

**NATIONAL CENTRE FOR CATALYSIS RESEARCH
INDIAN INSTITUTE OF TECHNOLOGY, MADRAS**



A National Centre sponsored and supported by

**DEPARTMENT OF SCIENCE AND TECHNOLOGY,
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SELF EVALUATION REPORT OF NCCR FOR 2009

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SELF EVALUATION REPORT OF NCCR FOR 2009

INTRODUCTION

National Centre for Catalysis Research was formed in the year 2006 from the grants from DST, Government of India and the Indian Institute of Technology, Madras. The centre has since then has been growing and expanding its activities. In this brief report, the centre's activities and realizations in the year 2009 are outlined for both self evaluation by the members of the Centre and also forms the basis document for future growth of the centre.

The centre had its Management and Advisory committee meeting chaired by Prof M M Sharma with Director, IITM, Secretary, DST, Drs. Paul Ratnasamy, T.S.R.Prasada Rao, Dr R.P.Verma and the Director NCL as honourable members of the committee. The committee reviewed the activities of the centre on June 22nd and the minutes of the meeting is attached to this document for ready reference.

(a) M TECH PROGRAMME

The major step of the centre in this year is the start of an academic programme M Tech in Catalyst Technology with the support of the Department of Chemical Engineering of IITM. The centre wishes to place in record the grateful thanks for the Chemical Engineering Department for kindly taking this initiative and for their cooperation in conducting this programme. The programme is going on so far without much problems. The Department of Chemical Engineering has also associated with NCCR in two prestigious fellowships called **IOCL fellowship** which were obtained as a special grant by NCCR from IOCL. The fellows have been selected and started their research work jointly supervised by both the faculties of NCCR and the department of Chemical Engineering, IITM.

(b) PROJECTS DURING THE YEAR 2009

The centre has been able to attract various projects during this year. The major ones are listed as follows:

- (a) Tata Chemicals has entered into an MOU for water splitting by photo-electrochemical route and this project will be jointly carried out by Dr Ramnarayanan of the department of Chemical Engineering, IITM and the faculty of NCCR.
- (b) SRF has entered in an MOU for the development of specific catalysts for the production of chloro-fluoro carbons.
- (c) An MOU is being finalized with NISSAN, Japan for the development of adsorbents.

- (d) Shell has sanctioned another project on the successful completion of the previous project which has resulted in a disclosure for adhesion of active catalysts on stainless steel grids.
- (e) GM has sanctioned another project to us to study the type of NO_x species in autoexhaust.

(c) ACADEMIC COLLABORATIONS DURING THE YEAR 2009

Academic collaborations have been established with a number of educational institutions. These can be listed as follows:

- (i) MOU with CRC of the Technical University of Munchen, Germany.
- (ii) MOU with NIMS of Japan for possible collaboration.
- (iii) MOU with the department of Chemical Sciences and Energy of Tezpur University, Tezpur, Assam
- (iv) MOU with the Kalasalingam University for academic cooperation.
- (v) MOU with Bharathidasan University is in the process of finalization.
- (vi) Have been discussing possible academic cooperation with other institutes like Department of Physical Chemistry, University of Madras.

(d) GRANTS RECEIVED DURING THE YEAR 2009

The centre has also been successful in obtaining grants from Governmental sources and the important ones are:

- (a) The grant for joint Indo Australian programme for value added chemicals from biochemical sources
- (b) The Indo-Hungarian programme was continued this year and the exchange of research fellows and visit of the scientists from both sides have taken place with positive effects.
- (c) Indo Taiwan proposal of the centre was approved and the exchange of visits from Taiwan has taken place.
- (d) The NMITLI programme of CSIR for conversion of glycerol to value added chemicals was continued this year and valuable contributions have been added to this project from NCCR.

(e) VISITS BY THE FACULTY AND STUDENTS OF NCCR

The faculty of NCCR has made visits to other countries in connection with on going projects and also for other scientific assignments. They can be listed as follows:

- (a) Prof Selvam and B.Viswanathan visited the University of Queensland and held discussions on the on going project during July 12 to July 19, 2009.
- (b) Prof Selvam also visited again the University of Queensland during november 2009 for discussion on the on-going project and finalization of some scientific documents.

- (c) Prof Selvam also visited countries like Russia under the ILTP programme and participated in the Indo Russian Seminar during 2009.
- (d) Prof Selvam also visited Brazil and France and presented papers in the seminar
- (e) Prof Selvam participated in the National meeting of the in Bangalore during December 2009.
- (f) Helen visited France and presented a paper in the symposium on Hybrid materials in Tours, France March 16-19 and visited Germany and Swiss.
- (g) Mr B Kuppan a Ph D scholar of the Centre has gone to the laboratory of surface science and catalysis of the Hungarian Academy of Sciences for research work for a period of 4 months from November 30, 2009.
- (h)

(f) VISITS BY OTHERS TO THE CENTRE

1. Prof N. Roesch of the CRC, Technical university visited the centre during Feb 5 to 8, 2009.
2. Prof Ogura visited the centre on Feb 17, 2009.
3. Dr Nobuko Miyairi and Ms Preeti Sinha of the Thomson Reuters visited the centre for discussion on their products namely Web of Science.
4. Dr Rajiv Kumar and Dr Mal of the Tata Chemicals visited the centre for discussion and subsequently Dr Mal came to the centre for testing their Fuel cell station.
5. Dr Seshan of the University of Twente, The Netherlands visited the centre

(g) PATENTS GENERATED BY NCCR DURING 2009

The centre is in the process of filing the following patents. These documents are in the various stages of processing.

