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# Research on sulfidic catalysts: Match between academia and industry

F. Parlevliet, S. Eijsbouts\*

Albemarle Catalysts Company BV, Research Centre Amsterdam, Nieuwendammerkade 1-3, P.O. Box 37650, 1030BE Amsterdam, The Netherlands

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#### Abstract

A data set comprising close to 9000 scientific publications and patents published in the past 20 years has been evaluated by using specialized software (AnaVist by STN). Data like author, corporate source (university or company name), year, country and language of publication, concepts mentioned in the text, technology indicators assigned to the publication, etc. can be analyzed by using this software. Research trends such as the number of open literature and patent publications by different publishers and authors, hot and disappearing topics, topical areas of different industrial and academic institutions etc. have been evaluated in this way. The goal of this evaluation was to assess if the interest of industrial and academic research institutions for the area of catalysis by sulfides is growing, stable or declining. In addition to that, the qualitative evaluation of the present data set is also an example of how a large set of literature references can be dealt with.

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Keywords: Metal sulfides; Hydroprocessing; Literature data mining

# 1. Introduction

During the 2004 MACS-III symposium, there were several informal discussions dedicated to the future of the research in the field of catalysis by sulfides. Quite a few scientists felt that, for different reasons, the interest in this research area was disappearing. Firstly, principal scientists from a number of research institutions are near their retirement and might not be succeeded. Secondly, because the research topics lack the hot buzz words such as nano or bio, it is increasingly difficult to obtain governmental funding for research projects. Thirdly, the industry fails to provide guidance to the academic research and, consequently, the academic research topics are not of commercial interest. Because of these concerns about the future of this research area, the match between the academia and the industry has become one of the focal points of the 2007 MACS-IV symposium. To provide a solid basis for the discussions, the present paper attempts to analyze the field of industrial and academic research on catalysis by sulfides.

A data set comprising approximately 9000 scientific publications and patents published in the past 20 years has been evaluated. The primary questions to be answered are:

Are the numbers of open literature publications and patents in this area growing, stable or declining?

Are the numbers of industrial and academic research institutions active in this field growing, stable or declining?

In addition to this simple quantification, the data set is analyzed in more detail. This is done using specialized software (AnaVist by STN [1]). Data like author, corporate source (university or company name), year, country and language of publication, concepts mentioned in the text, technology indicators assigned to the publication etc. can be analyzed by using this software. Research trends over the past 20 years, e.g. hot and disappearing topics, topical areas of different industrial and academic institutions, can be assessed in this way. This qualitative evaluation of the data set not only provides basis for more extensive answer to our initial questions. In our every day struggle to handle the ever-growing stream of information made available to the scientists by the internet, it is an example of how a large set of literature references can be dealt with.

## 2. Origin of the analyzed data set

A search was performed in the Chemical Abstracts database (CAplus) on the combination of several concepts: (1) metal sulfides—and molybdenum, tungsten, nickel and cobalt sulfides in particular and (2) oil refining, hydroprocessing

<sup>\*</sup> Corresponding author. Tel.: +31 20 6347360; fax: +31 20 6347653. *E-mail address*: Sonja.Eijsbouts@Albemarle.com (S. Eijsbouts).

and sulfur and nitrogen removal. Subsequently, the number of publications was limited by only looking at publications in the last 20 years. The set was further reduced in size by removal of documents that fell outside the scope of this study. The result was a set of 8991 unique publications containing both patents and open literature. This answer set was subsequently analyzed by new STN software called AnaVist [1].

Although the search and analysis were performed with care, it can neither be excluded that some papers that conceptually fall within the set of interest were missed nor that this set contains papers that fall outside the scope of this study. The analyses were performed on data like author, corporate source (university or company name), year of publication, concepts mentioned in the text etc. Due to spelling mistakes, differences in spelling, changes of format etc., some redundancy might be present. The large number of entries in each data field, however, makes correction by hand unfeasible.

#### 2.1. Search details

The search was performed on April 20, 2007 in the Chemical Abstracts database (CAplus) using STN software. The following search strategy was used:

FILE 'REGISTRY'

- L1 S M/ELS AND S/ELS AND 2/ELC.SUB
- L2 S (W OR NI OR CO OR MO)/ELS AND S/ELS AND 2/ ELC.SUB
- L3 S NITROGEN/CN
- L4 S SULFUR/CN

FILE 'HCAPLUS'

- L5 S 7727-37-9/REM OR L3/REM
- L6 S 7704-34-9/REM OR L4/REM
- L7 S METAL? (2A) (?SULFIDE? OR ?SULPHIDE?)
- L8 S TUNGSTEN OR COBALT OR NICKEL OR MOLYB-DENUM
- L9 S (TUNGSTEN OR COBALT OR NICKEL OR MOLYBDENUM) (2A) (?SULFIDE? OR ?SULPHIDE?)
- L10 S HYDROGENATION OR HYDRIDING OR HYDRO-GENOLYSIS
- L11 S DENITROGENAT? OR DESULFURI!AT? OR DESULPHURI!AT? OR DEAROMAT?
- L12 S (L5 OR L6 OR L10 OR L11) AND (L2 OR L9) AND (REFINING OR GASOLINE OR DIESEL OR OIL OR PETROLEUM OR KEROSINE) (1,127 hits)
- L13 S HYDRODENITROGENAT?
- L14 S HYDRODESULFURI!AT? OR HYDRODESULPHUR-I!AT?
- L15 S HYDROTREAT? OR HYDROPROC? OR HYDRO-CRACK?
- L16 S (L13 OR L14 OR L15) AND (L1 OR L2 OR L7 OR L8) (11,932 hits)
- L17 S (HYDRODEAROMAT? OR HYDRODEMETAL?) AND (L2 OR L9) (43 hits)
- L18 S (C10G1-06 OR C10G45-00 OR C10G47-00 OR C10G49-00 OR C10G65-00 OR C10G67-00 OR C10G69-00)/IC (1855 hits)

