

corresponding gases. Carbon molecular sieves with good selectivity for CO₂/CH₄ separation and showing acceptable CO₂ adsorption capacity were obtained.

06/00046 Catalytic partial oxidation of gasoline to syngas in a dense membrane reactor

Zhu, W. *et al. Catalysis Today*, 2004, 93–95, (1), 257–261.

In a previous work, it was shown that LiLaNiO/γ-Al₂O₃ was an excellent catalyst for partial oxidation of heptane to syngas in a fixed-bed reactor at high temperature and the selectivity of CO was about 93%. However, pure oxygen was used as the oxidant. The authors have developed a dense oxygen permeation membrane Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O₃ that can supply pure oxygen for the reaction. In this work, the membrane was combined with the catalyst LiLaNiO/γ-Al₂O₃ in one reactor for the partial oxidation of heptane that is typical component of gasoline. A good performance of the membrane reactor has been obtained, with 100% *n*-heptane conversion and >94% hydrogen selectivity at the optimized reaction conditions.

06/00047 CO₂ separation during hydrocarbon gasification

Lin, S. *et al. Energy*, 2005, 30, (11–12), 2186–2193.

Hydrocarbon can be gasified with steam into fuel gas, including CO, CO₂, H₂, CH₄, etc. For H₂ production, it is necessary to separate the other gases from hydrogen. In this study, hydrogen production by removal of carbon oxides during hydrocarbon gasification with CaO and other metal oxides was examined theoretically and experimentally. It was experimentally confirmed that when the hydrocarbon, water, and Ca(OH)₂ were set in a micro-autoclave at a temperature of 973 K and a pressure of 25 MPa, the only gas products were hydrogen along with a small amount of methane. CO was converted to CO₂, and CO₂ was absorbed by Ca(OH)₂ to form CaCO₃ completely. CaOSiO₂ can absorb CO₂ to form CaCO₃ under the same experimental conditions. Others such as MgO, SnO, and Fe₂O₃ were found to be unsuitable sorbents for CO₂ absorption in the gasifier at high temperature. By calcination, CaCO₃ can reform to CaO. Because the chemical energy contained in CaO can be released during hydrocarbon gasification, H₂ production efficiency as high as 70–80% can be expected.

06/00048 Fundamental studies on hydrogasification of Taiheiyu coal

Zhang, A. *et al. Energy*, 2005, 30, (11–12), 2243–2250.

Rapid hydrogasification of a Japanese Taiheiyu coal was performed in a specially developed laboratory scale batch type reactor under conditions similar to an industrial gasifier to obtain fundamental data and a comprehensive understanding of the process. The experiments were carried out at 1073 K, 7.1 MPa atmosphere, with varying reaction times from 1 to 80 s and hydrogen/coal ratio in the range of 0.05–0.30 g/g. It was found that coal conversion was promoted at a higher hydrogen/coal ratio. The amount of methane was seen to increase with reaction time, whereas most of the other products showed dynamic characteristics with maximum formation during the observed reaction time. A comparison with results of pyrolysis in helium indicated that hydrogasification is mainly composed of two steps, initial primary pyrolysis followed by secondary gas phase reactions, including hydrocracking of intermediate hydrocarbons and methanation of carbon oxides.

06/00049 Hydrogen generation from catalytic hydrolysis of sodium borohydride for proton exchange membrane fuel cells

Wu, C. *et al. Catalysis Today*, 2004, 93–95, (1), 477–483.

A novel hydrogen generation (HG) method for proton exchange membrane fuel cell (PEMFC) is developed. Carbon-supported platinum catalysts were synthesized by an impregnation method, and adopted to catalysis hydrolysis of NaBH₄ solution. These catalysts exhibit excellent hydrogen generation rates and approximate 100% efficiencies. A HG system with 100 mg 20% Pt/C catalyst has the ability to supply a 299 W PEMFC. Specific surface of the support is not a crucial factor affecting the HG performances of the catalysts, while Pt loading, Pt particle size and size distribution, and micropore structure play important roles in hydrogen generation reactions.

06/00050 Hydrogenation of 2-butyne-1,4-diol in supercritical carbon dioxide promoted by stainless steel reactor wall

Zhao, F. *et al. Catalysis Today*, 2004, 93–95, (1), 439–443.

