

scattering problems and associated mathematical techniques. A substantial amount of research work on water-wave scattering by vertical barriers, thin vertical barriers, and thin curved barriers was presented. The implication of the numerical results was discussed in the context of modelling of break waters which are constructed to protect a sheltered area from the rough sea. P. R. Sengupta (University of Kalyani) addressed some problems of mechanics of fluids with special reference to visco-elastic fluids. He also discussed the numerical results to find the maximum velocity of OLDROYDIAN fluid in a circular pipe. S. N. Bora (IIT, Guwahati) talked about second-order wave theory for a circular cylinder in finite water depth. He presented the second-order diffraction problem for the large vertical cylinder. Expressions for three second-order forces, namely waterline force, dynamic force and quadratic force were obtained. The first-order potentials contribute to waterline and dynamic forces, whereas the second-order potentials contribute to the quadratic force. Emphasis was more on the contribution of the second-order forces to the total force. R. Sircar (REC, Durgapur) discussed computer-based modified Fourier algorithm for solving problems in the

industry. He tried to explore the feasibility of applying the modified Fourier method (MFM) in solving linear programming problems with finite number of variables and constraints that are relevant to industrial problems. The MFM algorithm has been successfully implemented in an interactive computer program which also highlights the pros and cons against conventional simplex algorithm. V. Charles (REC, Warangal) discussed a branch-and-bound technique for linear stochastic fractional programming with joint probability constraints. R. K. Upadhyay (ISM, Dhanbad) presented a Gauss-type mathematical model to study the effect of predation on two competing prey species in which the predator species is influenced by the damage effect caused by crowding from the members of its own population in a diffusive system. S. Dey (ISM, Dhanbad) talked on useful mathematics in seismic studies and showed the effect of presence of initial stresses and gravity field on the propagation, reflection and refraction of seismic waves. He also said that non-homogeneous earth allows torsional surface waves to propagate and initiated the idea of construction of seismograms which can record torsional movements. Some selected papers, which appeared in dif-

ferent technical sessions are: (i) Genetic algorithm and its applications (M. Chakraborty and M. Rajasekar, ISM, Dhanbad); (ii) Solving numerical problems on parallel computers (P. K. Jana, ISM, Dhanbad); (iii) On the conservation laws of the magma equations (K. Singh, Hisar); (iv) Software metrics in fuzzy environment (D. Patel, RIT, Jamshedpur); (v) Diffraction of shear waves in a homogeneous medium (B. K. Rajhans, ISM, Dhanbad); (vi) MHD flow in a rotating channel (G. S. Seth, ISM, Dhanbad); and (vii) A new approach to the estimation of population mean in two-phase sampling (G. N. Singh and L. N. Upadhyaya, ISM, Dhanbad).

All in all, the atmosphere was lively and informal, the younger participants had an opportunity to make short presentations. The panel discussion prompted us to think more seriously about the development of new techniques to resolve real problems of the society, and new tasks in S&T.

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New horizons in heterogeneous catalysis*

Processes based on heterogeneously catalysed reactions have become one of the most powerful tools of today's petrochemical and refining industry, and are critical to environmental protection and public health. Advancements in the science and technology of heterogeneous catalysis are, therefore, crucial for the sustainable development of global society. Taking into account the growing significance of the subject, a national symposium on heterogeneous catalysis was organized to advance the knowledge base

and to identify the critical areas for future research. Nearly a hundred participants from within the country attended this symposium.

Inaugurating the symposium A. V. Ramaswamy (NCL, Pune) provided a chronological overview of the outstanding Indian contributions in the area of catalysis since 1927, and said that future challenge of the subject is to achieve 100% selectivity for the desired product. This will enable clean manufacturing with no hazardous waste products. P. Ramachandra Rao (Vice-Chancellor, BHU) in his Presidential address, referred to several important problems such as coking and regeneration associated with industrial catalysis. He also dealt with the potential and future applications of nanocrystalline materials. The construc-

tion of these materials in bulk quantities is at present a challenge, for which an understanding of their surface to volume ratio is of particular importance. He urged for exploiting these materials directly as catalysts without any further treatment or coating.

