; (6) BMEP=0.605 MPa,  $R_M=30\%$ ; (7) BMEP=0.242 MPa,  $R_M=0$ ; (8) BMEP=0.242 MPa,  $R_M=30\%$   
 (a)  $m(\text{NO}_2)/m(\text{NO}_x)$  vs.  $R_M$ ; (b)  $\eta(\text{NO}_x)$  vs.  $n(\text{NH}_3)/n(\text{NO}_x)$

### Desulfurization of High-Sulfur Petroleum Coke by Microwave Calcination

LI Zhiying ZHANG Nianbing SHEN Yifan

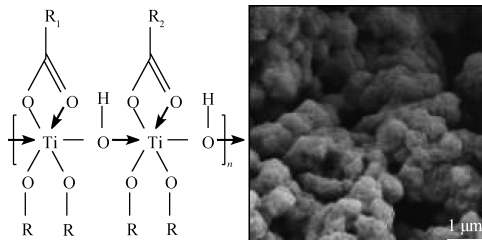
The effects of Na<sub>2</sub>CO<sub>3</sub> addition on desulfurization of high-sulfur petroleum coke were studied by the microwave irradiation calcination method. Compared with muffle furnace calcination, microwave calcination needs lower temperature and shorter time to obtain better desulfurization effect, which significantly improves the specific surface area and pore volume of coke.



### Shallow Analysis of Mechanism for Synthesis of Titanium Complex Grease

NIU Ming QU Jianjun

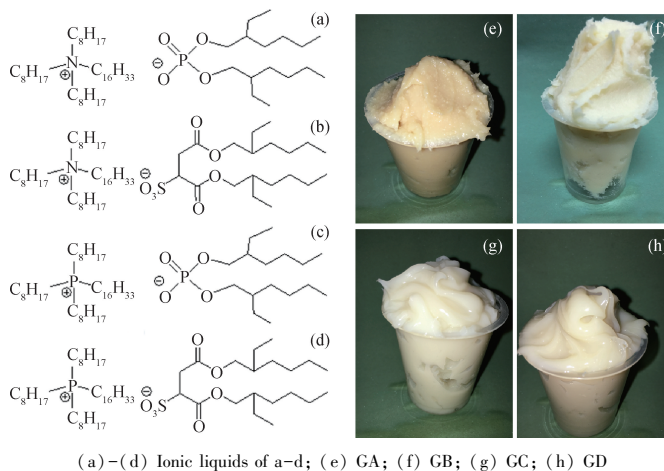
The mechanism of titanium complex grease was revealed based on the infrared spectroscopy, and it was found that two kinds of molecular generated were aggregate into titanium complex soap fibers. Moreover, appropriate interactions between titanium complex soap fibers and base oil are the mechanism for synthesis in another insight.



### Physicochemical and Tribological Properties of Four Oil-Soluble Ionic Liquid Complex Lithium Greases

YU Qiangliang ZHANG Chaoyang FAN Fengqi WANG Liping ZHOU Kang HUANG Qing ZHOU Xuguang  
CAI Meirong TANG Zhongping ZHOU Feng

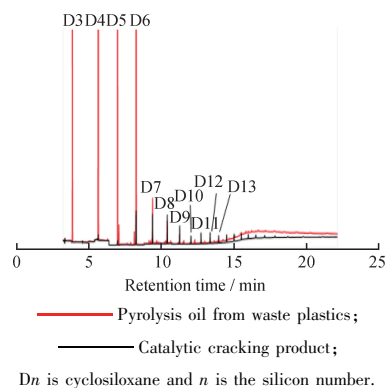
The effects of molecular structures of ionic liquids on the the ionic liquid complex lithium greases were systematically studied, and the results show that the addition of oil-soluble ionic liquid (D) hardly changes the physicochemical properties, but significantly improves the tribological properties.



### Qualitative and Quantitative Analysis of Silicon Species in Pyrolysis Oil From Waste Plastic

LIU Mingxing WU Mei LIU Zelong ZHANG Qundan

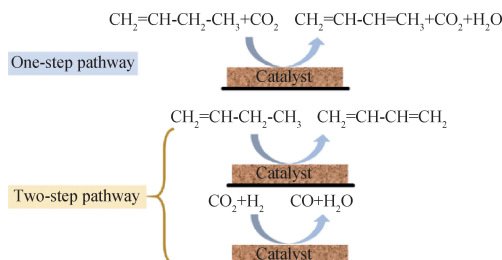
The silicon compounds in pyrolysis oil from waste plastics are mainly cyclorosiloxanes, concentrated in the low silicon number, and the cyclorosiloxanes in its catalytic cracking product are shifted to the high silicon number.