- L19 S (B01J8-00 OR B01J21-00 OR B01J23-00 OR B01J27-00)/IC
- L20 S (B01J29-00 OR B01J32-00 OR B01J35-00 OR B01J37-00)/IC
- L21 S (B01J38-00 OR B01J101-00 OR B01J103-00 OR B01J105-00)/IC
- L22 S L19 OR L20 OR L21
- L23 S L22 AND (L2 OR L9 OR L11 OR L13 OR L14 OR L15 OR L17) (373 hits)
- L24 S "GROUP VIII ELEMENTS" OR "GROUP VIB ELEMENTS"
- L25 S (L13 OR L14 OR L15) AND L24 (724 hits)
- L26 S L12 OR L16 OR L17 OR L18 OR L23 OR L25 (<u>14,433</u> hits)
- L27 S L26 NOT (PHOTOLYSIS?/CT,IT OR (FLUE (W) GAS?) OR WASTEWATER OR REDUCTION/CT,IT OR REDUCTION CATALYSTS/CT,IT OR POLYMERIZATION/IT,CT OR POLYMERIZATION CATALYSTS/IT,CT OR (OXIDATIVE (A) DESULFURIZATION) OR LUMINESC?/CT,IT) (13,681 hits)

L28 S L27 AND PY.B> = 1986 (8991 hits)

A description of the search in layman's terms comes down to the following: return all articles and patents in the CAplus database that mention metal sulfides (and molybdenum, nickel, cobalt and tungsten sulfides in particular) and also one or more terms (broadly) related to hydrotreatment of petroleum. Restrict the number by only returning those articles published in or after 1986.

# 2.2. Subject analysis

The AnaVist software allows the user to perform a subject analysis and a text analysis. Subject analysis or data mining is a statistical process to analyze structured data, in this case based on indexing terms used by the Chemical Abstracts Service (CAS) to index papers and patents. These terms are part of a CAS owned thesaurus including broader terms, narrower terms and related terms. Similar papers are indexed by CAS with the same indexing terms. Text analysis is an analysis on words used in the free text (title and abstract). Very common words are excluded. This analysis is very vulnerable to spelling mistakes and inconsistent use of terms.

We chose to use the indexing terms – in AnaVist referred to as "technology indicators" – to perform most if not all of our subject analysis. As these terms are added and reviewed by experts in the field and used consistently by the CAS employees they are considered to be the most reliable. Furthermore, they constitute an independent frame of reference that excludes "home made terms", spelling mistakes, popular terms or the improper use of terms by authors.

# 2.3. Patents in hydrotreatment

For the analysis of patents published in the area of hydrotreatment as mentioned in Section 3.2, a search was performed in the CAS database on the following IPC classes:

B01J sections 8/00, 21/00, 23/00, 27/00, 29/00, 32/00, 35/00, 37/00, 38/00, 101/00, 103/00 and 105/00 in combination with the search terms hydrotreating, hydroprocessing, hydrocracking, hydrogenolysis, (hydro)desulfurization or (hydro)denitrogenation and C10G sections 1/06, 45/00, 47/00, 49/00, 65/00, 67/00 or 69/00.

## 3. Global analysis of the dataset

# 3.1. Geographical distribution

The analysis of the geographical distribution of our dataset was carried out using the corporate source, i.e. the name of the publishing university, institute or company. The number of unique corporate sources was very high (1661). So, a more detailed evaluation was limited to 338 unique sources responsible for 80% of the total number of publications. Table 1 presents the numbers of publications from different geographical areas. Asia is the top-producer of papers in this area, followed by Europe and North America. Also the average number of papers per organization is higher for Asia (28) than for Europe (16), North America (15) and South America (16). However, multinationals have the highest average (50).

The top five publishing countries are shown in Table 2. Japan and China are in the lead followed closely by the USA, France and Russia. The average number of documents per organization is approximately the same for Japan (30), China (31) and France (30) and considerably less for the USA (16) and Russia (10). Switzerland (ranking 13th) has the highest average per organization (65), all 65 publications originating from the Swiss Federal Institute of Technology (ETH).

# 3.1.1. Languages

A feeling that is often expressed for chemistry in general is that more and more papers and patents are published in journals other than the "traditional" journals and in languages other than English. The output of China is certainly rising and that does have an effect on the other languages, in which the open literature papers and patents of the present data set are published. The top-10 most important languages in this study are shown in Table 3.

Fig. 1 shows the share of the five most important languages in this data set in the past ten years. The share of Chinese

Geographical distribution of open literature and patent publications over the continents

Continent	Number of documents	Number of organizations
Asia	2630	94
Europe	1649	104
North America	950	62
South America	128	8
Africa	20	2
Oceania	12	1
Multinational	1585	32
Unspecified	417	34

Table 2 Individual countries with the highest number of open literature and patent publications

Country	Number of documents	Number of organizations
Japan	1428	48
China	935	30
USA	610	38
France	533	18
Russia	239	23

Table 3
The 10 most frequently used languages in this study

Language	Total number of publications	Percentage (%)
English	5852	65.1
Chinese	1010	11.2
Japanese	971	10.8
Russian	399	4.4
French	254	2.8
German	229	2.5
Polish	74	0.8
Spanish	69	0.8
Korean	32	0.4
Romanian	27	0.3
Total	8917	99.2

language has indeed gone up, from 4% to 14% at the expense of Japanese (down from 20% to 7%) and, to a lesser extent, Russian (down from 9% to 3%). However, the English language remains relatively stable at approximately 65%.

