The Effect of Pt Particle Size on the Oxidation of CO, C₃H₆, and NO Over Pt/Al₂O₃ for Diesel Exhaust Aftertreatment

Platinum-based oxidation catalysts applied for diesel exhaust aftertreatment constitute a significant part of system costs. Effective utilization of platinum is therefore relevant to reduce costs while retaining performance. To this end, the influence of Pt particle size on catalytic activity for CO, hydrocarbon, and NO oxidation was studied. 1 wt% Pt/Al₂O₃ catalysts were prepared by wet impregnation, drying, and different calcination and thermal treatments, yielding Pt particles with diameters between 1.3 and 18.7 nm, as determined by CO pulse titration and transmission electron microscopy. Activity measurements for CO, C₃H₆, and NO oxidation showed an optimal Pt particle size with respect to the mass based activity between 2 and 4 nm for all three reactions. From measured turnover frequencies and site statistics of Pt particles, the reactions appear to be mainly catalyzed by terrace atoms, which are most abundant between 2 and 4 nm. The decrease in catalytic activity for large Pt particles is therefore due to the diminishing Pt surface area, while the decrease in activity for small particles is due to the lack of terrace atoms required for CO, HC, and NO oxidation.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, PILOT PLANT, Haldor Topsoe AS
Authors: Hansen, T. K. (Intern), Høj, M. (Intern), Hansen, B. B. (Intern), Janssens, T. V. (Ekstern), Jensen, A. D. (Intern)
Pages: 1333-1344
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Topics in Catalysis
Volume: 60
Issue number: 17-18
ISSN (Print): 1022-5528
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.55 SJR 0.974 SNIP 0.878
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.945 SNIP 0.789 CiteScore 2.41
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.989 SNIP 0.862 CiteScore 2.29
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.125 SNIP 0.837 CiteScore 2.67
ISI indexed (2013): ISI indexed yes
H2CAP - Hydrogen assisted catalytic biomass pyrolysis for green fuels

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Haldor Topsoe AS
Authors: Stummann, M. Z. (Intern), Høj, M. (Intern), Gabrielsen, J. (Ekstern), Jensen, P. A. (Intern), Jensen, A. D. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Links:
http://www.sustain.dtu.dk/

Bibliographical note
Sustain Abstract E-11
Publication: Research - peer-review » Conference abstract for conference – Annual report year: 2016
Bismuth molybdate catalysts prepared by mild hydrothermal synthesis: Influence of pH on the selective oxidation of propylene

A series of bismuth molybdate catalysts with relatively high surface area was prepared via mild hydrothermal synthesis. Variation of the pH value and Bi/Mo ratio during the synthesis allowed tuning of the crystalline Bi-Mo oxide phases, as determined by X-ray diffraction (XRD) and Raman spectroscopy. The pH value during synthesis had a strong influence on the catalytic performance. Synthesis using a Bi/Mo ratio of 1/1 at pH ≥ 6 resulted in γ-Bi₂MoO₆, which exhibited a better catalytic performance than phase mixtures obtained at lower pH values. However, a significantly lower catalytic activity was observed at pH = 9 due to the low specific surface area. γ-Bi₂MoO₆ synthesized with Bi/Mo = 1/1 at pH = 6 and 7 exhibited relatively high surface areas and the best catalytic performance. All samples prepared with Bi/Mo = 1/1, except samples synthesized at pH = 1 and 9, showed better catalytic performance than samples synthesized with Bi/Mo = 2/3 at pH = 4 and 9 and γ-Bi₂MoO₆ synthesized by co-precipitation at pH = 7. At temperatures above 440 °C, the catalytic activity of the hydrothermally synthesized bismuth molybdates started to decrease due to sintering and loss of surface area. These results support that a combination of the required bismuth molybdate phase and a high specific surface area is crucial for a good performance in the selective oxidation of propylene.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Karlsruhe Institute of Technology KIT, Haldor Topsoe AS
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Pages: 1554-1573
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information

Journal: Catalysts
Volume: 5
Issue number: 3
ISSN (Print): 2073-4344
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.44 SJR 0.928 SNIP 1.217
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.076 SNIP 1.246 CiteScore 3.45
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.683 SNIP 1.074 CiteScore 2.17
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.521 SNIP 0.582
Scopus rating (2012): SJR 0.471 SNIP 0.358
Original language: English
Catalysis, Physical and Theoretical Chemistry, Acrolein, Bismuth molybdate, Effect of pH, Hydrothermal synthesis, Propylene oxidation
Electronic versions:
catalysts_05_01554.pdf
DOIs:
10.3390/catal5031554

