
FUEL CHEMISTRY NEWS

Newsletter of the ACS Division of Fuel Chemistry

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<http://www.anl.gov/PCS/acsfuel/>

Fall 2006

Message from the Chair (Semih Eser)



Halfway through my term as Chair, I would like to take this opportunity to thank the Past Chair Marek Wójtowicz for his excellent and dedicated leadership in the Division. Marek has been a

great leader and a kind mentor along with other FUEL giants, including Phillip Britt, Katie Carrado, and Randy Winans. Their long association with and dedication to the Division have contributed much to the success of FUEL.

One of the highlights of the Atlanta meeting was launching a new vision for ACS: Improving people's lives through the transforming power of chemistry. I, for one, appreciate this new vision that reminds me to question what I do day-to-day to improve people's lives. It is an overwhelming question that extends to many circles from family and friends to the world at large. Making significant improvements in life usually requires more than an individual effort, and the synergy in FUEL membership stands out as an important potential to add to "transforming power of chemistry" through education, new developments, and improvements on the sources of power: Fuels. I copied below two of the five vision fields listed in the Strategic Plan of the Fuel Chemistry Division (See <http://www.anl.gov/PCS/acsfuel/fuel2015.pdf>).

- Our preprints and symposia will contribute to a strengthened and sound scientific basis for efficient and environmentally acceptable fuel production and use.
- We will promote public education and outreach in the area of fuel science.

I am happy to say that we have been successful in both endeavors, perhaps more successful in the first field.

On the preprint front, I am delighted to announce that FUEL members now have access to downloadable pdf files of all the preprints published from 1957 through present on the Division web page (<http://pubs.acs.org/meetingpreprints>). This effort initiated by Karl Vorres some years ago culminated in a project supported by a 2005 ACS Innovative Projects Fund Grant for Divisional Enhancement to finally place the preprint files on the web. Many thanks to Karl Vorres, Mercedes Maroto-Valer, Marek Wójtowicz, and Randy Winans for this monumental achievement.

Another 2005 ACS Innovative Projects Fund Grant that FUEL received will support a pilot program to provide travel support to graduate students and postdocs who will present a paper in FUEL symposia at the San Francisco meeting. Twelve individuals have been approved to participate in this program that is aimed at recruiting new and active members to the Division. I hope that in the future, we will be able to support such programs by donations from private and public institutions and the Division's own funds.

For the 2006 competition for ACS Innovative Projects Fund Grant for Divisional Enhancement, we have submitted a proposal entitled "Public Education and Outreach for Basic Literacy on Energy and Fuel Issues." The goal of the proposed project is to initiate a web portal for public education and outreach to introduce basic concepts and applications of science in the field of energy and fuels. Effective use of multimedia resources and presentations will make the science content easily accessible to a non-technical audience, but still interesting and informative to scientists and engineers. The introductory material on the web portal would also serve as a steppingstone to the topical symposia papers and presentations that will also be posted on the Division web site. An ad-hoc committee headed by Sarma Pisupati spisupati@psu.edu will take on this effort, hopefully with funding from ACS. Please contact Sarma or me if you would like to participate in this project as a

contributor, or reviewer.

The recipient of 2006 Henry H. Storch Award in Fuel Chemistry is Colin Snape. You may view the slides of the papers presented at the Storch Award Symposium in Atlanta at:

<http://www.anl.gov/PCS/acsfuel/2006%20Storch%20Award%20Symposium.htm>.

You will be happy to know that the executive committee has approved a proposal in Atlanta to offer Henry H. Storch Award annually thanks to good financial health of the Division and the willingness of the sponsor.

The Glenn Award winners for presenting the best paper at the 2005 Spring meeting in San Diego are Isabella Nova, Lidia Castoldi, Luca Lietti, Enrico Tronconi, and Pio Forzatti from Dipartimento di Chimica, Materiali e Ingegneria Chimica "G. Natta", Politecnico di Milano, Piazza Leonardo da Vinci 32, Milano 20133, Italy. The title of their paper is NOx Storage Mechanism over Pt-Ba/Al₂O₃ Lean NOx Trap Catalysts Professor Gianpiero Groppi accepted the award for the authors at the joint FUEL/PETR Dinner in Atlanta.