# 3.2. Patents versus open literature

The number of patents in this study is 3707 and the number of non-patents is 5284, the ratio between non-patents and patents being approximately 1.4. The ratio between academic sources (i.e. universities and dedicated research institutes) and industrial sources is 2.3 and the ratio of the number of academic papers to industrial papers is 1. These observations will be discussed in more detail in Section 3.3.

The five most publishing patent authorities in the studied area are, in descending order, the Japanese, the World, the Chinese, the European and the US patent office. In the open literature, most publications appear in "traditional" journals

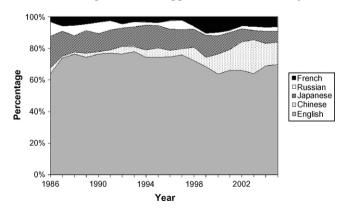


Fig. 1. The share of the five most important languages in the studied period.

Table 4
The top-15 sources in this study

	Source	Number of documents
Patent sources	Japanese Patent Office	699
	World Patent Office	550
	Chinese Patent Office	518
	European Patent Office	381
	US Patent Office	220
	Subtotal	2368
Open literature	Journal of Catalysis	347
sources	Applied Catalysis A	335
	Studies in Surface Science and Technology	267
	Preprints ACS Petroleum Division	255
	Catalysis Today	218
	Energy and Fuels	160
	Fuel	136
	Catalysis Letters	125
	Industrial and Engineering Chemistry Research	118
	Sekiyu Gakkaishi	105
	Subtotal	2066
	Total	4434

like Journal of Catalysis, Applied Catalysis A and Studies in Surface Science and Technology. The data on the top-15 sources are presented in Table 4.

An analysis of the trends for these sources shows that the World Patent Office, the US Patent Office and the Chinese Patent Office show a growth in the number of publications over the years, while the numbers of European and Japanese patents remain more or less stable (Fig. 2). The open literature sources show a more erratic output each year with big annual variations (Fig. 3). This is especially the case for sources such as Studies in Surface Science and Technology, Preprints ACS Petroleum Division and Catalysis Today, which publish symposium proceedings and/or reviews. The Journal of Catalysis and Applied Catalysis A have more stable output.

Contrary to the expectations, a strong shift from "western" sources towards "eastern" sources has not been observed. However, the top publisher in this study, the China Petroleum and Chemical Corporation, almost exclusively publishes in Chinese journals using the Chinese language (see Table 5). The

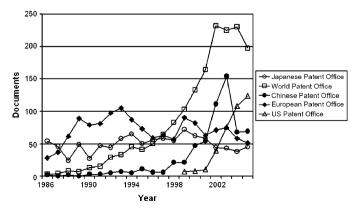


Fig. 2. Year publication trends of the five major patent issuing organizations.

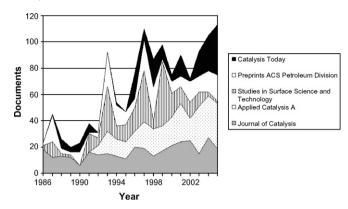


Fig. 3. Year publication trends of the five major journals.

World Patent Office is the most frequently used non-Chinese medium, in which the China Petroleum and Chemical Corporation publishes, but this only accounts for 1% of their publications.

#### 3.3. Academic versus industrial sources

Universities and dedicated research institutes together produce 47% of all publications, whereas industry accounts for 46%. The source of the remaining 5% remains unspecified. From the top-30 most publishing authors (Table 6), 25 work at academia or research institutes and 5 in industry (fully or for a part of the time). As already mentioned in Section 3.2, the ratio of publications of academic origin to those of the industrial origin is 1 and the ratio of non-patents to patents is 1.4.

The top-25 list of patent publishing organizations (Fig. 4) consists entirely of chemical companies. From this graph it is apparent that most companies publish their research results mainly in patents. With a few exceptions, most of the companies in this list publish patents only and almost nothing else.

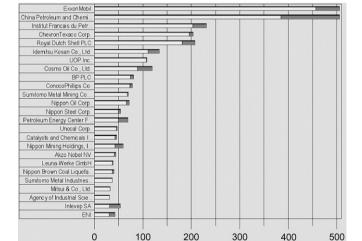
On the other hand, the top-25 list of open literature papers publishing organizations (Fig. 5) is strongly dominated by universities and research institutes. The exceptions here are the China Petroleum and Chemical Company in the 2nd position and ExxonMobil in the 14th position in this list. The academic organizations publish mostly open literature papers but hardly any patents. In fact, industry has a tendency to publish a higher percentage of their research in the open literature than academia in the patent literature. This explains why the non-patent to patent ratio is higher than the ratio of academic to industrial publications.