- (a) A patent for adhesion of active catalyst component on Stainless Steel grids. This patent will be filed by Shell Netherlands soon.
- (b) A patent document has been submitted to the Dean IC SR of IITM for the conversion of glycerol to value added ethers and it is in the process of evaluation.
- (c) A patent for hybrid membranes for fuel cell applications has been filed. The patent number is yet to be assigned.

2. THE INPUT AND OUTPUT OF HUMAN RESOURCE BY NCCR DURING 2009

The following persons have left the centre during this year

1. Ms Helen after completing her Ph D thesis went to Germany for her PDF position.
2. Ms Chandravathanam after submitting her Ph D thesis for her lecturer position in a local college.
3. Mr Jude Vimal Project associate to take up alternate job.
4. Dr P.P.George, PDF on obtaining a lecturer Job
5. Dr Navaladian, Post Doctoral fellow, after getting a PDF position in USA
6. Mr York R Smith from the University of Nevada, Reno left after completing his term of stay in December 2009.
7. **Prof A V Ramaswamy Chair professor left us for his position in Pune**
8. Ms Sumathi, Research Assistant left us for his work in Pune.
9. Dr Vidya Krishnan, DST Young scientist left us for her other assignments.
10. Dr Joyce, DST Young Scientist left for her lecture position in Bangalore.
11. Ms J Rajeswari, Ph D Scholar, left for her PDF position in USA, Colorado School of Mines.
12. Dr P S Kishore, Ph D Scholar left for his PDF in USA, Colorado School of Mines.
13. Mr R Kumaravel Research Assistant left for his further studies
14. Mr C Bennet from IOCL left after his assigned work is completed in NCCR to IOCL.

The following persons joined the centre during 2009:

1. **Prof K R Krishnamurthy as chair professor from RIL, Baroda**
2. **Dr.Raghuram Chetty joined NCCR as an adjunct faculty from Chemical Engineering Department**
3. Ms A Alagarasi as a research assistant
4. Mr Prakash as a research fellow in the Shell project
5. Ms K Gomathi joined as a research fellow in the GM Project
6. Ms V S Smitha joined as a research fellow in the GM Project
7. Ms S.Sandhya joined as a fellow in the SRF Project.
8. Mr Vinoth Kumar joined as a fellow in the SRF project

3. Publications for the year 2009

1. R.Mahalakshmi, P.Indraneel and B.Viswanathan, "Surface functionalities of nitric acid treated carbon - A density functional theory based vibrational analysis", *Indian J Chemistry A*, 48, 352-356 (2009).
2. B.Viswanathan, "Architecture of carbon support for Pt and Pd in direct methanol fuel cells", *Catalysis Today*, 141, 52-55 (2009).
3. G Muralidhar, L D Sharma B.Viswanathan and M. O. Garg, Guest editors of *Catalysis Today*, Vol 14, Issues 1 and 2 (2009).
4. P.Sangeetha, K.Shanthi, K.S. RamaRao, B.Viswanathan and P.Selvam, "Hydrogenation of nitrobenzene over palladium-supported catalysts - Effect of support ", *Applied Catalysis A* ,353, 160-165 (2009).
5. B.Viswanathan, "Fuel cells - challenges ahead", *Photo/electrochemistry and photobiology in the environment, Energy and Fuel*,2009,pp.1-14.
6. Jothiramalingam, B.Viswanathan and M.K.Wang, "Appraisal of heterogeneous solid acid base catalysts for Transesterification reaction ", *Photo/electrochemistry and photobiology for Energy fuel and environment, Research Signpost*, 2009 pp.15-46.
7. B.Viswanathan and M.Sankaran "Hetero atoms as activation centres for hydrogen absorption in carbon nanotubes", *Diamond and related materials*, **18**, 429-432 (2009).
8. S.Navaladian, B.Viswanathan, T.K. Varadarajan and R.P.Viswanath, "Fabrication of worm-like nanorods and ultrafine nanospheres of silver via solid-state photochemical decomposition", *Nanoscale Research Letters*, **4**, 471-479 (2009).
9. G.Magesh B.Viswanathan, R.P.Viswanath and T.K.Varadarajan, "Photocatalytic behaviour of CeO₂ -TiO₂ system for the degradation of methylene blue ", *Indian Journal of Chemistry*, 49A 480-488 (2009).
10. T.Maiyalagan and B.Viswanathan, "Electrochemical fabrication and characterization of poly(o-phenylenediamine) nanotubes by template method", *Indian Journal of Chemistry*, 49A, 198-201(2009).
11. Ch.Venkateswara Rao and B.Viswanathan, "ORR Activity and direct ethanol fuel cell performance of carbon supported Pt-M (M=Fe,Co and Cr) alloys prepared by polyol reduction method", *Journal of physical Chemistry*, Volume: 113 Issue: 43 Pages: 18907-18913 Published: OCT 29 2009.
12. K Joseph Antony and B.Viswanathan, "Single step synthesis and structural study of mesoporous sulphated titania nanopowder by controlled hydrolysis method ", *Applied Materials and Interfaces* , Volume: 1 Issue: 11 Pages: 2462-2469 Published: NOV 2009.
13. M.Helen, B.Viswanathan, and S Srinivasa Murthy, Polyvinyl alcohol (PVA) - Polyacrylamide (PAM) blends with cesium salts of heteropolyacid as polymer electrolyte for DMFC application, *Applied Polymer Journal* (in press)