Bibliographical note

This article belongs to the Special Issue Feature Papers to Celebrate the Landmarks of Catalysts
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Source: FindIt
Source-ID: 2281630096
Publication: Research - peer-review › Journal article – Annual report year: 2015
Systematic study on the influence of the morphology of α-MoO₃ in the selective oxidation of propylene

A variety of morphologically different α-MoO₃ samples were prepared by hydrothermal synthesis and applied in the selective oxidation of propylene. Their catalytic performance was compared to α-MoO₃ prepared by flame spray pyrolysis (FSP) and a classical synthesis route. Hydrothermal synthesis from ammonium heptamolybdate (AHM) and nitric acid at pH 1-2 led to ammonium containing molybdenum oxide phases that were completely transformed into α-MoO₃ after calcination at 550 °C. A one-step synthesis of α-MoO₃ rods was possible starting from MoO₃·2H₂O with acetic acid or nitric acid and from AHM with nitric acid at 180°C. Particularly, if nitric acid was used during synthesis, the rod-like morphology of the samples could be stabilized during calcination at 550°C and the following catalytic activity tests, which was beneficial for the catalytic performance in propylene oxidation. Characterization studies using X-ray diffraction (XRD), scanning electron microscopy (SEM) and Raman spectroscopy showed that those samples, which retained their rod-like morphology during the activity tests, yielded the highest propylene conversion.
Pyrolysis of biomass produces a high yield of condensable oil at moderate temperature and low pressure. This bio-oil has adverse properties such as high oxygen and water contents, high acidity and immiscibility with fossil hydrocarbons. Catalytic hydrodeoxygenation (HDO) is a promising technology that can be used to upgrade the crude bio-oil to fuel-grade oil. The development of the HDO process is challenged by rapid catalyst deactivation, instability of the pyrolysis oil, poorly investigated reaction conditions and a high complexity and variability of the input oil composition. However, continuous catalytic hydropyrolysis coupled with downstream HDO of the pyrolysis vapors before condensation shows promise (Figure 1). A bench scale experimental setup will be constructed for the continuous conversion of solid biomass (100 g/h) to low oxygen, fuel-grade bio-oil. The aim is to provide a proof-of-concept for the proposed process (Figure 1), to understand the reaction mechanisms of HDO, to develop highly active and durable catalysts for hydropyrolysis and HDO.
and to optimize the operating conditions; all in order to develop a sustainable production of green transportation fuels from biomass. To support the process development, the conversion of different bio-oil model compounds over a wider range of catalyst classes (reduced types, oxides, phosphides and sulfides) will be investigated. Special attention will be paid to operating conditions (e.g. temperature, \( \text{H}_2 \) partial pressure, residence time) and tolerance against water, sulfur, chlorine and potassium which are abundant in bio-oil.

**General information**

State: Published  
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Department of Mechanical Engineering, Thermal Energy, Stanford University, Haldor Topsoe AS, Karlsruhe Institute of Technology KIT  
Authors: Arndal, T. M. H. (Intern), Høj, M. (Intern), Jensen, P. A. (Intern), Jensen, A. D. (Intern), Clausen, L. R. (Intern), Grunwaldt, J. (Ekstern), Gabrielsen, J. (Ekstern), Studt, F. (Ekstern)  
Number of pages: 1  
Publication date: 2014

**Host publication information**

Title of host publication: Abstract Book - DTU Sustain Conference 2014  
Place of publication: Kgs. Lyngby  
Publisher: Technical University of Denmark (DTU)  
Main Research Area: Technical/natural sciences  
Conference: DTU Sustain Conference 2014, Lyngby, Denmark, 17/12/2014 - 17/12/2014  
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2014

Nitrene-carbene-carbene rearrangement. Photolysis and thermolysis of tetrazolo[5,1-a]phthalazine with formation of 1-phthalazinylnitrene, o-cyanophenylcarbene, and phenylcyanocarbene