Table 5
The most frequently used journals and patent offices by the China Petroleum and Chemical Corporation

Journal	Percentage (%)
Chinese Patent Office	81
Gongye Cuihua	4
Cuihua Xuebao	3
Shihua Jishu Yu Yingyong	2
Shiyou Xuebao	1
World Patent Office	1

Table 6
The top-30 most publishing authors

Author	uthor Organization	
Slavik Kasztelan	IFP	126
Hiromichi Shimada	Japanese Ministry of Economy	98
Isao Mochida	Shimane University	93
Chenguang Liu	University of Petroleum	91
Akio Nishijima	University of Tokyo	88
Roel Prins	ETH	88
V H J De Beer	Eindhoven University of Technology	88
Yuji Yoshimura	Japanese Ministry of Economy	85
Michel Vrinat	CNRS	84
Toshiaki Kabe	Tokyo University of Agriculture	81
Yahua Shi	China Petroleum and Chemical Corporation	81
Michele Breysse	CNRS	78
Hong Nie	China Petroleum and Chemical Corporation	78
Rob van Veen	Shell/Eindhoven University of Technology	77
Atsushi Ishihara	Tokyo University of Agriculture	76
Bernard Delmon	Universite Catholique de Louvain	69
Nobuyuki Matsubayashi	National Chemical Laboratory for Industry	67
Guohe Que	University of East China	66
Edmond Payen	University of Lille	65
Georges Marchal	IFP	62
Kinya Sakanishi	Kyushu University,	59
Chunshan Song	Pennsylvania State University	58
Dadong Li	China Petroleum and Chemical Corporation	57
J L G Fierro	Universidad Autonoma de Madrid	56
Eric Benazzi	IFP	54
Yasuaki Okamoto	Shimane University	54
Jean Grimblot	CNRS	53
Takashi Fujikawa	COSMO Oil Co. Ltd.	50
Muneyoshi Yamada	Tohoku University	48
Jacob Moulijn	University of Amsterdam, Delft University of Technology	46



Key Organizations/Assignees

Fig. 4. The top-25 patent publishing organizations. The length of the dark-grey bar represents the total number of publications for an organization; the white bar represents the number of patents.

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Count

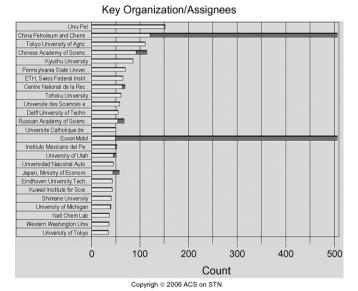


Fig. 5. The top-25 non-patent publishing organizations. The length of the dark-grey bar represents the total number of publications for an organization; the white bar represents the number of non-patents.

#### 3.3.1. Main authors

The top-30 most publishing authors, their document count and their organizations are presented in Table 6. It is apparent that the majority of the top researchers in this field works or worked at an academic or research institute when they produced the papers contained in the present data set. Only a few authors worked in the industry for the entire period or for a significant part of the studied period. Although the number of publications for each of these authors is impressive, it does not necessarily tell the whole story. The CAS database allows the registration of multiple authors for each publication and therefore it is hard to specify the "weight" of each author in this field. Furthermore, a number of the Japanese and Chinese top-authors appear less frequently in the classic catalysis journals and western patent literature but publish in Japanese and Chinese journals and patents. It is remarkable that a leading scientist in this field like Henrik Topsøe does not appear in the top-30 publishers in this study. Therefore we performed a separate search specifically on Henrik Topsøe as author. In the studied period (1986–2006) we found 50 articles that were (co)published by either Henrik Topsøe or H. Topsøe and which also mentioned concepts like hydrotreatment or related terms. Fifty publications would have put H. Topsøe in the top-30 list. However, in this study we specifically searched for hydrotreatment in combination with a metal sulfide and so only 32 out of these 50 were included in the search results. The only conclusion we can draw is that the other 18 articles were not indexed by CAS with "metal sulfide" keywords or that these keywords did not appear in the text of either title or abstract. In fact, the explicit use of certain keywords in title or abstract may strongly influence the assignment of indexing terms by CAS! Articles that are indexed specifically with the "right" keywords or which mention these keywords in title or abstract receive relatively more weight in this study and consequently their authors may end up higher in the ranking. We chose not to adapt the search strategy to avoid the possibility of obtaining large numbers of irrelevant articles. Neither did we choose to search for additional publications for a selected number of top-authors since this would probably increase bias. However, this case does show that a study like this can never be 100% complete and that the results depend strongly on the compatibility of the searcher's frame of reference and that of an author or indexer at CAS.

# 3.3.2. Top publishers

It is clear from Figs. 4 and 5 that the China Petroleum and Chemical Corporation and ExxonMobil take the absolute top position in this study. Both have published 506 papers and patents in the studied period and this is more than twice the input of the number three [Institute Francais du Petrole (IFP), 231 publications]. Therefore, the publication trends and topical areas of these two organizations were analyzed in more detail.

The China Petroleum and Chemical Corporation has not always belonged to the top-publishers in the studied area. The analysis of the top-10 most publishing organizations over the studied period shows that China Petroleum and Chemical Corporation does not appear in the top-10 before 1993. But

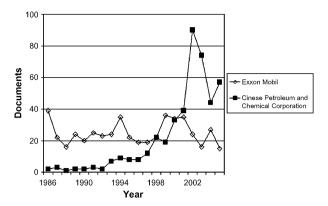


Fig. 6. Publication trends by the China Petroleum and Chemical Corporation and ExxonMobil.

from that year onwards it quickly took the first position and stayed there since 2001.

ExxonMobil shares the first place with respect to the total number of papers with the China Petroleum and Chemical Corporation though Exxon Mobil shows a much more regular output. Exxon Mobil was top-publisher in the period 1986–1997 but since then has been surpassed by China Petroleum and Chemical Corporation. Fig. 6 shows this development.

