

Molecular Structure of Heavy Oils and Coal Liquefaction Products

12-13 April 2007, IFP-Lyon, France

FINAL PROGRAM

Tuesday 12 April

- 8.30 Registration
- 9.15 **Welcome address**
P. Ungerer, Scientific Director (IFP, France)

Session 1: Aspect of exploitation, production and upgrading of heavy and extra heavy crude oils - Influence of their molecular structure

Chairpersons: J. Ancheyta (Instituto Mexicano del Petroleo, Mexico) and L. Nabzar (IFP, France)

- 9.30 **Keynote address - New challenges for production of extra heavy oils**
P. Montaud (Total, France)
- 10.10 **Keynote address - An overview of the improved oil recovery**
S. Thomas (PERL Canada)
- 10.50 *Break*
- Chairpersons: H. Zhou (Total, France) and P. Ungerer (IFP, France)*
- 11.20 **The colloidal approach: a promising route for asphaltene deposition modelling**
L. Nabzar, M. E. Aguilera (IFP, France)
- 11.40 **Principal regularities in compositions and structures of high-molecular compounds from crude oils and natural bitumens**
A. Golovko, J. Golovko, L. Gorbunova, V. Kamyranov, G. Pevneva, T. Filimonova (Institute of Petroleum Chemistry, Russia)
- 12.00 **Molecular structure of coal extracts produced from solvent de-ashing process**
T. Takanohashi, T. Shishido, I. Saito (National Institute of Advanced Industrial Science and Technology, Japan)
- 12.20 **Mechanisms of catalytic activity in heavily coated hydrocracking catalysts**
M. Millan, C. Adell, C. Hinojosa, A. A. Herod, R. Kandiyoti (Imperial College London, UK)
- 12.40 *Lunch*

Chairpersons: J. M. Shaw (University of Alberta, Canada) and H. Toulhoat (IFP, France)

- 14.10 **Challenges of modelling steam cracking of heavy feedstocks**
K. Van Geem, M. F. Reyniers, G. B. Marin (Ghent University, Belgium)
- 14.30 **Five-lump kinetic model for moderate hydrocracking of Maya crude oil**
S. Sanchez (Instituto Mexicano del Petroleo, Mexico), J. Ancheyta (Instituto Mexicano del Petroleo, ESIQIE-IPN, Mexico)
- 14.50 **Kinetic modelling of fixed bed residue hydrotreating**
K. Le Lannic, I. Guibard, J. Verstraete (IFP, France)
- 15.10 **An attempt to characterize the evolution of asphaltene structure during hydroconversion conditions**
I. Merdrignac, P. Danial-Fortain, A. A. Quoineaud, T. Gauthier (IFP, France)
- 15.30 *Break*

Session 2 - Part I: Chemical characterization of heavy oils and coal liquids

Chairpersons: O. R. Koseoglu (Saudi Aramco, Saudi Arabia) and J. Lynch (IFP, France)

- 16.00 **Keynote address - Chemical characterization of heavy fractions: modern approaches involving the combined use of multidimensional NMR and ultra-high resolution mass spectrometry**
P. G. Hatcher (Old Dominion University, USA), F. Behar, F. Lorant, E. Salmon (IFP, France)
- 16.40 **Applications and potential of fluorescence detection by intensity changes (FDIC) to the characterization of fossil fuel-derived products**
V. L. Cebolla (Instituto de Carboquimica, Spain), M. Matt (Université de Metz, France), M. P. Domingo (CNTA, Spain), E. M. Galvez, E. Mateos, L. Membrado (Instituto de Carboquimica, Spain), F. P. Cossio (Universidad des Pais Vasco, Spain), J. Vela (Universidad de Zaragoza, Spain)
- 17.00 **Molecular structure of hydrocarbon resources, a combined experimental and theoretical approach: QM calculations, spectroscopy, low temperature calorimetry**
V. Lastovka (University of Alberta, Canada), K. H. Michaelian (Natural Resources Canada), K. Schmidt (DK3 Scientific, Canada), J. M. Shaw (University of Alberta, Canada)
- 17.20 **Aggregation behavior of ultra-heavy component of coal extract**
M. Iino (National Institute of Advanced Industrial Science and Technology, Japan)
- 17.40 **Poster Session**
- 18.45 *Cocktail*

