高温高压下煤在溶剂中溶胀特性及动力学分析（1-7）

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摘要：根据溶胀测量原理，结合位移传感器，设计了一种可以在高温高压条件下测量煤样在溶剂中溶胀的装置.测量获得了不同颗粒粒度B3煤样在神华循环油中、N2气氛下溶胀比随温度的变化曲线，同时考察了初始压力、气氛和煤阶对煤样高温溶胀特性的影响，并采用非等温溶胀动力学方程对溶胀数据进行拟合分析.结果表明，不同颗粒粒度B3煤样的溶胀比随温度的升高而增大，在300 ℃时达到最大溶胀比，随着温度的进一步升高，溶胀比减小，煤层高度开始降低.增大初始压力和H2气氛下有利于煤样的溶胀.煤样在四氢萘中的溶胀比较在循环油中大.非等温溶胀动力学拟合分析表明，煤在溶剂中溶胀遵循简单级数反应机理函数，活化能在20 kJ/mol~60 kJ/mol之间.

关键词：循环油，四氢萘，溶胀，位移传感器，高温高压，非等温溶胀动力学

Kinetic Analysis and Swelling Behavior of Coal in Solvent at Elevated Temperature and Pressure

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ABSTRACT：According to the swelling measurement principle, combined with a linear variable differential transformer (LVDT) deformation transducer, an apparatus for measuring coal swelling in solvent at elevated temperature and pressure was made. Changes of swelling ratio of the different particle size B3 coal in N2 atmosphere in Shenhua recycle oil were measured. The effect of initial pressure, atmosphere, and coal rank was investigated, and non-isothermal swelling kinetic equation was used to fit the swelling data. The results show that the changes of swelling ratio of B3 increase with temperature increasing, achieve the maximum at 300 ℃ and decrease because of the coal cracking. The higher initial pressure and H2 atmosphere are helpful to coal swelling in solvent. The swelling ratios of the coals in tetralin are relatively higher than that in recycle oil. The non-isothermal swelling kinetics analysis show that the coal swelling in the solvent follows a simple series reaction mechanism and the activation energy is between 20 kJ/mol and 60 kJ/mol.

KEYWORDS：recycle oil, tetralin, swelling, liner variable differential transformer, high temperature and pressure, non-isothermal swelling kinetics

不同粒径褐煤的热解特性及煤焦结构（8-12）

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摘要：以内蒙褐煤为研究对象，于固定床反应器上，考察了粒径对褐煤热解过程中的产气率以及各气体组分含量的影响，通过XRD以及物理吸附等手段研究了热解后各煤焦的微观结构特性，并采用热天平探讨了不同粒径煤焦水蒸气气化反应活性的差异.研究表明，当原煤粒径增大，原煤热解产气率有所下降；对于各组分，CO，H2，CH4含量均随原煤粒径增大而减小，但CO2呈相反趋势.对于粒径越大的原煤，由于挥发分脱除不够完全，生成的煤焦碳化程度较低，使得煤焦石墨化程度越低，比表面积也越小；另外，不同粒径煤焦的水蒸气气化反应活性随着粒径的增大而明显降低.

关键词：粒径，固定床，热解，煤焦结构，气化反应活性

Pyrolysis Characteristic and Char Structures of Lignite with Different Particle Sizes

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ABSTRACT：The effects of particle size on gas yields and gaseous compound contents were investigated by Inner Mongolia lignite pyrolysis tests performed in fixed-bed reactor. The structural characteristics of chars were determined by methods of XRD and physical adsorption. Reactivities of chars of different particle sizes with steam were studied by a thermogravimetric analyzer. The results show that the pyrolysis gas yield decreases as the particle size increases. For gaseous compound contents, the content of CO2 increases with particle size, but contents of CO, H2, CH4 show opposite trends. The degree of graphitization and the specific surface area of the char with relatively large particle size are relatively low, due to the incomplete devolatilization of the char. In addition, the reactivity of char gasification with steam decreases as the particle size increases.

KEYWORDS：particle size, fixed-bed, pyrolysis, coal char structure, gasification reactivity

煤热解动力学分布活化能模型适用性分析（13-18）

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摘要：以三种不同升温速率下准东原煤样品的热解失重数据为研究对象，应用分布活化能模型(DAEM)法进行动力学计算，分析了此种方法在煤热解整体动力学研究中的适用性.结果表明，由于升温速率对热解过程的影响以及反应机理的转变，DAEM法对煤热解二次脱气阶段失重数据的适用性较差；失水脱气及二次脱气阶段失重的取舍对各转化率所对应的活化能值具有不同的影响，而对活化能分布函数则影响不大；在几乎整个热解过程中，频率因子和活化能之间均呈现明显的动力学补偿效应，且其具体表现形式仅取决于煤种，而与所选取的温度计算范围关系不大.

关键词：准东煤，热解，动力学，分布活化能模型，活化能分布函数

Analysis on Applicability of Distributed Activation Energy Model in Coal Pyrolysis Kinetics

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ABSTRACT：The weight loss data of temperature programmed pyrolysis of Zhundong raw coal at three heating rates were investigated and the kinetic parameters were calculated by using distributed activation energy model (DAEM) method. The applicability of this method in global kinetics research of coal pyrolysis was analyzed. The main conclusions are as follows: due to the effect of heating rate on pyrolysis process as well as the change of reaction mechanism, the applicability of DAEM method to the weight loss data of secondary degassing stage of coal pyrolysis is weak; inclusion or exclusion of the weight loss in the dehydration and degassing stage or the secondary degassing stage, has different effects on the activation energy values corresponding to various degrees of conversion, but little effect on the activation energy distribution function; the relationship between frequency factor and activation energy presents obvious kinetic compensation effect in the almost entire pyrolysis process, and the expression form of this effect only depends on coal type and is not associated with the selected range of temperature for calculation.

KEYWORDS：Zhundong coal, pyrolysis, kinetics, distributed activation energy model, activation energy distribution function

煤与生物质快速流化床共热解的协同效应（19-25）

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摘要：在自主搭建的千克级流化床装置上进行了油房梁煤(YFC)与秸秆(JG)的共热解反应，考察了掺混比和温度对共热解油品收率和品质的影响.结果表明：在压力为0.1 MPa，输送气量为15 L/mim，流化气量为25 L/min，下料速度为1.5 kg/h的条件下，当油房梁煤与秸秆以0.7∶0.3的质量比混合，温度为600 ℃，反应气氛为N2时，收率较高，为19.18%，此时对应的协同效应度最大，为35.87%，且共热解油品较煤焦油硫的质量分数由0.60%降低至0.31%，酚系物主要集中在苯酚(16.82%)、对甲酚(21.92%)和邻苯二酚(16.56%)等11种酚类物，便于油品中酚系物的提取和利用.

关键词：油房梁煤，生物质，掺混比，共热解，协同效应

Synergistic Effect of Co-pyrolysis of Coal and Biomass on Fast Fluidized Bed

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ABSTRACT：The pyrolytic reaction of YFC, straw and their mixture, and the effect of temperature and mixing ratio on the oil yield and quality were investigated on a self-built kilogram class fluidized bed. The results show that the corresponding highest oil yield is 19.18% with reaction pressure 0.1 MPa, conveying gas 15 L/mim, flow gas 25 L/min, the feeding speed 1.5 kg/h, mixing ratio 0.7∶0.3 (mass ratio), temperature 600 ℃, reaction atmosphere N2, and synergistic effect has a maximum value 35.87%. Then the corresponding sulfur content (mass fraction) reduces to 0.31% from 0.60%, and phenolic compounds are mainly concentrated in phenol (16.82%), p-cresol (21.92%), catechol (16.56%) and other 11 kinds of phenolic compounds for extraction using.

KEYWORDS：Youfangliang coal, biomass, mixing ratio, co-pyrolysis, synergistic effect

水热处理对褐煤热解焦油自由基的影响（26-31）

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摘要：采用高压反应釜对内蒙古褐煤(IML)进行了不同温度的水热处理，并利用电子顺磁共振(EPR)波谱仪考察了水热处理对褐煤热解焦油中自由基的影响.结果表明，经过水热处理后，煤热解焦油中自由基的含量明显降低，在处理温度为260 ℃时达到最小值，自由基含量降低了66.67%；随着处理温度的升高，焦油的g因子值不断减小，峰宽增加，但在300 ℃时峰宽低于原煤焦油的峰宽.结合气相色谱质谱联用仪(GC-MS)对焦油的组分进行了测定，结果显示，经过水热处理后，焦油中酚类物质减少，单环芳烃的质量分数由15.10%上升至18.24%，多环芳烃的质量分数由12.79%上升至13.95%.通过在一定的保存时间内(40 d)持续对焦油中自由基含量的分析，发现经过水热处理后的热解焦油中，自由基的含量在保存过程中增加的趋势较原煤焦油缓慢，并且更早趋于稳定.

关键词：电子顺磁共振，自由基，水热处理，褐煤，焦油，稳定性

Effect of Hydrothermal Treatment on Free Radical in Lignite Pyrolysis Tar

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ABSTRACT：Inner Mongolia lignite was treated at different temperatures in an autoclave. The effect of hydrothermal treatment on free radical in lignite tar was investigated by EPR (electron paramagnetic resonance) spectrometer. The results show that the content of free radical in tar decreases obviously after hydrothermal treatment and reach minimum at 260 ℃ (decrease 66.67%). With the increase of hydrothermal treatment temperature, the g factor value of EPR spectra of tar is decreased and the linewidth of that is increased. However, the linewidth of EPR spectra of treated lignite tar at 300 ℃ is lower than that of raw coal tar. Combined with gas chromatography and mass spectrometry (GC-MS) for the determination of tar components, it shows that the relative content (mass fraction) of phenols decreases while monocyclic aromatic hydrocarbons in tar increase from 15.10% to 18.24%, polycyclic aromatic hydrocarbons in tar increase from 12.79% to 13.95%. Moreover, the free radical in tar was analyzed by EPR continuously within a certain time (40 d). The results show that the content of free radical in tar after hydrothermal treatment increases more slowly and reaches stably earlier than that in the raw tar in the preservation process.

KEYWORDS：electron paramagnetic resonance, free radical, hydrothermal treatment, lignite, tar, stability

中压全馏分煤焦油加氢工艺及经济性分析（32-38）

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摘要：在3×500 mL固定床中试装置上进行了中压(氢气分压10 MPa)神木全馏分中低温煤焦油加氢实验，并考察了反应条件对加氢产品组成和性质的影响.确定最佳的操作条件为：总液体体积空速为0.2/h，氢油体积比为1 500∶1，加氢保护剂、精制催化剂和裂化催化剂床层平均温度分别为280 ℃，380 ℃和400 ℃.进一步通过研究反应条件对技术经济性的影响，发现技术经济性最高时采用的操作条件与中试实验结果相一致.原料和产品价格对技术经济性影响的大小程度为产品价格>煤焦油价格>氢气价格.以目前价格为基础，原料和产品价格均提高35%后，中压全馏分煤焦油加氢技术可实现盈利.

关键词：煤焦油，中压，加氢，技术经济性，投资回报率

Economy and Process of Whole Fraction Coal Tar Hydro-upgrading Under Medium Pressure

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ABSTRACT：The pilot plant test of hydrogenation of Shenmu middle and low temperature coal tar was performed in 3×500 mL fixed bed reactors under hydrogen pressure of 10 MPa, and the effects of reaction conditions on the yields and properties of products were investigated. The optimized product distribution is obtained at the total liquid hourly space velocity (LHSV) of 0.2/h, H2 and oil volume ratio of 1 500∶1 and the average reaction temperature of pre-hydrogenation, hydrofining and hydrocracking catalyst is 280 ℃, 380 ℃ and 400 ℃. Compared to the pilot-plant tests, the same reaction conditions are used to obtain the maximum technical economic profit. The degree of influence on raw material and product prices for technical economy follow in the order of product price>coal tar price>hydrogen price. Base on the current prices, the process of whole fraction coal tar hydrogenation at medium pressure would be profitable, when the prices of the raw materials and products are further increased by 35%.

KEYWORDS：coal tar, medium pressure, hydro-upgrading, technical economy, return on investment

乳液法假均相催化剂制备及在煤液化中的应用（39-45）

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摘要：以洗油/Span80-Tween80/水相制成W/O型S2-和Fe2+前驱体乳液，双乳液经硫化制备铁基假均相催化剂，并对乳液稳定因素、乳液法制催化剂机理、催化剂稳定性及其对西沟煤的液化性能进行了研究.结果表明：稳定乳液的制备条件为油水质量比9∶1，Fe2+乳液和S2-乳液复配乳化剂的加入量(质量分数)分别为15.61%和18.36%，HLB值(亲水疏水平衡值)分别为7.3和6.7，机械搅拌速率6 000 r/min，乳化时间15 min，乳化温度20 ℃~30 ℃.所制假均相催化剂体系，沉降速率为5.24×10-7 cm/h.TEM表征得到催化剂粒径在100 nm左右，呈球形形貌.该催化剂用于西沟煤加氢液化，油产率较使用普通商用Fe2O3时提高4.04%.

关键词：乳液，洗油，乳化剂，稳定性，假均相催化剂，液化

Preparation of Pseudohomogeneous Catalyst by Emulsion Method and Its Application in Coal Direct Liquefaction

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ABSTRACT：W/O type Fe2+ and S2- precursor emulsion were prepared with wash oil/Span80-Tween80/water, double-emulsion was mixed to prepare iron based pseudohomogeneous catalysts by vulcanization, and the emulsion stability factor, the mechanism of catalyst prepared by emulsion method, catalyst stability and the performance of Xigou coal liquefaction were investigated. The results show that the stable emulsion preparation conditions is m(oil)∶m(water)=9∶1 in Fe2+ and S2- emulsion system with the suitable dosage (mass fraction) of emulsifiers, which are 15.61% and 18.36% respectively, HLB values are 7.3 and 6.7 respectively; stirring rate is 6 000 r/min; emulsion mixing time is 15 min, and emulsion temperature is 20 ℃-30 ℃. In the pseudohomogeneous catalysts emulsion system, the sedimentation rate of catalysts granule is 5.24×10-7 cm/h, calculated by Stokes equation. TEM results exhibit that the average particle size is about 100 nm and the morphology of catalyst particles is similar to spherical particles. When Xigou coal is applied as objects to direct coal liquefaction experiments, in the pseudohomogeneous catalytic system, the oil yield is 4.04% higher than that by commercial Fe2O3 catalyst.

KEYWORDS：emulsion, wash oil, emulsifier, stability, pseudohomogeneous catalyst, liquefaction

煤直接液化重质产品油的催化加氢实验研究（46-52）

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摘要：在30 mL油品加氢实验装置上，进行煤直接液化全馏分油中重质油(＞320 ℃)加氢实验，考察反应温度、压力和体积空速变化对加氢生成油物性的影响.结果表明，油品的脱硫率和脱氮率与反应温度和反应压力成正比，与体积空速成反比；升高反应温度和反应压力或降低体积空速，都有利于加氢油品中单环芳烃和双环芳烃质量分数的增加、多环芳烃质量分数的减少.计算得到的油品供氢指数(*I*PDQ)增加，从而溶剂供氢能力增加.不同加氢条件下得到的油品物性表明，反应温度为380 ℃，压力为19 MPa，体积空速为0.8/h时，得到的重质馏分油作为煤液化循环溶剂使用时供氢性最好.

关键词：煤直接液化，重质油，催化加氢，供氢性能，溶剂加氢

Experimental Study on Catalytic Hydrogenation of Heavy Fraction from Coal Liquids

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ABSTRACT：The catalytic hydrogenation experiments of the heavy coal derived fraction (＞320 ℃) were carried out under different conditions. The influence of temperatures, pressures and liquid space velocities were investigated in 30 mL hydrogenation reaction device and the properties of hydrogenated products were examined. It is found that the rate of desulfurization and denitrification of the heavy fraction is positively related to temperature and pressure in the hydrogenation, and negatively related to the liquid space velocity. The results also show that the content of monocylic aromatics and binuclear aromatics in hydrogenation products increase and the content of polycyclic aromatics decrease with the elevated temperature and pressure and with decented liquid space velocity. The hydrogen donation ability of hydrogenation products increase with the proton donor quality index increasing. The hydrogenation products characteristics show that temperature 380 ℃, pressure 19 MPa, liquid space velocity 0.8/h are optimized hydrogenation conditions in which products show the best hydrogen donation ability for coal liquefacion.

KEYWORDS：coal derived liquefaction, heavy fraction, catalytic hydrotreating, hydrogen donating, solvent hydrogenation

微孔活性炭对对二甲苯的吸附和脱附性能（53-58）

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摘要：实验研究了两种典型活性炭对对二甲苯的气相吸附与脱附性能，分析了活性炭的孔隙结构、吸附与脱附温度对对二甲苯吸附量的影响规律.结果表明，随着吸附温度升高，活性炭吸附对二甲苯能力降低，吸附温度在30 ℃时，可以获得较高的吸附值；活性炭的中孔尺寸为1 nm~2 nm部分所占比表面积及比孔容越高，其吸附对二甲苯的性能越好.同时，两种活性炭气相吸附对二甲苯的量是其吸附升华萘量的1.10倍，表明用活性炭吸附对二甲苯方法来间接评价活性炭对萘的吸附量是可行的.