There is a clear trend towards more publications for the China Petroleum and Chemical Corporation. In fact, both the output in patents and in open literature publications have been growing, the number of patents even more so than that of non-patents. In 1986, the China Petroleum and Chemical Corporation published only two papers in the open literature on the studied subject. In 2005, the total number of publications increased to 57 and the patent to non-patent ratio had jumped to 7 (Fig. 7).

A closer look into the China Petroleum and Chemical Corporation topical areas (Table 7) shows that zeolites in general and surface area are amongst the most popular subjects if the used search terms and non-descriptive terms are omitted. The subjects that are published most frequently in open literature differ little from those in patents (Table 8). Further analysis of two subjects from the top-15 list (zeolites combined and surface area) again shows the increasing output of the China Petroleum and Chemical Corporation in the last decade (see Fig. 8).

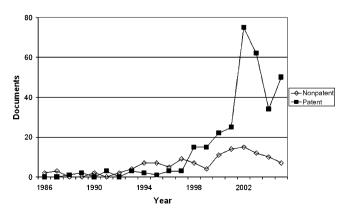


Fig. 7. Publication trends of patents and open literature for the China Petroleum and Chemical Corporation.

Table 7
The top-25 most popular subjects studied by the China Petroleum and Chemical Corporation

Petroleum hydrotreating catalysts         320           Petroleum refining catalysts         125           Hydrodesulfurization catalysts         122           Petroleum cracking catalysts         117           Diesel fuel         108           Petroleum hydrotreating         107           Petroleum refining         69           Gasoline         67           Y zeolites         66           Petroleum cracking         56           Naphtha         44           Group VIII elements         42           Hydrodesulfurization         42           Beta zeolites         41           Gas oils         40           Petroleum products         40           Petroleum refining residues         38           Hydrogenation catalysts         34           Group VIB elements         33           Zeolites         32           Surface area         31           Zeolite ZSM-5         27           Kerosene         26           Hydrocracking catalysts         25           Group VIII element oxides         24	Technology indicator	Document	
Hydrodesulfurization catalysts       122         Petroleum cracking catalysts       117         Diesel fuel       108         Petroleum hydrotreating       107         Petroleum refining       69         Gasoline       67         Y zeolites       66         Petroleum cracking       56         Naphtha       44         Group VIII elements       42         Hydrodesulfurization       42         Beta zeolites       41         Gas oils       40         Petroleum products       40         Petroleum refining residues       38         Hydrogenation catalysts       34         Group VIB elements       33         Zeolites       32         Surface area       31         Zeolite ZSM-5       27         Kerosene       26         Hydrocracking catalysts       25	Petroleum hydrotreating catalysts	320	
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Petroleum cracking         56           Naphtha         44           Group VIII elements         42           Hydrodesulfurization         42           Beta zeolites         41           Gas oils         40           Petroleum products         40           Petroleum refining residues         38           Hydrogenation catalysts         34           Group VIB elements         33           Zeolites         32           Surface area         31           Zeolite ZSM-5         27           Kerosene         26           Hydrocracking catalysts         25	Gasoline	67	
Naphtha       44         Group VIII elements       42         Hydrodesulfurization       42         Beta zeolites       41         Gas oils       40         Petroleum products       40         Petroleum refining residues       38         Hydrogenation catalysts       34         Group VIB elements       33         Zeolites       32         Surface area       31         Zeolite ZSM-5       27         Kerosene       26         Hydrocracking catalysts       25	Y zeolites	66	
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Hydrodesulfurization       42         Beta zeolites       41         Gas oils       40         Petroleum products       40         Petroleum refining residues       38         Hydrogenation catalysts       34         Group VIB elements       33         Zeolites       32         Surface area       31         Zeolite ZSM-5       27         Kerosene       26         Hydrocracking catalysts       25	Naphtha	44	
Beta zeolites       41         Gas oils       40         Petroleum products       40         Petroleum refining residues       38         Hydrogenation catalysts       34         Group VIB elements       33         Zeolites       32         Surface area       31         Zeolite ZSM-5       27         Kerosene       26         Hydrocracking catalysts       25	Group VIII elements	42	
Gas oils       40         Petroleum products       40         Petroleum refining residues       38         Hydrogenation catalysts       34         Group VIB elements       33         Zeolites       32         Surface area       31         Zeolite ZSM-5       27         Kerosene       26         Hydrocracking catalysts       25	Hydrodesulfurization	42	
Petroleum products       40         Petroleum refining residues       38         Hydrogenation catalysts       34         Group VIB elements       33         Zeolites       32         Surface area       31         Zeolite ZSM-5       27         Kerosene       26         Hydrocracking catalysts       25	Beta zeolites	41	
Petroleum refining residues       38         Hydrogenation catalysts       34         Group VIB elements       33         Zeolites       32         Surface area       31         Zeolite ZSM-5       27         Kerosene       26         Hydrocracking catalysts       25	Gas oils	40	
Hydrogenation catalysts       34         Group VIB elements       33         Zeolites       32         Surface area       31         Zeolite ZSM-5       27         Kerosene       26         Hydrocracking catalysts       25	Petroleum products	40	
Group VIB elements       33         Zeolites       32         Surface area       31         Zeolite ZSM-5       27         Kerosene       26         Hydrocracking catalysts       25	Petroleum refining residues	38	
Zeolites       32         Surface area       31         Zeolite ZSM-5       27         Kerosene       26         Hydrocracking catalysts       25	Hydrogenation catalysts	34	
Surface area       31         Zeolite ZSM-5       27         Kerosene       26         Hydrocracking catalysts       25	Group VIB elements	33	
Zeolite ZSM-5 27 Kerosene 26 Hydrocracking catalysts 25	Zeolites	32	
Kerosene 26 Hydrocracking catalysts 25	Surface area	31	
Hydrocracking catalysts 25	Zeolite ZSM-5	27	
	Kerosene	26	
Group VIII element oxides 24	•	25	
	Group VIII element oxides	24	