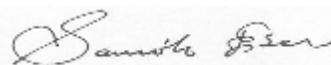
The technical program in Atlanta included eight symposia in addition to the Storch Award symposium. A major strength of FUEL division programming is the capability to organize symposia in diverse topical areas as illustrated in the following list.

Chemistry of Carbon Materials and Nanomaterials
Biofuels for Transportation
Nanoparticles in Energy Processes: Friend and Foe:
Combustion Synthesis: From Pollutants to Advanced
Materials
Science and Technology of Greenhouse Gas
Management
Nanoparticles in Energy Processes: Friend and Foe:
Environmental and Health Effects (co-sponsored by
I&EC)
Advances in Fuel Science and Technology
Environmental Issues in Energy and Fuels
Nanoparticles in Energy Processes: Friend and Foe:
Nanoparticle-based Catalysts and Sorbents (co-
sponsored by CATL)

The traditional FUEL/PETR divisions joint dinner was held at Atlanta Fish Market restaurant guarded by a giant fish statue at the front. About 80 people attended the event. Randy Winans presented the 2006 Henry H. Storch Award in Fuel Chemistry to Colin Snape. Semih Eser presented the Glenn Award for the best paper at the 2005 Spring meeting in San Diego to Professor Gianpiero Groppi who accepted the award on behalf of Isabella Nova and her co-authors.

In closing, I would like to acknowledge the magnificent job Robert Hurt has done as the 2006 Program Chair, as you may read about in this newsletter.

With warm greetings and best wishes,

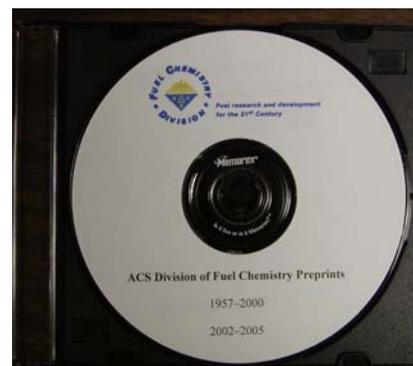
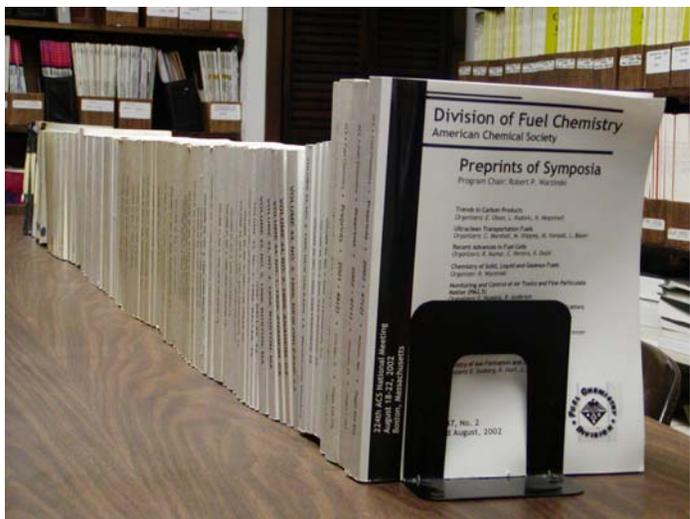


Semih Eser



2006 ChemLuminary Award Application

Archives of the Division of Fuel Chemistry Preprints (1957–2005)
Scanned and Now Freely Available on the Division Web Site



The ACS Division of Fuel Chemistry provides a forum for documentation and communication to the international community of research and development results, in order to promote efficient and environmentally acceptable fuel production and use.

Fuel Chemistry Division Strategic Plan

● [FUELS 2015](#)

[On-Line Preprints](#)

[On-Line Preprint Information](#)

[Preprint Archives 1957 - 2005](#) ^{NEW!}

<http://www.anl.gov/PCS/acsfuel/>

Pictures from the 2005 joint FUEL & PETROLEUM dinner



AWARDS – Colin Snape (Storch) and Gianpiero Groppi (Glenn) for Isabella Nova







Laboratory of Catalysis and Catalytic Processes
Dipartimento di Chimica, Materiali e Ingegneria Chimica
“Giulio Natta”, Politecnico di Milano

The Laboratory of Catalysis and Catalytic Processes is involved in the study of Catalysis and Chemical Reaction Engineering within several research projects on novel and environmentally benign processes for the production of energy, on the production of clean fuels and on the abatement of pollutants from stationary and mobile sources.