1-Azidophthalazine 9A is generated in trace amount by mild FVT of tetrazolo[5,1-a]phthalazine 9T and is observable by its absorption at 2121 cm\(^{-1}\) in the Ar matrix IR spectrum. Ar matrix photolysis of 9T/9A at 254 nm causes ring opening to generate two conformers of (o-cyanophenyl) diazomethane 11 (2079 and 2075 cm\(^{-1}\)), followed by (o-cyanophenyl)carbene 312, cyanoacycloheptatetraene 13, and finally cyano(phenyl)carbene 314 as evaluated by IR spectroscopy. The two carbenes 312 and 314 were observed by ESR spectroscopy (\( D|hc = 0.5078 \), \( E|hc = 0.0236 \) and \( D|hc = 0.6488 \), \( E|hc = 0.0195 \) cm\(^{-1}\), respectively). The rearrangement of 12, 13, 14 constitutes a carbene-carbene rearrangement. 1-Phthalazinylnitrene 310 is observed by means of its UV-vis spectrum in Ar matrix following FVT of 9 above 550 C. Rearrangement to cyanophenylcarbenes also takes place on FVT of 9 as evidenced by observation of the products of ring contraction, viz., fulvenallenes and ethynylcyclopentadienes 16-18. Thus the overall rearrangement 10 \( \rightarrow \) 11 \( \rightarrow \) 12, 13, 14 can be formulated. © 2013 American Chemical Society.

**General information**

State: Published  
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, University of Queensland  
Authors: Høj, M. (Intern), Kvaskoff, D. (Ekstern), Wentrup, C. (Ekstern)  
Number of pages: 7  
Pages: 307-313  
Publication date: 2014  
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Journal of Organic Chemistry  
Volume: 79  
Issue number: 1  
ISSN (Print): 0022-3623  
Ratings:  
BFI (2017): BFI-level 2  
Web of Science (2017): Indexed Yes  
BFI (2016): BFI-level 2  
Scopus rating (2016): CiteScore 4.59 SJR 1.976 SNIP 1.03  
Web of Science (2016): Indexed yes  
BFI (2015): BFI-level 2  
Scopus rating (2015): SJR 2.018 SNIP 1.174 CiteScore 4.69  
Web of Science (2015): Indexed yes  
BFI (2014): BFI-level 2  
Scopus rating (2014): SJR 2.003 SNIP 1.222 CiteScore 4.69  
Web of Science (2014): Indexed yes  
BFI (2013): BFI-level 2
One-step synthesis of bismuth molybdate catalysts via flame spray pyrolysis for the selective oxidation of propylene to acrolein

Flame spray pyrolysis (FSP) of Bi(III)- and Mo(VI)-2-ethylhexanoate dissolved in xylene resulted in various nanocrystalline bismuth molybdate phases depending on the Bi/Mo ratio. Besides alpha-Bi2Mo3O12 and gamma-Bi2MoO6, FSP gave direct access to the metastable beta-Bi2Mo2O9 phase with high surface area (19 m(2) g(-1)). This phase is normally only obtained at high calcination temperatures (>560 degrees C) resulting in lower surface areas. The beta-phase was stable up to 400 degrees C and showed superior catalytic performance compared to alpha- and gamma-phases in selective oxidation of propylene to acrolein at temperatures relevant for industrial applications (360 degrees C).
Selective oxidation of propylene to acrolein by hydrothermally synthesized bismuth molybdates
Hydrothermal synthesis has been used as a soft chemical method to prepare bismuth molybdate catalysts for the selective oxidation of propylene to acrolein. All obtained samples displayed a plate-like morphology, but their individual aspect ratios varied with the hydrothermal synthesis conditions. Application of a high Bi/Mo ratio during hydrothermal synthesis afforded γ-Bi2MoO6 as the main phase, whereas lower initial bismuth contents promoted the formation of α-Bi2Mo3O12. Synthesis with a Bi/Mo ratio of 1:1 led to a phase mixture of α- and γ-bismuth molybdate showing high catalytic activity. The use of nitric acid during hydrothermal synthesis enhanced both propylene conversion and acrolein yield, possibly due to a change in morphology. Formation of β-Bi2Mo2O9 was not observed under the applied conditions. In general, the catalytic performance of all samples decreased notably after calcination at 550 °C due to sintering. © 2014 Elsevier B.V.
Structure, activity and kinetics of supported molybdenum oxide and mixed molybdenum-vanadium oxide catalysts prepared by flame spray pyrolysis for propane ODH