14. B.Viswanathan, "Nurturing Scientific Temper", *One India One People*, September 2009 pp 8-10,
15. B.Viswanathan, "The relevance of the science of nano materials in catalysis", *Chemistry Industry Digest*, September 2009 ,
16. KJoseph Antony and B.Viswanathan, and A V Ramaswamy "Surface Area, Pore Size, and Particle Size Engineering of Titania with Seeding Technique and Phosphate Modification", *J Physical Chemistry C* 2009, 113 (31), pp 13750- 13757 ,
17. P. Satyananda Kishore B.Viswanathan, and T K Varadarajan "Silico-tungstic Acid Based Carbon Supported Noble Metal Electrodes for Energy Conversion Application", *J Physical Chemistry C*, 2009, 113 (29), pp 12918- 12925 ,
18. K Joseph Antony Raj and B.Viswanathan, ""Effect of surface area, pore volume and particle size of P25 titania on the transformation of anatase to rutile, *Indian Journal of Chemistry Section A* 48A,1378-1382(2009).
19. S.Sabiah and B.Viswanathan, Mo-amino acid complexes as analogs for molybdoenzyme: A DFT approach, *Indian Journal of Chemistry*, 48A,911-920 (2009).
20. K Joseph Antony Raj, R Shanmugam, R Mahalakshmi & B Viswanathan, XPS and IR spectra studies on the structure of phosphate and sulphate modified titania – A combined DFT and experimental study, *Indian Journal of Chemistry* 49A (2010) in press.
21. Ch.Venkatewara Rao and B.Viswanathan, Carbon supported Pd-Co-Mo Alloy as an alternative to Pt for oxygen reduction in direct ethanol fuel cells", *Electrochimica Acta* (in press).
22. K Joseph Antony Raj, Structural Study of Silica Modified Titania and its Photocatalytic Activity of 4-Chlorophenol Oxidation in Water, *Journal of Physical Chemistry C*, (Submitted)
23. K.Joseph Antony Raj York R Smith , Vaidyanathan (Ravi) Subramanian and B.Viswanathan, Catalytic Combustion of Diesel Soot Particles on Potassium and Sodium Titanates, *Journal of Physical Chemistry C*, (Submitted).
24. Viswanathan B, Neel PI, Varadarajan TK, Development of Carbon Materials for Energy and Environmental Applications, *Catalysis Surveys from Asia*, Volume: 13 Issue: 3 Pages: 164-183 Published: SEP 2009.
25. Kishore PS, Viswanathan B, Varadarajan TK, Electrochemical Oxygen Reduction Reaction by Pt Nanoparticles on Carbon Support Stabilized by Polyoxometalates, *Journal of Nanoscience and Nano technology*, Volume: 9 Issue: 9 Pages: 5188-5197 Published: SEP 2009.
26. Kumar, E. Anil, Maiya, M. Prakash, Murthy, S. Srinivasa, Viswanathan, B., Structural, hydrogen storage and thermodynamic properties of some mischmetal-nickel alloys with partial substitutions for nickel, *Journal of Alloys and Compounds*, Volume: 476 Issue: 1-2 Pages: 92-97 Published: MAY 12 2009.

27. Rajeswari J, Kishore PS, Viswanathan B, Varadarajan, T K., One-dimensional MoO₂ nanorods for supercapacitor applications, **Electrochemistry communications**, Volume: 11 Issue: 3 Pages: 572-575 Published: MAR 2009.
28. Navaladian S, Viswanathan B, Varadarajan TK, and Viswanath, R P., A Rapid Synthesis of Oriented Palladium Nanoparticles by UV Irradiation, **Nanoscale Research Letters**, Volume: 4 Issue: 2 Pages: 181-186 Published: FEB 2009.
29. Shanmugam S, Viswanathan B, Varadarajan TK., The preparation of metal oxygen molecular cluster embedded organic-inorganic nanocomposite and its rectification behaviour, **Materials Chemistry and Physics**, Volume: 112 Issue: 3 Pages: 863-868 Published: DEC 20 2008.
30. V, Udayakumar and S, Alexander and V, Gayathri and S, Shivakumaraiah and K R, Patil and B, Viswanathan (2010) Polymer-supported palladium-imidazole complex catalyst for hydrogenation of substituted benzylideneanilines. **J Molecular Catalysis A Chem**, 317 . pp. 111-117.
31. S.Chandravathanam, B.Viswanathan and T K Varadarajan, Effect of aminopyridine functionalization of carbon black, Bulletin of the Catalysis Society of India, 8, 143-148 (2009).
32. York R. Smith, K. Joseph Antony Raj, Vaidyanathan (Ravi) Subramanian, and B. Viswanathan, Sulfated Fe₂O₃-TiO₂ Synthesized from Ilmenite Ore: A Visible Light Active Photocatalyst, Applied Catalysis (submitted)
33. S. K. Badamali and P. Selvam, "Probing the Fe(III) sites in Mesoporous FeMCM- 41", *Catal. Today* **141** (2009) 103.
34. K Joseph Antony and B.Viswanathan, CuO, K₂O and V₂O₅ supported on ceria-titania: Synthesis, characterization and application on diesel soot combustion, J Molecular Catalysis (communicated)
35. K.Joseph Antony, M.G. Prakash and B.Viswanathan, Alkylation of phenol with *tert*-butanol over sulphated Fe₂O₃-TiO₂, J. Molecular Catalysis (Communicated).