The scientific programme commenced with the Professor Gopal Tripathi Memorial Lecture-2002 delivered by S. P. Sukhatme (Chairman, Atomic Energy Regulatory Board, Mumbai) who focused his attention to present India's production and reserves of various commercial and non-commercial energy sources. In view of the gradual decline in fossil-fuel reserves, he presented a comparative account of the two major alternative options such as solar energy and nuclear power. The Principal N. N. Godbole

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Memorial Lecture–2002 delivered by K. V. Raghavan (Director, Indian Institute of Chemical Technology (IICT), Hyderabad) highlighted new dimensions and opportunities in chemical engineering aspects of catalytic reactions. Nature of reaction engineering inputs that are required for studying complex gas–solid reaction system was the focal point of his talk. Importance of C_1 chemistry and catalysis in confined spaces was also discussed by him. Keynote speaker for the symposium, G. V. S. Sastry (BHU, Varanasi) spoke about the applicability of quasicrystalline materials as catalysts. Comparing the catalytic behaviour of quasicrystalline materials with conventional catalysts, he showed detailed results on systems consisting of Al-Pd and Al-Cu for methanol decomposition and on-board H_2 production.

The contributory presentations were included in nine thematic sessions: catalysis by oxides and sulphides; synthesis, characterization and modifications of zeolites; metal catalysts; novel catalytic technologies; solid acids and bases; biocatalysis and environmental catalysis.

Oxide and sulphide catalysts

Metal oxides on a molecular scale provide interesting opportunities for tailoring acidic and redox properties of oxidic catalysts, while sulphides are important catalyst components in a wide range of refinery processes. In an invited lecture, A. V. Ramaswamy (NCL, Pune) gave an overview on the designing of catalysts based on basic oxides such as MgO and Fe_2O_3 for the selective alkylation of phenol and showed that molecular modelling can be a useful tool in understanding the basis of adsorbed state of phenol on oxide surface. The work by S. Saravananurugan (Anna University, Chennai) showed that silica-supported $Ti(O^iPr)_4$ catalyst can be used for enantioselective epoxidation of allylic alcohol. Veda Ramaswamy (NCL, Pune) discussed the results of her findings on the synthesis, characterization and photocatalytic activity of nanocrystalline particles of anatase titanium dioxide. Vapour-phase methylation of pyridine over a few ferrites was presented by A. Radhe Syam (D.A. University, Indore). S. K. Samantaray (Regional Research Laboratory, Bhubaneswar) discussed the effect of phosphate and sulphate anions impregnated on titania in

alkylation of benzene, toluene and chlorobenzene with *iso*-propanol in a fixed-bed flow reactor. M. Kumar (Indian Institute of Petroleum (IIP), Dehradun) presented data on the effect of mixed oxide supports such as $TiO_2-Al_2O_3$, $SiO_2-Al_2O_3$, $ZrO_2-Al_2O_3$ and SiO_2-ZrO_2 on the reduction behaviour of Co/Mo hydrotreating catalysts.

Zeolite catalysts

Two separate sessions were devoted to discuss the trends in synthesis, characterization and modifications of zeolytic materials. S. R. Patwardhan (IIT, Mumbai) in his invited talk gave an overview on the preparation and characterization of mesoporous silicates molecular sieves and related materials of M41S family such as MCM-41 (hexagonal), MCM-48 (cubic) and MCM-50 (lamellar). A. Vinu and R. Savidha (Anna University, Chennai) showed the synthesis and characterization of Al, Fe and Zn substituted MCM-41 material for catalysing *tert*-butylation and regioselective isopropylation of phenol respectively. Emerging trends in synthesis and catalytic application of MCM-41 molecular sieves in reactions such as cyclization, alkylation and liquid-phase oxidation were discussed by S. J. Kulkarni (IICT, Hyderabad). He also reviewed the application of zeolites in the synthesis of speciality and fine chemicals. A. B. Halgeri (Indian Petrochemicals Corporation Limited, Vadodara) talked about the designing of zeolite catalyst through pore size engineering for the synthesis of *para*-dialkyl benzenes. G. Ravichandran (Indian Oil Corporation Limited, Faridabad) discussed the effect of variation in different components of a catalyst used in fluid catalytic cracking process. D. Srinivas (NCL, Pune) discussed a catalytic process using Y-zeolite encapsulated metal complexes for selective aerial oxidation of *para*-xylene. Presentations by K. K. Cheralathan and K. S. Priya (Anna University, Chennai) discussed the combined spectroscopic and catalytic study of modified β and Y zeolite in the alkylation and acylative cyclization of phenol respectively. With regard to the application of modified zeolite as catalysts in petroleum refining three presentations were made from IIP, Dehradun. The activity of hydrothermally-treated and Ga-exchanged HZSM-5 for aromatiza-