KEYWORDS

Catalysis, Fischer-Tropsch diesel, catalytic combustion, H₂ production, catalytic mufflers, SCR process, emission abatement

RESEARCH GROUP

Pio Forzatti, Enrico Tronconi, Luca Lietti, Gianpiero Groppi, Alessandra Beretta, Cinzia Cristiani, Isabella Nova, Lidia Castoldi

RESEARCH ACTIVITIES

Catalytic processes for energy and transport applications have been of growing importance in recent years in view of the reduction of the environmental impact and of the diversification of energy sources. Since more than a decade the Laboratory of Catalysis and Catalytic processes of Dipartimento di Chimica, Materiali e Ingegneria Chimica “G. Natta” has been involved in several research topics within these areas including: production of clean liquid fuels from natural gas, novel energy conversion system with minimal environmental impact; clean up processes of exhaust combustion gases. The role and the characteristics of the investigated processes are briefly described in the following along with some details on the performed researches.

“Gas to liquid” process

This process transforms natural gas in liquid fuels for diesel engines via the following steps: i) natural gas conversion to syngas; ii) syngas conversion to complex mixtures of higher hydrocarbons by Fischer-Tropsch synthesis; iii) production of diesel fuel by hydrocracking. Two targets are achieved: i) valorization of remote sources of natural gas, since gas to liquid conversion markedly reduces transportation costs; ii) production of sulphur free clean diesel fuels.

Research activity on this topic has been performed in cooperation with ENITECNOLOGIE. The aim is to clarify the mechanism and the kinetics of the complex

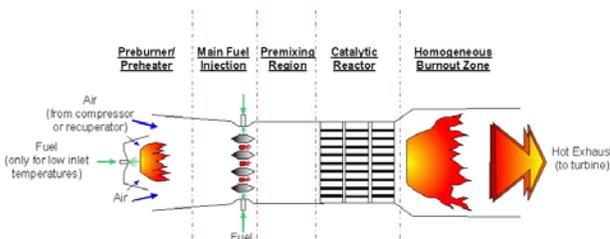
reaction network that occurs in the key step of the process: the Fischer-Tropsch synthesis. The study has been performed on last generation, cobalt based catalysts and will provide a key support to the development of pilot and demonstration plants.

Catalytic combustion for gas turbine applications

The use of catalytic combustors allows reducing the environmental impact of gas turbines systems by minimizing NO_x production (below 3 ppm) while stabilizing combustion so to guarantee CO and unburned hydrocarbon emission below 10 ppm.

Such a technology is based on close coupling of catalytic reactors, which ignite combustion and pre-heat the reactants, with homogeneous combustion that allows a rapid fuel burn out.

The research activities at the Laboratory of Catalysis and Catalytic Processes have been carried out with a combined approach including the development of novel catalysts (hexaaluminates, Pd-based systems) and the engineering analysis of the system by mathematical modelling. The research has been performed both from a fundamental point of view in inter-university projects financed by Italian Government and from an applied point of view in EU funded project and industrial contracts with world leading gas turbine manufactures (Alstom Power)



Catalytic combustor

Hydrogen production for fuel cell applications

Energy scenarios for the next decades predict a growing use of fuel cell for stationary and mobile applications. In the short-mid term the H₂ fuel required for such applications will be likely produced from fossil fuels. Among different strategies, catalysis plays a key role in those processes based on distributed H₂ production either in fuel stations or directly on board. In such cases due to economies of scale the small production volumes make conventional production processes too expensive, so that innovative solutions are required, based on catalytic processes such as partial oxidation and autothermal reforming.

On these latter topics the Laboratory of Catalysis and Catalytic Processes has recently started a research activity funded by Italian Government which is focused on Rh based systems, i.e. the most promising catalysts so far. The research activity is targeted to the evaluation of the catalyst stability and activity properties as a function of different choices on the support material and on the Rh deposition

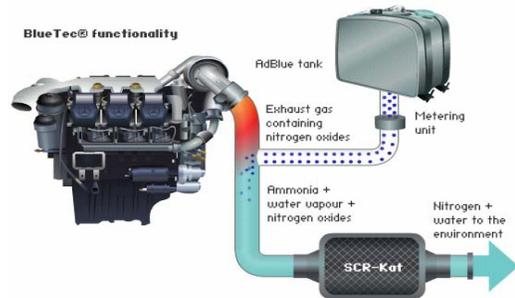
method. The research activity is also focused on gaining insight in mechanistic and kinetic features of several relevant reactions (combustion, partial oxidation, steam reforming) in order to obtain kinetic equations to be implemented in mathematical models suitable for reactor design.