关键词：活性炭，对二甲苯，萘，吸附，脱附

Performance of Adsorption and Desorption of P-xylene by Micropore Activated Carbon

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ABSTRACT：In this study, two types of activated carbon have been used to investigate their capacity to adsorb and desorb p-xylene. The experimental results showed that the saturated adsorption capacity of activated carbon for aromatic hydrocarbon molecules increased as the specific surface area increased with a specific pore volume of 1 nm-2 nm, but it decreased as the adsorption temperature increased. A relatively high adsorption value was obtained at 30 ℃. In addition, the adsorption of p-xylene is 1.1 times as much as the adsorption of naphthalene on two types of activated carbons. This study indicates that it is a feasible manner to appraise the naphthalene adsorption of the developed activated carbon by analysis of its adsorption of p-xylene.

KEYWORDS：activated carbon, p-xylene, naphthalene, adsorption, desorption

Al2O3对神东煤灰渣熔体特性的影响（59-64）

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摘要：向神东煤灰中添加Al2O3，通过煤灰熔融性测试，分析Al2O3对神东煤灰熔融温度的影响；通过激冷实验、X射线衍射(XRD)、热重分析及热力学软件FactSage，探究Al2O3对神东煤灰熔融特性的影响机理.结果表明，Al2O3始终起到提高煤灰熔融温度的作用.在Al2O3添加量(质量分数，下同)较低时，煤灰熔融温度升高趋势较为平缓；随着Al2O3添加量继续增大，煤灰熔融温度急剧升高.通过XRD检测及热力学软件FactSage模拟分析发现，Al2O3添加量较大时，在煤灰熔融过程中其与原煤灰中的SiO2(以石英形式存在)形成了莫来石(3Al2O3·2SiO2)，从而造成了煤灰熔融温度急剧升高.

关键词：神东煤，Al2O3，灰熔融，激冷实验，FactSage，热分析

Effect of Al2O3 on Shendong Coal Ash Fusion Characteristics

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ABSTRACT：The influence of Al2O3 on Shendong coal ash fusion temperature was investigated by adding various amounts of Al2O3. The impact mechanism of Al2O3 on Shendong coal ash fusion characteristics was explored using quench experiments, XRD, TG-DSC and thermodynamic software FactSage. The results show that with the increase of addition amount of Al2O3, the ash fusion temperature (AFT) rises gentle first and then zooms up. Through XRD and thermal analysis software FactSage, it is found that Al2O3 reacts with SiO2 derived from the original coal ash composition (in the form of quartz ) to form mullite (3Al2O3O2SiO2) in ash fusion process, which resulting in the sharp rise of coal ash fusion temperature with a higher added amount of Al2O3.

KEYWORDS：Shendong coal, Al2O3, ash fusion characteristics, quench experiments, FactSage, thermal analysis

基于TG-FTIR研究尾矿对褐煤的原位催化脱硝（65-69）

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摘要：针对褐煤燃烧过程中产生的NO及还原气体，采用热重红外联用技术研究尾矿加入后褐煤燃烧特性、NO生成量及还原气体的变化.结果表明，尾矿的加入对水分析出温度和挥发分燃烧温度的影响较小，但焦炭的起始燃烧温度相对降低，促进了焦炭燃烧阶段的进行.褐煤燃烧过程产生的还原气体主要为CH4，NH3，CO及脂肪烃类(—CH2)，尾矿的加入催化了NO与还原气体的反应，低温条件下以NH3还原NO为主，且尾矿催化存在选择性，其对CO还原NO的催化强度较其他几种气体弱.

关键词：热重红外联用技术，褐煤，燃烧，尾矿，NO，还原气

Study on In-situ Catalytic Denitrification of Lignite Using Tailings Based on TG-FTIR

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ABSTRACT：Point at NO and reduction gases generated from lignite combustion, the TG-FTIR was used to study the change of the combustion characteristic, NO generation and the reducing gas with the addition of tailings. The results show that the addition of tailings has no effect on the temperatures of water generation and the volatile combustion, but the initial combustion temperature of coke is reduced, so the phase of coke combustion has been promoted. The reduction gases generated from lignite combustion are CH4, NH3, CO and —CH2. The reaction between NO and reduction gases has been catalysed with tailings. At the low temperature, the main reaction is between NH3 and NO. The catalyst of tailings has selectivity, the catalyst effect on the reaction between CO and NO is not obvious compared with other reducing gases.

KEYWORDS：TG-FTIR, lignite, combustion, tailings, NO, reducing gas

脱腐植酸昭通褐煤残渣的热解特性（70-75）

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摘要：对抽提完腐植酸的云南昭通褐煤残渣进行热解，通过热解气产率、焦油产率和半焦产率研究其热解特性，考察温度、升温速率和热解气氛对褐煤残渣热解的影响，并对每组热解实验得到的气体产物进行气相色谱分析，研究热解气的主要成分和含量，用气质联用仪对焦油进行成分分析.结果表明，温度是影响褐煤残渣热解的最重要因素，温度越高，热解气和焦油产率越大，热解气中H2和CO越多，焦油中脂肪族物质增多，芳香族物质芳环数增大；升温速率越低，气体和焦油的产率越大；热解气氛对产物分布有着较大的影响，不同的热解气氛影响着热解气和焦油中主要组分的含量.

关键词：褐煤，残渣，热解，产物分布，气体组成

Pyrolysis Characteristics of Residue After Extracting Humic Acid from Zhaotong Lignite

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ABSTRACT：The pyrolysis of lignite residue after humic acid extraction in Zhaotong region of Yunnan Province was carried out, and the pyrolysis characteristics were analyzed through the pyrolytic gas yield, tar yield and semi-char yield. The effects of temperature, heating rate and pyrolysis atmosphere on residue pyrolysis were explored, the major components and content of pyrolysis gas were obtained by gas chromatography, and the composition of tar was revealed using gas chromatography-mass spectrometry. The results show that the temperature is the most important factor to affect residue pyrolysis, the higher of temperature, the greater yield of pyrolysis gas and tar, the more H2 and CO contained in pyrolysis gas, the more aliphatic compounds included in tar, and the number of aromatic ring in aromatic compounds will be increased accordingly; the lower of heating rate, the greater yield of gas and tar; pyrolysis atmosphere has prominent influence on product distribution, the content of major components of pyrolysis gas and tar is affected by different pyrolysis atmospheres.

KEYWORDS：lignite, residue, pyrolysis, product distributions, gas composition

煤制生物氢放大模拟实验研究（76-80）

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摘要：在5 L厌氧发酵罐内，控制温度为30 ℃，pH值为6.5，进行为期10 d的厌氧发酵产氢实验，对实验过程中液相的pH值、VFA(挥发性脂肪酸)摩尔浓度和COD值进行实时监控分析，并进行纤维素酶活性和氢化酶活性的检测.结果表明，氢气最大体积分数可达到52.3%，氢气最终产率为13.7 mL/g.pH值一直下降，最低降至5.46；VFA摩尔浓度基本呈上升趋势，与pH值变化相对应，发酵类型属于丁酸型发酵.COD值呈现先上升后下降的趋势，最高值为4 368 mg/L，且最终COD降解率为51.10%.纤维素酶活性在反应第4天出现最高值0.016 9 mg/(mL·h)，氢化酶活性最高值出现在反应第6天，为0.568 mmol H2/(min·mg).

关键词：厌氧发酵，煤制生物氢，累积产氢量，酶活性

Amplification Simulation Experimental Study on Coal Bed Hydrogen

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ABSTRACT：An experiment of hydrogen production through anaerobic fermentation was carried out under the condition of pH 6.5 lasting for 10 days, with temperature controlled at 30 ℃ in a 5 L anaerobic fermentation tank. The pH value, VFA molar concentration and COD value of the liquid phase during the experiment process were real-time monitored; meanwhile, cellulase activity and hydrogenase activity were monitored. The results show that the maximum volume fraction of hydrogen can reach 52.3% and the final production of hydrogen is 13.7 mL/g; pH value keeps dropping until it reaches the minimum value 5.46; VFA molar concentration basically tends to increase corresponding to the change of pH value, it belongs to butyric acid-type fermentation; COD value increases first then decreases, with maximum value 4 368 mg/L and the final COD degradation rate is 51.10%; the highest value 0.016 9 mg/(mL·h) appears in the fourth day for the active reaction of cellulase while the highest value 0.568 mmolH2/(min·mg) for the hydrogenase activity appears in the sixth day.

KEYWORDS：anaerobic fermentation, coal bed biohydrogen, cumulative hydrogen production, enzymatic activity

褐煤氧化自热过程中化学结构的演变（1-5）

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摘要：利用线性升温模拟褐煤由低温氧化到自燃的快速自热过程，结合FTIR，对比分析褐煤氧化自热过程中化学结构的变化.褐煤的氧化自热过程经历了四个特征温度，即自热起始温度(*t*sp)、交叉点温度(*t*cp)和燃烧温度(*t*c1，*t*c2).研究表明：褐煤氧化自热期间，—CH3和—CH2—的减少以及*n*(—CH3)∶*n*(—CH2—)的升高显示出氧更易攻击—CH2—；Ar—O—CO—R和R—O—CO—R随着氧化自热的加剧逐渐增加，而在*t*c1后发生水解；褐煤氧化自热初期不断增加的Ar—CO—Ar在*t*cp后大量分解生成气体氧化产物；褐煤的氧化自热经历*t*c1后，起初相对稳定的芳香族CC快速减少；Ar—COOH在*t*sp后逐渐增加，而在*t*c1后由于脱羧、脱水与酯化等反应的参与快速降低；Ar—COO—随着煤氧化自热的加剧而逐渐增加，在*t*c1后由于分解而减少.

关键词：褐煤，氧化，自热，FTIR，化学结构

Chemical Structure Changes During Oxidation Self-heating of Lignite

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ABSTRACT：A rapid self-heating of lignite during low temperature oxidation and spontaneous combustion was monitored by programmable changing oven temperature. Changes of chemical structure of the coal during self-heating was investigated by FTIR analysis. Temperature of the coal in air increased monotonically, successively exceeding the separation point temperature (*t*sp), the crossing point temperature (*t*cp) and combustion temperatures (*t*c1, *t*c2). The decrease of methyl and methylene and increase of *n*(—CH3)∶*n*(—CH2—) during self-heating of lignite indicate that the more methylene is attacked by oxygen during oxidation. Ar—O—CO—R and R—O—CO—R increase progressively, and decrease after tc1 in response to hydrolysis of the esters. The increasing Ar—CO—Ar during self-heating decomposes to generate gaseous oxidation products above *t*cp. Aromatic CC insignificantly changes up to *t*c1, and decreases thereafter. After coal temperature reaches to tsp, Ar—COOH increases gradually, and then decreases above tc1 because of the decarboxylation, dehydration and esterification. Ar—COO— increases gradually during self-heating, but decreases above *t*c1 because very high oxidation temperature enhances the decomposition of the group.

KEYWORDS：lignite, oxidation, self-heating, FTIR, chemical structure

镜质组随机反射率对焦炭热态强度的影响（6-10+15）

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摘要：将镜质组随机反射率*R*ran分为5个子区间，各区间所占百分比标记为*R*1，*R*2，*R*3，*R*4和*R*5，以这5个指标作为实验变量，在满足捣固炼焦对配合煤质量要求的前提条件下，实施了35组5 kg试验焦炉捣固炼焦实验.结果表明：*R*1，*R*2，*R*3，*R*4和*R*5这5个指标与*w*(Vdaf)值、*R*max值、*G*值和*Y*值之间都有着较强的线性相关性，相关系数*R*分别为0.933，0.976，0.858和0.564；采用*R*1，*R*2，*R*3，*R*4和*R*5预测焦炭反应性，预测精度高；*R*1含量增加会明显劣化焦炭热态强度，*R*3和*R*4含量增加会提高焦炭热态强度，同时，*R*1，*R*2，*R*3，*R*4和*R*5对CRI的影响程度大小为*R*1>*R*3=*R*4>*R*5>*R*2.通过调整*R*1，*R*2，*R*3，*R*4和*R*5的含量，使其分别为25%~35%，20%~30%，10%~20%，10%~25%和5%~15%，可以有效改善焦炭热态强度.

关键词：镜质组，随机反射率，焦炭，热态强度，预测模型，配煤

Effect of Vitrinite Random Reflectance on Thermal Strength of Coke

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ABSTRACT：The respective percentage of five subintervals of vitrinite random reflectance was defined as *R*1, *R*2, *R*3, *R*4 and *R*5 indicators. 35 groups of 5 kg test coke oven stamping coking experiments were carried out, with the five indicators as experimental variables and on the condition of meeting the blended coal quality requirements in tamping coking process. The results show that there is strong linear correlation between the five indicators and content of the dry ash-free volatile matter *w*(Vdaf), the mean maximum reflectance of vitrinite (*R*max), the caking index (*G*) and the maximum thickness of plastic layer (*Y*). The correlation coefficient is 0.933, 0.976, 0.858 and 0.564, respectively. And there is high prediction accuracy by using *R*1, *R*2, *R*3, *R*4 and *R*5 to predict the coke reactivity index. Moreover, the coke reactivity index improves obviously for the increasing of the content of *R*1, and reduces for the increasing of the content of *R*3 and *R*4. Meanwhile, the degree of impact of *R*1, *R*2, *R*3, *R*4, *R*5 on the coke reactivity index is *R*1>*R*3=*R*4>*R*5>*R*2. Therefore, the thermal strength of coke can be effectively improved by adjusting the respective content of *R*1, *R*2, *R*3, *R*4 and *R*5 to 25%-35%, 20%-30%, 10%-20%, 15%-25% and 5%-15%.

KEYWORDS：vitrinite, random reflectance, coke, thermal strength, prediction model, blending coal

离子交换法洗涤准东煤脱钠提质研究（11-15）

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摘要：针对新疆准东煤钠含量偏高，锅炉燃用时易发生水冷壁结渣、受热面高温腐蚀和烟道沾污积灰等情况，对准东煤的煤质特性进行分析，采用阳离子交换树脂洗涤准东煤，利用树脂的离子交换功能，使树脂的交换基团中的阳离子与准东煤的钠离子发生置换反应，达到脱钠的效果，并研究洗涤温度与洗涤时间对准东煤脱钠效果的影响.结果表明：在4 h，60 ℃的恒温洗涤条件下，准东煤脱钠效果达到最佳，可溶性钠脱除率达到90%以上，*t*s提高124 ℃，煤质特性得到改善.

关键词：准东煤，离子交换，洗煤，脱钠，提质

Ion Exchange Method of Coal-washing and Sodium-removing for Zhundong Coal Upgrading

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ABSTRACT：Zhundong coal is a typical high-sodium coal, which makes slag on cold water wall, high temperature corrosion in heated wall,pollution and dust contamination in flue pipe prone to take place when coal is burning in power plant. The characteristic of Zhundong coal was analyzed, cation exchange resin method was used to wash coal. The exchange function of resin made the displacement reaction occur between the cation in exchange group and sodion in Zhundong coal, so that the sodium in coal could be removed. The effect of temperature and time on the desulphurization efficiency of Zhundong coal was studied. The results show that the removal effect in condition of 4 h, 60 ℃ is optimum, sodium removal rate reaches to 90% and the soften temperature (*t*s) increase by 124 ℃, and the coal characteristics are improved.

KEYWORDS：Zhundong coal, ion exchange, coal-washing, sodium removal, upgrading

钙基高硫煤共热解焦中硫测定方法及分布规律（16-21）

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摘要：运用X射线衍射(XRD)、X射线光电子能谱(XPS)分别研究了焦炭中无机硫和有机硫的类型，尝试用一种新方法分析热解焦中形态硫，即碘量法测定焦中无机硫化物含量、且可以直接测定焦中有机硫含量的方法，并运用此方法考察了钙基添加剂对高硫煤高温热解后形成的焦中形态硫分布的影响规律.结果表明：钙基添加剂改变了煤热解后焦炭形态硫的分布，一方面，通过高温固硫作用，提高了焦中无机硫化物含量所占比例(其中无机硫化物主要以CaS形式存在)；另一方面，通过促进煤中有机硫的分解，降低了焦炭中有机硫含量所占比例.

关键词：高硫煤，高温热解，焦炭，钙基添加剂，形态硫

Change Rule and Measuring Method of Sulfur Forms in Coke Obtained by Co-pyrolysis of High Sulfur Coal and Ca-based Additives

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ABSTRACT：The inorganic sulfur and organic sulfur in coke were investigated and a method for determination of sulfur forms was established using X-ray diffraction, X-ray photoelectron spectroscopy analysis methods.With this method, effects of Ca-based additives on the distribution rule of sulfur forms in coke was researched during high sulfur coal pyrolysis. The results indicate that the distribution rule of sulfur forms in coke is changed by Ca-based additives. The proportion of inorganic sulfur content is improved through sulfur retention ability (inorganic sulfur mainly exists in form of CaS) and the proportion of organic sulfur content reduces by promoting the decomposition of organic sulfur in coke.

