Online Technology Exchange Workshop

Innovative Refining & Petrochemicals

Abstracts

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Modeling of Asphaltene Molecular Aggregation

Masato Morimoto
Energy Process Research Institute, National Institute of Advanced Industrial Science and Technology (AIST), 16-1 Onogawa, Tsukuba 305-8569, Japan

Crude oil contains asphaltene, which is defined as a component that is insoluble in heptane or hexane and soluble in toluene. Past studies have shown that asphaltene consists of tens of thousands of heavy hydrocarbons with atoms such as nitrogen, sulfur, and oxygen, and some metals such as nickel and vanadium. Asphaltene exists as a molecular aggregate, causing serious precipitation/deposition problems in petroleum processes such as oil-well plugging in crude-oil production, fouling in pipelines, and catalyst deactivation in refineries. Therefore, it is important to know their aggregation behaviors under different conditions.

Asphaltene molecules and their aggregation behaviors are modeled by ultra-high resolution mass spectrometry with column separation methods, Rayleigh scattering measurements, small-angle X-ray scattering (SAXS) measurement, and Hansen solubility parameter (HSP) analysis. The model enables us to determine the phase distribution of each molecule and the degree of aggregation of their molecules under various conditions, which is very helpful for engineering and improving the crude oil processes.

This research was supported by the Japan Petroleum Energy Center (JPEC) as a technological development project entrusted by Ministry of Economy, Trade, and Industry.

Speaker Name	***Masato Morimoto***
Present Position	Leader, Group
Organization	National Institute of Advanced Industrial Science and Technology (AIST)
Education	3/2008: Ph.D. (Engineering), Kyoto University
Experience	4/2008-3/2010: AIST Postdoctoral Researcher, AIST 4/2010-9/2012: Researcher, AIST 10/2012-3/2019: Senior Researcher, AIST 4/2019-Current: Leader, Group, AIST Asphaltene aggregation analysis, molecular structure analysis, Hansen solubility parameter analysis, light/X-ray scattering analysis, molecular dynamic simulation, and organic synthesis of model compounds.

RDS Catalyst Design Using Petroleomics Technology

Hiroshi Shintaku

JPEC

Residue desulfurization (RDS) is one of the key processes to produce higher value products from heavy fractions and effective to improve profitability of the refinery. Japan Petroleum Energy Center (JPEC) has been developing "Petroleomics" since 2011, which enables us to evaluate detailed chemical structures of heavy oils with FT-ICR MS. As one of application targets for Petroleomics, we are challenging to design sophisticated RDS catalysts based on big data from heavy oil components.

A series of Mo/Alumina based catalysts with different characteristics (pore diameter, amount and types of additives, and Nickel/Cobalt ratio) were prepared and evaluated by using 16-fold high throughput reactors. Properties of product oils were analyzed by FT-ICR MS and correlated with catalyst characteristics by means of support vector machine (SVM).

Petroleomics analysis revealed reaction characteristics of prepared catalysts in molecular level, e.g., Nickel/Cobalt ratio and the amount of support additive affected the selectivity of hydrogenation for aromatic species in residue. The obtained results give new insights for the catalyst design strategy to reduce polyaromatic compounds, which will lead to effective reduction of Conradson carbon residue (CCR).

The application of response surface method for the rapid optimization of RDS catalyst properties will also be presented.

Speaker Name	Hiroshi Shintaku
Present Position	Associate Senior Researcher
Organization	Japan Petroleum Energy Center (JPEC) JGC Catalysts and Chemicals Ltd.
Education	Doctor of Engineering (03/2015, Tokyo Institute of Technology)
Experience	04/2015-present. Researcher, JGC Catalysts and Chemicals Ltd. 04/2018-present. Associate Senior Researcher, Japan Petroleum Energy Center (JPEC)

Kinetics of the Promotional Effects of Oil Soluble Dispersed Metal Catalysts on Slurry Phase Hydrocracking of VGO

