

## Preface



The present issue of *Catalysis Today* is, once again, devoted to sulfidic catalysts. The papers included here are based on contributions to the 4th International Symposium on Molecular Aspects of Catalysis by Sulfides (MACS-IV), held on 13–17 May 2007, in The Netherlands. There, six keynote lectures, 26 oral presentations, and 28 posters were presented, the number of participants being 108. The generous financial support of Albemarle Catalysts BV, CRI/Criterion, ExxonMobil, Shell Global Solutions, Haldor Topsoe, Total, Chevron Lummus Global, Advanced Refining Technologies, and IFP is gratefully acknowledged.

The MACS-III meeting in Ascona, in 2004, left many of those present, with the feeling that perhaps the prospects of hydrotreating research were not as bright as they used to be. The number of participants was substantially lower than at the earlier symposia, and there were comments about insufficient interaction between academic research and industrial practice. Also, several principal scientists and heads of research groups were (and are) near retirement and not all of them would/will be succeeded. Finally, it looked increasingly difficult to get funding,

as the topics are apparently not “hot enough” for the policy makers.

That is why, besides continuing the MACS tradition of providing a forum for the dissemination of the latest results, MACS-IV was planned to address the future of research in the field of sulfide catalysis and to stimulate the interaction between academia and industry. In the event, a sense of optimism pervaded the meeting: the number of participants was again at the customary level, collaborations between academia and industry appear to be thriving, and funding is not a major problem—the retirement of a number of eminent people could still have an adverse effect on the number of groups that will be active in sulfide catalysis, but so far there is no sign of this—the geographical distribution of these groups (now heavily concentrated in France, Denmark, and The Netherlands) is likely to change, however (China!). In fact, the mood of the meeting could be caught in the following couple of quotes, “business is booming”, and “the field is as alive as ever”.

A total of 32 papers have been accepted for publication in this special issue of *Catalysis Today*. They are arranged

according to the symposium's technical program and divided into the following topical areas: (1) new preparations & new active materials, (2) characterization of the catalyst in its working state, (3) computational chemistry, (4) reaction mechanism/kinetics, and (5) future refinery and transportation trends and future of hydrotreating research.

In the last session of the symposium, there was some discussion about the topics to be pursued in the immediate future—the following list emerged:

- New & adapted supports—still a very important research area, as many improvements in catalyst performance over the last decennia came from improved carriers;
- Theoretical studies: it was concluded that (i) atomic scale properties of sulfide surfaces in HDS conditions can be modelled, generating views on promotor localisation (in combination with EXAFS, XPS, STM, IR) and reaction mechanisms (which should result in microkinetic models able to describe catalytic tests); (ii) concepts useful for experimentalists can be, and are being generated, *e.g.* morphology in reaction conditions, volcano curves (Sabatier revisited & better quantified)), mixed sites, support wetting; (iii) “design” of new active phases will be possible in the, not too distant, future—*ergo*, this line of research should be vigorously pursued;
- New tools—*e.g.*, STM, HAADF-STEM, in situ TEM, tomography, He-ion microscopy;
- Experimental validation: bridging the gap between the catalyst as seen in modelling & highly sophisticated tools, and as they might look in actual practice—our catalysts are non-equilibrium solids after all (Topsoe) and we do not, as yet, know very much about their state under (industrial) reaction conditions (*cf.* the possibility of the MoS<sub>2</sub> edges being carbided then);
- “Industrial issues”: (a) presulfiding (H<sub>2</sub>/H<sub>2</sub>S vs. liquid phase in its various guises), (b) inhibition: real feed behaviour, (c) H<sub>2</sub> activation, (d) deactivation phenomena, (e) design & dispersion of the active phase (this ties in, obviously, with the points above); reaction mechanism & kinetics are clearly relevant here. At the meeting consensus appeared to crystallize around Teh Ho's notion that with model feeds, one elucidates particular catalyst functionalities, while the final proof of the catalytic pudding lies in its behaviour in a real feed;
- “Novel” active phases: strictly speaking, this is much broader, in the hydroprocessing context, than sulfides, but still there are essentially two sides to this: generating new knowledge/concepts, and finding better catalysts—in the

latter case, a reality check is better carried out sooner rather than later (*cf.* John Armor, Appl. Catal. A 282 (2005) 1);

- Interaction with process engineering—new feeds, or new catalysts may demand, or open up, new processing schemes, and it is good to have an engineer in one's team to address such issues.

In principle, of course, sulfide catalysis is broader than hydroprocessing, and in the past we have had contributions on, *e.g.*, water–gas shift, and in the future we may have contributions on, *e.g.*, the hydrogen electrode reaction, but all papers in this issue address hydroprocessing issues. We trust that they will clearly convey the message that the field, although dubbed “mature”, is still exciting and has a bright future!

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