A series of molybdenum oxide (2 to 15 wt% Mo) and mixed molybdenum-vanadium oxide (4 to 15 wt% Mo and 2 wt% V) on alumina catalysts have been synthesized by flame spray pyrolysis (FSP). The materials were structurally characterized by BET surface area, X-ray diffraction (XRD), Raman and diffuse reflectance UV-vis spectroscopy and evaluated as catalysts for the oxidative dehydrogenation (ODH) of propane. The results show that samples with high specific surface areas between 122 and 182 m²/g were obtained, resulting in apparent MoOx and VOx surface densities from 0.7 to 7.7 nm⁻² and 1.5 to 1.9 nm⁻², respectively. Raman spectroscopy, UV-vis spectroscopy and XRD confirmed the high dispersion of molybdenum and vanadia species on γ-Al₂O₃ as the main crystalline phase. Only at the highest loading of 15 wt% Mo, with theoretically more than monolayer coverage, some crystalline molybdenum oxide was observed. For the mixed molybdenum-vanadium oxide catalysts the surface species were separate molybdenum oxide and vanadium oxide monomers at low loadings of molybdenum, but with increasing molybdenum loading interactions between surface molybdenum and vanadium oxide species were observed with Raman spectroscopy. The catalytic experiments showed that the most selective molybdenum oxide catalysts for the ODH reaction were those with high Mo loadings of 7 to 15 wt% Mo, while the most selective mixed molybdenum-vanadium oxide catalyst were at 4 wt% Mo, where separate surface species of molybdenum and vanadium oxide were observed by Raman spectroscopy. A simple kinetic model based on the propane ODH reaction, parallel combustion of propane and sequential combustion of propene described the experimental
results well and could be used to determine the optimal reaction conditions. © 2013 Elsevier B.V.
A series of five vanadia on alumina catalysts for oxidative dehydrogenation of propane to propene were synthesized by flame spray pyrolysis (FSP) using vanadium(III)acetylacetonate and aluminium(III)acetylacetonate dissolved in toluene as precursors. The vanadium loading was 2, 3, 5, 7.5 and 10wt.%. The catalysts were subsequently characterized by BET surface area, X-ray diffraction (XRD), Raman, UV–vis diffuse reflectance and X-ray absorption spectroscopy (XAS) as well as measurement of the catalytic performance. The catalysts had specific surface areas from 143 to 169 m²/g corresponding to average particles diameters from 9.0 to 10.9nm and apparent vanadia surface densities from 1.4 to 8.4 VOₓ/nm². The only crystalline phase detected by XRD was γ-Al₂O₃, except at 10wt.% vanadium where traces of crystalline vanadia were observed. Raman spectroscopy showed vanadia monomers at 2 and 3wt.% V (1.4 and 2.1 VOₓ/nm²), a mixture of vanadia oligomers and monomers at 5wt.% V (3.6 VOₓ/nm²) and mainly oligomers at 7.5 and 10wt.% V (6.0 and 8.4 VOₓ/nm²). Diffuse reflectance UV–vis and extended X-ray absorption fine structure (EXAFS) spectroscopy measurements supported the results of Raman spectroscopy. In situ X-ray absorption near edge structure (XANES) spectroscopy showed that the vanadia can be reduced when operating at low oxygen concentrations. The catalyst performance was determined in fixed bed reactors with an inlet gas composition of C₃H₈/O₂/N₂=5/25/70. The main products were propene, CO and CO₂, with traces of ethene and acrolein. Comparing propene selectivity as function of propane conversion the most selective catalysts were the 2 and 3wt.% V samples, which contained mostly vanadia monomers according to Raman spectroscopy. The best propene yield of 12% was obtained with the 2wt.% vanadium catalyst while the best space time yield of 0.78g-propene/(g-cat·h) at 488°C was obtained with the 3wt.% V catalyst.
Two-Nozzle Flame Spray Pyrolysis (FSP) Synthesis of CoMo/Al2O3 Hydrotreating Catalysts

Two-nozzle flame spray analysis (FSP) synthesis of CoMo/Al2O3 where Co and Al are sprayed in separate flames was applied to minimize the formation of CoAl2O4 observed in one-nozzle flame spray pyrolysis (FSP) synthesis and the materials were characterized by N2-adsorption (BET), X-ray diffraction (XRD), UV–vis diffuse reflectance spectroscopy, Raman spectroscopy, transmission electron microscopy, and catalytic performances in hydrotreating. By varying the flame mixing distances (81–175 mm) the amount of CoAl2O4 could be minimized. As evidenced by UV–vis spectroscopy, CoAl2O4 was detected only at short flame mixing distances, where the flame conditions resemble one-nozzle FSP. Raman spectroscopy revealed that β-CoMoO4 was a component of all the catalysts (in the as-prepared oxidic form) together with alumina supported MoO x surface species. The only phase detected with XRD was γ-Al2O3. The FSP synthesized oxidic catalysts were activated by sulfidation without further heat treatments. The hydrodesulfurization activity of the best two-nozzle FSP catalysts, compared to the one-nozzle FSP catalysts, improved from 75 to 91 % activity relative to a commercial reference catalyst and the hydrodenitrogenation activity improved from 70 to 90 % relative activity. This suggests that better promotion of the active molybdenum sulfide phase was achieved when using two-nozzle
FSP synthesis, probably due to less formation of the undesired phase CoAl2O4, which makes Co unavailable for promotion.