Catalytic processes for clean up of combustion exhaust gases from stationary and mobile sources. The role of catalytic processes in the abatement of combustion emissions is well established. Typical examples are selective catalytic reduction of NO_x by NH₃ (SCR process), which is widely used for NO_x abatement in thermal power station, and catalytic mufflers and or DPF systems for purification of vehicle exhaust gases.

However, since regulations on combustion emissions are getting stricter and stricter, research in this field is still very active and it is targeted both to the improvement of existing processes and to the development of novel one with superior emission abatement performances.

The Laboratory of Catalysis and Catalytic Processes has been active in this field since 1987, starting with a research on the SCR process performed in cooperation with ENEL. Within this project the research group has developed a wide experience on the preparation, characterization and mathematical modelling of industrial monolith catalysts. On the basis of this background the research activity has been recently re-focused on more innovative processes including: the SCONO_x process for abatement of NO_x emissions from gas turbine power stations (research funded by Edison Termoelettrica); the Toyota process for NO_x abatement in exhaust gases from gasoline and diesel engines with lean and high efficient combustion (research funded by Italian Government); selective catalytic reduction of NO_x by NH₃ or urea for NO_x abatement from heavy vehicle diesel exhaust gases (research funded by Daimler-Chrysler and Corning). This latter process closely resembles conventional SCR, although unsteady state operations characteristics of mobile applications pose peculiar problems on kinetics and on mathematical modelling of the reactor. Such

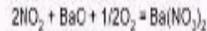
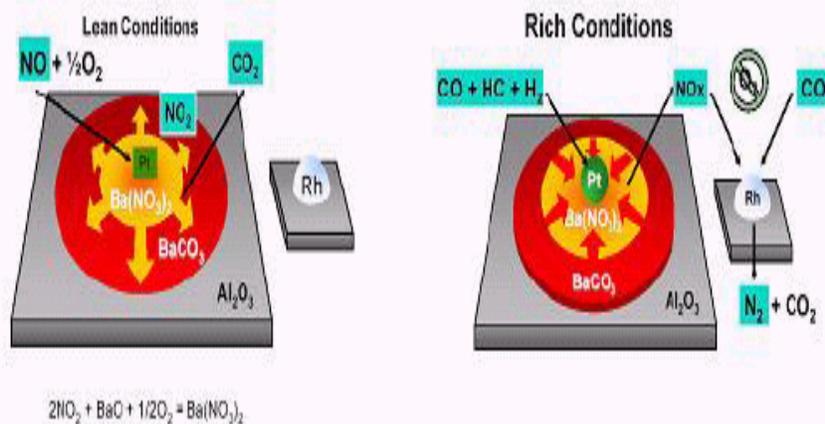
problems have been specifically addressed within the research performed at the Laboratory of Catalysis and Catalytic Processes.



Typical configuration of SCR device for heavy-duty vehicles

The SCONO_x and the Toyota process are both based on the lean DeNO_x concept which consists of alternate cycles between a NO_x storage phase on a alkaline sorbent during the normal lean (O₂ excess) operation regime of the engine and a short regeneration phase performed under rich condition in which adsorbed nitrates are reduced to molecular nitrogen. The research carried out on these processes has been focused to clarify the complex surface chemistry of the two phases with specific attention on the role of noble metals (Pt,Rh). The final target is the improvement of the performances and the reduction of the costs of the materials.

More recently new activities on removal of soot from exhaust gases have been undertaken.



Principles of storage and reduction/regeneration phase in lean DeNO_x processes

The Committee on Nominations and Elections

(N&E) is pleased to announce the final slate of candidates that will appear on the fall 2006 ballot. They are:

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Dr. James A. Walsh, Professor of Chemistry (Retired), John Carroll University, Treasure Island, FL

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Dr. Dorothy J. Phillips, Director, New Business Development, Waters Corporation, Milford, MA

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