KEYWORDS：high-sulfur coal, high-temperture pyrolysis, coke, calcium-based additive, sulfur forms

气氛及甲烷催化活化对流化床煤热解的影响（22-28）

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摘要：为了提高煤热解焦油的产率和品质，在小型流化床实验台上分别考察了N2，N2+H2，CH4+N2，CH4+H2等气氛及前置Ni/Al2O3催化剂对流化床煤热解的影响，结果表明：H2气氛会减少半焦产率，增加焦油产率；CH4气氛在800 ℃时反而会增加半焦产率，同时高温下CH4的分解对焦油产率的增加有促进作用，相比于N2气氛，焦油产率提高了35.8%；CH4+H2气氛下半焦焦油产率的总体趋势同H2气氛下相同.还原性气氛有利于焦油的轻质化：H2，CH4+N2，CH4+H2气氛下800 ℃时，轻质焦油的占比分别较N2气氛提高了29.1%，15.2%，24%.在CH4+N2和CH4+H2气氛下，采用前置Ni/Al2O3催化剂后，焦油产率都得到不同程度的提升.CH4+N2气氛下600 ℃时，催化剂可以使焦油产率较无催化剂时提高40%；CH4+H2气氛下800 ℃时，催化剂对CH4的催化效果更好，热解气中CH4含量明显减少，而焦油产率较无催化剂时提高了37%.Ni/Al2O3催化剂可以进一步提高焦油的品质，并且有利于焦油中芳香烃的生成.

关键词：热解，流化床，气氛，焦油，催化剂

Effect of Atmosphere and Methane Catalytic Activation on Coal Pyrolysis in Fluidized Bed Reactor

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ABSTRACT：In order to improve the yield and quality of coal tar, the effects of atmosphere and Ni/Al2O3 catalyst on coal pyrolysis characters were investigated in a fluidized bed in H2, CH4, N2 and mixed atmosphere. The results show that H2 can reduce semicoke yield and increase tar yield; CH4 can increase semicoke yield at 800 ℃. Due to the decomposition of methane, compared with N2 atmosphere, CH4 can increase tar yield by 35.8%. In CH4+H2 atmosphere, semicoke and tar yield have the same trend with H2 atmosphere. Reducing atmosphere is beneficial to improving the quality of the tar. In H2, CH4+N2, CH4+H2 atmosphere, light tar ratio increases by 29.1%, 15.2%, 24%, respectively. The Ni/Al2O3 catalyst placed before the reaction segment can improve semicoke and tar yield to different degrees. At 600 ℃, compared with coal pyrolysis in CH4+N2 atmosphere without catalyst, adding Ni/Al2O3 into CH4+N2 atmosphere increases tar yield by 40%. In CH4+H2 atmosphere, the Ni/Al2O3 has better catalytic effect on CH4 at 800 ℃, and CH4 in the pyrolysis gas decreased significantly, meantime tar yield increases by 37% compared that of without catalyst. Ni/Al2O3 can further improve the quality of the tar and is beneficial to the formation of aromatic compounds.

KEYWORDS：pyrolysis, fluidized bed, atmosphere, tar, catalyst

甘蔗渣与褐煤低温共热解产物特性分析（29-35+41）

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摘要：采用自制的低温热解装置研究褐煤与甘蔗渣(SB)共热解过程中添加甘蔗渣对褐煤热解特性的影响.结果表明：随着甘蔗渣掺混比的增加，热解油产率呈现先增大后减小的趋势.在甘蔗渣掺混比为20%(质量分数，下同)时，热解油产率达到最大值16.7%，比褐煤单独热解得到的焦油产率增加了13.7%，与焦油计算值产率出现0.57%的最大正偏差.热值分析得出共热解过程有利于褐煤和甘蔗渣的能量富集，共热解半焦比原煤半焦的热值大；焦油的FTIR谱表明，添加甘蔗渣会促进褐煤中—OH和—CH3官能团的断裂和分解，会使甘蔗渣中羧基官能团以其他含氧官能团形式转移到焦油中，有利于焦油轻质化；热重分析表明，热解过程分为三个阶段，甘蔗渣的添加对褐煤的快速热解阶段影响显著，使褐煤的最大失重速率增加，提高了8.96%，最大失重速率所对应的热解温度降低了98.8 ℃，甘蔗渣的添加一定程度上促进了热解反应的进行.

关键词：褐煤，生物质，共热解，焦油，半焦

Analysis of Low-temperature Co-pyrolysis Product of Sugarcane Bagasse and Lignite

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ABSTRACT：Low-temperature co-pyrolysis of lignite and sugarcane bagasse(SB) was undertaken in a homemade carbonization apparatus to study the effect of different SB ratio on pyrolysis characteristics in lignite. The results show that with the increase of SB blending ratio, the pyrolysis tar yield shows a trend of decrease after the first increase, and the peak value is 16.7% when the blending ratio of SB is 20% (mass fraction, the same below), which is 13.7% higher than that of lignite pyrolysis alone, and shows the maximum positive deviation of 0.57% to the calculated value of tar yield. The date analysis of lignite, SB and the blend was studied by caloricity analyzer. Results show that co-pyrolysis is conducive to the centralization of energy in lignite and bagasse, and the heat value of co-pyrolysis semicoke is higher than that of lignite pyrplysis alone. FTIR indicates that the addition of SB can promote the decomposition and fracture of —OH and —CH3 functional groups in lignite, and carboxyl functional groups in SB can be transferred to the tar in the form of other oxygen-containing functional groups, which is conducive to the conversion of heavy components in tar to the light ones. Thermogravimetric analysis shows that the pyrolysis process is divided into three stages and the presence of SB has a significant effect on the stage of rapid pyrolysis, the maximum weight loss rate of lignite increases by 8.96% and the pyrolysis temperature corresponding to the maximum loss rate decreases by 98.8 ℃. The addition of SB facilitates the pyrolysis reaction to a certain extent.

KEYWORDS：lignite, biomass, co-pyrolysis, tar, semicoke

O2/CO2气氛下煤与生物质混燃NO*x*的排放特性（36-41）

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摘要：在滴管炉上研究不同煤种(褐煤、烟煤、贫煤和无烟煤)与生物质(稻壳)混燃NO*x*的排放特性，分析不同燃烧气氛、生物质掺混比例和氧气体积分数对混燃NO*x*排放特性的影响.结果表明：在20%O2/80%N2气氛下，不同煤种和生物质混燃时，NO*x*沿程分布均呈现出先增大后减小的变化趋势，烟煤/稻壳的NO*x*排放量最高；在氧气体积分数为20%条件下，O2/CO2气氛比O2/N2气氛下NO*x*的排放量降低；在30%O2/70%CO2气氛下，随着混燃中生物质掺混比例的增加，不同煤种NO*x*的排放量逐渐降低，褐煤的NO*x*排放量下降最显著，由130.029 mg/m3下降到49.674 mg/m3；在O2/CO2气氛下，随着氧气体积分数的升高，NO*x*排放量增加.氧气体积分数由20%升高到30%，烟煤单燃时NO*x*排放的增加量较小，生物质和烟煤混燃时NO*x*排放的增加量较大.

关键词：生物质，混燃，O2/CO2气氛，滴管炉，NO*x*排放

NO*x* Emission Characteristics of Coal and Biomass Co-firing in O2/CO2 Atmosphere

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ABSTRACT：NO*x* emission characteristics of different kinds of coal (lignite, bituminous coal, lean coal and anthracite) / biomass (rice husks) blends combustion were studied using drop tube furnace. The effects of atmosphere, blending ratio of biomass, oxygen volume fraction on NO*x* emission characteristics were investigated in details. Experimental results show that: NO*x* emissions present a trend of firstly increasing and then decreasing for different coal/biomass blends along the furnace height. NO*x* emission of bituminite/rice husk co-combustion is the highest in the atmosphere of 20%O2/80%N2. NO*x* emission in O2/CO2 atmosphere is lower than that in O2/N2 atmosphere in the condition of 20% oxygen volume fraction; with increasing of the blending ratio of biomass, NO*x* emission gradually decreases, and that decreases most significantly for the lignite and biomass co-combustion, which decreases from 130.029 mg/m3 to 49.674 mg/m3 in the atmosphere of 20%O2/70%CO2; with the oxygen volume fraction increases, NO*x* emission increases. When the oxygen volume fraction increases from 20% to 30% in O2/CO2 atmosphere, the increase of NO*x* emisson of bituminous coal reduces, however the increase of NO*x* emission of rice husk/bituminite co-firing improves.

KEYWORDS：biomass, co-firing, O2/CO2 atmosphere, drop tube furnace, NO*x* emission

超声波预处理对煤-油临氢共炼的影响（42-46）

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摘要：在预设的超声条件下对不同煤-油共炼原料进行预处理，并在相同的反应条件下使用实验室自制的铁系催化剂进行煤-油共炼反应，考察煤液化率的变化，对液体产物进行元素和馏程分析以及对固体产物进行工业四组分分析，确定超声波预处理对煤-油临氢共炼的影响.结果表明：经过超声波预处理后，共炼原料结构发生改变，分别对油浆及使用安徽煤与油浆所配油煤浆进行超声处理，再进行共炼反应，安徽煤的液化率分别提高9.85%和12.42%；分别对煤焦油及对使用安徽煤与煤焦油所配油煤浆进行超声处理，再进行共炼反应，安徽煤的液化率分别提高7.99%和18.65%，固体产物的灰分、挥发分降低，固定碳含量增加，质量有所提高；液体产物的馏程分布基本没有改变.达到了在提高煤液化率的同时、保证共炼产物质量不变的目的.

关键词：煤-油共炼，超声波预处理，液化率，产物组成，馏程

Effect of Ultrasonic Pretreatment on Coal-oil Co-hydroprocessing

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ABSTRACT：Coal-oil co-hydroprocessing pretreatment experiment proceeded by using lab’s self-made iron-based catalyst to figure out the coal liquefaction rate. Analysis of liquid products, especially on its proceeding elemental and distillation range distribution was made. Industrial four component analysis of solid products was also made and the effect of ultrasonic pretreatment on coal-oil co-hydroprocessing was obtained. The results show that the structure of co-processing raw materials has changed through ultrasonic pretreatment. Liquefaction rate of Anhui coal has improved by 9.85% and 12.42% after processing oil slurry by ultrasonic and compounding oil-coal slurry with oil slurry respectively. Similarly, to the coal tar after ultrasonic treatment and oil-coal slurry compounded by oil-coal slurry, by using same sample,liquefaction rate has improved by 7.99% and 18.65% respectively. Obviously, ash content and volatile matter in solid product have decreased, and fixed carbon has improved after processing, while the distillation range distribution of liquid products has been basically stable. The coal liquefaction rate has improved and the quality of co-processing products remains unchanged.

KEYWORDS：coal-oil co-hydroprocessing, ultrasonic pretreatment, liquid yield, product composition, distillation range

煤液化沥青制备超级活性炭及其气体吸附特性（47-52）

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摘要：使用KOH作为活化剂，以煤液化沥青为碳源，制得比表面积在3 000 m2/g以上的活性炭材料.使用X射线衍射(XRD)、扫描电镜(SEM)、氮气吸附和脱附等方法对炭材料的物理化学特性进行了表征.结果表明：煤液化沥青基活性炭(ACCLA)对H2，CH4和CO2的吸附量最高分别为24.85 mmol/g(77 K，400 kPa)，4.62 mmol/g(298 K，400 kPa)和3.57 mmol/g(298 K，100 kPa)，发现超级活性炭在气体吸附方面表现出优异的性能和良好的应用前景；同时，对多孔结构特性与吸附量之间的对应关系进行了讨论.发现在测试条件下，H2在吸附量受材料比表面积大小影响很大，而对于CH4和CO2孔径尺寸的作用更显著.

关键词：煤液化沥青，超级活性炭，KOH活化法，孔隙结构，气体吸附

Preparation and Gas Adsorption of Super Activated Carbons Derived from Coal Liquefaction Asphaltene

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ABSTRACT：Activated carbons were prepared with coal liquefaction asphaltene as carbon source. After the optimization of the synthesis process, activated carbons with specific surface area more than 3 000 m2/g was successfully obtained. The physical and chemical characteristics of activated carbons from coal liquefaction asphaltene (ACCLA) were also investigated with X-ray diffraction (XRD), scanning electron microscope (SEM) and nitrogen adsorption-desorption methods. The adsorption of H2, CH4 and CO2 on these activated carbons were also tested, the relationship between the texture properties and adsorption capacity was discussed. The as-prepared samples show excellent performance and good application prospects in gas adsorption. It is found that the maximum adsorption of H2, CH4 and CO2 is 24.85 mmol/g (77 K, 400 kPa), 4.62 mmol/g (298 K, 400 kPa) and 3.57 mmol/g (298 K, 100 kPa), respectively. The relationship between the texture properties and adsorption was also discussed. Under test conditions, it is found that the adsorption of H2 is greatly influenced by the specific surface area of the material, and the pore size has a more significant effect on the adsorption of CH4 and CO2.

KEYWORDS：coal liquefaction asphaltene, super activated carbon, KOH activation, pore structure, gas adsorption

煤制合成天然气过程能量转换分析（53-58）

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摘要：基于分析法及黑箱模型理论，针对规模为14亿m3/a的煤制合成天然气的工艺设计，对其主要工段进行计算分析，得出不同工段及整个工艺的损失状况.结果表明：气化工段的普遍效率最低，甲醇洗工段的普遍效率最高，分别为84.75%和98.90%，系统的损失主要发生在气化工段，占整个工艺损失的77.78%；变换、甲醇洗和甲烷化工段分别占整个工艺损失的5.49%，4.04%和12.68%；在气化工段，增加副产蒸汽压力对于提高效率效果并不明显，提高效率应着重改善气化炉和洗涤冷却器的操作条件；对于甲烷化工段，增加副产蒸汽压力能明显提高效率，同时也能增大副产蒸汽量.



关键词：煤制合成天然气，加压气化，粗煤气变换，低温甲醇洗，甲烷化，分析，能量转换

Energy Transformation Analysis of Coal to SNG Process

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ABSTRACT：Based on exergy analysis method, for an actual process of coal to SNG with an annual scale of 1.4×109 m3, the distribution of exergy loss in each unit and in the whole process were investigated. The results show that general exergy efficiency of gasification unit is the lowest, 84.75%, and that of rectisol unit is the highest, 98.90%. The prime exergy loss occurrs in gasification unit, reaching to 77.78% of total exergy loss. The exergy losses in shift unit, rectisol unit and methanation unit are 5.49%, 4.04% and 12.68% of total exergy loss, respectively. In gasification unit, increasing byproduct steam pressure could not impact exergy efficiency effectively, it is more important to optimize the operating condition of gasifier and scrubber cooler. In methanation unit, higher byproduct steam pressure could improve exergy efficiency obviously and increase steam yield.

KEYWORDS：coal to SNG, pressurized gasification, shift of raw gas, rectisol, methanation, exergy analysis, energy transformation

铝基锰系催化剂的低温脱硝性能（59-64+80）

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摘要：在固定床反应器中对溶胶凝胶法制备的锰铈催化剂进行脱硝实验、氧化实验和脱附实验.结果表明：MnO*x*/γ-Al2O3催化剂在300 ℃达到最佳脱硝效率，添加CeO2后，最佳脱硝效率对应温度降至250 ℃.CeO2的添加提高了低温条件下催化剂表面的氧化活化能力，但温度高于300 ℃时，NH3会发生过度氧化生成N2O副产物.MnO*x*负载量的增加会使NH3在催化剂表面的吸附量增多，且会增加NO在多种活性位上的吸附，从而使催化剂在更宽的温度范围内均表现出较高的催化效率.

关键词：溶胶凝胶法，选择性催化还原，脱硝，氧化锰，氧化铈

Denitrification Performance of Mn/Al Catalysts at Low Temperature

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ABSTRACT：The denitrification performance experiments, oxidation experiments and desorption experiments have been carried out over MnO*x*/Al2O3 and MnO*x*-CeO2/γ-Al2O3 prepared by sol-gel process in a fixed bed reactor. The results show that MnO*x*/γ-Al2O3 catalysts reach highest NO removal efficiency at 300 ℃, after adding CeO2 into the catalyst, the optimum temperature reduces to 250 ℃. The addition of CeO2 improves the activation ability of the catalysts at low temperature, but can cause excessive oxidation of NH3 which generates by-products like N2O when the temperature is higher than 300 ℃. The increase of the MnO*x* content can raise adsorption quantities of NH3 over the catalysts, and can also promate NO adsorbtion on different active sites, therefore the catalysts have high NO removal efficiency in wider temperature range.

KEYWORDS：sol-gel method, selective catalytic reduction, denitrification, MnO*x*, CeO2

山西临汾褐煤微生物降解工艺条件的优化（65-72）

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摘要：对6株细菌和硝酸氧化的山西临汾褐煤进行菌-煤匹配降解实验，筛选出降解优势菌恶臭假单胞菌.在单因素试验的基础上，通过正交试验优化了恶臭假单胞菌降解临汾褐煤的工艺条件，得出的影响权重为：煤样粒度>煤浆质量浓度>培养时间>接种量.较优降解工艺条件为：煤样粒度<75 μm，煤浆质量浓度0.200 0 g/10 mL，培养时间14 d，接种量1.0 mL/10 mL.此条件下的降解转化率达到46.81%.对降解后的煤残渣和降解产物进行红外检测，结果表明：煤残渣在氧化煤既有波数处的吸收大部分已消失或者变弱，说明煤中的有机大分子已被恶臭假单胞菌降解成小分子，包含在降解后的黑色油状滤液中.滤液分级萃取物的GC-MS总离子流色谱证明了降解液中含有丰富的小分子有机物，且大多为脂肪烃、酯、羧酸及芳香族化合物.