**General information**

**State:** Published  
**Organisations:** Department of Chemical and Biochemical Engineering, CHEC Research Centre, University of Bremen, Haldor Topsoe AS  
**Authors:** Høj, M. (Intern), Pham, D. K. (Ekstern), Brorson, M. (Forskerdatabase), Mädler, L. (Ekstern), Jensen, A. D. (Intern), Grunwaldt, J. (Intern)  
**Pages:** 386-394  
**Publication date:** 2013  
**Main Research Area:** Technical/natural sciences

**Publication information**

**Journal:** Catalysis Letters  
**Volume:** 143  
**Issue number:** 5  
**ISSN (Print):** 1011-372X  
**Ratings:**  
- **BFI (2017):** BFI-level 1  
- **BFI (2016):** BFI-level 1  
- **Scopus rating (2016):** CiteScore 2.39 SJR 0.733 SNIP 0.768  
- **BFI (2015):** BFI-level 1  
- **Scopus rating (2015):** SJR 0.757 SNIP 0.757 CiteScore 2.27  
- **Web of Science (2015):** Indexed yes  
- **BFI (2014):** BFI-level 1  
- **Scopus rating (2014):** SJR 0.895 SNIP 0.937 CiteScore 2.56  
- **Web of Science (2014):** Indexed yes  
- **BFI (2013):** BFI-level 1  
- **Scopus rating (2013):** SJR 0.894 SNIP 0.935 CiteScore 2.45  
- **ISI indexed (2013):** ISI indexed yes  
- **Web of Science (2013):** Indexed yes  
- **BFI (2012):** BFI-level 1  
- **Scopus rating (2012):** SJR 1.016 SNIP 0.988 CiteScore 2.35  
- **ISI indexed (2012):** ISI indexed yes  
- **Web of Science (2012):** Indexed yes  
- **BFI (2011):** BFI-level 1  
- **Scopus rating (2011):** SJR 1.07 SNIP 0.993 CiteScore 2.47  
- **ISI indexed (2011):** ISI indexed yes  
- **Web of Science (2011):** Indexed yes  
- **BFI (2010):** BFI-level 1  
- **Scopus rating (2010):** SJR 1.07 SNIP 0.792  
- **Web of Science (2010):** Indexed yes  
- **BFI (2009):** BFI-level 1  
- **Scopus rating (2009):** SJR 0.996 SNIP 0.887  
- **Web of Science (2009):** Indexed yes  
- **BFI (2008):** BFI-level 1  
- **Scopus rating (2008):** SJR 1.113 SNIP 0.858  
- **Web of Science (2008):** Indexed yes  
- **Scopus rating (2007):** SJR 1.22 SNIP 0.925  
- **Web of Science (2007):** Indexed yes  
- **Scopus rating (2006):** SJR 1.285 SNIP 0.872  
- **Web of Science (2006):** Indexed yes  
- **Scopus rating (2005):** SJR 1.263 SNIP 0.966  
- **Web of Science (2005):** Indexed yes  
- **Scopus rating (2004):** SJR 1.35 SNIP 1.058
Flame synthesised vanadium and molybdenum oxide catalysts for oxidative dehydrogenation of propane

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre
Authors: Høj, M. (Intern), Jensen, A. D. (Intern), Grunwaldt, J. (Intern)
Publication date: 2012
Event: Abstract from 15th International Congress on Catalysis, Munich, Germany.
Main Research Area: Technical/natural sciences
Electronic versions:
ICC2012_Abstract_OxDehyd_Hoj_1.pdf

Bibliographical note
Poster presentation.
Source: dtu
Source-ID: u::5603
Publication: Research › Conference abstract for conference – Annual report year: 2012

Flame synthesized vanadia catalysts for oxidative dehydrogenation of propane

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre
Authors: Høj, M. (Intern), Jensen, A. D. (Intern), Grunwaldt, J. (Intern)
Number of pages: 1
Publication date: 2012
Main Research Area: Technical/natural sciences
Electronic versions:
Nordic_abstract2012_AJrev_JDGrev_1_.pdf
Source: dtu
Source-ID: u::4084
Publication: Research › Conference abstract for conference – Annual report year: 2012

