

## Preface

The European Workshop on Combinatorial Catalysis EuroCombiCat 2002 took place in the island of Ischia in Italy from 2 to 5 June, 2002. The 106 participants came from 16 countries, both from industry and academia, and not only from Europe but also from various other transcontinental countries. The workshop aimed at showing the state of the art and the most recent developments in the field of combinatorial catalysis (combicat) as well as the new experimental tools used for the related high-throughput experiment, some of them being exhibited by technology provider companies during the workshop.

Progress in combinatorial and high-throughput screening (HTS) methods in catalysis R&D has come to an impressive rate. Companies implementing these techniques have recognised their power and importance in increasing productivity and adding value to processes and products. Companies providing technologies, instrumentation, expertise are also expanding their effort, looking for a wider array of clients' needs. In parallel, academia which has initiated an effective approach of combinatorial research under a more fundamental basis during the last 5 years is now increasing its effort (tools, software, search for new concepts, understanding, etc.). However, only a limited number of academic institutions are deeply involved today in that research area.

The main combicat tools are needed for parallel synthesis, characterisation, screening and testing of catalytic materials including the chemical analysis of the reaction mixtures as well as management and analysis of the vast amount of data accumulated in the combicat process. All these tools were dealt with various contributions (6 plenaries, 17 oral communications, 23 posters) of which most are presented in the present special issue of Catalysis Today. In summary, it may be stated that, quite a significant progress has been

achieved during the last few years. Still some kind of common technological platforms is missing by which results from the various laboratories can be validated at a high-quality standard.

Particularly in data analysis exciting work has been more recently initiated. This concerns data storage and mining by using appropriate descriptors and by correlating input and output variables, like composition and structure of catalytic solids on one hand and catalytic results on the other one. Also various optimisation procedures for finding the best catalyst compositions in the combicat process are now already applied. One of these methods is an evolutionary approach using, e.g. a genetic-algorithm-based approach.

Of special interest were some success stories, i.e., illustrations of combicat for developing new or at least improved catalytic materials. From what has been discussed informally it can be expected that new results in this area will soon become public.

The meeting closed with a lively discussion lead by M.B. and C.M. in which about 60 scientists and engineers from industry and academe took part, half of them contributed to the discussion of which a few crucial points are mentioned.

- It was emphasised that combicat needs an interdisciplinary approach and besides the solution of experimental challenges with respect to synthesis, screening, testing and characterisation of the catalytic materials, data analysis will become the main issue in the near future. Thus, by enlarging the scope of fundamental catalysis, it may be anticipated that the relationships between catalytic performance and properties of the materials, which is derived from data mining or expert systems, e.g. neural networks correlating these variables with each other, will provide new basic insights.

- The high-throughput experimental tools developed for combiCat will also enable academia to more rapidly examine hypotheses, which are usually part of the conceptual process in catalyst development. Emphasis was put with respect to basic science that it would be extremely useful to collect descriptors for the materials and their catalytic data in a general format agreed upon among scientists and to put them in networked data banks for general use.
- Most of the work reported on the workshop dealt with heterogeneous gas-phase and gas–liquid-phase reactions. A cross fertilisation with bio- and homogeneous catalysis was highly recommended.
- From remarks of equipment providers it appeared that tools of even more sophisticated instrumental nature with respect to automation are to be expected. Particularly synthesis tools for a wide range of methods seem to be required.
- Finally, the issue of patents was focused on. Criticism was raised about various trivial claims, which came up in the recent patent literature. The controversy could not be resolved but the statement “apply for patents whenever you think it is patentable” may be taken as a general guideline not only for industry but also for academe.

Concluding, it may be stated that the workshop was a tremendous success to which not only the magnificent landscape of Ischia and the well-organised social programme contributed, but also the openness by which all contributions, i.e., plenaries, oral communications and posters were discussed and the significant support from the 11 sponsoring institutions and companies.

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