Mohammad Mozahar Hossain

Chemical Engineering Department, KFUPM

The present research aims at investigating the promotional effects that can be attained with dual water-soluble precursors and a bimetallic oil-soluble precursor for vacuum gas oil (VGO) hydrocracking in a slurry-phase reactor. The synergistic effects of NiLTM were investigated by employing it as a cocatalyst with a commercial hydrocracking catalyst.[1] The products analysis indicated that Ni-LTM significantly decreased the coke deposition on the supported catalyst as noticed by the SEM images. The dispersed catalyst provides high hydrogenation activity because of their small sizes that are similar to reactant molecules which reduces the formation of coke and minimizes the fouling of equipment. The high surface area-to-volume ratio of the dispersed catalysts reduced the mass transfer limitations by minimizing the gradients of concentration and facilitating the reactants diffusion inside the catalyst particles.[2]

A five-lump discrete reaction scheme was found suitable for the kinetic modeling of VGO hydrocracking over the cocatalytic system. The estimated kinetic parameters show that VGO has a higher probability of being converted to naphtha than distillate, which explains the high selectivity of naphtha compared to the other pseudoproducts. The catalyst decay constant decreased with the process severity indicating an enhancement of hydrogenation by the dispersed catalysts.[1,2]

References

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Speaker Name	***M. Mozahar Hossain***
Present Position	Professor, Chemical Engineering
Organization	King Fahd University of Petroleum & Minerals
Education	Ph.D. in Chemical Engineering, Western University
Experience	08/2009-Current: Professor (Asst. - 2009; Assoc.-2014), Chemical Eng., KFUPM 09/2008-08/2009: Sr. Research Engineer, Headwaters Tech. Innovation, NJ, USA 08/2007-08/2008: Research Engineer, CREC-UWO, Canada Oxidative dehydrogenation of HC to olefins, Chemical-looping, CO_2 capture and utilization, Gasification of heavy oil/biomass, Hydrotreating of heavy oil.

Machine-learning-aided Structure Determination of Catalyst Nanostructures

Toshiaki Taniike,[a,b] Gentoku Takasao[a], Toru Wada[a,b]

[a] Graduate School of Advanced Science and Technology, Japan Advanced Institute of Science and Technology, 1-1 Asahidai, Nomi, Ishikawa 923-1292, Japan
[b] Dutch Polymer Institute (DPI), P.O. Box 902, 5600 AX Eindhoven, The Netherlands

In spite of their importance, nanostructures of practical heterogeneous catalysts are hardly elucidated by experimental means. Recent developments in computers and DFT calculations have enabled realistic simulation of complicated systems. However, the bottleneck of the computational chemistry is at the fact that computational chemistry requires a molecular model of materials as an initial structure: For complex materials like heterogeneous catalysts, the construction of molecular models relies on physicochemical inference or limited experimental clues, and inaccurate molecular models fall in wrong local minima as a result of usual geometry optimization. A method for non-empirical structure determination has been desired in this respect.

Recently, we have developed a non-empirical structure determination program, which combines a genetic algorithm for global exploration and DFT calculations for local geometry optimization. The program was successfully applied to the nanostructure of $TiCl_4/MgCl_2$ as an olefin polymerization catalyst. The structure determination clarified that the adsorption of $TiCl_4$ as a catalytically active component accompanies a reconstruction of $MgCl_2$ nanoplates, and this also causes structural diversification of the system. The latter fact is plausibly related to the distribution of polyolefins produced by Ziegler-Natta catalysts.

The work of Toshiaki Taniike and Toru Wada forms a part of the research programme of DPI, project no. 802.

Speaker Name	***Toshiaki Taniike***
Present Position	Professor
Organization	Japan Advanced Institute of Science and Technology (JAIST)
Education	3/2003: Ph.D (Science), University of Tokyo
Experience	1/2013-9/2020: Associate Professor, JAIST 10/2020-Current: Full Professor, JAIST 4/2020-Current: Director of International Excellent Core for Materials Informatics

Refining R&D activities in Saudi Aramco

Dr. Omer Refa Koseoglu

Introduction to the Refining R&D Activities in Saudi Aramco

Speaker Name	***Omer Refa Koseoglu***
Present Position	Principal Scientist
Organization	R&DC, Saudi Aramco
Education	Ph.D., University of Toronto, 1988
Experience	July 2014 - July 2016: Sr. Research Science Consultant July 2001 - July 2016: Research Science Consultant, Science Specialist July 2000 - January 2001: Staff Research Engineer, Conoco September 1995 - September 1999: Technology Specialist, IFP North America May 1991 - September 1995: Technology Specialist, HRI Inc March 1988 – May 1991: Research Engineer, Shell Canada Limited