关键词：临汾褐煤，细菌，微生物降解，正交优化，GC-MS

Optimization of Technological Conditions for Microorganisms Degrading Shanxi Linfen Lignite

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ABSTRACT：The degradation matching experiments of Shanxi Linfen lignite with six kinds of bacteria had been investigated, showing that *Pseudomonas putida* is the most effective degrading bacterium. Based on single factor experiments, the degrading process conditions of *Pseudomonas putida* and Linfen lignite were optimized by orthogonal experiments. The results show that the effect-weight order of the factors for degrading rate is coal particle size > coal slurry mass concentration > incubation time > inoculum size, the best degrading technological conditions are coal particle size <75 μm, coal slurry mass concentration of 0.200 0 g/10 mL, incubation time of 14 d, inoculum size of 1.0 mL/10 mL. Under this technological conditions, the conversion rate reaches 46.81%. The coal residue and degrading product were tested, the infrared analysis shows that the absorption of coal residue at the wavenumber of oxidized coal has been disappeared or weakened, which further indicates that organic macromolecular in coal has been degraded by *Pseudomonas putida* into micromolecule containing in the black oily filtrate derived from the degradation. The total ion chromatogram of fractional extraction product of degradation filtrate demonstrates that it contains abundant small molecule organics, which mostly include aliphatic hydrocarbons, esters, carboxylic acids and aromatic compounds.

KEYWORDS：Linfen lignite, bacteria, microbial degradation, orthogonal optimization, GC-MS

CH4和N2在炭分子筛及13X沸石上的吸附分离（73-80）

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摘要：采用静态体积法测试了298.15 K，313.15 K和328.15 K时，CH4和N2在太西煤基炭分子筛(T-CMS)及13X沸石上的吸附量，并使用Langmuir模型对吸附量数据进行了线性拟合，分析了拟合参数饱和吸附量*q*m和吸附平衡常数*b*值的变化.结果表明：随着温度的升高，CH4在T-CMS上的饱和吸附量*q*m稍有减少，但变化不大，N2在T-CMS上的饱和吸附量*q*m呈增大趋势；CH4和N2在13X沸石上的饱和吸附量*q*m均呈减小趋势，CH4和N2在T-CMS及13X沸石上的吸附平衡常数*b*值均随温度的升高而减小；CH4和N2在T-CMS上的分离系数均大于其在13X沸石上的分离系数，分离系数均随温度升高而减小.吸附热力学分析表明，CH4和N2在T-CMS上的等量吸附热平均值分别为27.30 kJ/mol和22.43 kJ/mol，而在13X沸石上的等量吸附热平均值分别为12.96 kJ/mol和10.41 kJ/mol，两种吸附剂对CH4的吸附作用均强于其对N2的吸附作用，且均属于物理吸附.

关键词：CH4，N2，吸附量，分离系数，吸附热

Adsorptive Separation of CH4 and N2 on Carbon Molecular Sieve and 13X Zeolite

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ABSTRACT：Adsorption quantity of CH4 and N2 on T-CMS and 13X zeolite at 298.15 K, 313.15 K and 328.15 K were measured respectively, Langmuir model was used to fit the experimental data, and the change of fitting parameters, saturated adsorption capacity *q*m and adsorption equilibrium constant *b*, were analyzed. The results show that the *q*m of CH4 on T-CMS slightly decreases as the temperatures rise, but the variation is small; the *q*m of N2 on T-CMS increases; and the *q*m of CH4 and N2 on 13X zeolite decreases. However, the adsorption equilibrium constant *b* increases with the rising of temperature. Separation coefficients of CH4 and N2 on T-CMS are larger than that on 13X zeolite, and both decrease with the increase of temperature. The analysis of adsorption thermodynamics shows that the average adsorption isosteric heat of CH4 and N2 on T-CMS are 27.30 kJ/mol and 22.43 kJ/mol respectively, but that on 13X zeolite are 12.96 kJ/mol and 10.41 kJ/mol respectively. The studied adsorbents have stronger adsorption effect on CH4 than that on N2, which both belong to physical adsorption.

KEYWORDS：CH4, N2, adsorption quantity, separation coefficient, adsorption heat

不同类型酸作用下构造煤表面性的变化机理（1-7）

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摘要：以沁水盆地中南部霍尔辛赫井田的不同煤体结构煤为研究对象，用盐酸(HCl)、醋酸(HAc)和氢氟酸(HF)对煤样进行酸化处理，并运用低温灰化和X射线衍射等方法，对酸改造前后煤样的质量变化率、煤-水接触角和表面张力进行测试计算分析.研究表明：盐酸和醋酸作用后煤样的质量变化率在0.1%左右，而氢氟酸作用后煤样的质量变化率却高达7%；不同酸的作用对象不同，氢氟酸可与煤中大部分无机矿物质发生反应，效果最为显著；盐酸酸化后，煤-水接触角由59.75°减小为33.25°，表面张力由54.42 mJ/m2增至66.45 mJ/m2，含水性增强；而醋酸和氢氟酸酸化后，煤-水接触角由59.75°分别增至85.00°和84.50°，表面张力由54.42 mJ/m2分别减至39.34 mJ/m2和39.65 mJ/m2，疏水性增强；煤样经酸化处理后，煤-水接触角和表面张力变化明显.

关键词：构造煤，酸处理，接触角，表面张力，润湿性

Change Mechanism in Surface Properties of Treated Tectonic Coal by Different Acids

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ABSTRACT：The coal samples with different deformed degrees, collected from Huoerxinhe coalmine in Qinshui coal basin were treated by the different acids, including hydrochloric acid (HCl), acetic acid (HAc) and hydrofluoric acid (HF). Mass change rate and coal-water contact angel were measured, and the surface tension was calculated by low temperature ashing and X-ray diffraction methods. The results show that the mass change rate of the coal is about 0.1% by HCl or HAc treatment, while the mass change rate of the coal is 7% by HF treatment; the reaction objects are different for each acid, most of the minerals in the coal can react with HF, which is the most effective treatment method; after HCl treatment, the coal-water contact angel shows a obviously decreasing trend from 59.75°to 33.25°, but the surface tension increases from 54.42 mJ/m2 to 66.45 mJ/m2 to cause a stronger wettability. After HAc and HF treatment, the coal-water contact angel shows a correspondingly increasing phenomenon from 59.75° to 85.00° and 84.50°, the surface tension decreases from 54.42 mJ/m2 to 39.34 mJ/m2 and 39.65 mJ/m2 respectively. In general, the water-coal contact angel and surface tension of coal change significantly after the acid treatment.

KEYWORDS：tectonic coal, acid treatment, contact angel, surface tension, wettability

褐煤润湿性及水分复吸的量热法研究（8-14）

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摘要：利用量热法分别对褐煤、脱灰褐煤和常见矿物质的润湿热进行测定，考察水分复吸对褐煤润湿性的影响，并对干燥褐煤水分复吸动力学进行分析.结果表明：褐煤中有机质的润湿热远大于其矿物质的润湿热，是褐煤润湿放热的主体.褐煤中含氧官能团越多，润湿热值越大.酸洗脱灰降低了褐煤的亲水性.芒来褐煤脱灰后，润湿热由101.61 J/g降至66.79 J/g，褐煤矿物质中高岭石的润湿热高于方解石和石英的润湿热；干燥褐煤的水分复吸符合二级动力学模型，相关系数大于0.99；褐煤复吸水分越多，其润湿热越小，芒来褐煤复吸水分增加到28.76%(质量分数)时，其润湿热由101.61 J/g降至5.04 J/g.水分复吸过程中，在表面形成的单层吸附或团簇吸附是褐煤润湿热降低的主要影响因素，而孔隙吸附或毛细凝聚吸附对其润湿热影响较小.

关键词：润湿热，水分复吸，褐煤，量热法，矿物质，吸附动力学

Calorimetry Investigation on Wettability and Moisture Re-adsorption of Lignite

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ABSTRACT：The wettability of lignite and demineralized lignite and conventional mineral matter were evaluated by calorimetric measurement. The effects of moisture re-adsorption on the wetting heat of lignite were investigated and the moisture re-adsorption behavior of dried lignite was analyzed by dynamics models. The results show that wetting heat of organic components in lignite is much higher than that of mineral matter in lignite, indicating its dominated role for heat released of wetting process. The lignite with more content of oxygen-containing groups has a higher value of wetting heat. After the treatment by acid solution, the wetting heat of lignite decreases. For the Manglai lignite, the wetting heat decreases from 101.61 J/g to 66.79 J/g after demineralition. Among the mineral matter in lignite, wetting heat of kaolinite is higher than that of calcite and quartz. The moisture re-adsorption behavior was fitted properly by second-order dynamical model, and the correlation coefficient is greater than 0.99. With the increasing content of moisture readsorbed, wetting heat of lignite decreases. When the moisture re-adsorption reaches to 28.76%, wetting heat of the Manglai lignite decreases from 101.61 J/g to 5.04 J/g. The monolayer or cluster of water molecules adsorbed on surface of lignite is devoted to wetting heat decreasing, while the influence of water adsorbed in pores or capillary condensation is not obviously.

KEYWORDS：wetting heat, moisture re-adsorption, lignite, calorimetry, mineral matter, adsorption dynamics

基于热分析法的神府粉煤低温热解影响因素研究（15-20）

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摘要：利用TG-DTG热分析仪对神府粉煤热解特性进行实验研究，考察升温速率、煤样粒径和载气流速对神府粉煤热解过程的影响，并通过正交实验确定最大失重速率的最佳条件.热重实验结果表明：升温速率、煤样粒径和载气流速对热解失重均有影响.升温速率和载气流速增大，热解失重量减少.粒径对热解失重率的影响呈抛物线分布，最大热解失重量存在最佳粒径，本实验所研究的粒径小于0.84 mm的神府煤，热解过程中最佳粒径为0.25 mm~0.42 mm.正交实验结果表明：升温速率是影响煤热解过程的主要因素，其次是粒径，载气流速对热解影响最小；当神府煤的煤样粒径为0.25 mm~0.42 mm、升温速率为30 ℃/min、载气流速为120 mL/min时，热解失重速率最大，为4.95 %/min.

关键词：神府粉煤，热解，兰炭，正交实验，TG-DTG，失重率

Effect Factors of Shenfu Pulverized Coal Low-temperature Pyrolysis by Thermal Analysis Technique

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ABSTRACT：The pyrolysis process of Shenfu pulverized coal at different heating rate, with different diameter and at different flow rate of carry gas was studied by TG-DTG thermogravimetric analysis. The optimal condition of maximum weight loss rate was determined through orthogonal experiments. The thermogravimetric experiment results show that heating rate, diameter and flow rate of carry gas have effect on the pyrolysis weightlessness. It is found that the pyrolysis weightlessness decreases with the increase of heating rate and flow rate of carrier gas. The effect of diameter on pyrolysis weightlessness is a parabola distribution, so there is an optimal diameter when the pyrolysis weightlessness is a maximum. During pyrolysis the optimal diameter of Shenfu coal (d<0.84 mm) is 0.25 mm-0.42 mm. The results of orthogonal experiment show that during coal pyrolysis, the main factor is heating rate, next is diameter and then flow rate of carry gas. The fastest pyrolysis weight loss rate is 4.95%/min when diameter is 0.25 mm-0.42 mm, heating rate is 30 ℃/min, flow rate of carry gas is 120 mL/min.

KEYWORDS：Shenfu pulverized coal, coal pyrolysis, blue-coke, orthogonal experiments, TG-DTG, weight loss rate

改性ZSM-5对神东煤热解行为的影响（21-27+51）

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摘要：以自制的ZSM-5为载体，制备了NiW/ZSM-5及磷改性PNiW/ZSM-5负载型催化剂，通过XRD，ICP，BET，NH3-TPD和SEM等检测手段对催化剂进行系列表征.结果表明：绝大部分Ni，W和P活性组分被引入到载体上，且分散均匀，改性后分子筛的强酸性位数量明显减少.利用热重-红外联用(TG-FTIR)装置对神东煤在不同催化剂上的热解性能进行评价.结果显示，与原煤热解相比较，催化剂NiW/ZSM-5和PNiW/ZSM-5均使神东煤热解的最大失重峰温提前了8 ℃，失重率分别增加了1.2%和2.0%.FTIR谱显示，在ZSM-5作用下气相产物析出量无明显增加，而在NiW/ZSM-5和PNiW/ZSM-5催化剂作用下，CH4、CO、NH3、轻质脂肪烃和芳香烃的析出量增加明显，其中以PNiW/ZSM-5催化剂效果最佳.

关键词：热解特性，催化性能，过渡金属，产物分布，二次反应

Pyrolysis Characteristics of Shendong Coal on Modified ZSM-5 Catalyst

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ABSTRACT：NiW/ZSM-5 and PNiW/ZSM-5 supported catalysts were prepared on self-made ZSM-5 carrier. Catalysts were characterized by XRD, ICP, BET, NH3-TPD and SEM techniques. The results indicate that most of the active components of Ni, W and P have been successfully introduced into the carrier and disperse evenly, and the amount of strong acid sites decreases after modification. The catalytic properties of different catalysts on Shendong coal were evaluated by thermogravimetry-infrared (TG-FTIR). Compared with raw coal pyrolysis, NiW/ZSM-5 and PNiW/ZSM-5 catalytic pyrolysis can descrease the maximum weight loss peak temperature of Shendong coal by 8 ℃, increase the weight loss rate by 1.2% and 2.0%. The FTIR analysis results show that although ZSM-5 have no significant increase in the amount of gas-phase products, the contents of CH4, CO, NH3, light aliphatic and aromatic hydrocarbons increase significantly with NiW/ZSM-5 and PNiW/ZSM-5 catalysts, and PNiW/ZSM-5 catalyst has better advantages compared to NiW/ZSM-5.

KEYWORDS：pyrolysis characteristics, catalytic properties, transition metal, product distribution, secondary reactions

新疆淖毛湖长焰煤地下催化热解的反应特性（28-33）

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摘要：设计了适合于地下催化热解/气化的错时喷射催化剂添加装置，在卧式热解反应器中使用四种典型催化剂对新疆淖毛湖长焰煤进行地下催化热解模拟实验.结果表明：四种催化剂可有效提高热解气中H2和CO组分及气态产物产率，催化活性由大到小依次为8% Na2CO3溶液(8%为质量分数，下同)，10%Ca(OH)2溶液，10%CaO粉末，6%FNC(复合催化剂(Fe2O3-Na2CO3-Ca(OH)3))；活性较高的Na2CO3溶液和Ca(OH)2溶液使热解气中H2组分提高了19%(体积分数)，CO组分增加1.2倍，CH4组分在低温热解区有所增加，但在600 ℃以上热解时无明显效果.半焦和焦油产率较催化前分别下降30%和20%~70%，煤气产率提高1.4倍~1.6倍.从催化活性和成本分析，在地下催化热解过程中主催化剂可选择Ca(OH)2溶液，并配置活性最高的Na2CO3溶液作为辅助催化剂.

关键词：长焰煤，地下催化热解，催化剂活性，热解气，错时喷射

Underground Catalytic Pyrolysis Reaction Characteristics of Long Flame Coal from Naomaohu in Xinjiang

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ABSTRACT：Interleaved catalyst injection unit suitably for underground pyrolysis and gasification was designed. Four sorts of typical catalysts were used in the horizontal pyrolysis reactor for the simulation test of underground catalytic pyrolysis on the long flame coal of Naomaohu in Xinjiang. The results show that these four sorts of catalysts can efficiently improve the composition of H2 and CO, and the yield of gaseous products. The descending order of their catalytic activity is 8% Na2CO3 solution (8% is mass fraction, the same below), 10%Ca(OH)2 solution, 10%CaO powder, 6%FNC (compound catalyst (Fe2O3-Na2CO3-Ca(OH)2)). For Na2CO3 and Ca(OH)2 of high activity, these two catalytics increase the composition of H2 by 19% (volume fraction) in the pyrolysis gas and CO by 1.2 times respectively, and increase the composition of CH4 in the low temperature pyrolysis, but without sustainable effect during the pyrolysis over 600 ℃. The yield of semicoke and tar decreases by 30% and 20%-70% respectively, and gas yield can increase by 1.4-1.6 times compared to the yield before the catalytic pyrolysis. On the analysis of the aspects of catalytic activity and cost, Ca(OH)2 can be selected as the major catalyst for underground catalytic pyrolysis, and Na2CO3 of highest activity can be considered as promoter.

KEYWORDS：long flame coal, underground catalytic pyrolysis, catalyst activity, pyrolysis gas, interleaved catalyst injection

硅区尺寸对SAPO-34分子筛稳定性和酸性的影响（34-43）

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摘要：构建了SAPO-34分子筛中不同尺寸的硅区Sin(n=5，8，9，11，12，13，14)，并运用色散力修正的密度泛函理论(DFT-D)方法研究了SAPO-34分子筛中不同尺寸硅区形成的难易，以及所形成硅区对SAPO-34分子筛的稳定性和酸性的影响.计算结果表明：在SAPO-34分子筛中，含Si5和Si9的硅区容易形成.硅区尺寸越大，SAPO-34分子筛的结构越稳定，酸性越强.同时给出了预测含有不同硅区的分子筛中各酸性位强弱次序的规则.

关键词：SAPO-34分子筛，Brnsted酸，硅区，稳定性，酸性，密度泛函理论

Effect of Si Island Size on Stability and Acidity of SAPO-34 Molecular Sieve

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ABSTRACT：SAPO-34 molecular sieve with different sizes of Si islands Sin (n=5, 8, 9, 11, 12, 13, 14) was constructed and investigated using dispersion-corrected density functional theory method in order to study the formation of Si islands, and the effects on the stability and acidity of SAPO-34 molecular sieve were studied. It indicates that the Si islands including Si5 and Si9 are easy to form in SAPO-34 molecular sieve. In addition, the larger the Si island is, the more stable the structure is and the more acidity the Bronsted sites are. The rule is proposed to judge the acidic strength in SAPO-34 molecular sieve with different sizes of Si islands.