4. Presentations in the year 2009

1. B.Viswanathan, Nano materials in Catalysis, A lecture in the 14th national workshop in catalysis held at the Department of Chemistry, Tezpur University on December 21 (2009).
2. B.Viswanathan, Control of size of nano particles and their activity, Presented in the Indo Japan workshop at IICT, Hyderabad, on December 23, 2009.
3. B.Viswanathan, Science of nano materials in catalysis, Plenary lecture in the 6th National symposium and conference on Solid State Chemistry and Allied Areas ISCAS 2009 during November 20-21, VIT, Vellore.
4. B.Viswanathan, Nano materials for energy harvesting, in the nano materials for energy harvesting seminar at the Thiagarajar College of Engineering, Madurai held on December 2-4, 2009.
5. B.Viswanathan, The relevance of hybrid membranes for DMFC applications, in the International symposium on hydrogen in matter, held at IITM December 13-16, 2009.
6. P.Selvam, Platinum supported nitrogen containing ordered mesoporous carbons, Plenary lecture at the 14th National workshop on catalysis at the Tezpur University, December 21, 2009.
7. M.Helen, B.Viswanathan and S.Srinivas Murthy, Polyoxometalate based membranes for possible DMFC application, Hybrid Materials, First International conference on multifunctional hybrid and nanomaterials, March 15-19 (2009) Tours, France.
8. B. Kupan, B. Viswanathan, and P. Selvam, "Mesoporous Carbon Nitride Supported Platinum (Pt/MCN-1) Electrocatalyst for Methanol Oxidation" CATSYMP-19, Pune, January 18-21, 2009.
9. P. Selvam, B. Viswanathan and B. Kupan, "Platinum supported Nanoporous Carbon / Nitrogen containing Carbon Molecular Sieves: Promising Electrocatalysts for Methanol Fuel Cell Application", ICMAT-2009, Singapore, June 28-July 3, 2009
10. P. Selvam, "Uranyl-incorporated MCM-41: an efficient photocatalyst for the oxidation of volatile organic compounds" CATSYMP-19, Pune, January 18-21, 2009.
11. V. Kirishna, P. Selvam, and B. Viswanathan, "Chromium containing SBA-15: potential photocatalyst for the reduction of nitric oxide" CATSYMP-19, Pune, January 18-21, 2009.
12. T.M. Sankaranarayanan, M. Banu, R. Sumathi, J. Masih, G.Valavarasub, A. Meenakshisundaram, B. Sairam and S. Sivasanker, "End point reduction of a straight run diesel fraction using zeolite catalysts", *19th National Symposium on Catalysis, Pune, Jan. 18- 21, 2009 (oral paper)*.
13. S.Sivasanker, "Nano-structures in heterogeneous catalysis" Workshop on Nanotechnology, SSN College, Chennai 20th March, 2009 (Chief guest lecture).
14. K. Joseph Antony Raj, A.V. Ramaswamy and B. Viswanathan, Synthesis and characterization of organic-free, phosphate-modified anatase titania with high surface area, CATSYMP-19, Pune, January 18-21, 2009.
15. B.Viswanathan, Metal oxygen cluster compounds and their use in electrochemical devices, Presented in the International school on Nano Materials, Anna University, Feb 2009.

16. S.Chandravathanam, 'Enhanced utilization of Pt/C catalyst for methanol electrooxidation' in a National Seminar on 'Recent Trends in Chemistry, RTC- 3' conducted at Jayaraj Annapackiam College for Women, Periakulam, 26-27 Feb., 2009.
17. Vamshi Krishna, B.Viswanathan and P Selvam, Synthesis and Characterization of Novel Mesoporous (IITM-56) Silicates" in" Modern Trends in Inorganic Chemistry, MTIC-XIII" conference conducted in IISC, Bangalore,December 7 to 10, 2009.

5. Ph D theses submitted by the candidates of the centre during the year

1. **Ms Helen**, Development of hybrid membranes for application in Direct Methanol Fuel cells, April 2009 (Guides: S.Srinivasamurthy and B.Viswanathan)
2. **Ms. S. Chandravathanam**, Effect of pretreatment of electro-catalyst for Direct Methanol Fuel cell applications, August 2009 (Guide Prof T K Varadarajan and B.Viswanathan) (thesis submitted)
3. **Mr P. Indraneel**, Development and Exploitation of carbon materials from plant sources, December 2009 Guide Prof T K Varadarajan (thesis submitted)