Light Paraffinic Naphtha to BTX Aromatics over Metal-Modified Pt/ZSM-5

Ziyauddin S. Qureshi,[a] A. M. Aitani [a], M.N. Akhtar [a], H. Alasiri [a], O. Koseoglu[b], Yaming Jin[b]

[a] Center for Refining & Petrochemicals, KUPM, Dhahran 31261, Saudi Arabia

[b] R&D Center, Saudi Aramco, Dhahran 31311, Saudi Arabia

The main utilization of C5-C6 paraffinic naphtha has been as a feedstock for steam cracking (60%) plants for ethylene production and as an isomerate for gasoline blending (30%). However, currently light naphtha components find less use as gasoline blending because of their high vapor pressure and low-octane number.[1] The aromatization of light naphtha into benzene, toluene, and xylenes (BTX) aromatics has attracted interest from industry and academia because benzene and para-xylene are very important basic petrochemicals used in the production of several economic value chemicals and polymers.

The conversion of light paraffinic naphtha into BTX aromatics was conducted using 1.0 wt% Pt-M/ZSM-5 (modifier M = 1 wt% Zn, 2 wt% of Fe, La, Ga) prepared using wet-impregnation method. Our findings reveal dramatic differences in catalyst performance over the modified Pt-Ga/ZSM-5 catalyst, with aromatic selectivities enhanced by ~2-fold compared to H-ZSM-5. Collectively, this work provides new insights into the design of modified Pt-M/ZSM-5-containing zeolite catalysts for light naphtha upgrading.[2]

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Speaker Name	Ziyauddin S. Qureshi
Present Position	Research Scientist
Organization	Center for Refining & Petrochemicals, Research Institute, King Fahd University of Petroleum & Minerals (KFUPM)
Education	01/2012: PhD (Science), Institute of Chemical Technology, Mumbai, INDIA
Experience	03/2012-03/2013: Research Associate, NUS, Singapore 04/2013-04/2016: Postdoc Fellow, KAUST, Saudi Arabia 04/2017-Current: Research Scientist, Center for Refining & Petrochemicals, KFUPM, Saudi Arabia

Effects of a Matrix on Formation of Aromatic Compounds by Dehydrocyclization of *n*-Pentane Using ZnZSM-5–Al_2O_3 Composite Catalysts

Atsushi Ishihara, Kentarou Takai, Tadanori Hashimoto, Hiroyuki Nasu*

Mie University, Japan

Mesoporous alumina and Zn-exchanged ZSM-5 were combined and its effect on the activity and selectivity of aromatic compounds were investigated in dehydrocyclization of *n*-pentane. A conventional kneading method was used to prepare the composite catalysts with the weight ratios of ZnZSM-5, Al_2O_3 and a binder of 85:0:15, 75:10:15 and 65:20:15. Dehydrocyclization of *n*-pentane was performed using a fixed-bed reactor under the conditions, H_2 atmosphere and temperature range 450-550°C. ZnZSM/0A (85wt% ZnZSM-5, 0wt% Al_2O_3, 15wt% binder) exhibited the highest conversion. The selectivity for toluene and benzene increased with increasing temperature while it decreased in the order ZnZSM/10A> ZnZSM/0A> ZnZSM/20A. The result indicated that the use of mesoporous Al_2O_3 as a matrix would be very effective for this reaction and draw the maximum catalytic functions. When the reaction route was estimated from the amounts of methane, C2 and C3 fractions formed, it was proposed that active Zn species would catalyze the aromatization of olefins where benzene is formed from ethene and butene, toluene from propene and butene, and xylene from 2 molecules of butane.

Speaker Name	Atsushi Ishihara
Present Position	Professor
Organization	Mie University (2006-present time)
Education	PhD (1989, Kyoto University)
Experience	Assistant Professor (1989-1994) and Associate Professor (1994-2006) in Tokyo University of Agriculture and Technology