Nanoparticle synthesis using flame spray pyrolysis for catalysis

Roughly 85 to 90 % of the products from the chemical industry have been in contact with a catalyst and the production volume and financial turnover of the catalyst industry are expected to increase in the near future. This growth will be fueled by increasing demands for chemicals, new catalytic processes based on renewable feedstock, new or improved ways of preparing catalysts and a better understanding of the catalyst structure at operating conditions. This thesis explores flame spray pyrolysis (FSP) as a novel one-step preparation method for heterogeneous catalysts and investigates structure-activity-selectivity relationships. Specific catalysts studied are cobalt-molybdenum hydrotreating catalysts and vanadium and molybdenum oxide catalysts for oxidative dehydrogenation of propane (ODP). Hydrotreating is an established field in the petrochemical industry, driven by strict legislation on sulfur and nitrogen content in transportation fuels. Research is therefore performed to improve the commercial catalysts. In this thesis, FSP prepared catalysts are demonstrated to have an activity of up to
91% of a commercial reference. This is promising for a new synthesis method which has not yet been optimized. The catalysts structure was investigated by spectroscopy and electron microscopy. ODP is an exothermic, alternative process to current highly energy demanding propene production methods; however the propene selectivity is a major obstacle for commercialization. FSP prepared vanadia catalysts with low vanadium loadings gave propene yields of up to 13% at 33% propane conversion and space time yields of up to 0.88 gpropene/(gcat·h), which competes well with vanadia catalysts prepared by other methods. Kinetics of the reaction and the catalyst structure were investigated by in-situ and ex-situ by e.g. X-ray absorption and Raman spectroscopy.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre
Number of pages: 158
Publication date: 2012

Publication information
Publisher: Technical University of Denmark, Department of Chemical Engineering
ISBN (Print): 978-87-92481-96-2
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
PhD Thesis - Martin Høj, klar til trykning.pdf
Source: dtu
Source-ID: u::7363
Publication: Research › Ph.D. thesis – Annual report year: 2012

One and two flame synthesis of CoMo/Al2O3 and CoMo/Al2O3-SiO2 hydrotreating catalysts

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Haldor Topsoe AS, University of Bremen
Authors: Høj, M. (Intern), Brorson, M. (Ekstern), Pham, D. (Ekstern), Jensen, A. D. (Intern), Grunwaldt, J. (Intern)
Publication date: 2012
Event: Abstract from 15th International Congress on Catalysis, Munich, Germany.
Main Research Area: Technical/natural sciences
Bibliographical note
Poster presentation.
Source: dtu
Source-ID: u::5606
Publication: Research › Conference abstract for conference – Annual report year: 2012

CoMo/Al2O3 hydrotreating catalysts prepared by flame synthesis

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering, Haldor Topsoe AS
Authors: Høj, M. (Intern), Brorson, M. (Ekstern), Jensen, A. D. (Intern), Grunwaldt, J. (Intern)
Publication date: 2011
Event: Abstract from 10th EuropaCat Congress, Glasgow, United Kingdom.
Main Research Area: Technical/natural sciences
Electronic versions:
como.pdf
Source: orbit
Source-ID: 315579
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2011

Flame made V/Al2O3 propane oxidative dehydrogenation catalyst

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Authors: Høj, M. (Intern), Jensen, A. D. (Intern), Grunwaldt, J. (Intern)
Flame spray synthesis of CoMo/Al2O3 hydrotreating catalysts