6. Project proposals submitted during the year 2009

1. Studies on hydrogen storage in carbon materials, submitted jointly by NCCR, Physics department and CFCT (ARCI) to MNRE has been approved for funding.
2. Catalytic problems in alternative energy production – a joint Indo Hungarian Programme submitted by Prof P Selvam and B.Viswanathan
3. Under Indo Russian programme, P Selvam and B.Viswanathan has submitted a proposal entitled “Iron containing nanostructured catalysts for environmental protection” to DST jointly with Zelinsky Institute of Organic Chemistry, Moscow.
4. A Project proposal on Chemical mitigation of Carbon to fuels & chemicals is under consideration by HPCL – Submitted by Prof K R Krishnamurthy and B.Viswanathan

7. Books compiled in the year 2009 by NCCR

1. B.Viswanathan edited a book on nano materials and has been published by Alpha Science International, and Narosa Publishing house with the ISBN number 978-1-84265-494-1 (2009)
2. Prof D K Chakrabarty and B.Viswanathan wrote a text book on Heterogeneous Catalysis, published by New Age Science Limited with the ISBN number 978-1-906574-09-3 for the international market.
3. S Kaneco as editor in chief and B.Viswanathan and H Katsumata as associate editors a book on Photo/electrochemistry & photobiology in the Environment, Energy and Fuel was published by Research signpost with ISBN 978-81-308-0251-0 (2009)
4. B.Viswanathan edited a book on selected topics in Catalysis, published by Narosa publishing House with ISBN 978-81-7319-758-1
5. B.Viswanathan, P.Indraneel and T K Varadarajan, Methods of Activation and Specific Applications of Carbon Materials, **an e- book at the NCCR website** .
6. B.Viswanathan, Pollution Control strategies – A chemists' perspective an e-book to be placed in the NCCR web site soon.
7. B.Viswanathan with S Kannan and R C Deka, Catalysts and Surfaces: Characterization Techniques, Narosa Publishing house with ISBN 978-81-7319-735-2 (Under production).

8. Educational Activities in relation to Human Resource Development:

1. A M Tech programme in catalysis Technology has been started in the odd semester of this year and five students are undergoing this programme. Details are given in **Appendix 1**.
2. A four day special programme was conducted for the scientists of Nagarjuna Fertilizers and Chemicals limited from September 18 to 21, 2009. The details of the programme and also the response of the organization are given in **Appendix 2**.
3. The faculty of the centre has been participating in many other academic and teaching duties and the important ones are:
 - (a) B. Viswanathan has been sharing with Prof Ajit Kumar Kolar the M Tech course ME 770 Theory and Technology of Fuel cells.
 - (b) B.Viswanathan was a resource person for the Green Chemistry workshop held by the Department of Chemical Sciences and delivered 10 lectures during 4-9th June 2009.
 - (c) B.Viswanathan conducted the catalysis specialization course for the M Sc students of Tezpur University in the third semester during October 2009.
 - (d) B.Viswanathan and Prof P Selvam were resource persons for many courses conducted during the year and the typical ones are: Science city Madras two of their short term courses in the year 2009, NICE University, Thiagarajar college of Engineering, S V Nadar College, Madurai, International workshop in Anna University, MS University, Thirunelvali, Kalasingam University, Enrichment Programme in Science held at IITM,
 - (e) The centre has also conducted the Science programme in the summer April 2009 for the Childrens' Club, Mylapore on the theme Pollution Control Strategies –A chemists' perspective
 - (f) The 10th Orientation programme for the research Scholars of this country was held from November 28 to December 16, 2009 and 42 participants were selected all over from India.
 - (g) Two research scholars meet between Anna University , Madras University and NCCR were held in April, 11 and August 2009.
 - (h) Pre School on Electron Spectroscopy was held at NCL on behalf of the Catalysis Society of India during January 16 and 17, 2009 and B.Viswanathan coordinated the whole programme in addition to be the main resource person with Prof P Selvam.
 - (i) Pre School on Theoretical Methods in Catalysis was held at the Department of Chemistry, Gauhati University on 19 and 20th December, 2009 and B.Viswanathan coordinated the programme and was main resource person with Prof P Selvam.
 - (j) Bulletin of the Catalysis Society of India a catalysis journal 8th volume of this journal was brought out this year with 4 issues on behalf of the catalysis Society of India and B.Viswanathan was the Editor-in-Chief of this journal.
 - (k) In addition, B.Viswanathan is an editorial board member of the Indian Journal of Chemistry Section A and also Euroasian Journal of Chemical Technology.

Special Training Program

In addition, the faculty of the centre has participated in various educational and refresher programmes conducted by other institutions like Anna University (international school on nano materials, Tezpur University (Green Chemistry summer school), Kalasalingam University, Krishnankovil, and many other schools and some of the details of these are available in the section on presentations.

Special training in catalysis was offered to number students of sister organizations like Christian college, Chennai, Loyola college and University of Madras. Prof S Sivasanker supervised four summer research fellows (two students and two lectures) sponsored by the Indian Academy of Sciences Bangalore for about 2 months. Prof Selvam supervised a summer fellow from NISER, Bhubaneswar, (Mr. Jayanth K Ajay). Also the following persons have been trained for their summer programme at NCCR.