### Thermodynamic Analysis on the Reaction of Oxidative Dehydrogenation of 1-Butene to 1,3-Butadiene With CO<sub>2</sub> as the Soft Oxidant

CHEN Quanxin DOU Hongxin YAN Bing LIU Yiyin LIU Chunjing LI Jian JIANG Tao

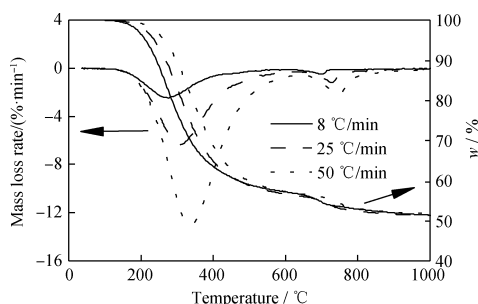
The thermodynamic studies show that the target reaction can not occur at room temperature, but it is reversible at 873.15 K. It is found that the isomerization reactions are more likely to occur than the oxidative dehydrogenation reaction thermodynamically. Inhibiting the isomerization reactions will effectively improve the catalyst catalytic performance.



## Pyrolysis Characteristics and Kinetic Analysis of Coal Tar Residue

CHANG Qiulian

In this article, thermogravimetric (TG) analysis method was used, and kinetic analysis was performed by the Freeman-Carroll method, to study the pyrolysis process of coal tar residue.

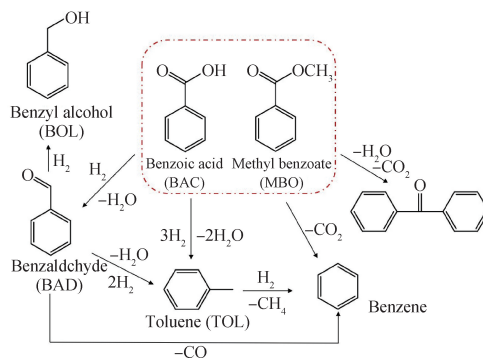


## Reviews

## Research Progress in Catalytic Hydrogenation of Benzoic Acid and Benzoate to Produce Benzaldehyde

GONG Xiaoxiao GAO Liang WEN Langyou ZONG Baoning

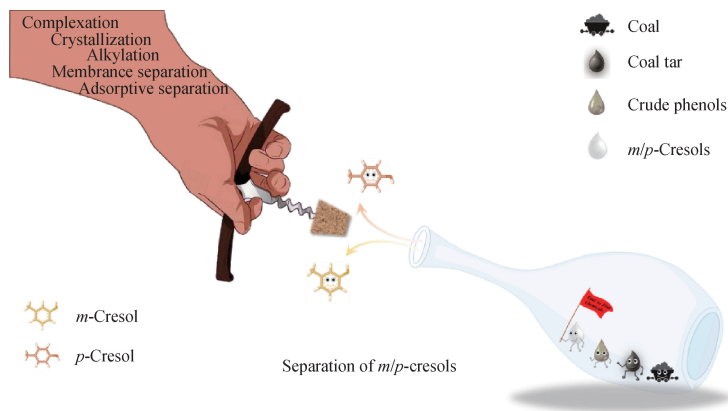
Reaction pathways reported in the literature for gas-phase hydrogenation of benzoic acid/methyl benzoate to benzaldehyde over oxide catalysts are shown as follows. Product composition is impacted by reaction conditions and catalyst characteristics, such as active sites, surface acidic and basic sites, oxide reducibility, etc.



## Research Progress on *m/p*-Cresols Separation Process and Technology

ZHANG Jingqi LIU Shuangtai FU Gang QIAO Jing ZHANG Shengjun MA Xiaoxun

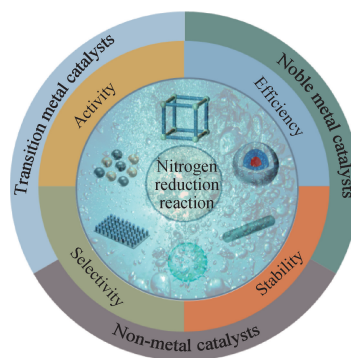
It is difficult to separate *m*- and *p*-cresols by conventional methods due to their very close boiling points. Different *m/p*-cresols separation methods, including alkylation, complexation, crystallization, simulated moving bed adsorption separation and membrane separation technologies, were reviewed to provide a direction for the future research on high value-added phenols from coals.



## Recent Advances in Electrocatalytic Nitrogen Reduction to Produce Ammonia Under Ambient Conditions

YIN Hongli LÜ Xianwei QIU Shuwei REN Tiezhen YUAN Zhongyong

The recent advances of the electrocatalytic nitrogen reduction reaction (NRR) to produce ammonia are reviewed. The structural-activity relationships of noble metals, transition metals and nonmetallic catalysts were discussed in detail, and the strategies to improve NRR efficiency were summarized, including enriching the number of active sites, regulating the electronic structure, inhibiting the hydrogen evolution reaction, and increasing the  $N_2$  concentration on the catalyst surface. It provides some ideas for improving the activity, efficiency, selectivity and stability of NRR catalyst in the future.



**特约英文编审:**范志明,加拿大不列颠哥伦比亚大学化学及生物工程博士,先后在加拿大自然资源部及加拿大国家研究院工作,现供职BP美国公司,研究领域包括重质油加工、石油加工过程中沥青质沉淀及石油化学等。

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