tion of *n*-heptane was discussed by O. S. Tyagi. Use of Pt-promoted HZSM-5 in conversion of straight light naphtha into high octane unleaded gasoline was presented by P. Vijayanand, whereas the role of NaY zeolite as support in formulating hydrotreating catalysts was the subject matter of discussion by K. S. Rawat.

Metal catalysts

Metallic catalysts are used on a large scale for petroleum refining, conversion of automobile exhaust and in many other processes. They constitute only about 1 wt% of the catalytic material, being applied in a finely dispersed form as particles on a high area porous support. The essence of this subject was discussed by N. M. Gupta (BARC, Mumbai) who in his invited talk reviewed the present knowledge on the particle size effect in heterogeneous catalysis. L. Dixit (IIP, Dehradun) reported the feasibility of $ZnAl_2O_3$ spinels as supports for bimetallic Pt-Sn dehydrogenation catalysts. P. Vijayanand, also of IIP, described the results of a highly active and selective catalyst for conversion of *n*-pentane to *iso*-pentane over WO_x/ZrO_3 promoted with both Pt and Fe. The transformation of agro-based ethanol directly to acetone with 99.5% selectivity by using Fe-Zn mixed oxide catalyst over silica gel support was discussed by D. J. Prakash (Osmania University, Hyderabad). R. Labroo (P. R. Engineering College, Ahmednagar) had studied the kinetics of the catalytic dehydrogenation of ethyl alcohol for manufacturing acetaldehyde on a mixed oxide catalyst consisting of CuO (93%), CoO (5%) and Cr_2O_3 (2%). N. K. Bhattacharya (Arora Mettley Limited, Kolkata) explained the reasons for catalyst deactivation and discussed the ways for its regeneration on the site of reactions, to make the process cost-effective.

Solid acids and bases

Though extensive studies have been made on heterogeneous solid acid catalysts compared to heterogeneous basic catalysts, research on the use of the latter in the synthesis of speciality and fine chemicals has substantially increased in recent years. In this context, S. Sivasankar (NCL, Pune) in his invited lecture dealt with the utility of solid base

catalysts such as supported alkali metal-loaded silica, MCM-41 and silicalites for different types of alkylation reactions such as C-alkylation of alkyl aromatic compounds, O-alkylation of hydroxy aromatic compounds and N-methylation of aniline. V. K. Gupta (Reliance Industries, Surat) discussed the use of metallocenes and non-metallocenes type of new generation catalysts to produce tailor-made polyolefin with enhanced end-product performance. V. K. Srivastava (Central Salt and Marine Chemicals Research Institute (CSMCRI), Bhavnagar) dealt with the use of several solid base catalysts for isomerization of 3-(4-methoxyphenyl)-1 to 1-(4-methoxyphenyl)-propene, an important perfumery chemical. The effect of various preparatory parameters on sulphated zirconia catalysts was studied by M. K. Mishra (CSMCRI) to establish a correlation of synthetic strategy on the structural and textural properties of catalyst. Pankaj Sharma (M.S. University, Baroda) reported the results on the esterification of *n*-butanol catalysed by heteropolyacid, $H_2PW_{12}O_{40}$ supported on activated alumina. Esterification of salicylic acid with phenol in presence of different solid acid catalysts such as Al_2O_3 , ZrO_2 , SiO_2 , amorphous $AlPO_4$ and zeolites (NaY, Na β and NaZSM-5) was the content of the talk by N. Nagaraju (St. Joseph College, Bangalore). M. Karthik (Anna University, Chennai) presented the results of *tert*-butylation of *m*-cresol with *tert*-butyl acetate over Al-MCM-41 catalyst. The effect of pH on acidity of partially sulphated metal oxides, TiO_2 and Al_2O_3 was discussed by P. C. Soni (BHU, Varanasi) in the light of XRD, IR spectroscopy and NH_3 desorption methods.