ExxonMobil, together with the China Petroleum and Chemical Corporation is the only company that appears in the list of 25 organizations that publish the most in open literature. In fact, it holds the 14th position (Fig. 5). The subjects ExxonMobil reported on in patents again do not differ very much from the subjects in their open literature publications (Table 9). Apart from these subjects, which are very general and non descriptive, ExxonMobil appears to have studied zeolites frequently.

The output of publications from ExxonMobil is remarkably stable in the studied period (see Fig. 9). Even when the publications are split up into patents and non-patents the output for both seems very stable. The number of non-patent publications seems to have declined but this might be a temporary phenomenon.

# 3.4. Main topics

The top-15 most frequently occurring technology indicators [1] are presented in Table 10. The terms used to define the dataset are printed in *italic* and **bold** (e.g. *hydrodesulfuriza*-

Table 8
Top-5 most important subjects for patents and non-patents for the China Petroleum and Chemical Corporation

Patent subjects	Non-patent subjects		
Petroleum hydrotreating catalysts	Petroleum hydrotreating catalysts		
Petroleum refining catalysts	Hydrodesulfurization catalysts		
Petroleum cracking catalysts	Petroleum cracking catalysts		
Hydrodesulfurization catalysts	Petroleum hydrotreating		
Diesel fuel	Diesel fuel		

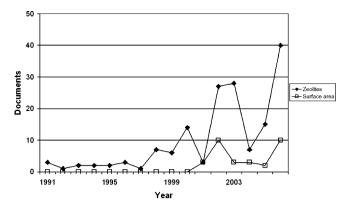


Fig. 8. Publication trends for two selected top-15 subjects of the China Petroleum and Chemical Corporation.

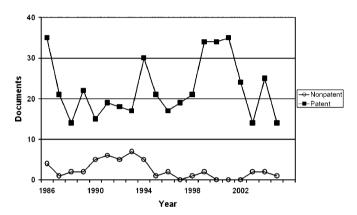


Fig. 9. Publication trends of patents and open literature for ExxonMobil.

tion, desulfurization, etc.). These terms clearly occur very frequently but are not specific enough for further topical analysis, nor are terms like Petroleum refining catalysts. Not surprisingly, the number of documents indexed with these terms is rather stable or even rising throughout the studied period (Fig. 10). So, only a few technology indicators are unambiguous and well enough defined to be suitable for further trend analysis. To these technology indicators belong coal liquefaction, sulfidation, zeolites and surface structure.

Coal liquefaction is a subject that shows strong trend sensitivity (Fig. 11). Coal liquefaction was particularly popular at the beginning of the studied period but the interest quickly disappeared around 2000. Maybe we can expect a similar pattern with terms such as "tar sands" or "biofuel" in the next 10 years if these or related terms will in fact be adopted by the Chemical Abstracts Service.

Table 9
Top-5 most important subjects for patents and non-patents for ExxonMobil

Patent subjects	Non-patent subjects
Petroleum hydrotreating catalysts	Petroleum hydrotreating catalysts
Petroleum refining	Petroleum refining catalysts
Petroleum refining catalysts	Hydrodesulfurization catalysts
Group VIII elements	Petroleum refining residues
Petroleum hydrotreating	Desulfurization catalysts

Table 10 Most frequently occurring technology indicators

Technology indicator	Number of documents	
Petroleum hydrotreating catalysts	3381	
Hydrodesulfurization catalysts	2511	
Petroleum refining catalysts	1659	
Petroleum hydrotreating	1285	
Petroleum refining	1082	
Petroleum cracking catalysts	1007	
Gas oils	941	
Hydrodesulfurization	927	
Petroleum refining residues	777	
Diesel fuel	743	
Gasoline	629	
Group VIII elements	615	
Petroleum cracking	580	
Desulfurization catalysts	570	
Zeolites	513	
Naphtha	502	
Hydrogenation catalysts	480	
Group VIB elements	457	
Coal liquefaction	400	
Sulfidation	395	
Y zeolites	380	
Petroleum products	363	
Coal liquids	343	
Hydrocracking catalysts	321	
Catalysts	315	

Zeolites, sulfidation and surface structure are of a more fundamental character than coal liquefaction and that is perhaps why the interest in those two subjects shows a relatively stable trend in the period 1986–2006. A remark should be made here though. Judging from our experience, we feel that the numbers of publications on both sulfidation and surface structure are rather low. This may be caused by synonyms that are not recognized as such. For example, sulfuration, sulfurization and sulfiding are used as synonyms for sulfidation. Furthermore, "a study into the NiMoS surface of . . ." might refer to the surface structure but is not indexed as such. Apart from browsing through a large number of articles by hand there seems to be no easy way to avoid this.