KEYWORDS：SAPO-34 molecular sieve, Bronsted acid, Si island, stability, acidity, density functional theory

煤液化柴油调和及发动机试验研究（44-51）

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摘要：对煤直接液化柴油(diesel of direct coal liquefaction，DDCL)和煤间接液化柴油(diesel of indirect coal liquefaction，DICL)的性质进行了分析，通过调和试验考察了二者的相容性、煤液化调和柴油的性质规律及其对润滑性改进剂的感受性；并通过发动机台架试验考察了煤液化调和柴油的动力性、经济性和排放性能.结果表明：DDCL与DICL有很好的相容性；煤液化调和柴油的密度和十六烷值与其中DICL的质量分数呈线性关系，能够实现二者的优势互补；其对润滑性改进剂具有良好的感受性；在国Ⅳ发动机上有很好的动力性，单位质量油耗略有优势，常规排放满足国Ⅳ排放标准，且在NO*x*、烟度和PM排放方面有较大优势.

关键词：煤液化柴油，调和，发动机，燃烧，排放

Study on Blending and Engine Test with Diesel of Coal Liquefaction

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ABSTRACT：The properties of diesel of direct coal liquefaction (DDCL) and diesel of indirect coal liquefaction (DICL) were analyzed, the miscibility of the two types of diesel, the properties of blending diesel and the effect of lubricity additives on the two types of diesel were studied by the blending experiment, and the mobility, economy and emission performance of the blending diesel were investigated by engine bench test. The results show that DDCL is well dissolvable with DICL, and the density and the cetane number of the blending diesel are both linearly related to the mass fraction of DICL. It indicates that the two types of diesel have complement advantages with each other very well. The blending diesel has good sensibility to the lubricant. It is found that the blending diesel of coal liquefaction has good dynamic performance, less fuel consumption per unit mass and less pollutant emissions on China Ⅳ engine. The regulated emissions of the blending diesel fuel meet China Ⅳ emission standard. It has great advantage in the emissions of NO*x*, smoke intensity and particulate matter.

KEYWORDS：diesel of coal liquefaction, blend, engine, combustion, emission

新疆地区低阶煤污水制浆及成浆特性（52-58）

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摘要：采用4种水样(含采油污水)对新疆地区3种低阶煤展开成浆特性、浆体流变特性及稳定性实验研究.结果表明：乌苏红山煤、乌苏四棵树煤和徐矿4煤的成浆质量分数分别可达66.5%，61.0%和53.4%.在污水制浆中，以含油量较高的重力除油入口水较合适，可促进成浆，相比重力除油出口水制浆，乌苏红山煤和乌苏四棵树煤浆体表观黏度分别可降低30.3%和66.8%，徐矿4煤成浆质量分数提升1.1%；重力除油入口水还可提高浆体热值，简化污水处理.3种煤浆稳定性差异较大，其中乌苏四棵树煤浆稳定性最好；影响浆体稳定性的主要是煤质和添加剂，水样对煤浆稳定性的影响较小.

关键词：油田污水，低阶煤，水煤浆，成浆特性，稳定性

Properties of Coal Water Slurry Prepared with Low-rank Coal and Oil-field Sewage from Xinjiang

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ABSTRACT：The properties of coal water slurry (CWS) prepared by low-rank coal and oil-field sewage were investigated. The results show that the maximal CWS mass fraction for each coal follows: Wusuhongshan coal (66.5%)>Wususikeshu coal (61.0%)>Xukuang 4 coal (53.4%). Compared with the CWS prepared by oil-free sewage, the CWS prepared by oil-bearing sewage for each coal have lower viscosity, which decrease by 30.3% and 66.8% for Wusuhong-shan coal and Wususikeshu coal respectively, and have larger mass fraction, which increase by 1.1% for Xukuang 4 coal. It indicates that the use of oil-bearing can promote the mass fraction and calorific value of CWS, as well as simplifying the treatment of oil-field sewage. Among three kinds of CWS, the Wusuhongshan CWS has the largest stability due to its high ash content. The stability of CWS is largely affected by coal type and additive, while the type of water or sewage shows little effect.

KEYWORDS：oil-field sewage, low-rank coal, coal water slurry, slurry properties, stability

型煤燃烧中改性活性氧化铝的固硫效果（59-63）

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摘要：基于等体积浸渍法和固硫理论，研究了以表面负载不同金属氧化物的活性氧化铝作为型煤添加剂的固硫效果，并通过SEM分析和XRD分析，分别考察了不同活性氧化铝的孔结构变化、原煤煤灰和负载CaO的活性氧化铝型煤煤灰的物相变化.结果表明：活性氧化铝和负载不同金属氧化物的活性氧化铝对型煤燃烧中SO2减排效果由高到低依次为负载CaO的活性氧化铝、负载CuO的活性氧化铝、负载BaO的活性氧化铝和活性氧化铝.通过SEM分析发现，活性氧化铝改性后提高了孔结构的热稳定性.通过XRD分析发现，负载CaO的活性氧化铝在型煤燃烧过程中会与SO2反应，生成耐高温络合物3CaO·3Al2O3·CaSO4，阻碍了部分CaSO4的分解，从而提高了其固硫性能.经实验对比发现，负载CaO的活性氧化铝的固硫效果比传统固硫剂CaO更优.

关键词：型煤，固硫剂，活性氧化铝，改性，CaO

Sulfur Retention Effect of Modified Activated Alumina During Briquette Combustion

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ABSTRACT：Based on the isometric impregnation and the theory of sulfur-fixation, the sulfur retention of activated alumina as briquette additive and loading with different metal oxides on the surface was studied. The changes of pore structure before and after modification were analyzed by using SEM, and the changes of phase transformation of raw coal ash and briquette ash were analyzed by using XRD, while activated alumina loading with CaO was used as the briquette sulfur fixing agent. The results show that the effect on reduction of SO2 emission by activated alumina loading with different metal oxide is activated alumina loading with CaO>activated alumina loading with CuO>activated alumina loading with BaO>activated alumina. The SEM analysis shows that loading different metal oxides on the surface of activated alumina has improved its heat stability. It is found by using XRD that CaO loading on activated alumina can react with SO2 and generate 3CaO·3Al2O3·CaSO4 with thermostability, which hinders the decomposition of CaSO4, thus can improve the sulfur retention effect. Compared with the sulfur retention effect of CaO, the sulfur retention effect of modified activated alumina is better in the experiment.

KEYWORDS：briquette, sulfur fixing agent, activated alumina, modification, CaO

新型梯级筛分内加热流化床CMC工艺能效分析（64-69）

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摘要：提出了一种梯级筛分和内加热流化床结合的新型CMC(coal moisture control)工艺(EN-CMC工艺)，其用高比热和高密度的热水作为载热介质，分离原有热烟气的载热和载湿功能，可彻底改变原有流化床CMC工艺的能质流程，并且与马钢投产运行的186 t/h新日铁流化床CMC工艺和宝钢投产运行的330 t/h蒸汽滚筒式CMC工艺(STD工艺)进行能效对比.结果表明：通过EN-CMC工艺处理后，减少焦炉供热量2.78×105 kJ/t(干煤)，折合9.50 kgce/t(干煤)，节能效果达到6.92 kgce/t(干煤)，比新日铁流化床CMC工艺的节能效果增强53.4%.

关键词：流化床，焦化，热力学，煤调湿，梯级筛分

Energy Efficiency Analysis on New CMC Technology of Cascade Sieving and Fluidized Bed with Immersed Heating Tubes

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ABSTRACT：A new CMC technology of cascade sieving and fluidized bed with immersed heating tubes (EN-CMC technology) was proposed. The energy and mass flow of the original fluidized bed CMC technology was completely changed by means of hot water as heat carrier which had high specific heat and density, and the previous heat and moisture carrying function of exhaust gas was divided. The energy efficiency among three kinds of CMC technologies was compared, including EN-CMC technology, 186 t/h Nippon steel fluidized bed CMC technology in MA steel and 330 t/h steam drum-type CMC technology in BAO steel. The results indicate that after the process of EN-CMC, coke oven heating quantity can decrease by 2.78×105 kJ/t (dry coal (DC)), with amounts to 9.50 kgce/t(DC). The energy-saving effect reaches 6.92 kgce/t(DC), which is 53.4% higher than Nippon steel CMC technology.

KEYWORDS：fluidized-bed, coking, thermodynamics, coal moisture control, cascade sieving

*n*(Na+)/*n*(Cl-)对烟气脱氯及脱硫废水零排放的影响（70-75）

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摘要：半干法脱氯是通过碱基物质将燃煤烟气中的大部分HCl固定到飞灰中，同时将大幅度减少的脱硫(flue gas desulfurization，FGD)废水作为碱基溶剂回喷烟道，从而可实现脱硫废水零排放.通过搭建实验台对碱基物质与烟气中HCl和SO2的反应效率随*n*(Na+)/*n*(Cl-)的变化进行了实验研究.结果表明：碱基物质与HCl的反应效率与*n*(Na+)/*n*(Cl-)呈正相关，且随*n*(Na+)/*n*(Cl-)的增大，其增长趋势逐渐变缓，在*n*(Na+)/*n*(Cl-)为4.8时，反应效率已经达到70%以上.针对一台660 MW燃煤机组进行计算，采用半干法烟气脱氯后，脱硫废水量显著下降，由8.01 m3/h降为2.31 m3/h；利用脱硫废水作为碱基溶剂回喷空气预热器后烟道，烟气温降较小，仅为2.49 ℃.半干法脱氯系统简单，运行成本较低，不会对粉煤灰的综合利用造成显著的不利影响.

关键词：燃煤烟气，氯化氢，半干法脱氯，脱硫废水，零排放，*n*(Na+)/*n*(Cl-)

Effect of *n*(Na+)/*n*(Cl-) on Semi-dry Dechlorination in Coal-fired Flue Gas to Realize Zero Emission of FGD Waste Water

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ABSTRACT：Semi-dry dechlorination technology is put forward to attach most chlorine in coal-fired flue gas to fly ash by spraying in alkaline solution to realize the zero emission of desulfurization waste water. Simultaneously, drastically reduced FGD (flue gas desulfurization) waste water was used as the solvent of alkali, which could help to realize the target of zero emission of desulfurization waste water. Effects of *n*(Na+)/*n*(Cl-) on reaction efficiencies of base material with HCl and SO2 were analyzed. It shows that the reaction efficiency of HCl is positively correlated with *n*(Na+)/*n*(Cl-). As *n*(Na+)/*n*(Cl-) continues increasing, there is a slower growth of HCl reaction efficiency. When *n*(Na+)/*n*(Cl-) is 4.8, reaction efficiency of HCl increases beyond 70%. For a 660 MW unit, after semi-dry dechlorination, the amount of FGD waste water decreases significantly from 8.01 m3/h to 2.31 m3/h, and the decrease of flue gas temperature is only 2.49 ℃ when waste water is sprayed back as the solvent of alkali. The system of semi-dry dechlorination is simple and the cost is relatively low. There is no significantly negative effect on the comprehensive utilization of fly ash after semi-dry dechlorination.

KEYWORDS：coal-fired flue gas, hydrogen chloride, semi-dry dechlorination, FGD waste water, zero emission, *n*(Na+)/*n*(Cl-)

烟道气碳化水镁石副产碱式碳酸镁碳捕集技术（76-80）

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摘要：以天然水镁石(Mg(OH)2)浆液为原料，在固液质量比1∶6，反应温度40 ℃，反应压力1.01×105 Pa，模拟烟道气的CO2体积分数为15%的条件下进行碳捕集，同时产出副产品碱式碳酸镁(4MgCO3·Mg(OH)2·4H2O)，此方法不仅降低了捕集成本，而且副产高附加值产品.对反应过程中体系的pH值和物质组成进行了检测，探讨了不同气速对反应时间的影响，并对最终产物进行了滴定分析和热失重分析.结果表明：反应终止的pH值为7.73~7.74，较适宜的气速为60 mL/min，此时CO2回收率达40.87%.最终产物碱式碳酸镁的镁含量达到43.16%(质量分数)，失重量达到56.26%，符合碱式碳酸镁产品的行业标准.

关键词：水镁石，烟道气，二氧化碳，碳捕集，碱式碳酸镁

Carbon Capture Technology of Basic Magnesium Carbonate as a By-product of Brucite Carbonized by Flue Gas

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ABSTRACT：Brucite(Mg(OH)2) as raw material, the carbon capture by absorbing carbon dioxide (15%, volume fraction) of simulated flue gas was carried out under the condition that the solid-liquid mass ratio was 1∶6, the reaction temperature was 40 ℃ and the reaction pressure was 1.01×105 Pa. The cost of capture was reduced by deputy producting high value-added products such as basic magnesium carbonate (4MgCO3·Mg(OH)2·4H2O). The changes of pH value and substance composition during the reaction were determined, the influence of gas velocity on reaction time was discussed, and the final product was analyzed by titration and thermogravimetric analysis. The experimental results show that the pH value of the termination reaction is 7.73-7.74, the suitable gas velocity is 60 mL/min, and the recovery rate of CO2 is 40.87%. The final product basic magnesium carbonate magnesium content reaches 43.16% (mass fraction of MgO), and its weight loss reaches 56.35%. Above results are complied with the industry standard of magnesium carbonate products.

KEYWORDS：brucite, flue gas, carbon dioxide, carbon capture, basic magnesium carbonate

基于HRTEM的煤分子芳香片层结构表征（1-6）

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摘要：利用MATLAB语言开发了简单易用的图形用户界面(GUI)程序VirtualFringe，此程序采用阈值与灰度的调整、高斯模糊、傅立叶变换、二值化、骨架提取、分枝剪切与修剪等方法，从煤的HRTEM图像中抽取出煤微观芳香片层的条纹结构，并通过条纹的外接矩形拟合，分析得出芳香片层的相对位置、角度和长度等信息.利用传统人工分析方法和固态13C NMR结构参数测定，证实了此程序的准确性与可靠性.本程序获得的煤芳香片层结构参数可以用于大尺度煤分子聚集体模型的构建工作.

关键词：MATLAB GUI，HRTEM图谱，图像处理，西山烟煤，芳香片层结构

Characterization Based on HRTEM for Coal Molecular Aromatic Sheets Structure

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ABSTRACT：An easy-to-use graphical user interface (GUI) program, VirtualFringe, was developed using MATLAB programming language. The aromatic fringes were extracted by the steps of thresholding and gray adjustment, Gaussian blur, Fourier transform filtering, binary image conversion, skeletonization and branches trim. And the parameters of positions, angles of declination and lengths were defined by fitting the enclosing rectangles of fringes. The reliability of this application has been confirmed by manual image analysis and structural parameters derived from solid state 13C NMR technique. The size and distribution of aromatic sheets obtained by VirtualFringe, can be used in the construction of large scale molecular coal model that meaningful molecular weight distribution and diversity of coal molecule have been incorporated.

KEYWORDS：MATLAB GUI, HRTEM image, image processing, Xishan bituminous coal, aromatic sheet structure

担载γ-MoNxCy的活性半焦在甲烷化反应中的应用（7-12+19）

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摘要：一定比例的六次甲基四胺(HMT)和钼酸铵(AHM)反应生成络合物，将络合物简单焙烧，成功制备了β-Mo2C.将上述络合物与霍林河(HLH)脱灰煤机械混合后热解，在煤热解的同时，原位生成担载γ-MoNxCy的活性半焦(ASC).采用XRD，SEM，HRTEM和元素分析等方法对催化剂进行表征，并对其在甲烷化反应中的催化行为进行考察.结果表明：尽管β-Mo2C的CO转化率较高，但CH4选择性较低且活性不够稳定；而在担载γ-MoNxCy的活性半焦中，由于活性半焦提高了金属活性组分Mo的分散度及C部分取代N所造成的晶格畸变提高了催化剂本身的催化活性，两者共同作用使单位质量Mo上CO转化速率由β-Mo2C的2.22 mol/(h·g)增加到17.47 mol/(h·g)，同时CH4选择性由β-Mo2C的33.52%(质量分数，下同)增加到49.54%.担载γ-MoNxCy的活性半焦在合成气气氛下实现了煤催化加氢热解与甲烷化反应的耦合.

关键词：β-Mo2C，γ-MoNxCy，活性半焦，甲烷化，加氢热解，耦合

Catalytic Performance of Activated Semi-coke Supporting γ-MoNxCy for Methanation

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ABSTRACT：The complex of hexamethylentetramine (HMT) and ammonium molybdate (AHM) was simply decomposed and bulk β-Mo2C was successfully prepared. In the meantime the complex was mechanically mixed with HLH de-ashed lignite, then the activated semi-coke (ASC) supporting γ-MoNxCy was generated in situ in the process of coal pyrolysis. The synthesized carbides were characterized by XRD, SEM, HRTEM, and elemental analyzer, and their catalytic performances on methanation were evaluated. The results show that the bulk β-Mo2C catalyst exhibits high conversion of CO(XCO), but the selectivity of CH4 (SCH4) is low and the catalytic activity is not stable; as for the activated semi-coke supporting γ-MoNxCy, because of the improved dispersion of Mo and the improved catalytic activity on account of more lattice defects caused by lattice distortion of γ-MoNxCy, the XCO on unit mass of Mo greatly increases from 2.22 mol/(h·g) on bulk β-Mo2C to 17.47 mol/(h·g) on activated semi-coke supporting γ-MoNxCy. In addition, the SCH4 increases from 33.52% on bulk β-Mo2C to 49.54% on activated semi-coke supporting γ-MoNxCy. The above results reveal that methanation can be coupled with catalytic hydropyrolysis of coal under syngas atmosphere on activated semi-coke supporting γ-MoNxCy.