The first alumina supported and unsupported cobalt molybdenum hydrotreating catalysts have been prepared by one-step flame spray pyrolysis (FSP) by spraying and combusting tris(acetylacetonato)aluminum, cobalt 2-ethylhexanoate and molybdenum 2-ethylhexaoate dissolved in toluene. The oxide particles produced contained varying amounts of transition metals (8, 16, 24 and 32wt.% Mo with atomic ratio Co/Mo=1/3 and 16wt.% Mo with atomic ratios Co/Mo=2/3 and 1/1) with alumina constituting the balance. In addition, an unsupported reference catalyst (atomic ratio Co/Mo=1/3) was produced. The particles obtained consisted mostly of γ-Al2O3 with some CoAl2O4, as evidenced by X-ray diffraction (XRD) and UV–vis spectroscopy. Bulk MoO3 was not detected by XRD, except at the highest molybdenum content (32wt.%) and in the unsupported sample, indicating that molybdenum is well dispersed on the surface of the support. The specific surface area as measured by nitrogen adsorption (BET) decreased from 221 to 90m2/g when going from the lowest loading supported catalyst (8wt.%) to the unsupported reference. Transmission electron microscopy (TEM) images showed that at low molybdenum loadings nanoparticle agglomerates with 5–10nm primary particles were produced. As the molybdenum loading on the alumina was increased from 8 to 32wt.% and for the unsupported reference the primary particle size increased to up to 20nm and the morphology became more irregular due to primary particle sintering and aggregation. After activation by sulfidation the activity of the catalysts were measured for the three hydrotreating reactions hydrodesulfurization, hydrodenitrogenation and hydrogenation using a model oil containing dibenzothiophene, indole and naphthalene in n-heptane solution. The best catalyst was the FSP-produced material containing 16wt.% Mo (atomic ratio Co/Mo=1/3), which did not contain crystalline MoO3 and only small amounts of CoAl2O4. The hydrotreating activity was approximately 75% of that of commercial cobalt molybdenum catalysts prepared by wet impregnation of pre-shaped alumina extrudates. Since the commercial catalyst is the product of years of development, this shows the potential of the flame spray pyrolysis technique. The Co–Mo–S phase, active for hydrotreating, is formed upon sulfidation of the flame made oxide precursor. TEM images of the spent catalysts showed that as the metal loading was increased from 8 to 32wt.% Mo the average length of supported MoS2 entities increased from 3 to 4nm (for the unsupported catalyst it was 8.5nm), while the average number of MoS2 layers per particle increased from 1.1 to 2.5. The increase in MoS2 particle size resulted in lower activity.

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering, Technical University of Denmark, Haldor Topsoe AS
Pages: 201-208
Publication date: 2011
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied Catalysis A: General
Volume: 397
Issue number: 1-2
ISSN (Print): 0926-860X
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.26 SJR 1.178 SNIP 1.311
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.203 SNIP 1.394 CiteScore 4.08
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.303 SNIP 1.574 CiteScore 4.04
Web of Science (2014): Indexed yes
Flame synthesized CoMo/Al2O3 hydrotreating catalysts

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering, Haldor Topsoe AS, Karlsruhe Institute of Technology KIT
Authors: Høj, M. (Intern), Brorson, M. (Ekstern), Jensen, A. D. (Intern), Grunwaldt, J. (Ekstern)
Publication date: 2011
Event: Abstract from 8th European Congress of Chemical Engineering, Berlin, Germany.
Main Research Area: Technical/natural sciences
Electronic versions:
flame.pdf
Characterization of Fe-zeolite catalysts for NH3-scr of NOx in diesel exhaust

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering, Department of Physics
Authors: Høj, M. (Intern), Beier, M. J. (Intern), Grunwaldt, J. (Intern), Dahl, S. (Intern)
Publication date: 2010
Main Research Area: Technical/natural sciences
Source: orbit
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2011

Nature of Active Sites of Fe-Beta Catalyst for NOx-SCR by NH3

A correlation of the reaction rate over Fe-Beta catalysts with a concentration of specific isolated Fe3+ sites represented by an ESR signal at g ≈ 4.3 and by UV adsorption bands with λmax <300 nm was observed. Blocking zeolite cationic positions with Ca2+ and investigation of "Fe-free" Beta-zeolites confirmed the idea of isolated Fe complexes in cationic positions being active sites for NH3-deNOx.
Keyword: Fe-Beta, UV-Vis, SCR, Iron zeolite, ESR, deNOx

General information
State: Published
Organisations: Zelinsky Institute of Organic Chemistry, Haldor Topsoe AS
Authors: Doronkin, D. E. (Ekstern), Stakheev, A. Y. (Ekstern), Kucherov, A. V. (Ekstern), Tolkachev, N. N. (Ekstern), Kustova, M. (Ekstern), Høj, M. (Intern), Baeva, G. N. (Ekstern), Bragina, G. O. (Ekstern), Gabrielsson, P. (Ekstern), Gekas, I. (Ekstern), Dahl, S. (Ekstern)
Pages: 1728-1733
Publication date: 2009
Main Research Area: Technical/natural sciences
Publication information
Journal: Topics in Catalysis
Volume: 52
ISSN (Print): 1022-5528
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.55 SJR 0.974 SNIP 0.878
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.945 SNIP 0.789 CiteScore 2.41
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.989 SNIP 0.862 CiteScore 2.29
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.125 SNIP 0.837 CiteScore 2.67
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.196 SNIP 0.851 CiteScore 2.49
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
The role of monomeric iron during the selective catalytic reduction of NOx by NH3 over Fe-BEA zeolite catalysts