#### 3.5. Publication year trends

According to popular belief, the research on metal sulfides in hydroprocessing is becoming less attractive for the research. However, the number of all publications in this field has not dropped in recent years but has risen from 425 in 1996 to 566 publications in 2005 (Fig. 12). To correct for the general increase of the number of published open literature papers per year, the total number of papers in three journals devoted to catalysis over the past 10 years was used for comparison (Fig. 12). For the selected journals – Journal of Catalysis, Applied Catalysis A and Catalysis Today – the trend is similar to the trend observed for the studied subject. Moreover, the same trend is observed for the number of patents on catalysis in general and the number of patents on hydrotreating.

An analysis of the number of organizations and authors publishing in this field (Fig. 13) also shows an overall upward

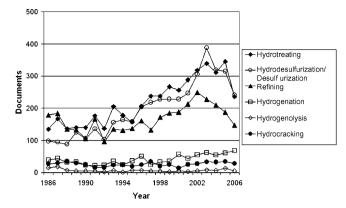


Fig. 10. Publication trends on technology indicators used for this study.

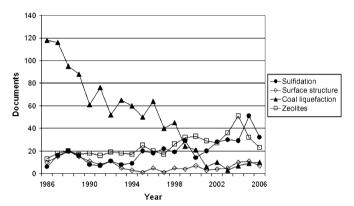


Fig. 11. Publication trends for coal liquefaction, zeolites, sulfidation and surface structure.

trend for both. Therefore, from these data it cannot be concluded that the studied area would have become less interesting.

Although the presented data show a steady increase in the number of publications, organizations and authors in this field we cannot draw any conclusions on the scientific impact of this growth. We are aware of the fact that the number of publications alone is not a correct measure of a field of research. However, it is nearly impossible to check the impact factor or citation index of each individual article/patent or author in this study by hand and the current software did not allow us to do so.

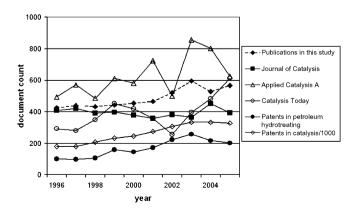


Fig. 12. Publication trends for a number of selected catalysis patents and journals.

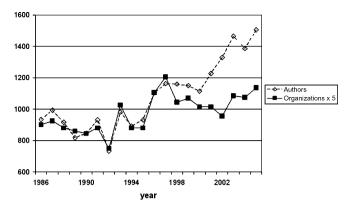


Fig. 13. Number of organizations and authors publishing on catalysis by metal sulfides.

#### 4. Discussion

# 4.1. Disappearing research groups?

While at least nine out of the top-30 most publishing authors have retired or are near their retirement, the number of authors in this study has increased (Fig. 13). As CAS allows for the registration of multiple authors for one publication, this trend does not have to mean that research in this area is growing. However, since the number of publications in this area and the number of publishing organizations are also growing (Fig. 13) there is no reason to assume that this field of research is disappearing.

There might be a side effect to the retiring principal scientists though. While the industrial groups will continue work on topics related to their core business, the research directions of the academic groups can change with a new professor. In addition to that, the academic research is very dependent on funding and therefore on governmental interest and focus.

# 4.2. Topical disconnect between academia and industry?

The top-10 most publishing organizations were analyzed with respect to the most frequently occurring research topics (as indicated by CAS). The exact search terms were excluded as

topics because while they appear frequently they are non-specific. The top four research subjects for the selected organizations are shown in Table 11.

The topics in Table 11 deviate to some extent from the most frequently occurring topics overall mentioned in Section 3.4. It seems that each company and academic institution has its own focus. Therefore, it is hard to conclude whether or not there is a disconnection between academia and industry in general. However, the data shown in Table 11 suggest that the focus of industry was on zeolites and related materials whereas academic institutes focused more on sulfidation and coal liquefaction.

An additional analysis was made of the top publishing organizations in each of the fields mentioned in Section 3.4—coal liquefaction, zeolites, sulfidation and surface structure (Table 12). This analysis reveals that 49% of the publications, published by the top organizations in coal liquefaction was of industrial origin, 39% of academic origin and 12% unknown. This roughly corresponds with the general industrial and academic share in this study. Similar trend can be found for zeolites, in which case 42% is of industrial and 53% of academic origin. Sulfidation and surface structure are subjects that appear to be studied by academia much more than by industry.

The data in Table 12 do not show a strong disconnection between industry and academia. The lower industrial share in the sulfidation and surface structure related publications is not unexpected as these two topics have a more fundamental character. However, to some extent, this can also be an effect of the different terminology used by academia and industry, i.e. due to different language used in open literature and patent publications.

### 4.3. Funding

The trends for funding of the traditional petroleum refining research can be illustrated by a number of examples. Industry R&D expenses on petroleum refining in the US are more or less stable [2], on average ca. 2.9 billion US\$/year between 2000 and 2004. (Top-3 are Pharmaceutical preparations with 37.4 billion US\$/year, Motor vehicles and car bodies with 29.3

Table 11 Most frequently occurring research topics for the top-5 publishing industrial companies and universities

Organizations	Topic <sup>a</sup>			
China Petroleum and Chemical Corporation	Y-zeolites (9)	Beta zeolites(14)	Zeolites(20)	Surface area (21)
Exxon Mobil	Lubricating oils (7)	Zeolites (8)	Beta Zeolites (11)	Zeolites ZSM-5 (13)
IFP	Zeolites (9)	Y-zeolites (11)	Clays (21)	Aluminosilicates (23)
Shell	Y-zeolites (9)	Zeolites (10)	Lubricating oils (11)	Aluminosilicates (18)
Chevron Texaco	Lubricating oils (7)	Zeolites (8)	Fischer-Tropsch reaction (19)	Silicoaluminophosphate zeolites (21)
Univ Pet	Catalyst supports (10)	Zeolite HZSM-5 (11)	Sulfidation (13)	Surface acidity (15)
Chinese Academy of Sciences	Sulfidation (6)	Zeolite MCM-41 (9)	Adsorption (10)	Zeolite HY (13)
Tokyo University of Agriculture and Technology	Sulfidation (5)	Isotope indicators (8)	Nitriding (9)	Coal liquids (14)
Kyushu University	Coal liquids (9)	Catalyst supports (11)	Zeolite HY (15)	Y-zeolites (20)
Pennsylvania State University	Zeolite MCM-41 (4)	Coal liquids (5)	Coal liquefaction catalysts (7)	Coal liquefaction (15)

<sup>&</sup>lt;sup>a</sup> Ranking in the list of topics for this company in brackets.