KEYWORDS：β-Mo2C, γ-MoNxCy, activated semi-coke, methanation, hydropyrolysis, coupling

流化-输送床中煤的气力分级数值模拟分析（13-19）

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摘要：为提高流化-输送床耦合装置气力分级过程中煤颗粒的品质，采用正交实验法，选择耦合装置的表观气速、进料口位置和进料速率三个参数为因素，每个因素取三个水平，考虑因素之间的交互作用，选取L18(37)正交表得到18组方案.运用计算颗粒流体力学(CPFD)软件，对煤颗粒气力分级过程进行数值模拟，结合气固流化-输送床耦合装置气力分级实验对分级过程进行研究，并以煤颗粒最优分级效率为指标，由极差综合分析法得出，耦合装置的输送床表观气速是影响煤颗粒气力分级的主要因素，输送床表观气速为8.30 m/s、进料口位置为输送床下部以及进料速率为22.5 kg/(m2·s)的最优组合.

关键词：流化床，输送床，气力分级，正交实验，数值模拟

Numerical Simulation Analysis of Pneumatic Classification of Coal in Coupling Device for Fluidized Bed and Conveying Bed

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ABSTRACT：In order to improve the quality of pneumatic classification of coal in the coupling device for fluidized bed and conveying bed, orthogonal test method was used to select three parameters, such as the apparent gas velocity of conveying bed, the feed inlet position and the feed rate, and each factor was taken at three levels, taking into account the interaction between the factors, and the L18(37) orthogonal array was chosen to be the 18 groups. Based on the computational particle fluid dynamics (CPFD) software,the pneumatic classification of coal was simulated, the pneumatic classification of coal in the coupling device for fluidized bed and conveying bed was studied using experimental measurements, and the optimum separation effect of coal particles was taken as the index. By comprehensive analysis of range method, the apparent gas velocity of conveying bed is the main factor affecting the pneumatic classification of coal and the best combination scheme for the pneumatic classification, which is the apparent gas velocity of conveying bed is 8.30 m/s, the feed inlet position is the lower part of the conveying bed, the feed rate is 22.5 kg/(m2·s).

KEYWORDS：fluidized bed, conveying bed, pneumatic classification, orthogonal test, numerical simulation

煤炭分级利用过程中清洁油品的生产技术（20-24）

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摘要：在催化剂装量100 mL的中型试验装置上，以煤焦油为原料，通过加氢方法得到了清洁柴油，柴油密度为0.83 g/cm3~0.86 g/cm3，十六烷值为42~52，硫含量低于2 μg/g；在千吨级固定床费托合成工业试验装置上，以合成气为原料，经费托合成高选择性地得到了液体烃类，在原料气转化率高于93%时，C5+选择性超过86%；在百万吨级工业装置上，以费托合成油为原料，通过加氢提质得到了密度低于0.77 g/cm3、十六烷值为76~81、硫含量低于1 μg/g的清洁柴油组分，同时还可以得到高品质液蜡、喷气燃料和溶剂油.煤炭分级利用过程中产生的煤焦油和荒煤气，通过合适的加工路线均可以得到硫含量满足国五标准的清洁油品.

关键词：煤焦油，费托合成，加氢，煤炭分级利用，清洁油品

Clean Oil Production in the Process of Coal Classification Utilization

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ABSTRACT：Coal tar can be hydrogenated to produce diesel with density 0.83 g/cm3-0.86 g/cm3, cetane number 42-52 and sulfur lower than 2 μg/g in 100 mL pilot plant, while liquid hydrocarbons can be produced by waste gas F-T synthesis with a feedstock gas conversion rate above 93%, selectivity of C5+ hydrocarbons above 86% in a 3 000 t/a fixed-bed F-T synthesis industrial plant, and further synthesis oil can be hydro-upgraded to gain diesel oil with density lower than 0.77 g/cm3, cetane number 76-81. Beyond that, waste gas can be used to produce high quality liquid wax, jet fuel and solvent oil. Choosing suitable process, coal tar and waste gas generated during the classification utilization of coal can produce clean and high value oils with sulfur content met the requirement of China V clean oil standards.

KEYWORDS：coal tar, F-T synthesis, hydro-upgrading, coal classification utilization, clean oil

n(H2O)∶n(Al)对Ni-W催化剂低温煤焦油加氢性能的影响（25-30+68）

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摘要：采用完全液相法制备以TiO2-AlOOH为复合载体，Ni和W为活性组分的浆状加氢催化剂，考察n(H2O)∶n(Al)对Ni-W催化剂结构与催化性能的影响，并利用XRD，BET，NH3-TPD等手段对催化剂进行表征.采用GC-MS，TG和元素分析对原料及产物的馏分分布及组成进行分析，结果表明：n(H2O)∶n(Al)为75时制备的Ni-W催化剂，产物中轻组分含量最高，加氢脱硫(HDS)活性及产物油的n(H)∶n(C)最高，对煤焦油加氢处理具有较优的加氢效果.

关键词：加氢，馏分，n(H2O)∶n(Al)，Ni-W浆态床催化剂，低温煤焦油

Effects of n(H2O)∶n(Al) of Ni-W Catalyst on Catalytic Hydrogenation Properties of Low Temperature Coal Tar

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ABSTRACT：Slurry hydrogenation catalyst with TiO2-AlOOH as the composite carrier and Ni and W as active components were prepared by a complete liquid phase method .The effect of n(H2O)∶n(Al) on the structure and catalytic properties of Ni-W catalysts were investigated and the catalysts were characterized by XRD, BET, NH3-TPD and so on. The fraction distribution and composition of raw materials and products were analyzed by GC-MS, TG and ultimate analylzer, the results show that the content of light component, the hydrodesulfurization (HDS) activity and the n(H)∶n(C) in the products are the highest when n(H2O)∶n(Al) is 75 in the catalysts. It indicates that Ni-W catalyst with n(H2O)∶n(Al) 75 has better hydrogenation effect on coal tar hydrotreating than that of the other value of n(H2O)∶n(Al).

KEYWORDS：hydroprocessing, fraction, n(H2O)∶n(Al), Ni-W slurry catalyst, low temperature coal tar

固载化吡咯烷酮离子液体催化合成聚甲醛二甲醚（31-38）

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摘要：以HMCM-22分子筛为载体，化学键合固载吡咯烷酮离子液体，并用于催化合成聚甲醛二甲醚(DMMn).XRD，FTIR及SEM结果表明：吡咯烷酮离子液体可以较好地固载于HMCM-22分子筛上.优选合成聚甲醛二甲醚的反应条件为：催化剂用量为总反应物质量的2.0%，甲缩醛与多聚甲醛的质量比(醇醛比)为2∶1，反应温度为120 ℃，反应时间为6 h，离子液体负载量为2.0.产物中的甲缩醛转化率和DMM3-8选择性分别可达55.41%和30.87%，与纯离子液体和分子筛催化剂的反应效果相比，DMM3-8收率得到较大提高，且反应结束后催化剂和产物可自动分离为两相，可直接回收催化剂循环使用.重复使用4次后负载型分子筛催化剂仍能保持很高的活性.

关键词：离子液体，HMCM-22分子筛，固载化，聚甲醛二甲醚，催化合成

Synthesis of Poly(oxymethylene) Dimethyl Ethers Catalyzed by Immobilized Pyrrolidone Acid Ionic Liquids to Molecular Sieve

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ABSTRACT：Pyrrolidone acid ionic liquids ([Hnmp]HSO4) was immobilized on HMCM-22 molecular sieves by chemical method and used as the catalyst for the synthesis of polyoxymethylene dimethyl ethers (DMMn). The catalyst was characterized by XRD, FTIR and SEM. The results show that the pyrrolidone acid ionic liquids ([Hnmp]HSO4) can be stability immobilized on HMCM-22. The optimum reaction condition is that the catalyst amount of 2.0%(mass fraction), feed mass ratio m(DMM)/m(PF) of 2.0, reaction temperature 120 ℃ and reaction time 6 h, m(Ionic liquid)/m(HMCM-22) of 2.0. The conversion of PF and selectivity of DMM3-8 reach 55.41% and 30.87%, respectively. Compared with the reaction effects of pure ionic liquids or molecular sieve, the yield of DMM3-8 is improved quite a lot. The catalyst can be separated from product phase naturally and exhibits high stability upon reusage. It still remains high activity even after being reused for four times.

KEYWORDS：ionic liquid, HMCM-22, immobilized, polyoxymethylene dimethyl ethers (DMMn), catalyst for synthesis

成核剂对中间相炭微球性能的影响（39-44）

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摘要：以煤液化沥青为原料，炭黑、石油焦、石墨和针状焦为成核剂，在410 ℃恒温5 h条件下，采用热聚合法制备中间相炭微球，并研究四种成核剂在相同热处理条件下得到的中间相炭微球，作为锂离子电池负极材料的性能.结果表明：以炭黑和石墨为成核剂可以制备得到粒度分布均匀、表面形貌较好的中间相炭微球.由电性能测试结果可知，首次可逆容量和首次效率分别为353.9 mAh/g与92.9%和346.5mAh/g与92.6%.对比商品化中间相炭微球指标，发现以炭黑和石墨为成核剂制备得到的中间相炭微球，其性能与国内同类产品的性能相近.

关键词：成核剂，煤液化沥青，热缩聚，中间相炭微球，电性能

Effects of Nucleating Agent on Properties of Mesocarbon Microbeads

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ABSTRACT：Mesocarbon microbeads were prepared by thermal polymerization using coal liquefaction pitch as raw materials and carbon black, petroleum coke, graphite and needle coke as nucleating agents at 410 ℃ for 2 h. The properties of mesocarbon microbeads as negative electrode material for lithium ion battery were studied. Results show that with carbon black and graphite as nucleating agent, the mesocarbon microbeads with uniform particle size distribution and good surface morphology can be prepared. The results of electrical performance tests show that the initial reversible capacity and the initial efficiency of mesocarbon microbeads are 353.9 mAh/g, 92.9% and 346.5 mAh/g, 92.6% respectively. Compared with the similar products in the domestic market, the mesocarbon microbeads prepared by carbon black and graphite as the nucleating agent are similar to those of similar products in China.

KEYWORDS：nucleating agent, coal liquefaction pitch, thermal polymerization, mesocarbon microbeads, electrical performance

神木煤与黏结煤配伍制气化焦的黏结特性（45-49）

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摘要：以神木煤与黏结煤为实验对象，探究神木煤与黏结煤配伍的配比对炼焦黏结特性的影响规律以及达到完全融合状态的配煤条件.在此基础上，研究了神木煤与气煤、肥煤和焦煤配煤时，其黏结性能与wO∶wH的关系.结果表明：随神木煤配比增加，配煤黏结性变差，配煤GRI值快速下降且其实验值远低于单种煤加和计算值；在一定的神木煤配入比例内，Y值与加和计算值基本吻合；配煤wO∶wH的影响与神木煤比例的影响一致；神木煤与气煤、肥煤和焦煤配伍时，当配煤达到完全融合状态时，神木煤的最大配比分别为30%(质量分数，下同)，50%和40%，配煤Y值≥10，且神木煤与气煤、肥煤、焦煤配煤的焦渣特征指数分别大于4，5，4.

关键词：神木煤，配煤，胶质层最大厚度，黏结指数，气化焦

Caking Property of Shenmu Coal and Caking Coal Blending Coals for Coke-making

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ABSTRACT：Shenmu coal was blended with caking coal and the compatibilities of Shenmu coal in blended coal samples were explored. For this purpose, the influence of blending ratio on the coking property and the coal blending parameters in the completely bonding state of char were obtained. Meanwhite, the relationship between the wO∶wH in blended coal and the coking pro-perty were discussed. The results show that an increase in blending ratio of Shenmu coal results in a rapid decrease in the GRI value of the blending coal, and the experimental GRI value is far less than weighted GRI value, while in the Shenmu coal blending range, experimental Y value can well fit the calculated value of single coal. The effect of wO∶wH in blended coal on the caking property is in agreement with that of Shenmu coal blending ratio. In addition, in order to obtain completely bonding state coke, the largest percentage of Shenmu coal blended with gas coal, fat coal and coking coal are 30%, 50% and 40% , respectively. The Y value is equal to or bigger than 10 and the char residue characteristic index is bigger than 4, 5, 4 when Shenmu coal is blended with gas coal, fat coal and coking coal respectively.

KEYWORDS：Shenmu coal, blended coal, maximum thickness of colloidal matter layer, caking index, coke for gasification

干熄焦炉环形风道内墙损毁的应力分析与修复（50-55+62）

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摘要：根据干熄焦炉内焦炭颗粒不同堆积情况，计算了焦炭对环形风道内墙产生的横向推力，并考虑炉内循环气体流动对内墙产生的压差，耦合热应力与结构应力，采用有限元方法对环形风道内墙耐火材料应力进行仿真模拟，分析了环形风道内墙损毁的应力因素.结果表明：随冷却风量增加，环形风道内墙温度梯度变大，热应力增加；热应力为结构应力的两倍以上，是内墙耐火材料变形开裂的主要因素.为避免内墙的继续开裂与外鼓，在环形风道内安装三角支撑梁，并通过阻力计算确定了合理的闸板开度，以保持炉内热工制度的稳定.

关键词：干熄焦炉，环形风道，损毁，有限元模拟，修复

Damage Analysis from Stress and Repair of the Annular Gas Channel Inner Partition of Coke Dry Quenching

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ABSTRACT：The transverse thrust loads of the annular gas channel inner partition caused by cokes were calculated based on the different packing situation of coke particles in the coke dry quenching. Stress fields of the annular gas channel inner partition were simulated by the finite element method with considering the pressure caused by the circulate cooling gas and coupling structure and thermal. The damage of refractories was analyzed from stresses. Results show that the temperature gradients and thermal stresses of annular gas channel inner partition increase with the increase of cooling gas flow rate; thermal stress is the main factor for deformation and crack of inner partition refractory materials because it is larger more than two times of structural stress. In order to avoid the further cracking and even collapse of inner partition, triangle support beams in the annular gas channel are installed. Then the suitable openings of different outlet plates for coke dry quenching are determined based on the calculated resistances to maintain the stability of furnace thermal system.

KEYWORDS：coke dry quenching, annular gas channel, damage, finite element simulation, repair

兰炭末水蒸气活化制备活性炭过程中反应温度的影响（56-62）

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摘要：以粒度为2.0 mm～3.2 mm的兰炭末为原料，采用水蒸气高温活化法制备颗粒活性炭，研究活化温度对活性炭结构与性能的影响，阐述活化过程中活性炭孔结构的形成机理，并利用SEM和全自动吸附仪对活性炭的表面形貌、比表面积和孔结构等进行分析表征.结果表明：随着活化温度的升高，活性炭的收率持续减小，碘吸附值呈现先增大后减小的趋势.当活化温度为900 ℃时，活性炭的收率为59.81%，其碘吸附值最大可达到812.86 mg/g，BET比表面积和孔容分别为529.66 m2/g和0.298 9 cm3/g.当活化温度为600 ℃时，水蒸气活化过程以通孔作用为主导，700 ℃～800 ℃时为造孔阶段，而800 ℃～1 000 ℃范围内主要进行扩孔反应.

关键词：兰炭末，活性炭，碘吸附值，活化温度，吸附

Effects of Reaction Temperature on Preparation of Activated Carbon by Steam Activation from Blue-coke Powder

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ABSTRACT：Granular activated carbon was prepared by steam-activated high-temperature method using blue-coke powder with particle size of 2.0 mm-3.2 mm as raw material. The effects of activation temperature on the structure and properties of activated carbon were studied and the formation mechanism of pore structure of activated carbon was discussed. The surface morphology, specific surface area and pore structure of activated carbon were characterized by SEM and automatic adsorption apparatus. The results show that with the increase of the activation temperature, the yield of activated carbon continue to decrease, and the iodine adsorption value increases first and then decreases. When the activation temperature is 900 ℃, the yield of activated carbon is 59.81%, the iodine adsorption value is 812.86 mg/g, the BET specific surface area is 529.66 m2/g, and the pore volume is 0.298 9 cm3/g. The steam activation process is dominated by through-hole when the activation temperature is 600 ℃. The pore-forming stage is at 700 ℃-800 ℃, and the hole-expanding reaction is mainly carriy out at 800 ℃-1 000 ℃.

KEYWORDS：blue-coke powder, activated carbon, iodine adsorption value, activation temperature, adsorption

基于响应曲面法模拟优化褐煤腐植酸碱提工艺条件（63-68）

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摘要：通过响应曲面模型的建立，考察变量因素之间的相互作用，在减少实验操作次数的基础上，模拟优化出最佳的提取条件.选取碱提工艺中的碱液质量浓度、液固体积质量比和溶出时间作为变量因素，以腐植酸的提取率为响应值，进行了三因素三水平的Box-behnken的中心组合设计试验.结果表明：预测的最优碱提工艺条件为碱液质量浓度0.049 8 g/mL，液固体积质量比10.44 mL/g，溶出时间3.4 h；腐植酸的预测提取率为17.51%，验证实验的平均提取率为17.05%，与模型预测值相吻合.