Hydrogenation of 2-butyne-1,4-diol to 1,4-butanediol promoted by stainless steel reactor wall has been investigated in supercritical carbon dioxide (scCO₂) as well as in conventional organic solvents in the absence of catalysts at 50°C. scCO₂ was found to be an effective medium at pressures higher than supercritical region (7.3 MPa). The influence of phase behaviour, pressure and reaction time has been discussed. The first step hydrogenation of butynediol (C≡C) to

butenediol (C=C) is slower but the second-step hydrogenation of butenediol (C=C) to butanediol (C—C) is faster in scCO₂ compared with the case of ethanol.

04 BY-PRODUCTS RELATED TO FUELS

06/00051 Adsorption of cationic–anionic surfactant mixtures on activated carbon

Xiao, J.-X. *Carbon*, 2005, 43, (5), 1032–1038.

This paper reported the adsorption of cationic–anionic surfactant mixtures, such as octyltriethylammonium bromide/sodium dodecylbenzenesulfonate (OTEAB/SDBS) and dodecylpyridinium chloride/sodium octanesulfonate (DPC/SOS), on activated carbon (AC) in deionized water and in mineralized water systems. The AC surface chemistry was characterized by X-ray photoelectron spectroscopy and ζ-potential determinations. It was observed that in deionized water solution, the addition of SOS obviously promoted the adsorption of DPC, while the existence of OTEAB increased the adsorption of SDBS first and then decreased that slightly with increasing SDBS concentration. In mineralized water solution, the addition of cationic (anionic) surfactants reduced the adsorption of anionic (cationic) surfactants. It was shown that the adsorption of the surfactants on the AC was predominated mainly by the hydrophobic interaction between AC surface and surfactants because of the low oxygen content and very low z-potential on the AC surface. There might exist synergism between cationic and anionic surfactants when adsorbing on AC in deionized water due to the electrostatic interaction between oppositely charged surface active ions. Such synergism might be greatly weakened when a large number of inorganic salts exist owing to the ‘screen’ effect of the counter ions of the salt on the electrostatic attraction of oppositely charged surface active ions.

06/00052 Characterization of activated carbon fibres using argon adsorption

Nguyen, T. X. and Bhatia, S. K. *Carbon*, 2005, 43, (4), 775–785.

This paper presents the results of the internal structure (pore size and pore wall thickness distributions) of a series of activated carbon fibres with different degrees of burn-off, determined from interpretation of argon adsorption data at 87 K using infinite and finite wall thickness models. The latter approach has recently been developed in the laboratory. The results show that while the low burn-off samples have nearly uniform pore size (<0.6 nm), the pore size distribution of the high burn-off samples becomes broader, with a significant increase in proportion of larger pores. The results of pore wall thickness distribution are generally consistent with development of porosity with increasing degree of burn-off. Further they show good correspondence with X-ray diffraction.

06/00053 Dynamic adsorption of trinitrotoluene on granular activated carbon

Marinovic, V. *et al. Journal of Hazardous Materials*, 2005, 117, (2–3), 121–128.

The effects of trinitrotoluene (TNT) dynamic adsorption on granular activated carbon produced by ‘Miloje Zacic’, Serbia, are presented. The main task was to determine the conditions for TNT dynamic adsorption in order to remove the dissolved TNT from wastewater. The effects of temperature, concentration and flow rate in the chromatographic system were examined. Flow rates between 1 and 4 dm³/h were used. The heights of activated carbon in the columns were 70 and 135 mm while the diameter was 12 mm. The experiments were conducted at different temperatures (10–60°C) and TNT influent concentrations ranging from 32.76 to 171 mg/dm³ were used. The adsorption capacity of the activated carbon increased with increasing temperature, but it decreased with increasing input concentration and flow rate. The results obtained indicate that the influence of temperature is greater than was expected and the bed height and the amount of GAC used could be significantly lowered by increasing the temperature. The possibility of desorbing TNT from saturated activated carbon was also investigated. The amount of TNT adsorbed per mass unit of adsorbent was calculated using a model that optimally agreed with the experimental data.

06/00054 Effect of different oxidation treatments on the chemical structure and properties of commercial coal tar pitch

Petrova, B. *et al. Carbon*, 2005, 43, (2), 261–267.