Table 12 Share of industry and academia in a selected number of subjects

Subject	Academic	Industrial	Unknown
Coal liquefaction	39	49	12
Zeolites	53	42	5
Sulfidation	72	22	6
Surface structure	86	8	6

billion US\$/year and Semiconductors with 15.1 billion US\$/year.) When expressed as a percentage of sales, petroleum refining is the industry sector with lowest R&D as a percentage of sales (on average only 0.32%) between 2000 and 2004. (Top-3 are Computer communication equipment with 18.5%, Prepackaged software with 17.6% and Semiconductors with 15.5%.)

The federal R&D budget for the fossil energy sector (Coal and Power, Oil, Natural gas) is relatively stable (on average 455 million US\$/year) between 2001 and 2006 [2]. However, the budget for oil related R&D has decreased from 67 million US\$/year in 2001 to only 32 million US\$/year in 2006. The requested budget for 2007 is 0. If unchanged this will have major consequences for the smaller independent producers of oil and natural gas without in-house technology development capabilities.

In Europe, a major source of energy related subsidies for R&D are the European Community Framework Programmes (FP) [3,4]. The recent European Union energy policy is based on:

- White Paper On Renewable Energy Sources (Res) (1997)
- Green Paper On Security Of Energy Supply (2000)
- Directive On Promotion Of Electricity From Res (2001)
- Green Paper On Energy Efficiency: Directive On Biofuels For Transport (2003)
- Green Paper On A European Strategy For Sustainable, Competitive And Secure Energy (2006)

The current FP7 (2007 to 2013) budget is 53.3 billion Euro with ca. 2.4 billion Euro allocated for Energy related projects. (For comparison, ca. 3.7 billion Euro is allocated for Nanotechnologies, materials and production.) The Cooperation Theme 5 - Energy should address sustainable development, security of supply, climate change and competitiveness. The objectives are: Diversified energy mix, Energy efficiency and conservation, Low carbon and less dependence on imported fuels. FP7 programs are brought about by extensive consultation of the Commission with external advisory groups, of which the European Technology Platforms (approx. 30) play a major role. The following Energy Technology Platforms exist: Hydrogen and fuel cells, Photovoltaics, Biofuels, Smart Grids, Zero-emission fossil fuel plants, Solar Thermal and Wind. The energy work program contains 94 topics in total divided over the following strategic areas: Renewables for Heating and Cooling, Renewable Electricity Generation, Renewable Fuel Production, Hydrogen and Fuel Cells, CO2 Capture and Storage, Clean coal technologies, Clean Coal, Cross-cutting actions, Smart Energy Networks, Energy Efficiency and Savings, Knowledge for Energy Policy Making and Horizontal Programme Actions. So, obviously, the traditional hydroprocessing research does not easily fit into the objectives of FP7, but the new strategic areas could offer opportunities for this excellent refinery technology.

The above examples of the trends in R&D funding show that, while the industrial R&D budgets related to fuel processing are stable, it is indeed increasingly difficult to obtain governmental funding for research in the field of conventional oil and petroleum refining.

# 5. Concluding remarks

Contrary to the general feeling, the use of metal sulfides in hydroprocessing is not a disappearing field of research. In fact, the number of publications has increased slightly, in accordance with the general rise in the number of (catalysis) papers. Both the number of organizations studying this subject and the number of authors have increased too. However, to obtain funding for research on catalysis by metals sulfides has become more difficult in the US as well as in Europe.

Academia and industry are responsible for almost equal shares in the number of publications. Academia prefers to publish the results of its research in the open literature and industry in patents. The subjects studied by both academia and industry overlap to a certain extent though each organization has its specific focus and the more fundamental subjects are mainly studied by academia.

The China Petroleum and Chemical Corporation has increased its research output remarkably in recent years. It takes a shared first position together with Exxon Mobil in the list of most publishing organizations in this study.

Most publications still appear in "classical" catalysis dedicated journals, although one Japanese journal appears in the top-15 of most popular journals. A major shift in the preferred language of publications is not observed though. English is still the language of choice with a stable share of around 65–70%. Chinese has gained influence—its share went up from approximately 4% to 14% at the expense of Japanese and Russian

Our study has uncovered the sensitivity of this type of data mining and analysis to bias. The classification of publications by the Chemical Abstracts Service (CAS) with "technology indicators" or the classification of patents with international patent codes (IPC) in combination with the chosen search strategy has a strong effect on the results. Therefore, the results of an analysis as described in this paper must always be regarded with a good deal of skepticism and conclusions can only be drawn within the frame set by all these parameters.

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- [2] Who will fund America's energy future (2006) by Interstate Oil & Gas Compact Commission, http://www.iogcc.state.ok.us/.
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