1. Mr. Abhishek ShivKumar MIT, Manipal, Karnataka
2. Mr.Raghul Raghavan, NIT, Trichirapalli
3. Mr.K.T.Vikesh, Thiagarajar college, Madurai
4. Mr.R.Shanmugam, Thiagarajar College, Madurai
5. S.Esskiammal, Thiagarajar College, Madurai

9. Special Lectures given at the Centre in the year 2009

1. Prof N Roesch of the university of Munchen visited NCCR and delivered a lecture on Hydrogen activation by Transition metal Species in Zeolites and also signed an MOU between NCCR and CRC of University of Munchen.
2. Prof Ogura visited the centre on Feb 17 and delivered a lecture on the synthesis of new functionalized zeolites from mesoporous silica.
3. Prof V Krishnan of IIT Delhi visited our centre and gave a lecture on the prospects of Fuel cells.
4. Prof Raghuram Chetty of the Department of Chemical Engineering, IIT M gave a lecture on Flexible Fuel cells on 15th May 2009.
5. DR Seshan of the University of Twente, The Netherlands visited us and gave a lecture on Production of Sustainable hydrogen production.

10. Appendix

Minutes of the third meeting of Management Advisory Committee (MAC) of National Centre for Catalysis Research, at IIT-M, Chennai

Date: 22nd June, 2009
Time: 2.00 p.m.
Venue: Board Room,
Administration Building,
IIT- Madras, Chennai

The following members attended the meeting.

| | |
|---|----------|
| Prof. M. M. Sharma | Chairman |
| Dr. T. Ramasami, Secretary, DST | |
| Prof. M. S. Ananth, Director, IIT-M | |
| Dr. S. Sivaram, Director, NCL | |
| Dr. Paul Ratnasamy | |
| Dr. T. S.R. Prasada Rao | |
| Dr. R..P. Verma | |
| Dr. P.S . Sai Prasad representing Director, IICT | |
| Prof. Lingappan representing VC, Anna University) | |
| Mr. Jacob V.V., Scientist, DST | |

The following investigators and others associated with the Centre were also present:

Prof. B.Viswanathan, Head, NCCR
Dr. S .Sivasanker , Chair Professor, NCCR
Prof. T. K.Varadarajan , Dept. of Chemistry
Prof. P. Selvam , Dept. of Chemistry
Prof. G. Ranga Rao, Dept. of Chemistry
Dr. R. Ramnarayanan , Dept. of Chem. Engineering
Dr. Raghuram Chetty , Dept. of Chem. Engineering

The meeting started with welcome of the participants by Prof. B.Viswanathan.

A. Prof. M.M. Sharma, Chairman of the MAC also welcomed the participants and initiated the discussions on the following points.

1. He enquired about space, faculty and other positions. On this point, the efforts made by NCCR / IIT-M were outlined. Importance of recruiting faculty for the National Catalysis Centre was stressed. The Director, IIT-Madras pointed out that there was a standing advertisement and as and when suitable candidates were available, new faculty would be recruited. Dr. Raghuram Chetty who has joined the Chem. Eng. Dept. recently was introduced to the members of the committee.
2. The Chairman enquired about the rationale for domiciling the new M. Tech. (Catalysis Technology) degree course in the chemical engineering department. The reasons for domiciling the new course in the chemical engineering

department and the advantages of running it as a M. Tech. programme of an engineering department were explained.

3. The Chairman emphasized the need for separate building for the centre. The details of space available and the steps being taken for more space were made available to the committee.

The Secretary, DST recommended that in future, the reports of NCCR may include a separate section on resource flow management plan. He outlined the benefits of presenting a resource management plan (including financial and manpower) to the MAC and seeking approvals of the MAC for any deviations or alterations or mid course corrections (if necessary). The Secretary, DST advised that the resource management plan for NCCR may be prepared and circulated among members of MAC within the next few months.

He stressed on the role of NCCR in Human Resources Development and the need for strengthening the faculty base. He also enquired about the industry contributions and whether any specific equipment requirement or changes in the approved equipment was required to be approved by the committee, taking into account of new equipment acquisition by IIT-Madras through other complementary programs. He suggested that MAC could be advantageously employed by the Center for seeking approvals for mid-course changes in resource allocation and priorities.

Dr. S. Sivaram suggested that efforts should be made to retain persons obtaining Ph.D's from the centre at the centre itself.

B. After these remarks, Prof. B. Viswanathan made a detailed presentation of the activities of the centre elaborating on the following aspects

1. Action taken report: The minutes of the last MAC meeting of July 7, 2008 and the action taken on the various points raised by the Chairman and Secretary, DST was outlined. MAC approved the actions taken.

2. Education and capacity building at NCCR:

Various steps taken by NCCR on capacity building were discussed. Secretary, DST pointed out the quantitative target of 250 students to be trained at NCCR. He wanted to know as to whether steps have been taken to match the quantitative targets set originally. The Chairman, at this point pointed out that (i) the regular Ph. D. students working at NCCR as reflected in the document appears to be small and there is scope for improvement, and (ii) he was of the opinion that the history of development of catalysts should be included in the M.Tech. curriculum. He also suggested for inclusion of Catalysis as an optional course in M.Tech – Chemical Engineering. Dr. P. Ratnasamy made a suggestion to attract persons without Ph.D in engineering to work in the area of Catalysis. The MAC appreciated the spread of the activities to various parts of the country especially to Tezpur, Assam.

3. Highlights of research:

The scope of the research areas covered by NCCR was analyzed at length. Dr. Paul Ratnasamy stressed on needs of a separate identity for the centre. He said that NCCR

should build brand equities. Prof. Sharma suggested that preparation methods for industrially useful acid clays should be developed. He also suggested focusing on “**Homogenous catalysis**” as a benchmark area.