Novel catalytic technology

Although many institutions are working towards modification in catalyst technology for various operating processes, only four presentations were made in this session. G. Murali Dhar (IIP, Dehradun) in his invited talk reviewed the progress made in catalyst improvement for ultra-

deep hydrodesulphurization of petroleum fractions. This process is meant to enhance the product quality of refinery streams by way of reducing its sulphur content, using H_2 . Ashutosh Agarwal (Jubilant Organosys, Bhartigram) described applications of silica-alumina, ZSM-5 and vanadia-based heterogeneous catalysts for commercial production of pyridine and its various derivatives. Uma Shanker (IIP, Dehradun) provided an overview of the recent trends in catalyst technology for Fischer-Tropsch synthesis to produce clean liquid transportation fuels. P. Shashikala (Osmania University, Hyderabad) elaborated a novel approach for oxidizing *ortho*-chlorobenzaldehyde to *ortho*-chlorobenzoic acid using quaternary ammonium compounds as phase-transfer catalysts. In another submission related to modelling, P. Goyal (BARC, Mumbai) discussed important issues related to passive catalytic recombination-based hydrogen mitigation system in the containments of nuclear power plants.

Biocatalysis

This session had two presentations. R. V. Jasra (CSMCRI) in his invited talk reported the utility of silicious mesoporous molecular sieves for immobilization of enzymes. Understanding and controlling the properties of immobilized enzymes opens a whole range of applications in the pharmaceutical industry. Use of microorganism for biodesulphurization reaction was shown by H. K. Goindi (IIP, Dehradun). She presented the results of desulphurizing activity of free as well as immobilized *Staphylococcus* species, which shows that free cells have marginally higher activity for diesel desulphurization.

Environmental catalysis

This session was related to a theme of current interest for its approach to the practice of green catalysis that advocates production of cleaner technology. M. V. Shankar (Anna University, Chennai)

explained the role of titania in photocatalytic decontamination of wastewater using an organophosphorous insecticide as model pollutant. Anima Mahata (Central Mechanical Engineering Research Institute, Durgapur) focused on the exploration of visible light-assisted catalytic transformation of organic molecules using TiO_2 semiconductor particulate system modified with thionine, Nile blue A and eosin Y. Vibha Chaturvedi (National Environmental Engineering Research Institute (NEERI), Nagpur), presented work about the photocatalytic colour removal from reactive dye containing dye-bath wastewater using stirred slurry and open-trough type reactors. Anurag Garg (IIT, Roorkee) reported the performance of $CuSO_4$ and Cu_2Cl_2 for the removal of phenol from wastewater effluent using catalytic wet air oxidation. An environmentally benign process for the synthesis of biphenyl urea in presence of metal aluminophosphates, $M-AlPO_4$ ($M = V, Fe, Cu, Ni, Cu$) was reported by G. Kuriakose (St. Joseph College, Bangalore). While the role of activators such as Pt, Pd and Cd on gas-sensing properties of SnO_2 was highlighted by P. M. Jadhav (BHU, Varanasi), M. N. Narayan of the same research group discussed the effect of various preparatory and post-preparatory parameters on the stoichiometry and band structure of CdS photocatalyst.

The programme concluded with a valedictory lecture by R. N. Singh (Director, NEERI) who stated that new developments in materials science create new opportunities for catalysis professionals. He exhorted the participants for an interdisciplinary approach to seek solutions for technological challenges in catalysis research.

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