关键词：褐煤，腐植酸，响应曲面法，工艺优化，模拟

Simulation-optimization of Alkali-extracting Process of Humic Acids from Lignite Using Response Surface Methodology

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ABSTRACT：Through establishing the response surface model, the interaction among different variables was investigated, and on the basis of reducing the operating times, the optimum extraction conditions were simulated. Taking three major factors, alkali mass concentration, liquid-solid ratio and leaching time as independent variables, the extraction rate as the response value, three factors and three levels of Box-behnken central composite test was adopted. The results show that the optimum condition as follows: alkali mass concentration is 0.049 8 g/mL, liquid-solid ratio is 10.44 mL/g, leaching time is 3.4 h and the predicted extration rate reach to 17.51%. As the experimental extration rate is 17.05%, the actual value is in a good agreement with the model predicted value.

KEYWORDS：lignite, humic acids, response surface methodology, process optimization, simulation

粉煤灰活性剂对焊缝性能的影响（69-73+80）

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摘要：进行了不同成分粉煤灰活性钨极氩弧焊实验，得到低碳钢Q235A焊接母材焊缝，利用万能试验机对焊缝的拉伸性能进行了检测，并利用静态腐蚀性能测试和电化学腐蚀性能测试对焊缝的耐蚀性进行了检测.结果表明：加入粉煤灰作活性剂得到的焊缝的抗拉强度与无粉煤灰时得到的焊缝的抗拉强度相比无大变化；对于静态腐蚀性能测试，在15% H2SO4溶液、10%NaOH溶液和3.5%NaCl溶液中，粉煤灰1活性焊缝的耐蚀性较常规焊缝的耐蚀性分别提高了1.90倍、1.29倍和1.81倍，粉煤灰2活性焊缝的耐蚀性较常规焊缝的耐蚀性分别提高1.44倍、1.20倍和1.47倍；对于电化学腐蚀性能测试，粉煤灰1活性焊缝和粉煤灰2活性焊缝的腐蚀速率均小于常规焊缝的腐蚀速率.粉煤灰作活性剂可以使材料力学性能不变，并细化焊缝显微组织，增强结构耐腐蚀性.

关键词：粉煤灰，活性钨极氩弧焊，金相组织，抗拉强度，耐蚀性能

Effects of Fly Ash on Properties of Welding Seam

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ABSTRACT：The welding seam of Q235A steel from the experiment of A-TIG (tungsten intent gas) was get, the tensile property of welding seam was checked using universal testing machine, and the corrosive property was checked through static corrosion test and electrochemical corrosion test. The results show that when fly ash is added as active agent, the weld seams have no big change in tensile strength compared with the tensile strength without surfactant; in static corrosion test, when fly ash 1 as surfactant，the corrosion resistance of the welding seam increases 1.90 times, 1.29 times and 1.81 times in 15% H2SO4, 10%NaOH and 3.5%NaCl solution than that of conventional weld seam respectively; when fly ash 2 as surfactant, the corrosion resistance of the welding seam increases 1.44 times, 1.20 times and 1.47 times in 15% H2SO4, 10%NaOH and 3.5%NaCl solution than that of conventional weld seam respectively; In electrochemical corrosion test,the corrosion rate of the active welding seam is smaller than that of conventional weld seam. The results show that adding fly ash as active agent can maintain the mechanical properties of the material and refine the microstructure to enhance the corrosion resistance.

KEYWORDS：fly ash, activating tungsten inert gas welding, microstructure, tensile strength, corrosion resistance

低温合成碳化钙的热力学分析与实验验证（74-80）

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摘要：为了降低碳化钙合成温度，研究了碳(C)和氧化钙(CaO)合成碳化钙(CaC2)过程所涉及反应的热力学，通过平衡常数法计算得到临界温度等热力学数据.计算结果表明：氧化钙与焦炭最低反应温度为氧化钙的塔曼温度(1 442 ℃)，但由于反应物浓度低，反应速度缓慢；提高反应温度至1 882 ℃，固态氧化钙可与碳反应生成碳化钙，并随着碳化钙的积累，局部产生相变，发生界面反应，表现为液态氧化钙与碳反应生成碳化钙，临界反应温度降低为1 753 ℃.继续升高温度至2 222 ℃，生成的碳化钙能自催化氧化钙与碳反应生成碳化钙，但是当氧化钙过量而碳含量不足时，生成的Ca蒸气不能及时被碳吸收，则会造成Ca的流失，降低电石品质.计算结果进一步表明：降低CO分压可大幅度降低电石的临界生成温度，当CO分压为0.01 MPa时，固态氧化钙与碳的临界反应温度可降低至1 700 ℃，此时CaC2的理论平衡摩尔分数为92.9%.不同条件下氧化钙与碳对比反应结果验证了热力学的分析，并且Ar气氛下1 620 ℃就可以合成CaC2也验证了低温合成电石的可能.

关键词：碳化钙，低温合成，热力学，理论摩尔分数，临界反应温度

Thermodynamical Analysis and Experimental Test of Calcium Carbide Synthesis

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ABSTRACT：In order to explore the possibility of the synthesis of calcium carbide at low temperature, the thermodynamics of calcium carbide synthesis from calcium oxide and carbon were studied, and the influence of reaction conditions on the CaC2 theoretical equilibrium concentration were discussed. Thermodynamic analysis results indicate that the lowest critical production temperature of CaC2 is the Taman temperature of CaO (1 442 ℃) and the reaction is very slow because of the restricted diffusion of the reactants. When the temperature is 1 882 ℃, CaC2 can be synthesized from solid CaO and C. With the increase of CaC2 content, solid CaO would change into liquid and the critical temperature of production will drop to 1 753 ℃. When the temperature is 2 222 ℃, CaC2 can act as an auto-catalyst to promote the formation of calcium carbide. When the content of CaO is excessive, the Ca vapor can not be absorbed by C in time, which can cause the loss of Ca and the quality reduction of calcium carbide. The further results show that the theoretical equilibrium molar fraction of CaC2 reaches 92.9% when the temperature is 1 700 ℃ and CO pressure is 0.01 MPa. The thermodynamic analysis is verified by the experiments and CaC2 is synthesized when the temperature is 1 620 ℃ at Ar atmosphere.

KEYWORDS：calcium carbide, low-temperature synthesis, thermodynamics, theoretical molar fraction, critical reaction temperature

两种西部煤的化学结构及加氢液化性能（1-6）

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摘要：为探究西部煤的加氢液化反应性能，对新疆淖毛湖煤和内蒙古不连沟煤在间歇高压反应釜中进行了加氢液化实验，借助固体13C-NMR和FTIR分析手段，对比研究了不同类型碳和官能团在两种煤及反应中间产物沥青质(PAA)中的分布.结果发现：淖毛湖煤的转化率和油产率分别为96.33%和47.86%，明显高于不连沟煤的转化率(76.18%)和油产率(23.44%).煤中脂肪碳和芳香碳所占比例是造成加氢液化反应转化率差异的主要因素，脂肪类和芳香类官能团的含量与反应性的关系分别呈正相关和负相关；液化油产率与原料煤中亚甲基碳和次甲基碳含量有关；与原煤相比，沥青质中的脂肪碳比例减少而芳香碳比例增加，说明脂肪碳是加氢过程中发生裂解加氢的主要活性结构.

关键词：西部煤，加氢液化，化学结构，官能团，固体核磁碳谱

Chemical Structure and Hydrogenation Liquefaction Performance of Two Kinds of Western Coal

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ABSTRACT：In order to study the hydrogenation liquefaction reactivity of western coal, liquefaction experiments of Naomaohu (NMH) coal and Bulian’gou (BLG) coal were carried out in high pressure batch autoclave. FTIR and 13C-NMR were used to study the distribution of functional groups and different kinds of carbon in the coal and the pre-asphaltene and asphaltene (PAA). The results show that the conversion rate and the oil yield of NMH is 96.33% and 47.86%, respectively, which is significantly higher than 76.18% and 23.44% of BLG. The proportion of aliphatic carbon and aromatic carbon in coal is the main factor affecting the conversion rate of hydrogenation liquefaction. The proportion of aliphatic functional groups is positively correlated with the reactivity while the proportion of aromatic functional groups has negative effect. High methylene carbon and methane carbon content are favorable to oil yield. The aliphatic carbon content in PAA is lower than that in raw coal, which indicates that the aliphatic carbon is the active structure in hydrogenation liquefaction process.

KEYWORDS：western coal, hydrogenation liquefaction, chemical structure, functional groups, 13C-NMR spectrum

钾对纤维素-煤共热解过程焦炭结构和热解特性的影响（7-13，20）

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摘要：在纤维素上负载K2SO4和K2CO3，采用热重-红外联用(TG-FTIR)对负载钾盐的纤维素与煤共热解特性进行了研究，并采用红外光谱表征了热解前后样品的化学结构.结果表明：在900 ℃热解后，焦样中含C，H，O有机官能团和高岭石的峰消失，其中有机官能团的消失与气体产物释放有关，高岭石的消失是由于热转化生成偏高岭石和石英.纤维素与煤共热解过程中发生了协同反应.钾盐的添加对共热解反应中焦炭产率、最大反应速率、反应温度区间和活化能等都有较大影响，还促进了CO和CO2的产量增加，并且使它们产生的温度区间移向低温区，其中K2CO3的作用更明显.K2SO4对酸类和酮醛类等含CO官能团的产物生成具有促进作用，而K2CO3具有抑制作用.钾盐对共热解CH4气体的生成有不同程度的抑制作用.

关键词：纤维素，TG-FTIR，共热解，钾盐，化学结构

Effect of Potassium on Char Structure and Characteristics of Co-pyrolysis of Cellulose and Coal

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ABSTRACT：K2SO4 or K2CO3 was loaded on a microcrystalline cellulose material. The co-pyrolysis characteristics of cellulose loaded with catalyst and coal were investigated by TG-FTIR, and the chemical structure of the samples before and after pyrolysis at 900 ℃ was characterized by FTIR. The FTIR results show that the absorption peaks of carbon-containing, hydrogen-containing and oxygen-containing functional groups and kaolinite disappear after pyrolysis at 900 ℃. The disappearance of organic functional groups is due to the release of gaseous products. The change of kaolinite is caused by thermal transformation into metakaolinite and quartz. Synergistic effect is observed during the co-pyrolysis of cellulose and coal. The load of potassium salt has a great influence on the char yield, the maximum reaction rate, the reaction temperature range, and the activation energy during the co-pyrolysis. The presence of potassium salt also results in an increase in CO and CO2 yields. Moreover, the temperature ranges of CO and CO2 generation shift to lower temperatures with the addition of potassium salt, particularly the K2CO3. In addition, K2SO4 has a positive effect on the evolution of products containing CO functional groups such as acids and ketals, while K2CO3 has a negative effect on it. K2CO3 and K2SO4 have different extent of negative effect on the release of CH4.

KEYWORDS：cellulose, TG-FTIR, co-pyrolysis, potassium salt, chemical structure

煤焦热解过程中产生NH3的量子化学研究（14-20）

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摘要：基于密度泛函理论和过渡态原理，使用Dmol3模块在分子水平上研究了含有吡啶型氮和吡咯型氮的Armchair和Zigzag型煤焦边缘模型热解过程中释放NH3的过程，并从能量和热力学角度分析煤焦中哪种氮的存在形式容易热解释放NH3.所涉及的基元反应均寻找到了过渡态，并得到每一步反应的活化能.通过吉布斯自由能的比较和反应能量对比发现，含有吡啶氮的煤焦模型第一步加氢吸附是放热的，而第二步加氢吸附则为吸热的；含有2-吡啶酮的吡咯氮煤焦模型氢的吸附过程是吸热的；无论是含有吡啶氮还是吡咯氮，Armchair煤焦模型相对于Zigzag煤焦模型来说更容易开环析出NH2基团；含有2-吡啶酮的吡咯氮煤焦模型相对于含有吡啶氮的煤焦模型来说更容易加氢析出NH2，进而形成NH3分子；四条反应路径中含有吡咯氮的Armchair模型最容易产生NH3.

关键词：热解，煤焦，NH3，吡啶，2-吡啶酮，量子化学

Quantum Chemistry Study on NH3 Formation in the Process of Char Pyrolysis

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ABSTRACT：Molecular modeling research based on transition state theory and density functional theory was performed to investigate the elemental reactions between hydrogen and the chars containing pyridinic-nitrogen or pyrrolic-nitrogen. Which the form of the nitrogen in char is more easily to release NH3 was studied from the point of energy and thermodynamics. The transition states of every elementary reaction were found. The enthalpy and activation energy of every step were also calculated. The results show that the first step in the hydrogenation adsorption is exothermic for Armchair and Zigzag char model containing pyridinic-nitrogen.However the second step in the hydrogenation adsorption is endothermic. As for Armchair and Zigzag char model containing 2-pyridine the hydrogen adsorption is endothermic. Whether pyridine-nitrogen or pyrrole-nitrogen, the Armchair configuration char is more easily to release NH2 than the Zigzag configuration char. Secendly the pyrrolic-nitrogen char containing 2-pyridine is more easily to release NH2 than the char model containing pyridinic-nitrogen. Finally the Armchair configuration char containing 2-pyridine is the pathway which is most easy to release NH3 in the four pathways designed in the paper. The formation of NH3 which is the NOx precursor is revealed in the paper.

KEYWORDS：pyrolysis, char, NH3, pyridinic, 2-pyridine, quantum chemistry

油溶性铁镍催化剂在煤/重油加氢共炼中的应用（21-26，33）

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摘要：以褐煤A为原料煤，以马瑞常压渣油为原料油，采用实验室合成的油溶性铁镍复合催化剂在高压釜中模拟煤/重油浆态床加氢共炼反应进行活性评价.采用XRD，SEM和TEM等表征手段分析催化剂的硫化产物及煤/重油加氢共炼体系产生的固体残渣，探究该复合催化剂与单金属催化剂之间产生活性差异的原因.结果表明：相比于油溶性单金属铁、油溶性单金属镍催化剂，油溶性铁镍复合催化剂具有更高的干基无灰煤转化率，可达87.37%.油溶性铁镍复合催化剂的硫化产物结晶度低，颗粒表面粗糙，分散度高，不仅存在铁、镍的单金属硫化物，而且形成了铁镍混晶的硫化物(Fe-Ni-S混晶).油溶性铁镍复合催化剂作用下得到的固体残渣，粒径小，结构松散，芳香度低，进一步证实油溶性铁镍复合催化剂促进了煤的深度转化.

关键词：煤/重油共炼，油溶性铁镍复合催化剂，硫化产物，干基无灰煤转化率，固体残渣

Study on Oil-soluble Iron-nickel Composite Catalyst in Coal/heavy Oil Co-processing

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ABSTRACT：A kind of lignite A and atmospheric residue from Merey were chosen as raw materials. The reaction activity of the synthesized oil-soluble iron-nickel composite catalyst in the lab were evaluated during the coal/heavy oil co-processing in a autoclave. The catalysts’ sulfides and the solid residues after the co-processing were analyzed by XRD, SEM and TEM, to explain the activity difference among the composite catalyst and the single metal catalysts. Results show that the oil-soluble iron-nickel catalyst has a higher coal conversion of 87.37%, compared with the oil-soluble single metal catalysts of iron and nickel. The sulfide of the iron-nickel composite catalyst has low crystallinity and coarse surface, forming not only the individual metal sulfides but also the iron-nickel mixed crystal sulfide (Fe-Ni-S mixed crystal). The solid residue obtained from the iron-nickel composite catalyst exhibits small particle size, loose structure, and low degree of aromaticity, which further prove the promotion for the deep conversion of coal.

KEYWORDS：coal/heavy oil co-processing, oil-soluble iron-nickel composite catalyst, sulfide, coal conversion based on dry ash-free, solid residue

低温煤焦油的制备液相分离及组分分析（27-33）

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摘要：利用制备液相技术对传统柱层析方法进行了改进，并采用正戊烷、二氯甲烷、乙酸乙酯/乙腈、甲醇四种溶剂作为流动相，实现了对霍林河褐煤650 ℃下热解产出煤焦油的不同组成的窄组分分离，利用GC-MS手段对各个分离组分进行了组成分析.结果表明，实验所用低温煤焦油以芳烃、含氧及含氮化合物为主要成分，含量分别为22.47%，31.19%和17.66%；还含有10%左右的杂多原子化合物及低于10%的烷烃和烯烃.同时各组分的组成表明，低温煤焦油的各个窄组分的分离原理是流动相按照化合物的极性及分子结构进行分组分离.

关键词：低温煤焦油，制备液相，色谱分离，GC-MS，组分分析

Preparative Liquid Chromatography Separation and Components Analysis of Low Temperature Coal Tar

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ABSTRACT：Silica-gel column chromatography was improved utilizing the preparative liquid chromatography technology with four mobile phases (n-pentane, dichloromethane, acetic ether/ethyl cyanide and methyl alcohol) to separate and quantify the group components in the low temperature coal tar (LTCT) derived from Huolinhe lignite prolysis at 650 ℃, and each eluted fraction was identified by gas chromatography-mass spectrometer (GC-MS). Results show that the main components in LTCT include aromatics, oxygen-containing and nitrogen-containing compounds, which account for 22.47%, 31.19% and 17.66% of the total mass of the LTCT, respectively. The mass fraction of polyheteromatics is approximately 10% while both the contents of alkanes and alkenes are less than 10%. The results from the LTCT components demonstrate that the improved method shows desirable performance for the separation of group components in coal-based liquid according to their polarity and molecular structures.