4. The self sustainability of the centre after the 5 year DST support was discussed by the Chairman, the Secretary, DST and others. Dr. Sivaram cautioned that optimism must be taken with care and the Secretary, DST said that the assessment could be made only after details of resource statement was correctly presented and discussed by MAC. Secretary, DST advised NCCR on aspects relating to building strategic alliances with international centers.

Other points that were considered include the following:

1. Dr. T. S. R. Prasada Rao pointed out that the quality of the publications can be improved and there are only a handful of good papers in reputed journals.
2. Regarding the FT work, there were various suggestions. The Chairman wondered if monolith reactors will have sufficient productivity. Dr. Ratnasamy pointed out that the proposed work included the development of catalysts for the slurry reactor.
3. The Chairman remarked that NCCR should aim at developing catalysts based on rare earths (like ceria) since vast deposits of the same are available in India.

Recommendations:

1. The Committee appreciated the work done so far by the Centre and expressed a hope that the centre will meet the objectives for which it was set up.
2. The Centre should recruit more faculty members on urgent basis.
3. The Centre should function from an independent building with enough space for future expansion.
4. A review may be made on number of personnels to be trained and enhancement of Ph.D enrolment. It should give more priority to Human Resource Development.
5. History of development of catalysts should be included in the M.Tech. curriculum. Effort may also made to include Catalysis as an optional paper in M.Tech in engineering.
6. The centre should appoint personnel/s to maintain/upkeep of the equipments.
7. Efforts to be made to enhance the quality of publications.
8. The report of the centre should include a section on resource management (including financial and manpower), and measurable/visible output indicators etc. It should capture contributions from industries etc and linkages with other institutions. A report including all these should be circulated in the next few months.

9. A sub-committee be formed to assess and guide the centre in its growth. The Sub-committee would be meeting more than 2 or 3 times in a year.

The meeting ended with the Chairman thanking the Director, IIT-M ; Secretary, DST and other members of the committee.

Appendix 1

M Tech Catalysis Technology

I Semester

| Course No | Title | L | T | P | C |
|-----------|---|----|---|---|----|
| CA 5010 | Fundamentals of adsorption and catalysis | 3 | 0 | 0 | 3 |
| CA5020 | Solids and Surfaces | 3 | 0 | 0 | 3 |
| CH5010 | Chemical Reactor Theory | 3 | 1 | 0 | 4 |
| CH5020 | Experimental and analytical methods in chemical engineering | 3 | 0 | 0 | 3 |
| | Elective I | 3 | 0 | 0 | 3 |
| | Elective II | 3 | 0 | 0 | 3 |
| | Total Credits | 18 | 1 | 0 | 19 |

Semester II

| Course No | Title | L | T | P | C |
|-----------|--|----|---|---|----|
| CA5030 | Experimental methods in Catalysis | 3 | 0 | 0 | 3 |
| CA5040 | Introduction to surface analysis | 3 | 0 | 0 | 3 |
| CH5030 | Transport Phenomena | 3 | 1 | 0 | 4 |
| CA5050 | Catalyst preparation and characterization Laboratory | 0 | 0 | 3 | 1 |
| | Elective III | 3 | 0 | 0 | 3 |
| | Elective IV | 3 | 0 | 0 | 3 |
| | Total Credits | 15 | 1 | 3 | 17 |

Semester III

| Course No | Title | L | T | P | C |
|-----------|-----------------|---|---|----|----|
| CA 5510 | Project Stage 1 | - | - | - | 6* |
| CA5520 | Seminar I | - | - | -- | 1 |
| | Elective V | 3 | 0 | 0 | 3 |
| | Elective VI | 3 | 0 | 0 | 3 |
| | Total credits | 6 | 0 | 0 | 7 |

Semester IV

| Course No | Title | L | T | P | C |
|-----------|------------------|---|---|---|-----|
| CA5510 | Project Stage II | - | - | - | 20* |
| CD5530 | Seminar II | - | - | - | 1 |
| | Total Credits | - | - | - | 21 |

- Includes the 6 credits in the third semester.

Electives I and II

| Course No | Title | L | T | P | C |
|-----------|---|---|---|---|---|
| CA5310 | Preparation and Properties of Catalysts | 3 | 0 | 0 | 3 |
| CA5320 | Homogenous Catalysis | 3 | 0 | 0 | 3 |
| CA5330 | Bio-Catalysis | 3 | 0 | 0 | 3 |
| CA5340 | Computational methods in Catalysis | 3 | 0 | 0 | 3 |

Electives III and IV

| Course No | Title | L | T | P | C |
|-----------|---|---|---|---|---|
| CA5350 | Catalysis in Petroleum Technology | 3 | 0 | 0 | 3 |
| CA5360 | Catalysis in production of chemicals | 3 | 0 | 0 | 3 |
| CA5370 | Nano-Materials in Catalysis | 3 | 0 | 0 | 3 |
| CH516 | Chemical and Catalytic Reaction engineering | 3 | 0 | 0 | 3 |

