## **Prologue**

In the past decade the chemical industry has experienced a rapidly changing environment. Traditional activities for the design and manufacture of bulk commodity chemicals are now complemented with a significant focus on the design and manufacture of specialty, high value-added chemical products. As a result, the scope of computer-aided design has expanded from process design to important issues in product and process design.

FOCAPD 2004 (Foundations of Computer-Aided Process Design) is the 6th international conference, held every five years, in a distinguished series that focuses on computer-aided design. The major theme of the FOCAPD 2004 conference, "Discovery Through Product and Process Design", reflects this remarkable shift in the industrial sector.

The primary objective of the FOCAPD 2004 conference has been the triptych of: providing an in-depth review and critical assessment of the current state of the art; discussing the current and future needs of research, education and training; and identifying new directions, opportunities, and challenges in product and process design.

An important aim of FOCAPD 2004 has been to bring together and foster interaction among world-renowned experts from academia and industry, researchers and practitioners from government laboratories and several industries, graduate students, and postdoctoral associates. Participants from product and process oriented industries such as chemicals, petrochemicals, pharmaceuticals, biochemicals, food and beverages, electronics and materials, energy and environmental, will present and discuss recent advances, challenges, and emerging opportunities in product and process design. FOCAPD 2004 is organized under the auspices of the CACHE Corporation and it cosponsored by CACHE, AIChE, and the CAST Division of AIChE.

In these proceedings, the invited papers (keynote and plenary) are contributions by leading researchers in academia and industry and they cover an important and diverse set of topics. These include: integrated product and process design; education, training and industrial needs in product and process design; modeling and simulation as enabling technologies in product and process design; optimization methods and applications; product and process design for energy and the environment; process operations; and challenges and opportunities in systems biology. The contributed papers reflect state-ofthe art refereed contributions and their accompanying short oral presentations and poster presentations have been classified into four broad categories: (a) process design and synthesis, (b) product design and discovery, (c) process operations: control, identification, planning, and scheduling, and (d) modeling, optimization, and uncertainty. Four awards for the best contributed papers have been established through the generous donations of Aspentech, BASF, ExxonMobil, and Process Systems Enterprise. It is hoped that the scientific contributions presented at this conference and included in these proceedings will stimulate new advances and innovations in product and process design.

We would like to acknowledge the financial support and express our gratitude to the National Science Foundation, Princeton University (School of Engineering and Applied Sciences, and Department of Chemical Engineering), Air Products and Chemicals, Aspentech, BASF, Bristol-Myers-Squibb, Eastman, ExxonMobil, Invista, Mitsubishi Chemical, Optience, and Process Systems Enterprise. We would like to thank the members of the advising and organizing committee, the keynote and plenary speakers, the authors of the contributed papers, the co-chairs of the plenary sessions, and the co-chairs of the contributed papers session (Costas Maranas, Rafiqul Gani, Shinji Hasebe, and Jose Pinto). Finally, we are indebted to the excellent assistance and coordination provided by the conference manager Robin Craven, the great help of Dale Grieb (Princeton University), Lillian Clark (Princeton University), Eric Hamblin (Princeton University), Linda Clos (Princeton University), Stacy Janak (Princeton University), Scott McAllister (Princeton University) and Jodi Ray (Omnipress).

Additional information on the FOCAPD 2004 conference can be found at the web site: http://www.focapd.org/FOCAPD2004.

Christodoulos A. Floudas Princeton University Co-Chair FOCAPD 2004 Rakesh Agrawal Air Products and Chemicals, Inc. Co-Chair FOCAPD 2004