Friday 13 April

8.30 Registration

Session 2 - Part II: Chemical characterization of heavy oils and coal liquids

Chairpersons: O. C. Mullins (Schlumberger, USA) and I. Merdrignac (IFP, France)

- 9.00 **Keynote address - Recent advances in the characterization of heavy petroleum by FT-ICR mass spectrometry**
R. P. Rodgers, D. F. Smith, J. M. Purcell, P. Juyal, K. Do-Gyun, A. G. Marshall (Florida State University, USA)
- 9.40 **Overview of sulfur speciation in carbonaceous materials such as coal, kerogens and asphaltenes**
S. Mitra-Kirtley (Rose Hulman Institute of Technology, USA), O. C. Mullins (Schlumberger, USA)
- 10.00 **Comparing the pentane-soluble and toluene-soluble fractions of a petroleum residue and several coal derived liquids by size exclusion chromatography and UV-fluorescence spectrometry**
F. Karaca, M. Millan-Agorio, T. J. Morgan, **A. A. Herod**, R. Kandiyoti (Imperial College London, UK)
- 10.20 **Characterization of hydrocracking unit feedstocks by Fourier Transform Ion Cyclotron Resonance Mass Spectrometry**
A. A. Ai-Hajji, H. Muller, **O. R. Koseoglu** (Saudi Aramco, Saudi Arabia)
- 10.40 *Break*

Session 3: Colloidal structure characterization of heavy and extra heavy oils

Chairpersons: J. Buckley (PRRC, USA) and D. Espinat (IFP, France)

- 11.00 **Keynote address - The structure of oil reservoirs and the colloidal structure of crude oil**
O. C. Mullins (Schlumberger, USA)
- 11.40 **Keynote address - Asphaltene stability and precipitation and the asphaltenes-resins interaction**
G. Gonzalez (Petrobras Research Center, Brazil)
- 12.20 **Solution properties of asphaltenes**
L. Barré, S. Simon, T. Palermo (IFP, France)
- 12.40 **Nano fluidics of bitumens and heavy oil**
B. Zhao, M. G. Chodakowski, M. A. Hasan, M. Fulem, F. Lange, **J. M. Shaw** (University of Alberta, Canada)
- 13.00 *Lunch*

Chairpersons: R. P. Rodgers (Florida State University, USA) and T. Palermo (IFP, France)

- 14.30 **Small Angle Neutron Scattering (SANS) studies of asphaltene nanostructure: aggregate shape, solvent entrainment and emulsion films**
V. Verruto, Gawrys, P. Kilpatrick (North Carolina State University, USA)
- 14.50 **The effect of the molecular topologies on the aggregation of asphaltenes of the archipelago type**
J. Murgich (C. de Quimica, Venezuela), O. P. Strausz (University of Alberta, Canada)
- 15.10 **Influence of asphaltenes on heavy oil flow properties: viscosity, thermal and pressure dependence, foaminess**
I. Hénaut, P. Abivin, J. F. Argillier (IFP, France), M. Moan (UBO, France)
- 15.30 **Pulse ¹H-NMR study on the relaxation behaviors of asphaltene aggregates**
H. Kumagai (Hokkaido University, Japan), R. Tanaka, E. Sato (Idemitsu Kosan Co., Japan), T. Takanoashi, S. Sato (AIST, Japan)
- 15.50 *Break*

Chairpersons: P. Kilpatrick (North Carolina State University, USA) and L. Barré (IFP, France)

- 16.20 **Separation rate of an asphaltene-rich phase near the onset of instability**
J. Buckley (PRRC, USA), J. Wang, J. Creek (Chevron Energy Technology, USA)
- 16.40 **A SANS study of the adsorbed asphaltene layer in water in hydrocarbon emulsions**
J. Jestin (CEA Saclay, France), S. Simon, T. Palermo, L. Barré (IFP, France)
- 17.00 **Destabilisation of water-in-crude oil emulsions by silicone copolymer demulsifiers**
D. Daniel-David, I. Pezron (Université de Technologie de Compiègne, France), C. Dalmazzone, C. Noik, L. Barré (IFP, France), L. Komunjer (Université de Technologie de Compiègne, France)
- 17.20 **Phase transitions in asphaltenes using Temperature Modulated Differential Scanning Calorimetry (TMDSC)**
Y. Maham, K. Tran, J. W. Shaw (University of Alberta, Canada)
- 17.40 **Closing address**
D. Espinat (IFP, France)

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