KEYWORDS：low temperature coal tar, preparative liquid chromatography, chromatographic separation, GC-MS, component analysis

两种细菌降解内蒙古褐煤过程及液相产物分析（34-40）

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摘要：以少动鞘脂单胞菌和红城红球菌对氧化的内蒙古褐煤(氧化煤)进行了降解实验研究.通过测定这两种细菌每天降解氧化煤后离心液相产物的pH值和降解率，发现降解率与pH值有密切的联系，当pH值在8.1~8.2之间，两种细菌均表现出较好的降解效果；当pH值大于8.4时，细菌的生物活性降低，导致氧化煤被降解效率受到抑制.少动鞘脂单胞菌和红城红球菌的最大降解率分别为50.86%和52.86%，说明这两种细菌均能有效降解氧化煤，其中红城红球菌的降解率高于少动鞘脂单胞菌的降解率.通过紫外光谱(UV)、红外光谱(IR)和气相色谱-质谱联用(GC-MS)等方法对降解的液相产物进行分析，结果表明，两种细菌对氧化煤降解的液相产物主要包含酯类和酰胺类物质.

关键词：少动鞘脂单胞菌，红城红球菌，内蒙古褐煤，气相色谱-质谱联用仪，液相产物

Degradation Process and Liquid Products Analysis of Inner Mongolia Lignite by Two Kinds of Bacteria

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ABSTRACT：Oxidized Inner Mongolia lignite was degraded by two kinds of bacteria Sphingomonas Polyaromaticivorans and Rhodococcus Erythropolis. The pH value and degradation rate of centrifugal liquid product of degradated oxidized lignite were detected every day. The results show that the degradation rate is closely related to the pH value, when the pH value is in the range of 8.1 and 8.2, both bacteria show better degradation effect, and the degradation rate is inhibited when the pH value is greater than 8.4. The degradation rates of Sphingomonas Polyaromaticivorans and Rhodococcus Erythropolis is 50.86% and 52.86%, respectively, which indicate that both of these bacteria can effectively degrade oxidized lignite, and the degradation rate of Rhodococcus Erythropolis is higher than that of Sphingomonas Polyaromaticivorans. By ultravio-let spectrum (UV), infrared spectroscopy (IR) and gas chromatography-mass spectrometry (GC-MS) techniques, the liquid products of degradation were analyzed. The results show that the liquid products of degradation mainly include esters and amides.

KEYWORDS：Sphingomonas Polyaromaticivorans, Rhodococcus Erythropolis, Inner Mongolia lignite, gas chromatography-mass spectrometry, liquid product

KOH添加量对煤基电极材料结构与性能的影响（41-47，55）

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摘要：采用KOH-HNO3联合法对自制煤基电极进行改性处理，主要研究了KOH添加量对煤基电极材料结构和吸附性能的影响.采用扫描电子显微镜(SEM)、傅立叶红外光谱(FTIR)和N2吸附法对煤基电极的形貌特征、表面官能团及孔径分布进行分析表征.研究表明：随着KOH添加量的增加，煤基电极材料的碘吸附值逐渐增大，而抗压强度与收率则逐渐减小，比表面积、总孔容和微孔孔容逐渐增大.当KOH添加量为15%(质量分数)时，碘吸附值达810.8 mg/g，抗压强度为4.47 MPa，活化收率为59.5%，比表面积为377 m2/g，总孔容为0.187 cm3/g，微孔孔容为0.160 cm3/g，微孔率达到85.56%.微孔和中孔数量及表面含氧官能团的增加，导致形成发达的蜂窝状孔结构，有利于电解液进入形成双电层结构.电化学测试表明，KOH添加量越大，煤基电极的扩散阻抗越小，比电容越大.以煤基电极为阴阳极，活性炭为粒子电极，采用三维电极体系处理氰化废水，当电压为4 V、时间为5 h时，处理后的废水中离子的去除率均达到95%以上.

关键词：KOH，煤基电极材料，改性，氰化废水，吸附性能

Effects of KOH Addition on Structure and Properties of Coal-based Electrode Materials

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ABSTRACT：Using KOH-HNO3 combined method to modify the coal-based electrode, the effects of KOH addition on the structure and adsorption properties of coal-based electrode materials were mainly studied. The appearance, surface functional group and pore size distribution were characterized by scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FTIR) and N2 absorption method. The results show that the iodine adsorption value of coal-based electrode material gradually increases, while the compressive strength and yield decrease gradually, and the specific surface area, total pore volume and pore volume increase gradually as the KOH addition increases. When the KOH addition is 15% (mass fraction), the iodine adsorption value reaches 810.8 mg/g, the compressive strength is 4.47 MPa, the activation yield is 59.5%, the specific surface area is 377 m2/g, the total pore volume is 0.187 cm3/g, the pore volume is 0.160 cm3/g, and the porosity is 85.56%. With the increase in the number of micropore, mesopore and oxygen-containing functional groups on the surface，coal-based electrode material will form a well-developed honeycomb pore structure, which is conducive to the entering of electrolyte and the formation of electric double layer structure. Electrochemical tests show that the greater the KOH addition, the smaller the diffusion resistance of the coal-based electrode, and the larger the specific capacitance. The self-made coal-based electrode materials is used as the anode and cathode, and activated carbon is used as a particle electrode to treat cyanide wastewater，when the voltage is 4 V and the time is 5 h, and the removal rates of ions in wastewater is more than 95% by three-dimensional electrode system.

KEYWORDS：KOH, coal-based electrode materials, modify, cyanide wastewater, adsorption property

高铁煤灰的黏温特性及熔渣矿物质研究（48-55）

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摘要：以七种高铁煤灰为研究对象，采用高温黏度计测试煤灰的黏温特性，按煤灰黏温特性的特征对样品进行分组，采用X射线荧光光谱仪(XRF)、X射线衍射仪(XRD)和扫描电子显微镜及能谱(SEM-EDS)研究黏温特性与熔渣矿物质的关系.结果表明：高铁煤灰存在低灰熔点高黏度现象，样品的黏温特性曲线均呈现出结晶渣或接近结晶渣的特征，且存在不同程度的波动.Fe含量与煤灰黏温曲线的波动程度有一定的关联，随着煤灰中铁钙镁比(w(Fe2O3)/w(CaO+MgO))的增加，其黏温曲线的波动增大.当铁钙镁比<0.7时，煤灰黏温曲线没有波动或波动较小；当铁钙镁比在0.7~1.0之间时，煤灰黏温曲线有一定的波动，波动主要集中在黏度值为15 Pa·s~60 Pa·s之间；当铁钙镁比>2.0时，煤灰黏温曲线有较大的波动.样品熔渣的背散射(BSE)照片表现出明暗相间部分，明暗不同的区域元素的富集程度不同.Fe和Mg主要富集于明亮区域，Si和Ca主要富集于较暗区域，Al在两种区域中均有较多分布.研究证实高铁煤灰黏温曲线波动与铁尖晶石或镁铝铁氧化物的生成有关.

关键词：高铁煤灰，熔融特性，黏温特性，结晶渣，矿物质

Study on Viscosity-temperature Characteristics and Viscosity Minernal Behaviors of High-iron Coal Ash Slag

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ABSTRACT：Seven kinds of high-iron coal ash were selected as samples. The viscosity-temperature characteristics of high-iron coal ash were tested by high-temperature rotational viscosimeter. The samples were grouped according to the viscosity-temperature characteristics of coal ash. X-ray fluorescence (XRF), X-ray diffraction (XRD) and scanning electron microscope coupled with energy dispersive spectroscopy (SEM-EDS) were adopted to study the relationship between the viscosity-temperature characteristics and slag mineral. The results indicate that although the ash melting temperatures of high-iron coal ashes employe in this study are low, their critical viscosity temperatures are oppositely high. The viscosity-temperature curves of these samples show the characteristics of crystal slag and exhibit different fluctuation. The mass fraction of iron is related to the fluctuation of coal ash viscosity-temperature curve. With the increase of the ratio of w(Fe2O3)/w(CaO+MgO), the viscosity-temperature curves of coal ashes show more obvious fluctuation, which is mainly due to the formation of hercynite or magnesium aluminium iron oxide. When the ratio of w(Fe2O3)/w(CaO+MgO) is lower than 0.7, the viscosity-temperature curve shows none/little fluctuation. When the ratio of w(Fe2O3)/w(CaO+MgO) is between 0.7 and 1.0, certain fluctuation concentrated on viscosity value from 15 Pa·s to 60 Pa·s is exhibited. When the ratio of w(Fe2O3)/w(CaO+MgO) is higher than 2.0, significant fluctuation on the viscosity-temperature curve is observed.The brightness difference of back scattered electron (BSE) images indicates the variation of element enrichment. Fe and Mg are mainly enriched in brighter area, Si and Ca are mainly enriched in darker area, and Al is detected in these two areas.

KEYWORDS：high-iron coal ash, ash fusibility, viscosity-temperature characteristics, crystal slag, mineral

负载复合金属催化剂的活性半焦脱除烟气中NO的非等温动力学研究（56-62）

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摘要：对负载复合金属催化剂的活性半焦脱除烟气中NO进行了非等温动力学研究，并对其反应机制进行了探讨.使用热重分析仪进行程序升温脱硝实验，采用Flynn-Wall-Ozawa(FWO)，Kissinger-Akahira-Sunose(KAS)和Coats-Redfen(CR)非等温动力学方法，计算纯活性半焦和负载金属催化剂的活性半焦脱硝的表观活化能.使用X射线衍射仪(XRD)对催化剂脱硝前后的金属活性相进行了分析.结果表明：在活性半焦上负载铜铁复合金属催化剂后，降低了脱硝反应的表观活化能、反应所需温度和反应能耗；当活性半焦的碳转化率≤0.3时，脱硝过程主要由化学反应控制，当碳转化率＞0.3时，脱硝过程转向扩散控制为主；通过XRD结果分析可知，金属催化剂的低价态活性相具有较高的催化活性，随着脱硝反应的进行，金属活性相被氧化成为活性较低的高价态；复合金属氧化物铁酸铜能在反应过程中分解成为活性更高的金属活性相，提高了脱硝性能.

关键词：复合金属，催化剂，活性半焦，烟气脱硝，非等温动力学

Reaction Kinetics of NO with Carbon Catalyzed by Activated-char-supported Composite Metals During Flue Gas Cleaning

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ABSTRACT：The kinetics of reaction between NO and carbon during flue gas denitrification catalyzed by activated-char-supported composite metals were investigated under non-isothermal conditions. The apparent activation energy of the catalytic denitrification reaction by activated-char was calculated using Flynn-Wall-Ozawa (FWO), Kissinger-Akahira-Sunose (KAS) and Coats-Redfern (CR) methods using TGA data. The catalyst phases before and after denitrification reaction were analyzed using X-ray diffraction (XRD). The results show that the apparent activation energy of the denitrification reaction and the reaction temperature decrease after loading of copper and iron composite metal catalysts onto chars. When the carbon conversion of the activated char is less than 0.3, the denitrification process is limited by chemical reaction rate. When the carbon conversion is higher than 0.3, the denitrification process turns to diffusion controll. During the denitrification process, the deactivation of the catalysts is caused by the oxidation of the active metal phases.

KEYWORDS：composite metals, catalyst, activated-char, flue gas denitrification, non-isothermal kinetics

活化时间对加氢半焦气化废水吸附性能的影响（63-70）

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摘要：以加氢半焦为原料，利用下落床和固定床装置，高温水蒸气活化直接制得廉价的活性焦，并对其进行高浓度和低浓度气化废水处理实验.在优化的制备条件下，分别考察了活化时间对活性焦吸附指标和废水吸附性能的影响.结果表明：随着活化时间由5 s增加到120 min，所制备活性焦的苯酚吸附值和碘值先增加后略微下降，总比表面和总孔容增加.未活化的加氢半焦吸附指标较低且废水吸附效果较差.采用下落床活化，活化时间为5 s时，活性焦吸附性能提高不明显；而采用固定床活化，活性焦吸附性能明显提高.当活化时间为90 min时，活性焦的苯酚吸附值和碘值达到最大值，分别为97 mg/L和588 mg/L，总比表面积和总孔容分别可达675.53 m2/g和0.631 2 cm3/g.当活化时间>30 min时，自制活性焦对高低浓度气化废水中COD、总磷、TOC的去除率和吸附容量与市售活性焦相近，而活化时间在30 min~120 min范围内变动导致COD、总磷、TOC的去除率和吸附容量变化范围均<5%，活化时间对高低浓度气化废水中COD、总磷、TOC的去除率和吸附容量均影响不大.

关键词：加氢半焦，活性焦，水蒸气，活化时间，气化废水，吸附

Effect of Activation Time on Performance of Hydrogenation Char for Adsorption of Gasification Wastewater

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ABSTRACT：Cheap activated coke was directly prepared by using drop-tube reactor and fixed bed reactor under optimum preparation condition with high temperature steam activated method from hydrogenation char, and was used as adsorbent to treat high and low concentration gasification wastewater. The results show that with increasing activation time from 5 s to 120 min, the adsorption for iodine and phenol adsorbance of activated coke both first increase and then decrease slightly, while the specific surface and total pore volume of activated coke increase. Hydrogenation char without activation has poor performance both in adsorption index and treatment for wastewater. Activated coke prepared by using drop-tube reactor with activation time of 5 s has not obvious change in adsorption properties, while adsorption properties of activated coke prepared by using fixed bed reactor increase obviously. When activation time is 90 min，the adsorption for iodine and phenol of activated coke reaches the highest, 97 mg/L and 588 mg/L respectively, and the specific surface and total pore volume of activated coke reach 675.53 m2/g and 0.631 2 cm3/g respectively. When activation time is more than 30 min, the activated coke has good performance on the removal rate and absorption capacity of COD, phosphorus and TOC, similar to commercially available activated coke, while with the activation time changing from 30 min to 120 min, the variation range of removal rate and absorption capacity of COD, phosphorus and TOC are less than 5%, the activation time has little influence on the removal rate and absorption capacity of COD, phosphorus and TOC.

KEYWORDS：hydrogenation char, activated coke, steam, activation time, gasification wastewater, adsorption

O2/CO2气氛下生物质三组分的燃烧特性（71-77）

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摘要：采用热重分析法对生物质三组分(纤维素、半纤维素和木质素)进行O2/CO2燃烧特性实验，分析了不同气氛(O2/N2和O2/CO2)、氧体积分数(10%，21%和40%)和升温速率(10 ℃/min，20 ℃/min和30 ℃/min)对三组分O2/CO2燃烧特性的影响.结果表明：与O2/N2气氛相比，在O2/CO2气氛下三组分燃烧过程存在不同程度的延迟，主要体现在焦炭燃烧阶段；由于木质素焦炭质量分数较高，因此其燃烧延迟相较于纤维素和半纤维素更加明显.O2/CO2气氛下，由于三组分氧含量较高，氧体积分数增大对三组分挥发分燃烧阶段影响较小；而氧体积分数增大对焦炭燃烧阶段产生了明显的影响，使其向低温区移动，综合燃烧特性明显改善.O2/CO2气氛下，升温速率增大，三组分燃烧过程整体向高温区移动；在挥发分析出燃烧阶段，纤维素与半纤维素的失重速率显著增加，在焦炭燃烧阶段，木质素失重速率显著增加；三组分综合燃烧特性得到改善.相比于纤维素与半纤维素，木质素综合燃烧特性指数较低，综合燃烧特性相对较差.

关键词：纤维素，半纤维素，木质素，O2/CO2燃烧特性，热重分析

Combustion Characteristics of Three Biomass Components in the O2/CO2 Atmosphere

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ABSTRACT：O2/CO2 combustion characteristics of cellulose and hemicellulose and lignin were studied using thermogravimetric analyzer. The influence of the combustion atmosphere (O2/CO2, O2/N2), oxygen volume fraction (10%, 21% and 40%) and heating rate (10 ℃/min, 20 ℃/min and 30 ℃/min) on O2/CO2 combustion characteristics were investigated. The results show that the three-biomass components combustion process appeare varying degrees of delay in O2/CO2 atmosphere compared that in O2/N2 atmosphere and it mainly reflects in the coke combustion stage. The lignin combustion delay is more obvious than that of cellulose and hemicellulose, due to the higher lignin coke content. In O2/CO2 atmosphere, the increase of oxygen volume fraction has less influence on volatile matter combustion, due to the high oxygen content of the three biomass components. However, there is a remarkable impact on coke combustion with the increase of oxygen volume fraction, and the coke combustion stage moves to the low temperature zone, the comprehensive combustion characteristics improve significantly. In O2/CO2 atmosphere, the combustion process of three biomass components move towards higher temperature zone with the heating rate increasing. There are significantly increasing of weight loss rate of cellulose and hemicellulose in the stage of volatile separating out; in the stage of coke combustion, the weight loss rate of lignin increase significantly. The comprehensive combustion characteristics of three biomass components improve. Compared with cellulose and hemicellulose, lignin combustion reactivity and combined combustion characteristics are relatively poor.

KEYWORDS：cellulose, hemicellulose, lignin, oxygen-enriched combustion characteristics, thermogravimetric analysis