Electives V & VI

| Course No | Title | L | T | P | C |
|-----------|--|---|---|---|---|
| CA5380 | Catalysis in green chemistry and environment | 3 | 0 | 0 | 3 |
| CA5390 | Photocatalysis | 3 | 0 | 0 | 3 |
| CH6040 | Chemical reactor design for process plants | 3 | 0 | 0 | 3 |
| CH6120 | Particle Characterization | 3 | 0 | 0 | 3 |
| CH6150 | Multiphase reactors | 3 | 0 | 0 | 3 |
| CY672 | Chemical and Electrochemical energy systems | 3 | 0 | 0 | 3 |
| CY676 | Principles of Surface Chemistry | 3 | 0 | 0 | 3 |

Appendix 2

| Date | 8.30 to 10.00 | 10.30 to 12.00 | 14.00 to 15.30 | 16.00 to 17.30 |
|----------------------------|-----------------------------------|------------------------------------|--|---|
| Friday, 18 Sept. 2009 | Kinetics & Catalysis L1 (BV) | Selection of catalysts L2 (AVR) | Adsorption/ Diffusion L3 (BV) | Industrial Rxn Homogeneous L4 (AVR) |
| Saturday, 19 Sept. 2009 | Preparation: Homogeneous L5 (AVR) | Preparation: Heterogeneous L6 (SS) | Preparation: Heterogeneous L7 (SS) | Polymerization: Esters, etc. L8 (AD) |
| Sunday, 20 Sept. 2009 | Catalyst Characterization L9 (BV) | Catalyst Characterization L10 (PS) | Thermal methods L11 (PS) | Testing of Catalysts L12 (KRK) |
| Monday, 21 Sept. 2009 | Activation of Catalysts L13 (KRK) | Catalyst Deactivation L14 (SS) | Catalyst regeneration, reactivation L15 (SS) | General Discussions: Concluding session |

Proposed coverage for each lecture:

- L1: Introduction, kinetic study of catalytic reactions, catalyst activity and selectivity
- L2: Homogeneous and heterogeneous catalytic reactions, Selection of catalysts (Metal/Ligand) for specific reactions, electronic and steric factors
- L3: Adsorption on solid surfaces, Physical adsorption, Chemisorption, external and internal diffusion
- L4: Industrially important reactions using homogeneous catalysts: Hydroformylation, Carbonylation, Wacker oxidation, adipic acid, etc.
- L5: Typical examples of preparation of organo-metallics, ligand synthesis, application Biphasic/phase transfer reactions
- L6: General methods of preparation of solid catalysts, role and choice of supports, Impregnation/incorporation of active metals
- L7: Catalyst formulation: the complex nature of commercial catalysts, examples, Catalysts shapes and sizes vis-à-vis the process/reactor design
- L8: Polymerization: Ziegler-Natta to metallocenes: polyester synthesis
- L9: Characterization of porous materials: BET surface area, pore volume, distribution, Particle size, density, metal surface area, dispersion, etc.
- L10: Structural characterization (XRD), surface characterization (XPS), other spectral Techniques (diffuse reflectance), etc.
- L11: Thermal methods (TG/DTA/temperature-programmed techniques) in characterization of catalysts.
- L12: Testing of catalysts for specific reactions: Different types of laboratory reactors for screening of catalysts, micro reactors, differential and integral reactors, Pulse technique, batch reactors, on-line analysers, how to test a catalyst?
- L13: Activation of catalysts in industrial reactors, endo- and exothermic reactions and start-up procedures (examples), start of run conditions, steady state conditions
- L14: Factors responsible for catalyst deactivation, coking, fouling, poisoning, mechanism of coking, reversible and irreversible poisoning, indicators, examples
- L15: Regeneration of industrial catalysts, decoking procedures, semi-regenerative and

continuous regeneration of catalysts and reactor designs. Reactivation of catalysts

L12: Testing of catalysts for specific reactions:

Different types of laboratory reactors for screening of catalysts,
micro reactors,
differential and integral reactors,
Pulse technique,
batch reactors, on-line analysers, how to test a catalyst?

L13: Activation of catalysts in industrial reactors, endo- and exothermic reactions and start-up procedures (examples), start of run conditions, steady state conditions and prediction of catalyst life.

Faculty:

1. Prof. B. Viswanathan
2. Dr. A.V. Ramaswamy
3. Dr. S. Sivasanker
4. Dr. A. Deshpande
5. Prof. P. Selvam
6. Dr. K.R. Krishnamurthy

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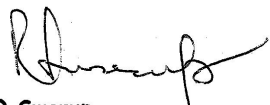


Certificate

This is to certify that the training program on catalysis conducted during the month of September 2009 by NATIONAL CENTRE FOR CATALYSIS RESEARCH (NCCR), INDIAN INSTITUTE OF TECHNOLOGY, MADRAS (IITM) has been very useful in knowledge and skill set development of scientists of Nagarjuna Fertilizers and Chemical Ltd (NFCL). The theoretical and practical aspects of the training session are well received and truly appreciated by the NFCL scientists and management.

On behalf of NFCL, I sincerely thank Prof. B. Viswanathan and NCCR team for the commendable work performed as part of the training program. I also thank IITM management for the cooperation, support and warm hospitality extended to my team mates during this program. We hope to continue this fruitful interaction with IITM and NCCR in future, as well.

Sincerely,



R Swarup

29.09.09.

CIO & Head - Nagarjuna Innovation Center