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering, Haldor Topsoe AS
Authors: Høj, M. (Intern), Beier, M. J. (Intern), Grunwaldt, J. (Intern), Dahl, S. (Ekstern)
Pages: 166-176
Publication date: 2009
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied Catalysis B: Environmental
Volume: 93
Issue number: 1-2
ISSN (Print): 0926-3373
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 8.86 SJR 2.583 SNIP 2.12
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.26 SNIP 2.081 CiteScore 7.72
Web of Science (2015): Indexed yes

Scopus rating (2011): SJR 1.346 SNIP 0.977 CiteScore 2.89
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.492 SNIP 0.91
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.269 SNIP 0.907
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.225 SNIP 1.015
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.522 SNIP 1.382
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.59 SNIP 1.202
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.444 SNIP 1.17
Scopus rating (2004): SJR 1.374 SNIP 1.136
Scopus rating (2003): SJR 1.229 SNIP 0.915
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.233 SNIP 0.874
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.451 SNIP 1.087
Scopus rating (2000): SJR 2.482 SNIP 1.684
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.43 SNIP 1.163
Original language: English
DOIs:
10.1007/s11244-009-9327-9
Source: orbit
Source-ID: 276150
Publication: Research - peer-review › Journal article – Annual report year: 2009
Tetrathiafulvalene-functionalized triptycenes: synthetic protocols and elucidation of intramolecular Coulomb repulsions in the oxidized species

A large selection of triptycenes functionalized with tetrathiafulvalene (TTF) units as well as triptycenes containing extended TTFs as a part of the triptycene core have been synthesized utilizing new triptycene di- and tetraaldehydes as well as bis-, tetrakis- and hexakis(bromomethyl) derivatives. The largest scaffold contains a total of 12 TTFs around the central triptycene core. From spectroelectrochemical and chemical oxidation studies, we have elucidated the extent to which an increasing number of electrostatic interactions among oxidized TTF units exert an influence on the absorption characteristics.

General information
State: Published
Organisations: Academy of Sciences of the Czech Republic, University of Copenhagen
Projects:

Catalytic Cracking of Sugars for Production of Chemicals
Department of Chemical and Biochemical Engineering
Period: 01/11/2017 → 31/10/2020
Number of participants: 4
Phd Student:
Schandel, Christian Bækhøj (Intern)
Supervisor:
Høj, Martin (Intern)
Osmundsen, Christian Mårup (Intern)
Main Supervisor:
Jensen, Anker Degn (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Novel catalysts for the oxidation of methanol to formaldehyde
Department of Chemical and Biochemical Engineering
Period: 01/11/2017 → 31/10/2020
Number of participants: 4
Phd Student:
Thrane, Joachim (Intern)
Supervisor:
Høj, Martin (Intern)
Thorhauge, Max (Ekstern)
Main Supervisor:
Jensen, Anker Degn (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Hydrogen assisted catalytic biomass pyrolysis for green fuels
Department of Chemical and Biochemical Engineering
Period: 01/10/2015 → 30/09/2018
Number of participants: 5
Phd Student:
Stummann, Magnus Zingler (Intern)
Supervisor:
Høj, Martin (Intern)
Jensen, Peter Arendt (Intern)
Sundet, Jostein K. (Ekstern)
Main Supervisor:
Jensen, Anker Degn (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD
Next Generation Methanol to Formaldehyde Selective Oxidation Catalysts

Department of Chemical and Biochemical Engineering
Period: 01/10/2015 → 30/09/2018
Number of participants: 3
Phd Student:
Raun, Kristian Viegaard (Intern)
Supervisor:
Høj, Martin (Intern)
Main Supervisor:
Jensen, Anker Degn (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed
Project: PhD

New catalysts for hydrodeoxygenation of biomass pyrolysis oil

Department of Chemical and Biochemical Engineering
Period: 01/04/2014 → 27/11/2017
Number of participants: 4
Phd Student:
Dabros, Trine Marie Hartmann (Intern)
Supervisor:
Grunwaldt, Jan-Dierk (Intern)
Høj, Martin (Intern)
Main Supervisor:
Jensen, Anker Degn (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Nanoparticle synthesis using flame spray pyrolysis for catalysis

Department of Chemical and Biochemical Engineering
Period: 01/09/2009 → 28/01/2013
Number of participants: 7
Phd Student:
Høj, Martin (Intern)
Supervisor:
Elmæe, Tobias Dokkedal (Intern)
Grunwaldt, Jan-Dierk (Intern)
Main Supervisor:
Jensen, Anker Degn (Intern)
Examiner:
Fehrmann, Rasmus (Intern)
Christensen, Kurt Agerbæk (Ekstern)
Schomäcker, Reinhard (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD