CHEMRAWN XVI
Innovation: From Pure to Applied Chemistry
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CHEMRAWN XVI Conference Welcome
Dr. Parry Norling, Dupont, USA

The CHEMRAWN series of conferences are different than other conferences because they involve not just scientists, but public and private industry, media, NGOs, and industrial and academic R&D sectors, all focused on a major world need. During a CHEMRAWN conference, a future actions committee develops a set of actionable recommendations. After the conference, this committee works on follow up activities.

Since 1978, thirteen conferences have been held:

- I Toronto, Canada (1978) "Future Sources of Organic Raw Materials”
- II Manila, Philippines (1982) "Chemistry and World Food Supplies: The New Frontiers”
- III The Hague, Netherlands (1984) "Resource Material Conversion: (Bio) Chemical Process Bridges to Meet Future Needs"
- IV Keystone, Colorado, USA (1985) "Modern Chemistry and Chemical Technology Applied to the Ocean and its Resources"
- V Heidelberg, Germany, (1986) "Current and Future Contributions of Chemistry to Health"
- VI Tokyo, Japan, (1987) “Advanced Materials for Innovations in Energy, Transportation, and Communications”
- VII Baltimore, Maryland, USA (1991) "Chemistry of the Atmosphere: Its Impact of Global Change"
- VIII Moscow, Russia (1992) "Chemistry and Sustainable Development: Towards a Clean Environment, Zero Waste, and Highest Energy Efficiency"
- IX Seoul, Korea (1996) "The Role of Advanced Materials in Sustainable Development"
- X Budapest, Hungary; Washington DC, USA; Honolulu, Hawaii, USA; and Brisbane, Australia (1999-2000) "The Globalization of Chemical Education—Preparing Chemical Scientists and Engineers for Transnational Industries"
- XI Montevideo, Uruguay (1998) “Latin American Symposium on Environmental Analytical Chemistry"
- XIV Boulder, Colorado, USA (2001) “Towards Environmentally Benign Processes and Products"
- XVI Ottawa, Canada (2003) “Innovation: From Pure to Applied Chemistry"

The following conferences are planned for the years ahead:
Senegal or South Africa - "Chemistry, Sustainable Agriculture, and Human Well Being in Sub-Saharan Africa"
Pune, India "Cleaner Energy"
Paris, France "Chemistry and Water"
Kingston, Ontario, Canada "Greenhouse Gas Mitigation"

Today’s event deals with one of the drivers of future development in society: innovation. The R&D process is in turn part of the overall more general innovation process. Here innovation means taking ideas and turning them into something unique and tangible and something that has utility.

Despite the obvious complexity, some companies are still trying to measure the impact of the innovative process by simply analyzing the number of new products introduced during a given time period. Such analyses are made without standard methodology and it is difficult to objectively judge the impact of the innovative process and even compare results from different industries. It is clear that innovation is the key to growth in the U.S. chemical industry. The task of to-days meeting will be to explore the innovative process in the chemical industry and try to answer the following questions:

- Is the current state desirable or not?
- What are the enablers?
- What are the barriers?
- Are there some specific actions that can be taken?

We want to enlighten some perspectives and elaborate on the recommendations. This is an ambitious plan, but it is the task of the CHEMRAWN Committee to carry it out.

Content o f the Proceedings

Papers Summaries

Topic A: Innovative Process and its Modalities

<u>Paper 1: Transformation of the Old Process: Ethylbenzene to Styrene with CO_2 Dilution</u>

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Origin of the Innovation

This invention originated from the use of carbon dioxide, a representative global warming gas, as the soft oxidant in oxidative catalysis. Previous studies of the catalytic conversion of CO_2 have concentrated on utilizing it as a carbon source through catalytic reduction processes with hydrogen. However, this approach was found to be economically unfeasible unless a more efficient process for H_2 production could be developed. So, a group of chemists from the Korea Research Institute of Chemical Technology (KRICT), working under the leadership of Dr. S.-E. Park, developed an alternate approach that utilizes oxygen atoms of a CO_2 molecule. This approach produces not only the oxidant used to abstract hydrogen atoms in the dehydrogenation of hydrocarbons, but it also produces an oxygen transfer agent in the partial oxidation of hydrocarbons. The C-H bond dissociation through the hydrogen abstraction with oxygen is generally accepted to be the rate-determining step in dehydrogenation of hydrocarbons. Therefore, the model for an industrial process was obvious: ethylbenzene dehydrogenation to styrene.

Presently, about 20 Mt of styrene are produced worldwide every year (over 10% is from South Korea), mainly through the direct dehydrogenation of ethylbenzene using potassium-promoted iron oxide catalysts. This is one of the 10 most important industrial processes. The reaction is generally carried out in vapor phase at 600 ^{o}C–650 ^{o}C, with large amounts of excess superheated steam as the heat carrier of the endothermic reaction. As a result, this commercial process is expensive. The steam consumes a large amount of latent heat upon condensation at a liquid-gas separator following the reaction. Moreover, it is thermodynamically limited besides energy consuming. By using the traditional oxidant, oxygen, the thermodynamic limitation can be overcome. However, a process that utilized oxygen directly for oxidative dehydrogenation has not been realized yet because of the significant loss of styrene selectivity by the production of carbon oxides and oxygenates. Judging from the reasons described above and the characteristics of CO_2, the utilization of CO_2 as the soft oxidant can offer many beneficial advantages in styrene production.

Table 1: Comparison of Carrier Gases for Dehydrogenation of Hydrocarbons

Characteristics	Steam	Oxygen	Carbon dioxide
Function	Diluent	Strong oxidant	Soft oxidant, Diluent
Heat capacity	Medium	Low	High
	37.0 J/mol.^{o}K at 673^{o} K	33.2 J/mol.^{o}K at 673^{o} K	49.1 J/mol.^{o}K at 673^{o} K
Advantages	High selectivity	High activity	High selectivity
	Catalyst stability	Exothermic	Activity enhancement
	Coke removal	Less derivatives	Higher equilibrium
			Cheap carrier gas
Disadvantages	High cost of diluent	Low selectivity	Partially endothermic
	Highly endothermic	Dangerous	Second reactor for off-gas
	Latent heat losses	Hot spot	Catalyst deactivation

Thus, CO_2 could play a role as the soft oxidant as well as the dilution agent in the dehydrogenation of ethylbenzene. However, before using CO_2 on a large scale, it must be determined how to obtain it in sizable amounts, and from where. Fortunately, there are many processes that produce CO_2 as a by-product in high concentrationa (e.g., in the petrochemical industry, gas-phase partial oxidation, reforming, etc.). Based on these ideas, researchers at KRICT developed a novel process for dehydrogenation of ethylbenzene to produce styrene using carbon dioxide as the soft oxidant. This process is referred to as the KRICT-SODECO$_2$ process, abbreviated from Soft Oxidative Dehydrogenation of Ethylbenzene with CO_2. In addition to the above advantages, this process uses very cheap CO_2 as a by-product of petrochemical oxidation or the reforming process without further purification, instead of using expensive steam dilution agents. The dehydrogenation catalyst employed comprises oxygen-deficient iron oxide and many promoters with transition metal oxides.

Table 2: The New Catalyst Basic Components

Function	Component	
Active phase	Fe_3O_4	V_2O_5
Activity promoter	Mn	-
Stability promoter	Mo	Sb
Structural stabilizer	Ca,Mg	Mg
Catalyst support	Promoted Al_2O_3 - ZrO_2	

Process Development Modalities

The KRICT- SODECO$_2$ process is under verification through a pilot-scale application so that process and engineering data necessary for industrial application may be collected further. An onsite mini-pilot plant is operating at Samsung General Chemicals Co., Ltd. (SGC). The scale of the pilot plant is 100 kg of styrene monomer per day. When using CO_2 as the oxidant, high selectivity for styrene (>97%), activity enhancement (> 30%), and a drop in reaction temperature (50^{o}C) through equilibrium alleviation have been accomplished compared with the conventional dehydrogenation process. Researchers are working on a more rational design utilizing sufficiently stable catalysts for industrial applications.

Table 3: Comparison of Catalytic Performance Between Commercial and SODECO$_2$ Processes

Catalyst	Commercial	SODECO$_2$
Temperature ^{o} C	SOR 625-575 (600) EOR 655-605 (630)	SOR 525-575 EOR Not fixed
Pressure atm.	0,75	0,75
Space velocity LHSV, h^{-1}	0,75-1	1,0
Carrier/Ethylbenzene molar	8-12	2-10
Styrene yield per pass %	60-66	55-65
Selectivity to styrene %	94,0-96,5	97,0-98,0
Catalyst lifetime years	2	In research

By-products	Hydrogen, BTX	BTX, CO/H_2 10-1,5

Project Funding

The project to develop and establish the KRICT-SODECO$_2$ process was performed for the Greenhouse Gas Research Center, one of the Critical Technology-21 Programs funded by the Ministry of Science and Technology of Korea. Daebo International Company is also a sponsor of and participant in the research. SGC, which joined the project as a cooperating company, has constructed a pilot-scale demonstration unit in the Daesan Petrochemical Complex and is still testing catalyst performance for this process.

Preliminary Assessment of Profitability

The use of steam as a dilution agent in the present ethylbenzene dehydrogenation process causes a number of problems: the need for a diluent recycle, owing to the low conversion achieved per pass (due to thermodynamic limitations); the need for operation at high temperature (up to 650 ^{o}C), and the need for high steam-to-hydrocarbon ratios. It has been demonstrated that a decrease by up to 50^{o} C in reaction temperature through equilibrium alleviation could be accomplished using CO_2 as the oxidant. The preliminary evaluation of the process efficiency is given below.

Table 4: Economic Efficiency of the New Process

Parameters	SODECO$_2$	Conventional
Temperature ^{o} C	560	600
SM Selectivity % Raw material savings USD/t	96.5 4.5	95.0
Loss of latent heat %	66%	100%
Energy savings USD/t	11.0	
Total savings in 0,6 Mt/year unit USD million	9.3	

A preliminary assessment shows that this new process would reduce energy costs by 33% (6.5 M dollar for 0.6 Mt-SM/year) compared to the conventional process. Now, the KRICT inventors are trying to verify these results in mini-pilot-plant work at petrochemical complexes.

Paper 2: Use of X-Ray Imaging in the Innovative Development of BP's Leap™ Technology

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Origin of the Innovation

In the mid 1990s, BP embarked on a fundamental restructuring of its European chemicals operations to create strategic, world-class assets. The acetyls business needed to replace two small vinyl acetate monomer (VAM) plants (Baglan Bay, Wales and Porto Marghera, Italy) with a new plant in Hull in the Northeast of England, which was to be fully integrated with feedstocks of BP ethylene and acetic acid. However, in the mid-1990s the cost of a conventional fixed-bed process did not make the investment attractive. Conventionally, such processes pass through a "demonstration" phase, which is, effectively, a small-scale commercial unit. Building such a unit would have meant an additional cost of USD20-30M and an unacceptable delay of three to four years in commercial implementation.

The option of exiting the market was even less attractive; therefore, BP researched how to ramp up development of a new fluidized bed route as a more cost-effective solution. The potential savings in the new process—branded as Leap™ technology—came from process simplification and intensification made possible by use of a fluidized bed process, which required only a single reactor compared with two fixed bed reactors. In 1995, the Leap™ technology had only been demonstrated at microreactor scale. The challenge was to scale up the process by 2001.

Process Development Modalities

In order to solve this problem, a virtual-team was set up with BP technologists in Hull and Sunbury in the UK, and Warrensville (and later in Naperville) in the USA, to work on different aspects of catalyst screening, preparation and testing. Expertise was also drawn from other relevant technologies such as BP's acrylonitrile and polyethylene businesses. The development team broke the challenge into its individual steps and developed techniques to understand each step.

The key technical challenges in development of this process were:

- formulation of precious-metal catalysts in fluid bed form
- establishing reaction kinetics and optimum conditions
- establishing the fluid dynamics and reactor design criteria
- constructing all embracing models

Fluid bed processes are notoriously difficult to scale up, as the complex interactions between process chemistry and fluid dynamics are difficult to establish at actual operating conditions. In addition, there are no proven theoretical predictions, which makes PC models unreliable. In order to design the new fluid bed reactor, it was imperative that the physical properties of the fluidized catalyst were assessed within a fluidized system. X-ray imaging at BP's unique VIPA (visualization imaging and analysis) center was used to observe the behavior of the fluidized process inside a reactor. The VIPA center studies processes under full temperature and pressure conditions. It uses the data to accelerate process development and optimize engineering designs.

The imaging equipment consists of an x-ray gun and receiver mounted on a fully programmable suspension system which can be moved in 3-D around a hydrodynamic test rig. Very high power x-rays are pulsed through the reactor and videos are taken of the images at 50 frames per second. The most promising catalysts were identified on the small scale and then scaled up and assessed in a small pilot plant (module 70x), which was used later to develop the reaction kinetics and optimum operating conditions (module 14,000x commercial scale).

The main elements of the bed were identified:

- grid design for gas distribution into the bottom of the bed
- systems to distribute the reactants within the bed
- cooling coils to remove heat from the exothermic reaction
- systems for capturing fines and returning them to the reactor

Throughout the process development, models were developed and finessed as new or refined data came in. Modeling assessed the combined effect of the chemistry and the process dynamics to determine the shape of the final process. The main models produced included the following:

- overall heat and mass balance of the process
- model of the catalyst management strategy
- reactor model giving local compositions within the reactor

The Result

The first time the full process was put to the test was when the plant started up at the end of 2001. During the start up, the process operation could be monitored on six screens—including a wall-sized display. The oxygen was turned on and the team watched as the temperature rose. A few hours later, on specification vinyl acetate was being produced and moved into bulk storage. The decision to go to a fluidized bed saved 30% in capital costs. The plant, the worlds first fluidized bed process for VAM, is rated at an annual capacity of 250,000 tons and output volume can be increased further in line with market penetration. Research work continues and options for further capacity increases are under development. Because over 80% of today's VAM plants are more than 20 years old, the Leap™ competitive edge will continue to increase as other VAM manufacturers face similar decisions on investing in new plants based on costly fixed-bed facilities.

The success of BP's innovative development of the Leap™ Technology was recognized in June 2002 by the Institution of Chemical Engineers (UK) when they awarded BP the Aspentech Award for Business Innovation.

Paper 3: New Innovation Concept at Degussa: Project Houses and New Business Development

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Positioning Degussa AG

Degussa is a multinational corporation with sales of EUR 11.8 billion and a workforce of some 48 000. It is Germany´s third-largest chemical company and the world market leader in specialty chemicals. In fiscal year 2002, the corporation generated operating profit (EBITA) of more than EUR 900 million. Degussa´s core strength lies in highly effective system solutions tailored to the requirement of its customers in over 100 countries throughout the world. The corporation is led by the vision "Everybody benefits from a Degussa product—every day and everywhere."

Table 1: Sales by Regions

Region	% of sales
Germany	26
Rest of the Europe	30
NAFTA	25
Asia	14
Latin America	3
Others	2

The industrial activities of Degussa are oriented towards specialty chemicals, such as admixtures for concrete, foaming stabilizers, probiotic cultures, crosslinking agents, and special polymers like polymethylacrylimide. For the customers of such specialty chemical products, the cost/risk factor of substituting possibly cheaper products is so high that changing suppliers is less probable than with other commodities. Therefore, R&D activities create the foundation for sustainable growth of the business in the following ways:

- taking care of the product portfolio and defending the market share
- establishing new technology platform for growth in existing markets
- developing new markets/new applications for existing technologies
- developing new technologies for future markets

R&D Operational Management

Worldwide, Degussa operates more than 50 R&D sites that employ over 3 300 people and have annual expenditures of 343 M Euro (about 3% of sales). These R&D operations have obtained 47 000 patents and established a large network of cooperative research through 500 cooperative activities (year 2002).

The R&D responsibilities are divided in three parts:

1) Business Unit (BU) Innovation Management
   - allocation of BU's R&D budgets according to the BU strategy
   - R&D portfolio management
   - R&D project management
2) Corporate Innovation Management
   - corporate guidelines (best practices)
   - allocation of corporate funds according to the company strategy
   - provides a check and balance of BU's technology positions regarding SMP, investments, M&As
   - supports BU innovation through coordinating of internal/external R&D networks and R&D information systems
3) Creavis Technologies and Innovation (special corporate organization independent of BUs)
   - strategic radar, technology watch
   - idea management
   - new business development (outside existing portfolio)
   - supervision of a project house and corporate funded R&D
   - management of corporate venture capital

R&D funding levels are established to motivate sustainability on the one hand and on the other hand responsibility for fund utilization:

a) Operative R&D, in the framework of BUs related to the core competencies of Degussa and new markets, is 100% financed by individual BUs.
b) Projects with high risk related to the emerging markets and new technologies are financed by sharing the costs (50:50) between the corporation and BU.
c) New businesses development outside the existing portfolio is financed by the corporation at 10% of the BU's R&D budget. Corporate R&D activities with long-term and strategic relevance are performed independently. These projects are run by the Creavis organization. They are focused on product or market segments outside the current portfolio that have high growth and revenue potential.

Every R&D project is implemented in a certain sequence allowing for control and elastic decision making. The so-called Project Houses implement R&D projects according to a specific pattern:

- explore technology in high-risk areas
- establish a joint effort of several BUs with Creavis
- ensure 50% funding from corporation
- delegate projects team members from BU to a central location (campus)
- share company knowledge and infrastructure
- cooperate with academia and other R&D institutions

Under company rules, these projects may only continue for for three years after which time they are either cancelled, integrated within an existing BU, or a new business is started.

Project Houses

Innovation management enhances the efficiency of R&D by creating and supporting corporate technology platforms. The Project House methodology ensures the R&D process is more efficient than with standard R&D projects.

Table 2: Project Houses Pattern of Operation

Standard Projects	Project House
R&D related to one BU	R&D projects link several BU
little interdisciplinary cooperation	interdisciplinary approach is a success factor
"daily work" has priority	strategic projects only
limited transfer of know-how from universities	fast and direct transfer of know-how from universities
limited time for basic research	basic research as a chance for visionary potential identification
low cross-linkage with customers	high cross-linkage with customers

The first Project House was related to nanomaterials. As a result of its activities, the following marketable products have been developed:

- ZnO
- In_2O_3/SnO_2 (ITO)
- CeO_2
- Fe2O3@SiO2
- Composites
-

In 2003, the following projects were carried out in Project Houses:

a) biotechnology
    - started January 2001
    - 8 BUs participating
b) catalysis
    - started June 2001
    - 7 BUs participating
c) functional polymers

Creavis is also responsible for supporting start-ups with venture capital. This is a strategic way for the company to establish leadership in emerging technologies. Creavis helps start-up companies in the following ways:

- validating business models
- supporting the generation of business plans
- searching for strategic partners
- validating strategic partners
- searching for strategic acquisitions
- realizing exit strategies

4. Conclusions

The Degussa strategy in the R&D area may be summarized as follows:

a) have a strategy to do right things
b) keep focus and balance resources
c) apply most modern techniques, organize interdisciplinary teams
d) use available information
e) manage projects in a well organized manner with well-established go/exit milestones

Paper 4: Innovation in the U.S. Chemical Industry

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Chemical Industry in the USA

The chemical industry in the United States represents an important segment of the national economy. Annual shipments amount to 400 USD billion, nearly 2% of the U.S. GDP. Around 50% of the chemical industry output serves other manufacturing industries. U.S. plants account for 24% of the total world chemical industry. These results were achieved thanks to intensive R&D and innovative processes.

The U.S. chemical industry has grown to its current size because industry understood how to take products of science and create value. Entire industries have resulted from research in magnetic resonance, superconductivity, lasers, and antibiotics, just to name a few. A study sponsored by the Council for Chemical Research found that for each dollar invested in chemical R&D in the USA produces 2 dollars of income over a seven year period—a 17% rate of return.

Concern Today

Despite the benefits of R&D, the "traditional" chemical industry (excluding life sciences) has seen its innovation rate dive during the past decade, as its R&D intensity (ratio of R&D spending to sales) has declined from 6% to 4%.

Table 1: Major Product Advances in the "Traditional" Chemical Industry

Years	Number of innovative products
1930-1949	40
1959-1969	20
1970-1989	2
1990-2000	2

Although the drops in the innovation rate and R&D intensity are relatively small, they pose certain questions about the future of the chemical industry:

- Are we walking away from discovery research and breakthrough technologies?
- Will innovation be a means to remain competitive?
- Are the new directions clear in R&D for the chemical industry?

It must be considered, as the Council for Chemical Research study has shown, that chemical technology is essential to such non-chemical industries as computers and peripherals, semiconductors and electronics, telecommunications, biotechnology, and pharmaceuticals. Patents for chemical technology arise from many different manufacturing industries.

As the U.S. chemical companies looks forward, they must decide whether mature businesses need to be replaced and whether they should invest in emerging areas such as advanced materials or nanotechnology. During 2004, the U.S. government increased investments in R&D by 123 billion, up 7% from 2003.

There are a number of enabling tools that are being employed by the U.S. chemical industry in efforts to spark innovation:

- **Modeling and simulation:** Significant advances are being made in computational chemistry and modeling and simulation techniques. A number of modeling and simulation packages are now available.
- **Green chemistry and bio-based processes:** CHEMRAWN XIV focused on green chemistry and the 2003 RAND report on "Next Generation Environmental Technologies: Benefits and Barriers," looks at manufacturing processes derived from green chemistry. Many of these processes are bio-based, using enzymes as the reaction catalyst.

- **Combinatorial chemistry and high-throughput experimentation:** This methodology has enormous impact on the number of feasible options and solutions.

Green Chemistry
Green chemistry is a multifaceted concept devoted to the invention and application of chemical products and processes designed to reduce or to eliminate the use and generation of hazardous substances. environmentally benign and sustainable chemistry. Green chemistry can be an alternative to end-of-the-pipe pollution prevention.

The RAND report presents 24 case studies and 47 examples of bio-based processes and covers the following issues:

- sectors affected now and in future
- immediate and long term benefits
- barriers to commercialization
- government role

The report shows that innovation is not a linear process, but involves many activities in idea development and concept/technology development. The report evaluates interesting case studies in the following areas:

1) use of supercritical or liquid CO_2 as solvent
    - solvent of surfactants in the dry cleaning
    - production of fluoro-polimers
    - computer chip manufacture
    - ibuprofen short synthesis (three steps instead six)
2) Bio-based processes (47)
    - genetically modified Echerichia Coli producing adipic acid, catechol, and substitute for BHT
    - 1,3 propanediol from glucose
    - biopulping
    - biocatalytic conversion of 5-cyanovaleramide
    - removal of metals from mine water
3) Pulp and paper processes
    - non-chlorine pulp delignification and bleaching
    - activation of hydrogen peroxide with species which mimic enzymes
4) Production of polylactides
5) Production of hydrogen peroxide directly from H2 and O2 in CO2
6) Synthesis of key intermediate for Monsanto Roundup
7) Sentricon termite colony elimination system

Modeling and Simulation
Modeling technology has been available to scientists for several decades, although it become more powerful every year. Large-scale interactive, intrinsic, and iterative models are now used for climate modeling, material sciences, fluid and solid mechanics, biological systems, and testing the interaction of new drugs with cells and bacteria. The sequence of modeling and simulation in principle is rather universal and include the following steps:

- understand the system
- prepare a mathematical interpretation of system
- prepare the model
- operate the model in a discrete or continuous manner to determine the functions of system and interaction of parameters and variables.
- analyze the results and adjust the model

Combinatorial Chemistry
The combinatorial methodology in general, and in chemistry in particular, includes preparation and use of libraries of materials and their properties, including permutations of variables. The use of these libraries ensures high throughput of experimentation. This methodology has been advanced by the establishment of a new government center that helps industry develop high-throughput methods to measure material properties of polymers.

The fields of application for combinatorial chemistry are continuously growing. The following areas of research have benefited from combinatorial chemistry:

- Drug discovery methodology has improved due to advances in synthesis, purification and analysis.
- In the field of catalysis, typically spots representing a matrix of catalyst compositions are prepared by robot or in plates of micro-reactors. The array is then put into a reaction chamber from which measurements are taken and sent directly to a computer that manipulates the data and creates a graph visualizing the results.

A recent success story in this field is that of the four-year cooperative effort by Symyx Technologies, Exxon Mobil, and Dow that yielded the discovery of a new class of single site catalysts for olefin polymerization. Currently, considerable activity in the field is carried out outside the USA by the companies:

- Avantium Technologies with Degussa
- Pfizer and Millenium
- HTE with BASF

The challenges for combinatorial chemistry have to do with software development. However, advances in this area are very quick; tools used today did not exist 18 months ago. This acceleration is expected to mean faster results in complicated areas of research.

Conclusions

- The chemical industry is moving into new domains.
- A number of new tools and approaches are enabling chemical companies to be more effective in their R&D efforts.

<u>**Paper 5: Peculiarities of the Innovation Process in Russia and Siberia**</u>

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Introduction

Siberia as a geographic area is an important part of today's Russia.

Table 1: The Geographic Features of Siberia

Countries/features	Russia	Siberia	Canada	USA	China
Area sq.km x1000	17 075	9 653	9 976	9 373	9 597
Population x1000	148 306	25 530	28 434	263 814	1 203 097
Population density men/sq.km	8,7	2,7	2,9	28,1	125,4

Siberia possesses the majority of the natural resources in Russia.

Table 2: Siberia's Share of Russian Natural Resources

Resources	Share in %
Crude oil	65
Natural gas	85
Coal	75
Hydroenergy	45
Timber	>50

In addition to the resources listed in the table, significant deposits of iron ore, non-ferrous metal ores, noble metals, and diamonds are present in Siberia. In an effort to develop these resources and make them useful to the entire country, a major scientific program has been organized by the Russian Academy of Science (RAS) through its Siberian Branch (SB) centers located in 11 cities . Eight of the locations are international research centers. Chemistry research is carried out at seven of the SB centers. Nearly 100 field stations are now operational for studying geo-cosmophysics, seismology, permafrost geography, and biospheric areas of research.

Peculiarities of the Innovative Process

The social and economic transformation that occurred in Russia after the dissolution of the Soviet Union had a significant role in changing the functions of the Russian Academy of Science. The previous scheme of developing innovations from the academic institute through the industrial institute has changed due to the lack of central financing for academic and industrial research. Under the current scheme, a pilot producing unit in the academic institute and the results, as well the processes or even final products, are offered to industrial enterprises. Obviously, this change has required that research be concentrated on the most advanced technologies and production equipment. Below, two examples of research and implementation of the innovative process are given.

Oxide Crystals

The LTG Cz technique has been developed and practically applied to produce laser crystals. This technique has the following advantages:

- During the entire process, the grown crystal stays inside the crucible.
- Weighting control is assured at all the stages of the process, including seeding.
- Temperature gradients are within 0.05-1.0 deg/cm. The temperature fluctuations in melt are not observed.
- Evaporation and decomposition processes are suppressed by the special pipe socket that works as a diffusion barrier.
- The faceted interface develops, and layered growth mechanism prevails.

More than 2 different laser materials of the general structure:

$M^{+} Ln (WO_4)_2$

where M= Na, K, Cs and Ln= Y, La, Nd, Gd, Ho,Er has been synthesized and applied.

The temperature of growth could be controlled between 735 ^{o}C to 1170^{o} C and different crystalline structures were possible (e.g., monoclinic, tetragonal, and rhombic, with crystal sizes starting from d=10mm L=30 to the size of tetragonal 60mmx60mmx150mm). The laser parameters were extraordinarily stable and in line with operational requirements of wave length and density of light.

The crystals have been used in a gamma-ray instrument in the BGO VETO Shield in the Imager IBIS on board the ESA mission INTEGRAL. Also, they have been used in the Belle Detector in KEK Tsukuba Japan.. Special tests have been conducted of the Cd WO_4 crystal at the NASA Godgard Space Flight Center, which show extraordinary stable transmittance through the diapason of the wave length between 350-600 nm.

Power Electronics

Silicon systems are the basic structural element of power electronics. They are used in :

- production of electricity
- transportation of electricity
- use of electricity

The program "Power Electronics of Siberia" is a multilateral approach to complex solutions, involving the regional government, SB RAS, Ministry of Atomic Energy, and Ministry of Electronics. The program consists of the following components:

- starting materials
- wafers and structures
- power electronic devices
- power electronic systems
- application of power electronic:
  - system planning
  - economics
  - legal support
  - ecology

The following table shows the types of silicon research carried out by the program.

Table 3: Silicon Research Program

Products Researched	**Research Program**
Raw material	New types of raw material New process of SiO_2 reduction
Metallurgical silicon	Direct hydratation of M-silicon
Chlorosilanes	Different ways of $SiCl_4$ conversion
Poli-silicon	Perfection of single crystal growth Optimizing the reduction process and recycling of products
Single crystalline Si	New processes of IC's

In the raw materials area, SiO_2 instead of $SiCl_4$ has been used along with LiH, to produce SiH_4. On the other hand, a new electronic beam device with an adjustable irradiation dose of 20 to 320 Mrad was used to irradiate $SiCl_4$ in the presence of hydrogen.

Power electronics research is also being conducted on an industrial scale. One innovation of note is the ERATON semiconducting electric drive, which continuously adjusts the rotational speed of AC and DC electric motors. It increases the life of the drive, saves electric power, and increasing the productivity of the system. It is available for capacities from 2.2 kW to 315 kW at the frequency of 1-100 Hz. Another example of innovative and ambitious research is to modify automobile electronics. At present, electromechanical power steering and a new starter generator are being tested.

The SB of RAS is ready to cooperate internationally in the field of power electronics and in particular in the following directions:

- high-quality silicone
- thermoelectric materials

- storage batteries
- portable phone communication systems
- automobile electronics engineering
- crystal chips production
- crystal chips encapsulation
- the household electrical appliances.

-

3. Conclusions

At present, intensive research is being carried out, supported by local industries and government organizations, in the following areas:

- production of monosilane and polysilicon (20 t/year)
- pilot-scale production of single silicon crystals
- starting production of epitaxial structure for MOSFET (wafers and structures)
- IGBT transistors and modules
- drivers for IGBT at voltage 1200V
- optoelectronic devices for drivers of high voltage
- high-voltage controllers for motors over 400 kW
- frequency converters for metal working machines

power electronics for automobiles (ignition system, engine control system, voltage controllers for 42 V, electromechanical power steering, starter- generator system, etc.)

Topic B: Instruments of Support in the Process of Transforming Inventions into Innovative Processes

Paper 1: Innovation Tools for Commercializing Process Technology

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Abstract

The worldwide process industry, which includes chemicals, petrochemicals, and petroleum refining, is a complex and interconnected global business. It achieved tremendous growth and development in the 20th century, driven primarily by innovation in chemistry and engineering. The industry also evolved in an era of relatively cheap energy and a seemingly limitless supply of raw materials.

Today, innovation in the process industry must not only seek to improve beyond the very high level of technology sophistication which already exists but also must recognize the limits articulated by sustainable development. As a leading technology supplier, UOP LLC must continuously renew its process technology portfolio. UOP employs a suite of innovation tools to enhance and accelerate its technology commercialization process. These tools are applied all along the commercialization path, providing fundamental knowledge that is essential to making correct decisions in a gated process for technology delivery. This paper provides an overview of these innovation tools and presents examples of their application at various stages of the commercialization of process technologies.

Background

The history of the process industry is a story of technical accomplishment and innovation. Achievements during the last century have led to both tremendous growth and a high level of process development. In the hydrocarbon processing industries, UOP has been a leader in developing and commercializing process technology for more than 80 years. UOP's first technology for license was the Dubbs thermal cracking process, which made possible a variety of important oil-derived products. Subsequently, UOP has contributed processes in many areas, including motor fuels, plastics, detergents, synthetic fibers, and food preservatives. UOP has become the largest process licensing organization in the world, providing more than 65 processes for license.

With the exception of the Sulfolane™ process, which was commercialized in the 1960s, UOP's "top-ten" petroleum refining processes in Table 1 were all commercialized between 1930 and 1960. Over the ensuing decades, innovations in materials, catalysis, and engineering have generated continuous improvements.

Table 1: Top 10 Refining Processes Licensed by UOP

Process	Description	No. of Units
1. Merox™	Mercaptan Extraction & Oxidation	1650
2. Platforming™	Naphtha Reforming	753
3. Unionfining™	Hydrotreating	675
4. Catalytic Polymerization	Oligomerization of Light Olefins to Gasoline	301
5. Fluid Catalytic Cracking	Gas Oil & Residue Conversion	212
6. Unicracking™	Hydrocracking of Petroleum Fractions	126
7. Sulfolane™	Extraction of Aromatics	106
8. HF Alkylation	Isobutane Alkylation with Light Olefins	105
9. Catalytic Condensation	Oligomerization of Light Olefins to Distillate Fuel	101
10. Isomerization	Conversion of normal C_5/C_6 paraffins to branched paraffins	99

As a result of innovation, refining processes are now at a high level of maturity, as demonstrated by the Platforming and Fluid Catalytic Cracking (FCC) processes for gasoline production. A parameter for evaluating the efficiency of a gasoline process is the "Octane Barrel" yield. Octane Barrels are defined as the Research Octane Number times the relative volume of gasoline produced:

Octane Barrels = RON x Barrels of Gasoline Product per 100 Barrels of Feed

The Platforming process was commercialized in 1949 as the world's first process for the catalytic reforming of naphtha via noble metal catalysis. The theoretical yield of Octane Barrels from naphtha reforming is 8600 to 9300, depending on feedstock composition. In the 1950s, the Platforming process was achieving approximately 80% of theoretical yield. Today, catalyst and process innovations produce yields that are greater than 90% of theoretical, along with substantially lower capital and operating costs. Historical advances in performance are given in Table 2.

Table 2: Platforming Process Historical Performance

Decade	@ 81 LV% Gasoline Yield		@ 99 Research Octane Number	
	Research Octane	OB	Gasoline Yield, LV%	OB
1950s	91	7400	-	-
1960s	96	7780	76	7520
1970s	99	8020	81	8020
1980s	102	8260	83	8220
1990s	105	8500	86	8510

FCC is another key refining process that has undergone continuous improvements in efficiency since its introduction in the late 1940s. Standard feedstocks are vacuum gas oils, for which theoretical yields are typically 6200 octane barrels. Amorphous catalysts were used in the early years of FCC, providing good octane and 4900 to 5100 octane barrels of gasoline. The introduction of zeolite catalysts in the late 1960s provided a step increase in yield to about 5300 octane barrels. The high activity of zeolite catalysts permitted lower residence times, leading to reactor improvements such as extended risers. In the 1970s and 1980s, ultra-stable Y zeolites, ZSM-5 zeolite additives, and many engineering innovations further increased octane barrels. Greater than 95% of theoretical yields have been achieved since the 1990s.

In the 20th century, principal focal points for process innovation in the hydrocarbon processing industries were yield and energy efficiency. In the 21st century, sustainable development has also become a key driver for innovation. For the production of transportation fuels, the challenges presented by sustainable development include cleaner fuels, alternatives to crude oil as a feedstock, and minimization of environmental impact. Cleaner fuels require cost-effective processes that yield products with zero sulfur and low nitrogen; new gasoline specifications demand a reduction in aromatics and olefin content while maintaining high octane. Alternatives to crude oil as a feedstock include renewable resources as well as increased utilization of natural gas. Minimizing environmental impact requires refineries to continue reducing emissions and to have better options for handling, disposal, and recycling of spent catalysts. With these new challenges, UOP must maintain its historical emphasis on innovation in order to preserve its leadership position in process licensing.

Technology Delivery Process

Innovation at UOP is supported by the work process in Table 3. It was designed specifically for new product/process development. It is accompanied by necessary experimental tools for materials and process innovation.

Table 3: UOP Gated Technology Delivery Process

Step 1:	**Idea Generation and Management** ***Gate 1: Project Selection***
Step 2:	**Idea Validation** ***Gate 2: Business Plan Approval***
Step 3:	**Business and Technology Development** ***Gate 3: Full-Scale Production Approval***
Step 4:	**Finalized Technology Package** ***Gate 4: Product Launch Approval***

Step 5: First Commercial Installation
Gate 5: Customer Acceptance

In order for a new idea to be successfully transformed into a new commercial product or process, it must pass through five gates of approval. At each gate, there are technical and business criteria that must be met. The first step is Idea Generation and Management, where ideas are sought from sources external to UOP as well as from employees participating in internal idea generation campaigns. Collected ideas are reviewed at the Project Selection gate. The criteria for approval ensure that approved projects are aligned with UOP's strategic business goals.

At each succeeding step in the work process, the gate criteria become more quantitative. Step 2 is Idea Validation, which requires laboratory experimentation. Prototype products (catalysts or adsorbents) are prepared and tested in screening experiments. The results must meet technical milestones established in a preliminary economic analysis.

In Step 3, Business & Technology Development, both product and process development are underway, requiring pilot-plant testing and the development of kinetic and process models. If rigorous business and technical criteria are met at Gate 3, the Finalized Technology Package is prepared in Step 4. Product scale-up is demonstrated via trial runs in UOP manufacturing plants. Commercial prototype products are tested with commercial feedstocks in pilot plants that incorporate all features of a commercial design, including recycle loops. Pilot-plant data are used to validate the design so that capital costs of a commercial plant can be estimated. When Gate 4 criteria are met, the new UOP process and/or product are launched. Step 5, the final step, is the First Commercial Installation of the new technology, with UOP working closely with the customer to ensure commercial success. The final gate criteria are satisfied when the technology has met UOP's guarantees and has been fully accepted by the customer.

The methodology of Six Sigma is utilized throughout the Gated Technology Delivery Process. The combination of UOP's work process and Six Sigma has proven to be very effective in internal projects and now is also facilitating collaborations with other companies. Examples of past collaborative development programs are given in Table 4.

Table 4: UOP Processes Developed in Collaboration with Others

Process	UOP Partner	Application
1. Cyclar™	BP	LPG to Aromatics
2. Detal™	CEPSA	Fixed Bed Alkylation for Detergents
3. Ethermax™	Hüls and Koch	Etherification
4. MTO	Norsk Hydro	Methanol to Olefins
5. Phenol	Sunoco	Cumene Oxidation
6. Tatoray™	Toray	Toluene Transalkylation
7. Thiopaq™	Paques Natural Solutions	Biodesulfurization of Caustic

Materials Innovation Tools

UOP processes employ proprietary catalysts and adsorbents which are expressly formulated from materials whose properties enhance the desired reactions and separations being performed. When a new material is discovered, it must be characterized, modified and screened for potential process applications. If an application is found, the preparation of the material must be scaled-up for commercial production. Materials innovation tools are applied at all stages, from discovery to manufacturing.

At the materials discovery stage, the pursuit of new synthetic zeolites has been ongoing for over 50 years. Zeolites are microcrystalline or nanocrystalline, porous aluminosilicates. They have become important materials for catalysis and adsorption in many process applications. Zeolites offer high-acid site density (low Si to Al ratio) for catalytic applications, as well as ion-exchange and compositional diversity for separation applications. Table 5 is a summary of zeolite discovery and application:

Table 5: Zeolite Discovery and Use by Decade

Decade	Known Structure Types	U.S. Patents (Composition or Use)	Commercialized Structure Types
1950-1969	27	2,900	3
1970-1979	11	4,900	1
1980-1989	26	7,400	2
1990-1999	61	8,200	5
Totals	125	23,400	11

New zeolites continue to be discovered, and there are now 145 structure types recognized by the International Zeolite Association. Knowing the crystal structure of a zeolite provides better understanding of its catalytic and adsorptive properties and of potential applications. Selected tools for solving the structure of a zeolite are given in Table 6.

Table 6: Structure Solution Tools

Problem to be Solved	Tools Applied
1. Primary Building Unit	Elemental Analysis
2. Secondary Building Unit	Fourier-Transform Infrared Analysis Nuclear Magnetic Resonance Probe Molecule Adsorption
3. Superstructure and Defects	Powder Diffraction Electron Diffraction Transmission Electron Microscopy High Resolution Transmission Electron Microscopy
4. Model Building and Verification	Distance Least Squares Refinement Rietveld Method

A zeolite's primary building units are single TO_4 tetrahedra, where T is a tetrahedrally coordinated atom in the framework. Up to 16 T-atoms form a secondary building unit. The entire framework, or superstructure, of the zeolite is constructed from a repeating combination of secondary building units. Powder diffraction data are analyzed by DLS Refinement or the Rietveld Method to build and verify framework models.

New and improved tools have significantly reduced the time required to solve the structures of nanocrystalline zeolites. In the comparison in Table 7, the structure of UZM-5, a new UOP zeolite, was solved in only 10 months. By contrast, Beta zeolite required a time period of over 10 years.

Table 7: Acceleration of Structure Solution

Event	Beta Zeolite	UZM-5 Zeolite
1. First Synthesized	1967	1999
2. Time to Solve Structure	>10 years	10 months
3. Structure Reported	1988	2002

The crystals of UZM-5 have plate-type morphology and typically are in the 2-20 nm size range. Although UZM-5's structure solution was not routine, it was greatly accelerated by applying electron diffraction and high-resolution transmission electron microscopy to the task. The material has two-dimensional channels that are approximately 0.4 nm in diameter. This pore size is consistent with the observed adsorption of normal butane in UZM-5 and the relative exclusion of isobutane.

The external surface contains cavities that are 0.8 to 0.9 nm in diameter. These cavities are sites where catalytic reactions such as xylene isomerization or benzene alkylation can occur, involving molecules that are excluded from the 0.4 nm pores.

The primary tool now being used for the discovery of new materials at UOP is the End-to-End™ combi-chem system jointly developed by UOP and SINTEF. Preparation and treatment steps can significantly change the properties of a heterogeneous catalyst. With UOP's combi-chem system, materials in a synthesis tray can be taken through all of the steps required for catalyst evaluation. The experimental design can also include multi-variable studies within a preparation step with a single material. The final step is catalyst screening, where the formulations are tested for activity and selectivity in a catalytic reaction. Table 8 shows the five steps in the system and the procedures that can be conducted at each step.

Table 8: End-to-End Combi-Chem System

Input: Hundreds of Ideas	
Step 1: Combinatorial Synthesis:	One-Shot Synthesis of Libraries of Materials
Step 2: Post Synthesis Processing:	Ion Exchange, Metals Addition
Step 3: Finishing:	Oxidation, Steaming, Oxychlorination
Step 4: Pretreatment:	Reduction
Step 5: Screening:	Parallel Screening of Catalytic Formulations
Output: 2 to 5 Leads for Scale-Up	

The End-to-End combi-chem system allows UOP to quickly and efficiently select the most promising candidates for scale-up and testing in pilot plants, to reduce the overall time spent on development, and to increase the probability of producing a superior product. The overall time for catalyst and process development is thereby reduced, resulting in a higher throughput of technology commercialization.

PI-242™ catalyst is an example of a UOP product developed from a combi-chem discovery. The combi-chem goal was to discover scale-up candidates for development into a new catalyst for the isomerization of C_5 and C_6 alkanes:

Table 9: Isomerization of C_5 and C_6 Alkanes

Feed	Feed RON	Products	Product RON
n-Pentane	61.7	i-Pentane	93.5
n-Hexane	31.0	2-Methyl Pentane	74.4
		3-Methyl Pentane	75.5
		2,2-Di Methyl Butane	94
		2,3-Di Methyl Butane	105

Alkane isomerization proceeds via a carbonium ion mechanism and is conducted in the presence of hydrogen. Branched alkanes have significantly higher RON (or research octane number) than normal alkanes and are thermodynamically favored at lower temperatures. A desirable isomerization catalyst will also promote benzene saturation, so that any benzene in the feed will undergo saturation to cyclohexane, isomerization to methyl cyclopentane, and ring opening to normal hexane. These reactions do not provide a net octane boost, but they have the advantage of reducing benzene in the product in order to meet gasoline specifications.

Commercial C_5/C_6 isomerization catalysts can be classified as either "high-activity" or "low-activity." High activity is preferred so that isomerization can be conducted at lower temperatures, which promotes the formation of higher-octane products. The high-activity catalysts are chlorided aluminas. Their reactor systems require a relatively high capital investment because the metallurgy must be resistant to acidic chlorides. The low-activity catalysts do not utilize added chloride to sustain acidity. Their reactor systems have lower capital cost, but the low activities require higher temperatures to achieve the necessary rates of reaction. The combi-chem program was seeking non-chlorided, high-activity catalysts for lower-capital reactors.

A prior R&D project screened 271 experimental isomerization catalysts in 3 years with conventional equipment before identifying the most promising candidate for scale-up. In the combi-chem project for PI-242 catalyst, 512 experimental catalysts were screened in only 5 weeks, and three promising candidates were identified. The relative performance of the final commercial product is shown in Table 10.

Table 10: Catalyst Activity Comparison

Catalyst	**Temperature, ^oC**	**C_5+ RON**
Commercial UOP Chlorided Alumina	120	82.4
PI-242	150	81.6
Commercial UOP Sulfated Zirconia	165	81.4
Commercial UOP Zeolitic	270	79.4

In Table 10, catalyst activity is measured by the temperature required to achieve a close approach to thermodynamic equilibrium at fixed pressure and liquid hourly space velocity. The data were obtained from a UOP pilot plant processing a commercial C_5/C_6 feedstock. Commercial zeolitic and sulfated zirconia catalysts are lower in activity than commercial chlorided alumina catalyst and hence require higher operating temperatures and yield lower octane products. PI-242 catalyst is a high-activity catalyst for lower-capital reactors, meeting the goal of the combi-chem program.

Many other innovative tools are used in the Gated Technology Delivery Process. Advanced characterization tools examine the active sites on a catalyst and guide modifications. Probe reactions are conducted to resolve reaction intermediates and catalytic cycles. For rapid catalyst/adsorbent scale-up, UOP employs diverse crystallization methods for zeolites and a variety of forming technologies.

Process Innovation Tools

UOP's Gated Technology Delivery Process also makes use of process innovation tools. Pilot plants are key tools that are essential for process development. UOP has over 75 pilot plants in continuous operation, ranging from quick screening tests to extended process demonstrations with integrated gas and liquid recycle streams. Automated data acquisition, on-line product analysis, and informatics software make information quickly available to R&D personnel.

Kinetic modeling is a fundamental innovation tool and is begun at an early stage of process development. Kinetic models are developed from pilot plant data and are used to develop the most appropriate design for commercial reactors. Table 11 correlates kinetic criteria and reactor design for 10 UOP processes.

Table 11: ***Reactor Design from Kinetic Modeling***

Reaction Kinetics Time Constant	Catalyst Deactivation Time Constant					
	Seconds	**Minutes**	**Hours**	**Days**	**Months**	**Years**
Hours				Ebulating Bed		Fixed-Bed Axial Flow: *Hydrocracking*
Minutes		Liquid Transport: *Alkylene*		Cyclic Fixed-Bed Axial Flow: *Detal*		
Seconds		Fixed Fluid Bed: *MTO*				
Milliseconds	Vapor Riser: *FCC*			Moving-Bed Radial Flow: *CCR Platforming Oleflex, Cyclar*		Fixed-Bed Radial Flow: *SR Platforming, Pacol*

UOP's Alkylene™ process provides an example of kinetic modeling's key role in process development. Alkylene is an alkylation technology for reacting isobutane with a light olefin, typically a C_4 olefin, to form a high-octane branched C_8 paraffin, such as 100 RON 2,2,4 trimethylpentane. A commercial C_4 olefin feedstock is a mixture of isobutene and normal butenes, yielding a product blend of trimethyl pentanes and dimethylhexanes. The feedstock may also contain propylene and C_5 olefins. The alkylate product typically has an octane of approximately 92 and is excellent blending stock for increasing the octane of a refinery's gasoline pool. Furthermore, it contains no olefins and has low vapor pressure, meeting specific requirements for cleaner fuels.

An objective of UOP's alkylation R&D program was to develop a process that utilized a novel heterogeneous catalyst rather than a liquid acid catalyst for the alkylation chemistry. UOP pioneered alkylation with hydrofluoric acid in the late 1930s and early 1940s. As shown in Table 1, HF alkylation is one of the top 10 processes licensed by UOP. The Alkylene process is a substitute for HF alkylation. It addresses environmental concerns associated with the continued use of HF and is in accord with sustainable development goals.

The kinetic parameters of the Alkylene catalyst place it in a unique location in Table 11. In order to achieve an economic balance between the rates of reaction and deactivation, UOP developed a liquid transport reactor for the Alkylene process. Olefin feed joins isobutane and catalyst in a riser at the bottom of the liquid-full reactor.

The alkylation reaction proceeds as reactants pass upflow with catalyst through the riser. Upon exiting the riser, liquid velocity is reduced, causing catalyst to disengage from the liquid. The liquid product is sent to fractionation, where LPG and alkylate are removed and excess isobutane is recycled.
Disengaged catalyst is stripped with feed isobutane and hydrogen in the annular space between the riser and the reactor wall. Stripped catalyst in isobutane flows down the annulus to the bottom of the riser, where the cycle is repeated.

Another important tool for developing the liquid transport reactor was a cold-flow model. It was used to study the effects of catalyst density on fluidization, disengagement, and attrition, and to optimize the design of the riser, liquid distributors, and other mechanical equipment. Residence-time-distribution experiments were conducted in the model to establish design parameters. The cold flow modeling was supplemented with Computational Fluid Dynamics.

Summary

The tremendous growth of the process industry in the 20th century was made possible by continuous innovation. An innovation slowdown began as processes reached a high level of technical sophistication and maturity. In the hydrocarbon processing industries, many processes achieved product yields in excess of 90% of theoretical. In the 21st century, the call for sustainable development has introduced additional challenges for hydrocarbon processing. These challenges include cleaner fuels, alternatives to crude oil as a feedstock, and minimization of environmental impact.

UOP follows a Gated Technology Delivery Process for generating and validating new ideas, conducting business and technology development, finalizing a technology package, and gaining customer acceptance of a first commercial installation. As part of this work process, innovation tools are applied to new catalytic and adsorptive materials and associated process technology. Materials innovation tools start with a combi-chem system for discovery and screening, and comprise a suite of techniques for solving crystal structure, characterizing active sites and elucidating reaction mechanisms. Process innovation tools include pilot plants, kinetic models, and cold flow models for developing an optimal reactor design. Innovation tools have proven to be very effective for accelerating process development and commercialization.

Paper 2: Invention to Innovation Bridge—Heuristic Rules

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Introduction

The term “innovation” has multiple interpretations (more than 100 could be found in literature) in science and engineering. However, this paper considers two categories of innovations [1]:

a) intrinsic
b) extrinsic

Intrinsic innovation is related to the product itself and its application, process, and manufacturing system. Extrinsic innovation is related to marketing, pricing, sales, and use by consumer.

Intrinsic innovation procedures transform the invention (or R&D know-how) through a practical manufacturing system. The procedures and their efficiency have a decisive influence on the competitiveness of the product. A review has shown that only about 5% of inventions (or R&D know-how) are finding their way to the market. This means that investigation of parameters of intrinsic competitiveness are including the bulk of information which leads to the rejection of the majority of invention as not meeting the required market parameters. Only when the intrinsic character of the innovation is tested and confirmed than the extrinsic innovative procedures should be searched to place the product on the market. This logic is leading to the search of parameterization of the innovation as quick as possible after invention has occurred. The milestones of the intrinsic innovation process are well known: 1) idea characterized by the newness of the approach to the R&D problem, 2) concept characterized by scientific positive assessment of the idea and 3) R&D and design: a) process functions design, b) process structure design, and c) process valuation.

Efforts by industry to streamline operations and become more efficient depend on the patterns of the innovative process inside individual companies.

The tables below show published data on R&D expenditures:

Table 1: New Products as Related to the R&D Effort [2]

Industry	Total R&D expenditures as % of sales	Percentage of total annual sales represented by new and improved products commercialized within past five years
Wood, paper, and allied products	1,3	13
Industrial inorganic materials	3,7	20
Plastic materials and synthetics	4,4	18
Drugs and pharmaceuticals	11,2	25
Soap, cleaners, and toiletries	3,4	28
Industrial organic chemicals	3,1	10
Agricultural chemicals	9,1	23
Miscellaneous chemical products	5,1	12
Median	2,8	23

Table 2: Europe, USA, and Japan in Research [3]

Comparative parameter	Europe	USA	Japan
Number of researchers per thousand people	4,7	7,4	8,0
Share of publications % 1993	32	36	8
Total R&D spending Euro mln 1994.	121 882	142 047	104 009
Total R&D a % of GDP 1995	1,91	2,45	2,95
Expenditures per capita Euro 1994	329	545	833
Number of researchers 1993	774 071	962 700	526 501
Patents 1995-1996	40 069	109 646	215 100

	-informatics 19,5% -biotechnology 29,7 -farmacology 25,8%	-informatics 67,4% -biotechnology 57,1% -farmacology 59,8%	

Macroeconomic Aspects of the Innovative Process

The data presented above show the importance of innovation to the modern economy. Observation of the research development and its direction orientation to the technology development and quick industrial application and amount of financial resources invested in the technology development show that there is some relation between the information value and growth parameters. This is interesting to remark that technology as a soft component of the industrial development is created by the information stock expansion. The development of technology requires projections of future market demand; it means there is need to understand what would be necessary for further social and economic development: new pharmaceuticals and new methods of communication allowing increase of the economic efficiency. This view or projection is not created by labor or capital in classic sense. This is created in the human brain by the logic analysis and evaluation of numerous options. Obviously not always the selection is adequate to the trend of development, but in macroeconomic terms it is the fuel for successes. Other element of the research is the search for new application of existing products, of the new products and of the new methods of production. This is made again by the human brain and respective instrumentation of research. However, even the most advanced and sophisticated instrumentation could not ensure the successful invention that is again the information parameter. This parameter has been present always in the development process as a condition of use of capital and labor.

However, its influence has been distributed over much longer period of time and therefore it was difficult to observe its influence on the basis of statistical research which were always the basis for the economy parameterization and obviously accuracy of these observation is limited.

Therefore considering these remarks as the initial observation requiring the proof accordingly to the mathematical instrumentation of the problem the hypothesis is proposed that the growth equation should be expanded by the third parameter: information. The classic Cobb-Douglas equation relating the production to the labor and capital, later improved by numerous researchers e.g. Solow [4] or Johnson [5] reviewed by Stoleru [6] by introduction so called technical progress coefficient into original Cobb-Douglas equation could not be fully proved statistically and at present time it is less chance to prove them now. It must be also observed that previously large influence of the labor in the equation is not more valid. The growing labor productivity and continuous relative decrease of labor forces should be a reason to review of its mathematical format in the production equation. Therefore continuing the research based on the classic econometric theory the information element should be introduced as a crucial factor of growth, exchanging the place in Solow equation with labor. Than the equation in its simplest form may look like:

$$Y = L_o e^{bt} I^{1-a} K^{a}$$

where: L_o - initial labor component of the production function
- b - coefficient of the dynamics of the labor productivity
- t - time considered for review
- I - information parameter of the production function
- K - capital parameter of the production function
- a - transformation coefficient of value 0-1

The transformation of the equation to the format allowing statistical evaluation requires advanced mathematical treatment and development of new methods.

Definition of Area of Interest

The impact of the innovative process on the world economy is changing and at present, new features and its patterns are observed. The globalization of the chemical market is introducing new challenges to the R&D process in particular in Europe [7]:

1) Research should be viewed in the world context.
2) The cost of research, which typically has a 5% yield, is beyond the means of a majority of small- and medium-sized companies
3) The practical exploitation of results requires large-scale investments and enormous marketing efforts.

The main R&D problem facing Europe life-sciences companies is the lack of “incubator” companies capable of developing good research ideas and bridging the gap between the research and commercialization.

Currently, two specific features are observed in the R&D process:
1) Application of the modern instruments of screening of the product (e.g. new catalysts). The results of research using these instruments allow identification of the promising molecule and furthermore the possible ways of its synthesis. Very often well-established methods of molecule identification are used in planning new catalysts. Above that, new instruments used in molecular modeling as well as combinatorial chemistry are implemented to speed up the R&D process and increase the number of successful programs.
2) However, the sequence of the process units must be established and their capacity calculated. Here, computer aided design is widely used. The unit processes design based on chemical engineering science is a key to evaluation of the technological process starting in the early 1930s. However, this was not an answer to the design of efficient technological units and after the early 1950s, the concept of the process engineering expanding the ideas of the chemical engineering has been introduced to the research and practice of design. The difference was obvious: process engineering has been searching for the optimum structural and functional properties of the technological unit, but chemical engineering was aiming for optimization of the process units.

In the early 1970s, the technological systems synthesis concept later called “flowsheeting” was developed using sophisticated computer programs [8]. At early stages they were basing on chemical engineering of the process units modules and by trial and error composed into technological unit. The specific deficiency of this approach is need for multiple approximations in case of one or more recycling flows. Parallel to this approach the equation – oriented process simulation has been researched.

The basic difference from previous approach was the dynamic simulation of the unified networks of the process units basing on linearization of equations as well as including the extended mathematical Newtonian or quasi-Newtonian (gradient based) methods of optimization search. Both approaches at that time were limited to the computer capacities (memory and speed) therefore it is no wonder that they are very much compatible presently and much more useful than in early 80-ties.

The general deficiency of all approaches and inaccuracy of gradient estimate is leading to the conclusion that only investigation of all variations of potential solutions (giving results in the frames of initial data and functions) is not possible. Even to-day when computation capability is exponentially higher than in early 80-ties this is not feasible considering need for step by step search for efficiency at different stages of R&D process. Therefore, the new R&D instruments are not excluding the structuralization of the process and evaluation of the potential structure or structures. Again, either very expensive evaluation instruments would be applied or stepwise application of heuristic rules.
The problem posed at this forum is the way to the innovation. Obviously the starting point to innovation is as defined above the invention covered by patent or by the specific know-how.

Invention as a part of innovative product or process.
Requirement to obtain patent is to prove the efficiency of the new process solution either usefulness of the product or its substitutive character. However, the invention very rare covers the whole process or the further processing needs or costly components of the product may deplete integrity of the product, therefore efficiency of the invention. This means that after invention will be accepted for inclusion into company R&D program it is necessary to find out the answer to the complete efficiency of the new product or process and control it during the whole life of the project.
Here starts the problem of efficient instruments of economic evaluation of the new product or process and sequence of respective R&D steps (pilot plant, basic engineering, market active research etc.) before the investment decision. These instruments may be based on very costly procedures or using to the certain step of the project advancement empirical, heuristic rules.
These rules are oriented towards selection of the sequence of process units providing the information allowing assessing the process or product conditions of acceptance by the market and will be discussed later.

b) Procedure of transformation of the invention into innovation
The transformation of inventions into innovative product or process as stated above is an activity of very low yield. Accordingly to the different research sources maximum 5% of the inventions find the way to the market. It means

that it is impossible to carry out R&D process through all stages of development process (from idea to the product/process) for all inventions available. Therefore, every R&D institution (decision making body) must have a screening system allowing at certain stages of the R&D process to abandon part of research goal which is not meeting the established criteria. The screening system has to be established in specific way ensuring equal judgment of the results. Companies at large have their own evaluation system, some are subcontracting this task to a specialized companies under specific terms of agreement. Whatever are the modalities of evaluation they must be based on similar or even exactly same level of information as well as using similar evaluation instruments. In practice the following elements of screening system are considered obligatory :

a) Technological flowsheet characterized by parameters of consumption of all inputs and algorithm of transformation of these inputs into uniform value
b) Estimate of structural elements cost and algorithm of transformation of this costs into investment cost
c) Select the integrated system of evaluation and evaluate results in strictly comparative modality
d) Control evaluation of the exogamic elements of the system through statistical analysis or prognostic statement

Mentioned above shows that at majority of the research periods the design problem is a fuzzy problem, considering that average chemical process is defined by dozens of thousands of variables, constraints and parameters estimated with different accuracy (at the beginning very low and growing only after expensive research efforts e.g. after establishment of the pilot plant) established by technology itself as well as by the potential technical applicability. The fascination of the growing capacity of computers as well as availability of more and more sophisticated (but less controlled) software in many cases is acting against the possibility of choosing the optimum design for innovation (innovative process).
The some of deficiencies are as follows:
- the different approach to the periodic and continuous processes
- the number of options surpass the acceptable evaluation costs
- the doubtful origin of the dynamic functions of the variables or parameters
- the differences between the results of functions parameterization and available structure
- the non-uniform approach to the valuation at different stages of R&D process

The design theory and practice of engineering rules application allows to diminish the impact of the deficiencies and provide the instruments for transformation of the invention into innovative process.
To transform invention into innovation, in particular at early stages of the product/process development above the developed sophisticated instruments of evaluation requiring large scale set of information and expensive instrumentation some specific instruments are necessary to ensure competitiveness and timely exposure of the product to the market.
Those are heuristic rules of design.

Patterns of the heuristic rules at different stages of the innovative process
Evaluation at early stage of development process
The goals at this stage are:
increase the statistical value of the success from 5% to higher value
decrease the time of implementation from 10 years to shorter time
This stage of evaluation is one of the most difficult and responsible from the point of view of the efficiency of the R&D process. The basic necessary information originating from R&D and exogamic sources (market assessment) assuming that there are not enough data to prepare basic engineering is as follows:
yield of the product
- price of the raw material
- expected price of the product
- statistical data on investment cost
- company cost structure

More than one thousand processes is described in detailed form available in the literature or could be provided by consulting companies. Establishing the sequence of the process units it is necessary to investigate the existing processes. The tested by practice at the large scale the unit processes sequence could be useful indication to resolve new process and implement innovation into operational stage.

The preliminary selection of the reaction system and capacity allows the heuristic evaluation of the invention for purpose of further research or abandoning the project.

4.2 Heuristic rules at the functions selection [9]

Before entering the discussion of the relations between algorithms of design and heuristic rules (concepts) of design the following considerations have to be taken into account:

a) The advanced chemistry using specialized computerized systems in many cases could design molecule with desired properties as well as reactions sequence of the total synthesis. The discussed below process design system is not related to the design of molecules but processes of their production.
b) The exogamic matters like market of the product, its application, potential substitution as well as marketing instruments introducing product to the market are not a part of the process design system

Design could be applied to any system of relations between the elements of specific actions changing the parameters of flow. In our case we are interested in the area of the chemistry and process of transformation of the invention in pure chemistry into innovative technological process. To analyze the option of application of the heuristic rules to the design of the processing function P it is necessary to define the elements of the system. For purpose of this exercise we are considering the following definitions:

c) The technological process is a set of processing elements interconnected by the specific relations between them (sequential, parallel, etc). The final output of the technological process is well defined product.
d) The processing unit is a structural unit having the isogamic properties f (Mi, Ni, Oi,…Pi) originating from the possession of the processing elements ability to change the properties of the flow from the level p(o) to p(i). The output from process units is a defined flow g(i) characterized by specific combination of parameters F (Xi, Yi, ….Zi).
e) The processing element is a physical component allowing establishment of the processing unit.

The output of the processing element is specific property of structural element Mi, Ni….Oi.
The number of functions is limited and their chain defines the process. Functions represent the thermodynamically defined potential of the process at every step of transformation. Further selection of the structure for each function defines the operation capability of the process.
The functions of the process unit and direction of changes through the process are given in the following table.

Table 3: Chemical Engineering Process Functions

Function	Direction of change	Direction of change
Energy level Temperature	Increase	Decrease
Energy level Pressure	Increase	Decrease
Reaction	Synthesis	Decomposition
Composition	Mixing	Separation
Sizing	Reduction	Enlargement
Linking functions	Transportation	Storage

When the new process or product is developed than the result of invention is possibly reaction defined by inputs as well as the thermodynamically parameters. At this stage of research the sequence of functions must be determined to provide information on unresolved process problems. Obviously it does not exist an algorithm for selection of sequence of functions and stochastic search is also not applicable. Therefore it remains only rationale approach derivative of the empirical, heuristic knowledge.
The algorithms of the calculation of the size of the structure of each process unit are well known and permanently improved to reach optimum values. However, the standardization process as well as the possibility of the establishment operational unit requires always the adoption of the heuristic rules.

Table 4: Examples of Models for Process Functions and Structures

Process function	Process Unit	Model of function estimate f(X,Y,...Z)	Model of structure estimate ? ? ? ? ?
Reaction	Isothermic plug flow reactor	(G? ?ln $(1-x_a)/k$	(n ? ?D^2 L)/4
Intensification of the flow	Heat exchanger	G c_p $(t_k - t_o)$	n ? ?D L ? ? ?k

Separation of mix	Distillation column	{4L (R+1)}{f(R+1)N}/? ? w	? D^2 , H

Obviously the models given in the table are simplified only for illustration purpose.

The design problem of the technological unit is divided into two stages:

- process synthesis
- process units adjustment (establishment of the structure of the functional units)

The goal of the process synthesis is to establish sequence of process units performing functions over the flow from input values F (Xo,Yo,…..Zo) to output values F (Xk,Yk,….Zk).
The goal of the process units adjustment is to select process units fulfilling conditions established F (Xi,Yi,…Zi) by the process synthesis but using the f(Mi, Ni,….Oi) effectively available in the shopping list.
The first stage of the process development is establishment of the sequence of functions. At the early stage of process development very limited information is available to assess the risk of further research. Here the heuristic rules are very helpful in avoiding expensive modalities of the process evaluation. As mentioned before the process is composed from the functional process units. Every process unit represents specific function and may be implemented in multiple structures.
The next stage is to establish structure of the functional process units
The algorithms of the calculation of the size of the structure of each process unit are well known and permanently improved to reach optimum values. However, the standardization process as well as the possibility of the establishment operational unit requires always the adoption of the heuristic rules.
The initial heuristic step to the establishment of the technological process is to select the sequence of functions. The standard structure is the first assumption:

S→TPA→R→TPA→VSS→S→LSS→S→SSS→TPA→S

where:
S - storage
TPA - temperature, pressure adjustment
R - reaction
VSS - vapor (gas) fractions separation
LSS - liquid fractions separation
SSS - solid fractions separation
This structure is statistically dominating in the chemical industry. Obviously the thermodynamic and kinetic parameters of the reaction are established by calculations and experiment as basis of invention.

1) TPA process units selection

Table N 5 Process units at the entrance to the reactor

TPA	Temperature adjustment	Pressure adjustment
Process units	Heat exchangers	Compressors, pumps

The functional size of the process units is calculated by the any of available CAD system.
The functional size is not yet implementable due to the lack of number of data and is later corrected at the structural size determination.

2) Reactor selection

From the point of view of the thermodynamics two options of reactors are available:
Isothermal reactor (IR)
Adiabatic reactor (AR)

From the point of view of kinetics other two options are available:
Plug Flow Reactor- PFR
Continuous Stirred Tank Reactor - CSTR

The selection is not obvious and depends on many specific modalities of the reaction, however the primary rules are allowing to omit not desirable solutions.

Table 6: Selection of the Type of Reactor

Reaction	Heat load MJ/h	Reactor isothermal	Reactor adiabatic *\
Exothermic	6,3 - 8,4	PF	PF

Endothermic	6,3 - 8,4	PF	CSTR or CSTR+ PF
Exothermic	>8,4 MJ/h	Not applicable	PF **\
Endothermic	< 6,3 MJ/h	CSTR	PF with heat carrier

*\ at DT between the entrance and outlet <15%
**\ with limited conversion
Regeneration of the catalyst can be made periodically or in continuous reactor-regenerator system where catalyst in adiabatic reactor is playing role of the heat carrier.
The selection of the type of reactor allows the functional size calculation by CAD system.

3) Flows stabilization
The flows through the reactor system are defining the size of the plant which could be much larger then its capacity. That depends on the volume of the recycle of the raw material.

Table 7: Recycling Principles

Conversion	Yield	Flow system
High	High	One-through
High	Low	Change the catalyst or parameters
Low	High	Recycle
Low	Low	Recycle or change the catalyst or parameters

The case High/Low is producing substantial quantities of by-products increasing the size of basic installation as well as make longer the basic functional sequence of the process units.
The case Low/Low is increasing size of installation in case of recycle and also expanding the functional sequence of the technological process.

1) Separation and purification of the products
The next TPA depends on the composition of the outlets from the reactor and general parameters of the reaction. Therefore below are given selections of the separation processes in order of structural enlargement.
Table N8 Order of selection of separation processes

Products	G	L/G	L	S/L
Unit processes	Transformation into liquid Absorption Adsorption PSA Other	Flash Absorption Adsorption	Flash Evaporation Distillation Extraction Azeotropic distillation Extractive distillation	Crystallization Filtration Drying Leaching Sublimation

Products of reaction: G- gaseous, L/G -liquid/gaseous, L-liquid, S/L- solid/liquid

The sequence of search to select process units after reactor are related to the phase status of the products.
In case of gaseous products we apply the VSS steps;
a) cooling to the 20 ^{o}C
b) pressurizing to the 0,5 MPa with cooling
c) flash separation
d) deep cooling (propylene condense)
In principle in all cases the L/G mixtures are obtained from which gaseous fraction is further treated by absorption or adsorption at the condition that it contains no more than 5% of liquids
The separation of the light components from the liquid phase may be organized in specific process unit of distillation character but specifically organizing the flows of light components. Those options are;
a) partial condensation
b) pasteurization
c) stabilizing

The typical and most common process of liquids separation is the distillation. The condition of applying distillation as a separation method is the value of relative volatility $a_1/a_2 > 1,1$.

The number of optional distillation schemes is growing exponentially in regard to the number of components and sequential calculations of the mixtures over four are not practical and heuristic methods are applied with very small difference from feasible optimum.
In case of higher number of components the following rules are applied [10]:

a) select the sequence in order of decreasing volatility
b) select the sequence where components' flows are equal
c) as key components select the neighbor relative volatility
d) preference is given to the high level of separation accuracy
e) the most difficult separation should remain last

In practice about 40 rules are applied in logical sequence eliminating the costly schemes.
They are divided in four groups of rules:
A) Related to the composition of the mixture (concentrations of components0
A) Related to the separation parameters e.g. relative volatility
B) Related to the process conditions (design modalities)
C) Related to the system operation parameters (e.g. recycles)
Other separation systems
When distillation is not feasible or not possible there is a sequence of other L/L separation processes:

a) extraction solving one of components
b) azeotropic distillation introducing the third component to impose deviation (negative or positive) from the Raoult's law.
c) extractive distillation to alter relative volatility of the components

These systems have always a deficiency by introduction of the third component which must be separated in additional separation system.

Heuristic Rules at the Structure Selection
The functional structure of the chemical process is not yet giving the possibility to make evaluation of its profitability after all necessary research has been carried out and process scheme has been designed.
In many countries there exists standards of the process elements entering the structure of the process unit and in all cases the machinery industry has their own prescriptions included in the catalogues of company.
Below are given tables of the most common parameters of the process elements.

a) intermediary vessels (about 20 parameters)

Table 9: Structural Parameters of the Intermediary Vessels

Parameter	Value
L/D	2,5 - 5
Holdup	60 min at 90% of volume
Thickness of wall 2MPa	9 mm

All parameters are later calculated accordingly to the engineering standards

b) columns (about 30 parameters)

Table 10: Structural Parameters of the Columns

Parameter	Value
Maximum height	50m.
L/D	20-30
Thickness of the wall P.=0,12MPa	8 mm
Height of column	3-5 m. over the plates/filling
Plates used at the diameter	over 1m.

All parameters are later calculated accordingly to the engineering standards

c) continuous stirred tank reactors (about 15 parameters)
d)

Table 11: Structural Parameters of the Stirred Tanks

Parameter	Value
H/D	1,0-1,5

Power requirement	0,3 kW/m3
Power requirement with internal heating/cooling	1kW/m3
Power requirement with reaction	2 kW/m3
CSTR cascade of 5	Equivalent to PF reactor
Diameter of the propeller	0,3 D

All parameters are later calculated accordingly to the engineering standards

d) heat exchangers - tube -shell (about 40 parameters)
e)

Table 12: Structural Parameters of the Heat Exchangers

Parameter	Value
Condensing components	Shell side
Linear speed of component in tubes	Higher
Length of the tube	Max. 6 m. (stepwise every 0,5 m.)
Tube diameter	15 mm stepwise every 5 mm
Tube distribution	Hexagonal with t=26-32 mm
Maximum HE surface (mounted)	4650 m2
Maximum HE surface (dismounted)	920 m2

All parameters are later calculated accordingly to the engineering standards

For purpose of preliminary evaluation of the heat exchanger surface the following heat transfer coefficients could be used:

Table 13: Assumed Heat Transfer Coefficients

Cooled component	Heated component	K [W/m2 ^{o}K
Water	Water	1420-2480
Water solutions	Water solutions	1420-2480
Light organic	Light organic	230-430
Medium organic	Medium organic	110-340
Heavy organic	Heavy organic	60-230
Light organic	Heavy organic	170-340
Heavy organic	Light organic	60-230

Although, to-day CAD packages are giving quick calculation of heat transfer coefficient however are requiring quite large number of physical data of flows.
Special packages are provided for optimization of the heat usage by special design of the heat exchangers system, but this is possible after general structure of heat exchange would be established.

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Paper 3: Predicting Profitability in the Chemical Industry

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Introduction

The Process Economics Program (PEP) provides in-depth technical and economic evaluation of both commercial and emerging technologies for the chemical and refining industries. The tools used in this evaluation are as follows:

- process simulation
- equipment sizing
- investment estimation
- reliable operating cost forecasts

This software instrument has a multipurpose character. It serves the comparative evaluation of the competitive processes, selection of the production profile of the expansions and restructuring, establishment of new industries, as well as the evaluation of the potential developments and preparation of the R&D programs in promising technological niches. The present library of SRI covers about 1000 processes in all areas of technology.

Table 1: The Statistical Presentation of SRI Sources (PEP reviews)

Area	Number of PEP reviews
Specialty chemicals	9
Polymers	16
Refining technologies	11
Life Science	2
Environmental technologies	3
Information technologies	5
Bio-technologies	3

Above the reviews, SRI is preparing PEP Review Studies (above 60). A list of these studies is available upon request.

Potential "Breakthrough" Technologies Covered in 2003

Assessments are provided below of the potential technologies that may be of interest to investors during this period of expanding globalization. This assessment gives the possibility to direct the R&D efforts in the catalyst area and engineering to be made to achieve the efficiencies assumed in the studies.

Mega Reforming

Large-scale natural gas reforming installations are providing raw material for the production of methanol, ammonia, Fisher-Tropsch (hydrocarbons), and dimethylether (DME). In order to be profitable, the installations need to provide natural gas at the competitive price of 0.5 cents per MCF. With conventional technology, capacities are between 1000MTPD to 2000 MTPD. It is expected with new technology, installations can achieve capacity of 15,000 MTPD. A number of projects are reviewed in the Middle East, Carribean, and Australia. Companies such as Lurgi, Eneas, Haldor-Topsoe, Shell, Mitsui, Exxon, Methanex, and JGS are exploring alternative processes for compact reforming, autothermal reforming, combined two-stage reforming, and hot-gas reforming to maximize yields.

The investment costs are very high and the natural gas price is critical to the success of this mega project.

Table 2: The Capital Investment Cost of the Methanol Plants

Capacity	Technological unit USD million	Off-site USD million	Total USD million
USGC	100	105	205
2300 MTPD	100	105	205
4600 MTPD	150	170	320
9200 MTPD	260	210	470

Table 3: The Production Cost of the Methanol in Mega Projects

Capacity	Variable cost USD/t	Fixed cost USD/t	ROI USD/t	Total USD/t
USGC At 3,0$/MSF	85	40	75	200
2300 MTPD at 0,5 $/MSF	15	35	65	115
4600 MTPD at 0,5$/MSF	15	25	50	90
9200 MTPD at 0,5$/MSF	15	20	45	80

Obviously the return on investment for this project may be substantially lower under different macroeconomic conditions. However, the natural gas price of 0,5 $.MSF is reasonable only in the Carribean and may be in some Arabic countries. The licensors evaluation shows similar results of 75 USD/t at a capacity 10,000 MTPD. Only at the capacity of 2,500 MTPD, does the ICI process show an advantage but optional price is about 125 USD/t.

Steam Cracking.
The steam cracking of naphta and ethane is one of the largest production operations in the chemical industry, requiring more than 300 million ton/year of raw material. Two products are essential: ethylene and propylene. The process is carried out in specially designed furnaces assuring very high temperature and very short residence time. The recent introduction of ceramic furnaces should ensure longer operating times throughout the year.

Table 4: Investment Comparison of the Furnaces in the Steam Cracking Process. Capacity:xxxxxx

Capacity	Technological unit USD million	Off-site USD million	Total USD million
Ceramic furnace	250	150	400
Conventional	280	140	420

Table 5: Production Cost of the Steam Cracking . Capacity:xxxxxx

Capacity	Variable cost cents/pound	Fixed cost cents/pound	ROI cents/pound	Total cents/pound
Ceramic furnaces	15	3	4	22
Conventional	16	3	5	24

Non-Phosgene Routes to Polycarbonate
Diphenylcarbonate (DCP) is an intermediate product on the route from phenol to polycarbonates. The classic route is the carbonylation process phosgene. This reaction poses security, safety, and environmental problems. Environmental problems are related to the estimated 300 kg of HCl produced per ton of DCP. The disposal of this by-product is difficult because of organic impurities. The absorption of HCl in water produces hydrochloric acid, which is one of the most corrosive species.

Currently, research is being carried out to substitute the phosgene with carbon dioxide in the catalytic system. Fixed bed and fluid bed carbonylation are being tested on an industrial scale to produce DCP from DMC (dimethyl carbonate).

A number of companies (e.g, Bayer, Dow, GE, Idemitsu, Mitsubishi, MGC, Tejin, Ube, Asahi, and Daicel) are working on these processes. SRI has evaluated potential processes showing that fixed and fluid bed catalytic carbonylation by carbon dioxide is competitive to other options.

Table 6: Investment Comparison of the Carbonylation Processes. Capacity: xxxxxx

Process	Technological unit USD million	Off-site USD million	Total USD million
Fixed bed	20	20	40

Fluid bed	20	20	40
DMC	34	26	60
Phosgene	37	28	65

Table 7: Production Cost of the DCP by Different Carbonylation Processes Capacity: xxxxx

Process	Variable cost USD/t	Fixed cost USD/t	ROI USD/t	Total USD/t
Fixed bed	600	250	250	1100
Fluid bed	600	250	250	1100
DMC	650	300	450	1400
Phosgene	700	300	400	1400

This assessment shows the need for concentrating R&D efforts on the direct carbonylation processes.

Propylene Production Options

The market analysis and comparison of future demand with expanded capacities show that marketing propylene will be tight in the near future. This condition is apparent for short periods when the capacities of the steam cracking facilities become limited due to renovations or closures due to accidents. Increasing the capacities of the steam crackers is not feasible because of parallel production of ethylene, which has an equal market demand and capacities. Therefore, options are open for the MTO process oriented towards maximizing the production of propylene.

Active R&D activities in this area are carried out by Lummus, Lurgi, UOP, Synopec, and Stone& Webster.

Table 8: Investment Comparison of the Propylene Production Processes. Capacity: xxxxxx
Alternative methanol (MTO) to steam cracking

Process	Technological unit USD million	Off-site USD million	Total USD million
Methanol based	180	170	350
Ethane cracking	200	180	380
Naphta	350	200	550

Table 9 Production Cost of the Propylene by Different. Capacity: xxxxx
Alternative methanol (MTO) to steam cracking

Process	Variable cost annual value USD million	Fixed cost annual value USD million	ROI annual value USD million	Total annual value USD million
MTO at 25 c/gallon	80	120	250	450
MTO at 40 c/gallon	380	120	270	770
Ethane	170	160	270	600
Naphta	180	220	380	780

Table 10: Investment Comparison of the Propylene Production Processes. Capacity: xxxxxx
Alternative methanol (MTO) to methatesis

Process	Technological unit USD million	Off-site USD million	Total USD million
Methanol based Lurgi	180	170	350
Methanol based UOP	200	185	385
Methatesis	350	230	580

Table 11: Production Cost of the Propylene by Different. Capacity: xxxxx
Alternative methanol (MTO) to methatesis

Process	Variable cost annual value USD million	Fixed cost annual value USD million	ROI annual value USD million	Total annual value USD million
Lurgi at 25 c/gallon	180	70	110	360
Lurgi at 40 c/gallon	350	60	130	540
UOP at 40 c/gallon	160	120	200	480
Methatesis	360	20	25	405

There is also an option for integration of the naphta cracker with methatesis process.

Table 12: Comparison of the Propylene High Yielding Option

Products	Naphta cracker	Naphta cracker & methatesis
Ethylene (kmta)	1 000	850
Propylene (kmta)	500	920
Butylene (kmta)	300	-
Olefin value ($MM/year) *\	855	885
Investment $MM	1 000	1 080

*\ Ethylene& Propylene- 500 USD/t, Butylene- 350 USD/t

The selection of the option depends on the local economic feasible conditions of the supply of the NG (e.g flare gas), company structure (e.g. supplier of NG is a shareholder) and logistics of the market considering the high capacity that assuming much longer radius of supply of the products to the final processing.

Polystyrene Process Potential Development

Polystyrene is one of high tonnage polymers of the second level of capacity. Polystyrene has very wide application, from General Purpose (GP) and Foamed Grade (FG) packaging to structural applications in the construction and automobile industry where the High-Impact grades and copolymers, such as ABS are used. The production process is well established, and includes suspension polymerization and from early 70-ties in block polymerization as free radical initiated polymerization. An obvious alternative is anionic polymerization, but there is a lack of substantial progress in Ziegler-Natta initiated anionic polymerization. The rate of the polymerization is very rapid and considering the highly exothermic reaction, it may become explosively non-controllable. However, there are companies investigating the process, such as Dow, Mitsubishi etc.

SRI has compared the traditional process with expected anionic process.

Table 13 Investment comparison of the polystyrene production processes. Capacity:68 000 t/year

Process	Technological unit USD million	Off-site USD million	Total USD million
Free radical GP	20	22	42
Free radical HI	35	22	57
Anionic GP	15	23	38
Anionic HI	22	33	55

Table 14: Production Cost of the Polystyrene. Capacity: 68 000 t/year

Process	Variable cost USD/t	Fixed cost USD/t	ROI USD/t	Total USD/t
Free radical GP	600	160	100	860
Free radical HI	700	160	200	1060
Anionic GP	580	140	100	820
Anionic HI	600	160	120	880

The anionic polystyrene would be produced at lower cost with lower residual monomers (10 ppm compared with 200ppm for free radical polymer) and higher strength in all mechanical resistance parameters.

Integration of Olefin Manufacturing Sites
One can expect that continued globalization will produce new sites of extreme integration using different raw materials (naphta, LPG, NG, etc supplied buy the pipe system) producing not only monomers but also polymers, aromatics, and chemicals at the capacities requiring mega infrastructures. These sites with the capacities of olefins over 3 million t/year structured at the cost more than 10 billion USD must be efficiently operated. The refining industry has introduced instruments such as the LP system that is providing savings over 5% of total revenue. At present, some large companies are developing instrumentation and control equipment for the petrochemical industry's integrated sites. Companies such as Aspen, SymSy, Honeywell, Invensys, SRIC, and many more, are active in the area and new developments are expected.

Conclusion
The instruments of the prospective investigation of the economics of the new processes and search for technological option could be used as an instrument in strategic planning of the R&D activities and concentrating efforts on new profitable alternatives.

Paper 4: Proactive Policies for the Promotion of Innovation in the Productive Sector and Entrepreneurship in Students and Alumni

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Features of the Activities of the Facultad de Quimica

In the mid-1980s, after 13 years of military dictatorship, the priority at Uruguay's Facultad de Quimica was to build a strong research base through qualified personnel development. From 1984 to 2002, the number of staff at the Facultad de Quimica with doctoral degrees increased from 8 to 75. In 2001, the total number of staff was 98, of which 14 were full professors. The majority of lecturers have doctoral degrees. This obviously had influence on the scientific position of the faculty. The number of published papers increased from about 10 per year in the 1980s to 65 in 2000, which represents about 25% of all papers produced by the university. The Facultad de Quimica produces one of every five Uruguayan scientific papers indexed in the international data bases and 50% of the patent applications from the whole university. However, this has reached a saturation point because the possibility of establishing new post-graduates positions has drastically diminished.

Table 1: The Faculty of Chemistry Budget (USD)

Source of financing	1998	1999	2000
Budget	2 109 931	2 109 168	1 981 414
External from abroad	91 401	45 594	99 679
External national	167 475	237 016	147 638
External public national	330 930	270 109	268 308
Total external	589 806	552 719	515 625
% of external funding	22%	21%	21%

Faculty provide technological advisory services to a number of industries.

Table 2: Orientation of the Technological Advisory Services of the Faculty

Sub-sector of industry	% of services
Pharmaceutical industry	44
Private health industry	13
Public health industry	10
Food industry	7
Private services	5
Other industries	10
Other	17

These services are becoming a source of financing. However, this cannot be the final solution either for the post-graduate programs or to cover the needs for development in a competitive chemical industry.

International Aspects of R&D Features

Obviously, during industrial development specific patterns developed in R&D financing and execution. Looking for solutions for Uruguay, these patterns were evaluated and taken into consideration as a pattern for local application.

Table 3: Distribution of R&D Financing in Selected Countries as % of the GNP (approx. Figures)

Countries	Total R&D financing	Public R&D financing	Industrial R&D financing
USA	2,75	1,20	1,55
Japan	2,85	1,05	1,80
Republic of Korea	2,80	1,05	1,75
Germany	2,30	1,20	1,10

France	2,20	1,15	1,05
Great Britain	1,85	1,05	0,80
Italy	1,15	1,00	0,15
Spain	0,85	0,75	0,40
Brazil	0,905	0,65	0,25
Uruguay	0,30	0,28	0,02

In particular, the pattern of implementing scientific programs in USA is interesting.

Sources	Who pays in %	Who does in %
Government	39	8
Industry	61	82
University	0	6
Other non-profit	0	4

b) Applied Research

Sources	Who pays in %	Who does in %
Government	39	14
Industry	55	66
University	4	18
Other non-profit	2	2

c) Basic Research

Sources	Who pays in %	Who does in %
Government	62	10
Industry	18	18
University	12	62
Other non-profit	8	10

Obviously this pattern has a macro-economic character and is related to the economic policies as well as to the general strategy of the country. From the point of view of the Uruguayan economy and the National University, it would be more effective to evaluate the patterns in countries with different levels of industrial development.

Table 5: R&D Private Investment in Countries with Different Levels of Industrial Development

Advanced country	% of private investment	Middle development country	% of private investment	Less advanced country	% of private investment
USA	64	Portugal	41	Argentina	15
Canada	56	Spain	48	Brazil	18
				Chile	30

These and other data discussed at the conference led to the following conclusions that must be considered for further scientific development in Uruguay:

a) Developed (industrialized) countries show a larger participation of the private sector in R&D funding and implementation compared with less advanced countries.
b) In industrialized countries, the private demand for knowledge promotes the growth of R&D funding. In less advanced countries this process is driven by the public R&D sector.
c) In the period of import substitutions there was not private demand (market) for knowledge in less advanced countries. The protected markets were satisfied by introducing mature (outdated but cheap) technologies from abroad.
d) The recent opening of national markets (globalization) and the accelerated obsolescence of applied technologies has not so far pushed less advanced countries companies to include R&D in their business strategies.

Instruments to Reverse the Orientation of the Strategy in Chemical Companies in LAS Countries
The assumptions behind the proposals and activities of the Faculty of Chemistry of the University of the Republic (Uruguay) are as follows:
a) In the mid and long term, the educational system may promote new attitudes (e.g., entrepreneurship, risk assessment, sense of cooperation, transparency, professional approaches) that may help create socially responsible modern local businessman.
b) In the short term, the university may play an active role by facilitating the generation of private demand for knowledge through strategic associations in the private sector.
c) University R&D policy should promote the vitality of local industries, increase employment, and improve the quality of life of common citizens, while sustaining the sustainability of university research activities and related MSc. and Ph.D. programs.

These assumptions have lead to practical actions inside and outside the university:
1) creation of a Support Foundation (FUNDAQUIM) to communicate with external actors from a private business legal basis
2) new curricula including business and entrepreneurship courses for undergraduates
3) creation of a Technology Pool

The Technological Pool
The structure of the Technological Pool is a decisive factor for success; it must include all the important actors of the R&D and industrial scene with decision-making power.

The following organizations are part of the Technological Pool:
1. Technological Department of the Faculty of Chemistry
2. Business Incubator
3. Center of the Technological Services
4. Consortium for Technological Strategy & Innovation (CESTI)

The CESTI is composed of management representatives of FUNDAQUIM & Urutec, an external Advisory Board and Executive Board.

The Advisory Board is composed of the following:
- 2 members of FUNDAQUIM
- 1 member from Urutec
- 2 members from paper and resins industries
- 1 member from pharmaceutical industry
- 3 members of the food industry (dairy, beer, wine)
- 1 member from banking sector

The Technological Pool strategy is to facilitate the introduction of independent R&D to industrial companies through strategic associations between the Pool and industry. Every partner contributes specific inputs to the Technological Pool:

- FUNDAQUIM is providing researchers, investment in installations, administration, a network of international research centers, and information.
- Participating companies provide funds for operational expenses, planning, and marketing of products resulting from research projects.
- Consortium provides joint definition of R&D strategy and business plans, joint management and follow-up of R&D, joint fund raising, and shared appropriation of the R&D results.

The activities of the Technological Pool are based on the experiences of a cooperative arrangement between FUNDAQUIM and CONAPROLE, the largest dairy industry in the country. The consortium, active since May 2001, has the following functions:
a) providing analytical services
b) carrying out projects of applied research

c) qualification and research training of the CONAPROLE staff
d) basic organizing of the future CONAPROLE R&D sector

Conclusions : Faculty of Chemistry--Future?
It is assumed that the present plans for the **Facultad de Quimica** at the University of Uruguay will have the following impacts:

a) Teaching impact: The university will produce graduates with the knowledge and skills necessary for the global economy.

b) Research impact: The program will improve scientific production, particularly in applied fields. It is expected that a larger volume of patents will be filed due to the stable financial position of FUNDAQUIM.

c) Industrial impact: Cooperation will allow the formation of independent R&D groups in local industries, which should encourage new processes and products, encourage more international cooperation and connections, and improve employment possibilities for graduates.

Topic C: Regulatory Problems for the Implementation of Invention

Paper 1: Modalities for Promoting Innovation in Agricultural and Petrochemical Sectors in Nigeria

Ikenna Oneyido, Department of Chemistry and Center for Agricultural Technology, University of Agriculture, Makurdi, Nigeria

Introduction

Nigeria is Africa's most populous country with a population of 129.9 million according to the latest World Bank estimate, and a landmass of 923,800 sq. km. It has a GDP of $37.1 billion, an average per capita income of $200, a growth rate of 2.2%, and life expectancy of 51 years for men and 52 years for women.

The chemical industry in Nigeria is in an infant state. Much of the activity in this area is in packaging and marketing of imported finished products. The economy is dominated by petroleum export which accounts for about 90% of the country's foreign exchange earnings. Thus, we have a mono-cultural economy that relies heavily on exportation of finished crude oil. It is against this background that we wish to discuss the modalities for innovation in the petroleum and agricultural sectors. Emphasis will be placed on research and development as well as the importance of private-sector leadership and encouraging industrial activities that can generate self-sustaining momentum.

What Are the Problems and the Opportunities?

Nigeria is OPEC's sixth larger producer of crude oil. The bulk of crude oil is exported. Unfortunately, Nigeria's refining capacity falls far below national demand, with the result that petroleum products are imported to augment the output of local refineries, which run significantly below capacity. A petrochemical plant has been on the drawing board and at the vestigial stage for decades. With a reasonably well-trained technical work force and the right policies and healthy macroeconomic environment, Nigeria should be able to take advantage of its oil supply to expand the chemical industry at home and export refined products to neighboring West African countries.

Although part of Northern Nigeria is under threat of desertification, the entire southern and middle-belt areas of the country have good arable land with a wide diversity of agricultural production. An entrenched system of high-yielding agriculture would ensure food safety and self-sufficiency for other African countries as well as provide raw material for the agro-base industries.

The Petrochemical Sector

The main bottleneck to the successful take-off of the petrochemical industry is the direct involvement of the government in the venture in a monopolistic sense. Experience in Africa and many parts of the world attest to the fact that government per se is always a notoriously inefficient entrepreneur. The starting point for ameliorating this situation is for the government to divest itself completely of an active role in this sector, which is an inescapable condition for free enterprise. The thrust of the government's role should be that of providing and enabling a hospitable environment for the industry. Foreign investment in terms of applicable technology and venture capital is needed to stimulate and sustain activity in the short and medium term. What is envisaged is strong support from government in the form of tax incentives, investment incentives (e.g., concessions duties on the import of machinery and equipment), export incentives, and improvement in the quality of chemical scientists and engineers. This can be accomplished through funding university training programs aimed at strengthening the technical base. The goal should be to take complex technologies to this sector (and indeed other sectors too) and make them more efficient and environmentally friendly.

In addition, the petrochemical sector needs to be planned and operated to be a part of an integrated chemical industry with linkages to the polymer, textile, and electrical sectors. In addition, the petrochemical sector should play the strategic role of supplying chemicals for the export industry. A clear example of success in this area is the Taiwanese experience of combining strong government support with an abundant supply of well-trained personnel.

The Agricultural Sector

As stated above, Nigeria has the potential to be food self-sufficient and to export the food to neighboring African counties. Beyond the production and marketing of food and export crops, there are other issues of interest and importance for the national economy.

One of the areas that can benefit tremendously from an innovative approach is in the provision of industrial raw materials. The lush tropical vegetation is a huge resource that has not yet been tapped for industrial/economic benefit, especially in the area of import substitution. I have come across several project reports in Nigerian universities that have investigated the use of non-edible vegetable oil such as linseed oil, castor oil, etc. for use in the manufacturing of soap, cosmetics, and pharmaceutical preparations. There are also inedible oils from rubber and other varieties of tropical plants that have been shown to have good properties for industrial use. Substitution of the traditional edible oils (palm oil, ground nut oil, etc.) with these non-edible oils will severe foreign exchange and generate indirect employment. The Indian experience in this regard with upgrading non-conventional oils for use in the manufacture of soap and cosmetics in partnership with Unilever Ltd. is an example of a successful transfer of innovation from the laboratory to the pilot plant, with huge payoffs for the industry and economy.

The other area, which I do not want to dwell on at any length, is the use of plant products and pesticides. There is a lot of activity going on in this area in many Nigerian universities and quite a lot of information is now available. The identification of the active principle is often hampered by poor scientific infrastructure, but practices evolving in which the crude plant extracts or powders have been shown to have pesticidal activity are administered in farming system with good results. The difficulty in the present context appears to be in setting up industrial research and development and networking with government and academic laboratories.

Concluding Remarks

These are just a few examples of the rewards that can flow to a country like Nigeria with the appropriate technology transfer and technology adjustment. To make these rewards a reality in the Nigerian situation, the government needs to adopt a more favorable approach to free enterprise and the necessary educational and research development infrastructure need to be in place. In the final analysis, the change that is needed to start the process is tied to some extent to the national macroeconomic frame.

Paper 2: Innovation in the Japanese Chemical Industry

Makoto Imanari, Mitsubishi Chemical Corporation, Japan

The Japanese Government's Plans

The Japanese chemical industry has been facing increased competition and reduced profits. In reaction to these circumstances, the Japanese government has developed plans to strengthen the competitiveness of Japanese industry, including the chemical industry. The following table illustrates the main science and technology policy issues and and proposed counter measures.

Table 1: Japanese Science and Technology Current Policies

Main Issues	Countermeasures
R&D does not lead directly to strengthening of competitiveness	Economy activation project
Lack of human resources (managers) with MOT [define] sense and skills	Nurturing of human resources with MOT sense and skills
Hoarding of " R&D fruits"	Promotion of spin-off venture businesses
Indispensability of activation of fundamental R&D institutes such as universities	Reformation of competitive fund system and academia
Necessity of government budget execution in accordance with R&D characteristics	Through performance-related evaluation agile and flexible budget execution
Lack of industry's MOT innovation model responding to a new age	Presentation of MOT innovation model

The necessity of good technology judgment and industrialization strategy, has been acknowledged among U.S. industry. Over 200 MOT courses were carried out, with about 10 000 graduates, in the USA. Similar MOT training is planned for about 10 000 managers in Japan because there is a lack of technology management systems. The METI [define] is supporting 39 universities in establishing MOT courses.

In addition, the Competitive Fund System has been instituted to increase competition and maximize researchers' creativity. Under this system, universities have full power to decide plans for their departments. In METI, a special program for directors has been established in competitive fund execution supervision.

A project directly related to the commercialization of inventions has been established with funding of 36.7 billion USD for FY 2003. The project has the following priorities:

Table 2: Priorities in Science and Technology in FY 2003 in Japan

Priority	Funds in billion of USD
Life Science	8.8

e.g Sugar cane engineering Bio-IT fused instrument	
Environment e.g new generation energy saving PDP high functional materials in photocatalysis	4.4
Information and telecommunication e.g IT based advanced software development chips for semiconductor application	17.3
Nanotechnology and materials e.g carbon nanotube FED ultimate function of diamond	6.1

The Reformation, Renovation, and Topics in Mitsubishi Chemical Corporation (MCC)

The Mitsubishi Chemical corporation is one of the largest chemical companies in Japan, with sales of 1,887,5 billion yen in 2003; 7,853 employees; and capital of 145,1 billion of yen. The R&TD activities are organized structurally in segments (chemical branches). Altogether, 28 laboratories, employing over 3500 researchers, are operational in the framework of MCC activities. The R&TD expenditures for consolidated output are 94 billion yen. The specialized Science and Technology Office is supervising Mitsubishi Group Science and Technology RC. The main orientation of the research is synthetic materials, materials technology, polymer technology, process system engineering, production technology, and computer science. R&TD activities are based on the Technology Platform with a specific Stage Gate System of decision making. The specific sequence of gates is as follows:

After exploratory research, outsourcing is a gate through which only prioritized product development projects will pass. When a project shows successful results it is passed through the next gate to business development projects. Afterwards, selected projects are commercialized.

The following pipeline examples shows the orientation of MCC in the R&TD area.

Table 3: Pipeline R&TD projects at Stages of Development

Stage	Projects
Business Development Projects	Nano-carbons Photoelectronics\Display Components Environmental Benign Plastics

	Designed Chemicals
Prioritized Products Development Projects	High Functional Polymers Energy related Inorganic Materials Biochemicals

The projects are executed by project teams composed of several researchers belonging to different technology laboratories of the MCC Group that have the necessary technological orientation. The mission of the project teams is to create new products and processes and improve existing products and processes according to the principles of the technology platform.

With academia and other companies, the cooperation is organized in "virtual" laboratories by dividing tasks between the partners in the agreed-upon project execution. In the area of electronics, the MCC group cooperates in "virtual laboratories" with UCSB, Kyoto University, as well as with companies like Rhom, Pioneer, NTT, and Hitachi.

Examples of Computer Simulation for R&TD Speed Up in MCC

Following are examples of the application of different tools for speeding up research results.

a. model-based solvent selection for the case resolution of diastereomer salts

b. protein crystallization

c. chemical reaction investigation

In the case of modeling solubility, the task was to find a solvent that maximizes the RS/SS solubility difference of diastereomer salts. The group contributions were analyzed and selected with the aid of UNIFAC models. Then follows the molecular simulations in discrete and continuum areas. The last is using the new computerized product COSMO-RS giving the sigma profile of the solvent. The experimental validation of the models has confirmed simulations for the case of toluene and paraffins C7-C10.

The protein crystallization example shows the linkages between biology, chemistry, and chemical engineering. To the synthesized protein the theory, crystallization modelling as well the experiments using the HT allowed to design the experiments where the protein single crystals of size 0,1-0,3 mm has been obtained and through X-ray diffraction the protein 3-D structure has been identified.

The chemical reaction investigation shows the case where process has shown low conversion, low yield, producing unknown by-product. The process was the reaction of ethyld ester where substitution of group X should be exchanged by cyan group. In the process of the research the micro-flow reactor has been used, and products were IR analyzed combined with chemometric. Then the kinetics evaluation (Reaction Analysis Studio) has been made giving possibility of optimization of the reactor. The by-product has been identified as a natrium salt.

The evidence of efficiency of applied procedure is given in the following table.

Table 4: The Procedure of the Chemical Reaction Investigation

Procedures	**Results**
micro-flow reactor	accurate experiment for rapid reactions
in-situ measurements (IR) and chemometrics	determination of complicated reaction mechanism

Reaction Analysis Tool (RAS)	high-performance kinetic estimation and optimization

4. Conclusions

1. The Japanese Government is improving science and technology policy.
2. Mitsubishi Chemical Corporation is improving its R&TD policy.
3. Mitsubishi Chemical Corporation has successfully utilized many kinds of computer simulation technology for speeding up R&TD.

Paper 3: The Role of Professional and Learned Societies in Chemical Innovation

John M. Malin, 2004-2005 Chair, CHEMRAWN Committee, American Chemical Society

Abstract

Providing a forum through its meetings, publications, and educational activities, the professional society plays an important role in catalyzing creativity and scientific innovation. Programs are discussed that demonstrate how major professional societies foster communication, consensus, and development of community. The professional society fills a special niche, encouraging collaboration and development of new ideas among all components of the chemical enterprise.

Introduction.

Successful innovation requires not only the generation of new ideas, but also the communication of those ideas to the scientific and technical community. The role of professional and learned societies in the innovation process is to catalyze interactions among the other components of the chemical enterprise. Academe, industry and government all depend upon the efficient exchange of new ideas, both within their own communities and cross-community.

Professional and learned societies function as communication nodes by channeling and filtering information, principally by means of professional meetings, publications, and educational programs. They also innovate in their own way, by developing new modes of communication:

a) Professional meetings. The desire to develop and contribute new research results is an important driver for the innovation process. Professional and learned societies perform a particularly important service for the community through the organization of professional meetings at which innovators can present new ideas to their peers and receive both comment and recognition. In many cases the first public exposure of a new idea or concept is at a professional meeting.

b) Discussions following presentations can be as important as the presentations themselves. Indeed, many scientists say that what they learn from colleagues over coffee or relaxing in the hallway between lectures is as useful to them as the material presented formally. Large chemical societies such as the American Chemical Society typically bring some 15,000-20,000 scientists together at a single national meeting, providing many opportunities for interaction. Professional and learned societies also catalyze the innovation process through workshops and small conferences.

c) Publications. Most major professional and learned societies publish one or more journals, which are the main mechanism of establishing and archiving new knowledge—the goal of the innovation process. Increasingly, this process now takes place on-line, which allows faster processing of articles, compact storage of data, and a much more effective search capability.

Publications support innovation by helping to establish the priority of research, giving recognition to the first to publish and, therefore, augmenting the pace of research. The publications peer-review process provides a major mechanism for evaluation of research results. Peer review aids the innovation process by helping to identify incomplete or incorrect results before publication. Also, recording the details of work done and the results obtained is crucial to verifying experimental reproducibility, which is a foundation of innovation through the scientific method.

c) Education. Educational activities are extremely important in developing a spirit of innovation among students and teachers. Professional and learned societies are in the forefront of recognizing and publicizing new areas of education, such as green chemistry and sustainable development, in which burgeoning interest has generated many innovative ideas. Educational activities cover a full spectrum of client ages, from preschool to continuing education. Professional and learned societies create symposia, workshops and publications describing new educational principles and techniques that enrich the chemical enterprise worldwide.

Professional and learned societies provide educational opportunities for established professional scientists by offering short courses. The American Chemical Society Short Course program provides specialized training in some 60 topics covering many fields of chemistry. These are offered in several hundred sessions each year at public venues such as ACS national meetings and the PITTCON meeting, and also as in-house courses at industrial and other sites. The courses catalyze interdisciplinary innovation by training established scientists to work in new fields or with new techniques.

d) Recognition: Professional and learned societies give innovators the opportunity to be recognized through national and international awards. Almost all learned societies worldwide present general or discipline-specific awards that encourage members of the scientific community to be part of the innovative process.

Government Liaison. Government leaders in many countries recognize professional and learned organizations as a source of accurate scientific information. In this role, the societies form part of the infrastructure for innovation, providing a basis for improved regulatory and funding decisions.

Conclusions

The community of professional and learned societies is an important component in the innovation process. These organizations tend to encourage democratic participation, helping to establish a "public commons" of ideas and a general validation of societal consensus in their fields. Through their meetings, publications programs, educational activities, awards, and government liaison, professional and learned societies help the scientific community to foster, recognize, and reward innovation.

The ideas and opinions expressed in this article are those of the author and do not necessarily reflect the policy or opinion of the American Chemical Society.

Paper 4: The Changing Face of Chemistry in the United Kingdom

Dr. Alan Smith, United Kingdom

The Past
The structure of the chemical industry in the United Kingdom has changed substantially during the last 20 years. In 1980, there were 31 companies registered under UK ownership. In 2000, 16 were registered under U.S. ownership, 6 French, 5 German, and 4 Swiss. Considering the sectoral-wise division of the chemical industry among pharmaceutical and other chemical companies, the number of chemical companies registered on the London stock-exchange has changed very much.

Table 1: Structure of the Chemical Companies Registered on the London Stock-Exchange

Years	1992	2002
Pharmaceutical companies	2	34
Other chemical companies	31	18

The Present
The sectoral breakdown of the chemical industry by value in the European Union is given below.

Table 2: Structure of the EU chemical industry (1999)

Sector	% of the production by value
Pharmaceutical	26
Specialty and performance chemicals	22
Rubber ,plastics, man-made fibers	16
Petrochemicals feedstocks, basic chemicals	13
Soaps, detergents, cosmetics and toiletries	13
Inorganic, chlor-alkali, gases, nuclear,	5
Fertilizers, agrochemicals	5

The R&D expenditures of large-scale companies are much higher in the pharmaceutical sector than in chemical industry. The median for the pharmaceutical industry (11 large-scale companies representing sales of about 180 billion British Pounds) is 12,5 % of R&D expenditures at 25% of the operating profit. There are cases of very high R&D expenditures, such as 20% of R&D on about 35% operating profit (Eli Lilly).

A substantially different picture is observed in the chemical industry. The median is located at 4% of the R&D expenditures at about 10% of the operating profit. There are some exceptions like Dupont and Lonza, which have about 7% of R&D expenditures at 30% of the operational profit. In the UK, the structure of R&D expenditures is similar.

Table 3: UK R&D expenditures

Sector	Year 1990 in %	Year 2000 in %
Pharmaceutical	26	36
Other chemicals	3,5	2,7
Other manufacturing	2,0	1,7

However, in the EU these expenditures do not bring the expected reward. A study by CEFIC titled "Barometer of Competitiveness" showed numerous factors penalizing innovation in the EU chemical industry:

- regulatory requirements for R&D
- spending on R&D
- regulatory principles
- number and cost of notifications for substances
- time required to meet all regulatory requirements

The cost to bring new products to market is 10 times higher in the EU than in the USA, and it takes three times longer.

The Future

The industry is facing pressure from all sides:

- global markets and competition
- rapid pace of technological change
- high cost and risk of R&D
- stock-holder demand for near-term profit
- government regulation
- customer pressure on costs
- technology/product complexity
- competing materials

The UK chemical industry must meet all these challenges to continue to be an export-oriented industry. It currently has a positive balance of payments of 5,5 billion British Pounds (about 10% of the turnover). The requirements for R&D and services proportions must be understood and kept under control.

Table 4: The R&D and services requirements in specific sectors of the chemical industry

Type of requirements	Pharmaceuticals	Effect chemicals	High volume	Custom synthesis
R&D intensity	High	High	Low	Low
Service requirements	Low	High	Low	High

The following innovation metrics are currently used to keep the industry competitive:

- amount spent on R&D per annum
- proportion of turnover coming from new products (< 5 years old)
- proportion of the profit coming from new products (< 3 years old)
- number of extra employees arising from new product introductions

In the UK specifically, universities are largely contributing to innovations. The spin-outs from 28 chemistry departments are related to 63 innovations applied in British industry. Also, materials science departments are contributing in particular to the following fields: nanotechnology (six start ups < than 3 years old), healthcare (5 start ups < than 3 years old), and new materials (4 start ups < than 3 years old). All together there are 23 new start ups less than 3 years old.

To organize better the impact of university research on the development process, the Faraday Partnership concept has been implemented in the UK following the example of the Fraunhofer Gesellshaft of Germany. Faraday Partnerships promote improved interaction between the UK science, engineering, and technology base and industry.

The specific logic of the technology road map must be considered when planning the innovation process. The following questions must be addressed and answered:

- Where are we now? Where do we want to be?
- What new processes/products will be needed to get there?
- What technology will be needed to achieve those products/processes?

Numerous technology-specific and product-specific roadmaps have been produced for different sectors of industry. These roadmaps provide companies with some answers to the following challenges:

- how to reduce the cost and risk of R&D
- ways to leverage technical resources
- how to guide technology investments
- how to boost the company image
- how to capitalize on existing research

- ways to co-ordinate access to R&D funding resources
-

In the USA, the specific fields such as advanced materials, molecular biology, and information science are poised for explosive intellectual and commercial growth.

The key themes for the UK are as follows:

- energy
- medical (imaging, tissue engineering)
- information and communications (photonics)
- systems for life (water, food safety, security)
-

An excellent summary of the innovation process is given in the book *Fourth Generation R&D* by W.L. Miller and L Morris: "Innovation is a difficult and complex problem that is constrained in many dimensions, but it is also an important activity and its mastery is vital for the long-term well-being of nations, companies, communities, and families. Only innovation increases the size of the pie, which means that only innovation leads to improved standards of living."

Paper 5: Policy Measures to Speed up Innovation Promotion in the EU

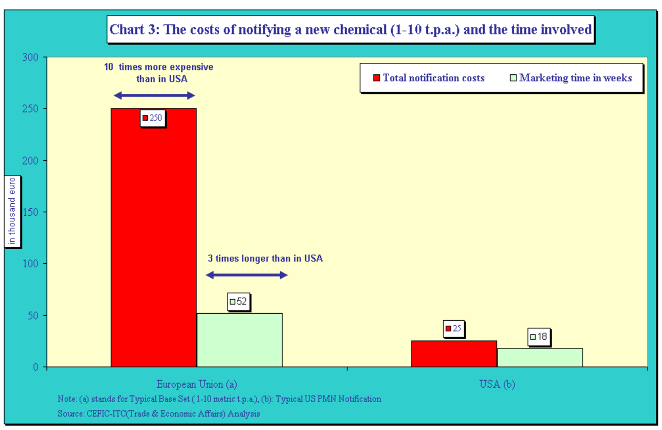
Collin Humphris, CEFIC, Belgium

Cefic Research & Science has two main activities. Through its LRI program, Cefic sponsors research into the health and environmental impact of chemicals. It also works to actively stimulate innovation that supports the sustainable development of the industry. There are two areas of public policy relevant to Cefic's work, which often seem to be in conflict. On one hand, there is no question that effective regulation is needed to protect human health and the environment, but on the other hand economic growth through innovation must continue to be stimulated.

Every year Cefic, publishes a "Barometer of Competitiveness," which focuses on issues that affect the European chemical industry. In 2000, this project looked at innovation and in particular the impact of regulations relative to other regions of the world. It identified a number of factors penalizing Europe:

- regulatory restrictions on research itself
- impact of the overall business environment on companies' profitability and ability to invest in innovation
- comparison of the blanket European approach to testing to establish risk compared with prioritized approaches elsewhere
- scope to innovate (i.e., reformulate) in speciality areas given lower numbers of new notifications
- actual cost per notification and the time it takes to complete the technical and notification dossiers

The stark facts are that in comparison with the US, it costs 10 times as much and takes three times as long to complete the technical work. Base costs are typically €250k <10 tonnes per annum, plus additional €500k up to 100 t.p.a, & over €1000k for over 1000t.p.a. This heavily penalizes low-volume chemicals which are typically the products of smaller companies. So what has the impact been and what is the outlook?



Manfred Fleischer (WZB) has shown that regulations arising from the 6th and 7th Amendments of the Dangerous Substances Directive have led to the following situation. European notifications have averaged 143 per annum over the past 15 years, whereas in the US, where the industry is of comparable size, the average has been 425.

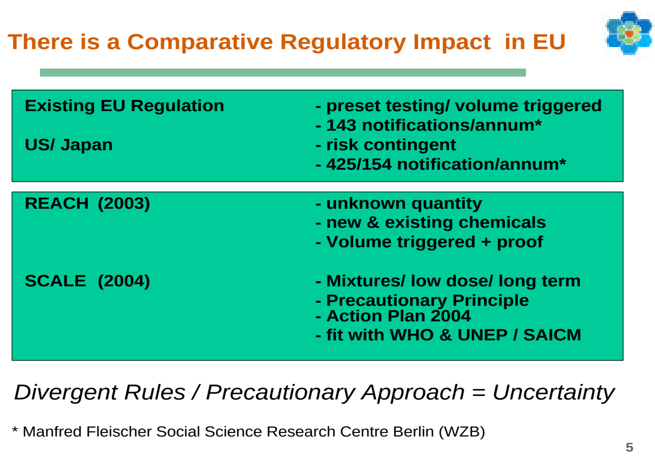
Things could potentially become worse. New regulations, known by the acronym REACH, have been proposed that are intended to tidy and simplify previous legislation and find the right balance between control and enterprise. REACH relates to:

- registration of all substances above 1 tpa
- evaluation of all substances above 100 tpa and all of high concern
- authorization of all especially hazardous chemical substances

These proposed regulations would introduce a burden of proof that a particular use of a substance is not harmful. Authorizations would be use specific. REACH is within the consultation period and the final details are unclear, but additional regulations are also being proposed.

Less familiar will be a new proposal for chemicals known as SCALE, which is moving rapidly towards an action plan in June 2004. This proposal focuses on the impact of chemicals and environmental factors, at low doses over long periods of time, on the most susceptible group of people—children. The stated intention is to bring good Science to bear on factors affecting Children's health and the environment, to raise Awareness of the environmental threats, to Legislate as necessary, and to set up continuous Evaluation (i.e., bio-monitoring) of environmental health issues across Europe. The danger is that such an ambitious vision simply takes an excessively precautionary approach.

This is not simply a European development. There is a good fit with WHO interests and the developing UNEP proposals for a Strategic Approach to International Chemicals Management. Overall, the cost and time involved with divergent approaches and increasing uncertainties around the world should concern all those interested in promoting innovation.



Cefic fully supports sound regulation that both protects human health and the environment and encourages enterprise. Cefic's concern is that REACH does not achieve the right balance between protection and competitiveness. A tiered risk approach is essential to making the system workable and affordable with a clear need to focus on category 1 and 2 carcinogens, mutagens, and reproductive toxicants. On SCALE, Cefic is now fully engaged in the process of establishing a meaningful and relevant Action Plan.

But is regulation the only public policy issue relevant to innovation? Last year, a major project was undertaken in the UK to look at innovation and growth in the UK chemical industry. This multi-stakeholder activity involved a broad cross-section of people from government, industry, cities, academia, unions, and NGOs, as well as customers. The work recognized the good work going on in many areas, but real concerns for the future remain. The work set out to introduce new thinking to supplement existing activity and to make clear the responsibilities of industry and what a supportive government could look like. The report was published last December and is available on the DTI website

The CIGT looked at four broad drivers:

- the market outlook and the economic outlook for the UK relative to other manufacturing regions
- the interplay between the very poor reputation of our industry and the licence this gives governments to regulate it in the absence of trust
- the skills the industry needs and the ability to attract the most able

and lastly, and by no means least, innovation and what can be done to stimulate it

These factor clearly interact. The reputation of the industry influences career choices and subjects of study. The market affects the interest to innovate which we have seen is directly impacted by regulation but which is also influenced by the availability of bright creative chemists and engineers. It is a multifaceted issue.

Looking at the Innovation there are very good things going on. The government recognises the importance of an innovative manufacturing sector and the role the Chemicals industry plays in this. The UK is thinking forward and has some excellent schemes to promote knowledge transfer between the science base and industry. This interest and support is both national and focussed on the special interests of the different regions.

It was also clear that many things could be better. The management of the science, innovation, and chemicals industry agenda are not well aligned and the processes to do this relatively weak. There is a concern that knowledge transfer is relatively under-funded and that with too many schemes (40 were identified), too little is spread too thinly for good effect. Industry was concerned that typically the costs of engagement were high and success uncertain and that the scope of work did not include proof of concept (typically at pilot-plant scale).

These same concerns are shared at the European level—mainly the Commissions Framework programs and the work of Eureka. For whatever reason, the industry is under represented in the current Framework programs and has no active work within Eureka.

In response there is a lot of activity. The UK is in the process of establishing a Chemicals Innovation Centre, which will have the role of helping companies engage, network, and define industry priorities. A forum has been established chaired by a government minister to bring more alignment to science, innovation, and industry priorities.

Cefic is starting comparable work at the European level. It is working to clarify a future vision for the industry and within this the innovation priorities. These will be in two distinct areas.

- topics of generic interest to the industry typically relating to HSE
- topics that will be fertile areas for competitive interest by individual companies

Cefic is in dialogue with the commission to develop what are being called “technology platforms,” technical themes important for the future. Cefic is proposing three pilot technology platforms:

- alternatives to animal testing
- biotechnology routes to simply synthetic process steps
- the role the industry has to play in water use and supply

Conclusions

Regulation in Europe demonstrably penalizes innovation and things could get worse. The role of a representative body such as Cefic is to work to influence thinking to protect health and the environment while also protecting enterprise. More can be done to stimulate innovation if governments and industry work together constructively through public/private partnerships. The key is for the industry to be clear where its priorities lie—easy for a company; much more complex for an industry.

Paper 6: Chemical Education and Chemical Industry in Turkey

Ayhan Ulubelen, Faculty of Pharmacy, University of Istanbul, Turkey

University Education in Turkey—Historical Overview

Until the late 18th century, higher education in Turkey (Ottoman Empire) was organized in theological schools (Medrese). In 1734, the first math and geometry school was founded; high school (Idadi) graduates were accepted in this higher education center. In 1774 a naval engineering school was established and in 1795 a civil engineering school was started. The first university (Darul- funun- gate of sciences) was opened in Istanbul (capital city of the Ottoman Empire) in 1915. Professors from Germany and Austria were invited (e.g., Prof. A. Arndt, Prof. von Hosch, Prof Fester, and others).

The university system in the Turkish Republic had three stages of development:

1. from 1915 until 1933
2. from 1933 until 1981
3. from 1981 until the present

During the first period, some professors had degrees while others did not. It was not compulsory for professors to carry out research. It was considered satisfactory for them to give lectures, have examinations, and carry out lab experiments for teaching purposes. If somebody wanted to carry out research it was considered a voluntary activity.

The second period started in the tenth year of the young republic and involved some revolutionary changes. After their examinations, hundreds of students were send abroad to Germany (majority), France, Italy (to study Latin law and art), England, and to the USA. From 1930 to 1950 a number of Jewish professors came from Germany by invitation of the Turkish government. The country was lucky to have known these wonderful scientists in medicine, chemistry, physics, and other fields. The Turkish students who had studied in Europe, some of whom had obtained doctoral degrees, came back to Turkey and worked with these professors. But because of World War II, research was limited at the five universities in Turkey.

After 1960, a jump in activity occurred across the sciences. Many university graduates from different science fields went to American universities to obtain masters or doctoral degrees. Some of these students returned to Turkey, bringing with them sophisticated research knowledge. However, the pace of activity slowed down after student protests in 1968. Higher education suffered more setbacks in 1980 when the military took control of the country and blamed unrest on university students.

During the third period, the Higher Education Council was formed, which resulted in a major loss of academic freedom. The law accorded many right to university presidents and deans, who were not always impartial in judging the merits of teaching personnel. However, the fact that their terms eventually expire has caused them to act in a more neutral manner.

Also during this time, a new method for assessing the merits of professors was instituted. It involved checking the number of papers published in SCI journals. Partly due to this system, and partly due to competition among young scientists, Turkey rapidly climbed in the rankings of SCI citations by country, going from number 46—with 250 publications—in 1981 to 22—with 9321 publications—in 2002. In 2003, Turkey is expected to have over 12 000 publications in SCI journals. Over this same time period, Turkish scientists have also doubled their publications in non-SCI journals.

In 1960, the TUBITAK “Scientific and Research Council for Turkey” was formed, with branches in Ankara and Istanbul. The Marmara Research Center was established in 1963. The TUBITAK supports basic and applied research on the basis of submitted projects. There are seven areas that the council supports: Information Technology, Genetic, Highly Technological Materials , Biotechnology, Molecular Biology, Environment, and Industry-University Innovative Relation. The Marmara Research Center is a well equipped institute for basic and industrial research. The center helps small- and medium-sized industry solve problems, often in innovative ways.

Another important step in the growth of the Turkish sciences was the establishment of the Turkish Academy of Science in 1993. Although the Academy is a young establishment, its members works with enthusiasm in social and other fields. The Academy provides grants to young scientists for important research projects. One important project is a “Cultural Inventory of Turkey.” This project started in four locations—two in the eastern and two in the western parts of the country—and covers different aspects of the culture such as archeology, history, ethnography, architecture, and ethnobotany. The Turkish Academy of Science is part of the European Organization of Science Academies (European Academies Assemble).

Turkish Chemical Industry
The chemical industry in Turkey is rather new. The first cement plant started in 1911 in a small town near Istanbul. Small cotton and silk mills existed during the Ottoman Empire.

Because there was a lack of private capital when the Turkish Republic was established in 1923, the government established sugar factories (now over 30 operate), cement factories, paper mills, cotton and silk mills, as well as the textile industry. After 1950, the private sector established small- and medium-sized industrial operations. The government developed the petroleum and petrochemical industry, establishing four large petrochemical centers, which are supposed to be privatized.

The pharmaceutical industry was developed by private groups and now is an important part of the chemical industry, selling to the local and international markets and also establishing joint-venture plants in Africa, Russia, and in other post-soviet republics. In the inorganic area, chromium and boron are the dominate minerals, although most of the minerals are sold unprocessed. There is also a house-hold chemicals industry operated by the private sector. Lastly, the glass industry, which was started in 1935 and is a very important source of exports for Turkey, involves the production of crystal glass ware and flat glass.

Innovative Process
The research is carried out in universities supported by different foundations and grants. The idea of developing new technology is rather new to Turkish industry. The industry was oriented towards the purchase of proven processes from licensors abroad. However, three technology parks were established to develop technologies for small-scale industry:

a) Istanbul TUBITAK Gebze
b) Istanbul at Technical University
c) Ankara in the Middle East technical University

The important work carried out at these parks should provide the innovative support the chemical industry needs to make a significant economic step by the time the Turkish republic celebrates its centennial in 2023.

Paper 7: A Ternary Approach to the Innovative Process

Raymond Hamelin, Paris, France

Innovation as an Interactive Structure Changing in Time

The innovative process depends on an interactive structure composed of three elements: science, technology, and society. The impact of each element has changed during the centuries of human development. Before the 17th century, the impact of science was very small and the application of technology to society was exclusively due to craftmanship. During the 18th century, science started to grow and progressively became an equal partner in the triad through the successive industrial revolutions.

It is interesting to note that the concept of "progress" appeared at the same time. In 1750, Turgot said that scientific knowledge will be the source of technical progress, leading humanity towards happiness in an undefined future. This concept was developed by Condorcet and some of the "Encyclopédists," such as Voltaire, but not all of them (Rousseau). The 19th century saw the development of several scientific fields supporting the industrial revolution (i.e., the technical progress announced by Turgot). A confusion appeared between two meanings of the concept "progress". For a majority of philosophers (positivists) progress meant a road, the only road to happiness for everybody. For the scientists and the industrialists, progress was a quantitative measure of economic and social development. The misundestanding has increased with time and is particularly acute nowadays. The so-called "Two Cultures" phenomena of C.P. Snow was born in 1750 in a Turgot lecture.

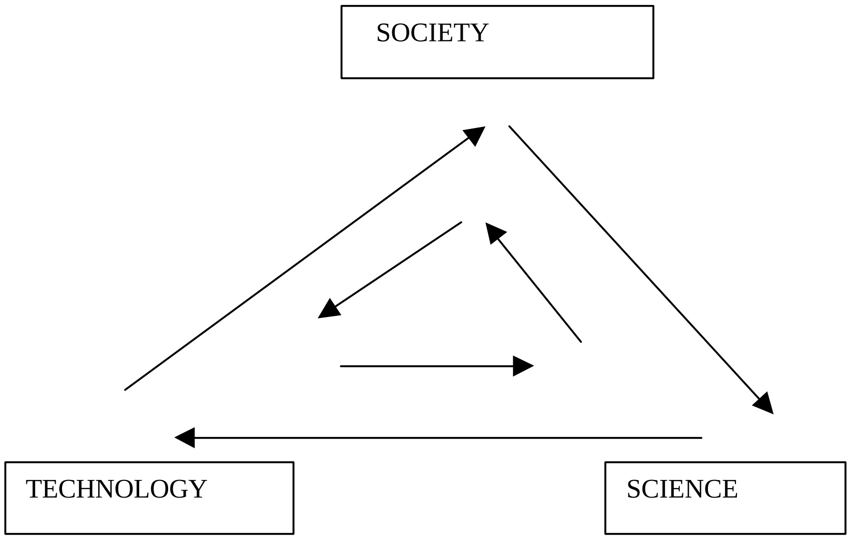
Until the third quarter of the 20th century, the innovation process has been ruled according to a cartesian rationalism in the format of a linear model:

Scientific research **-** Technology development **-** Societal application (incl. business)

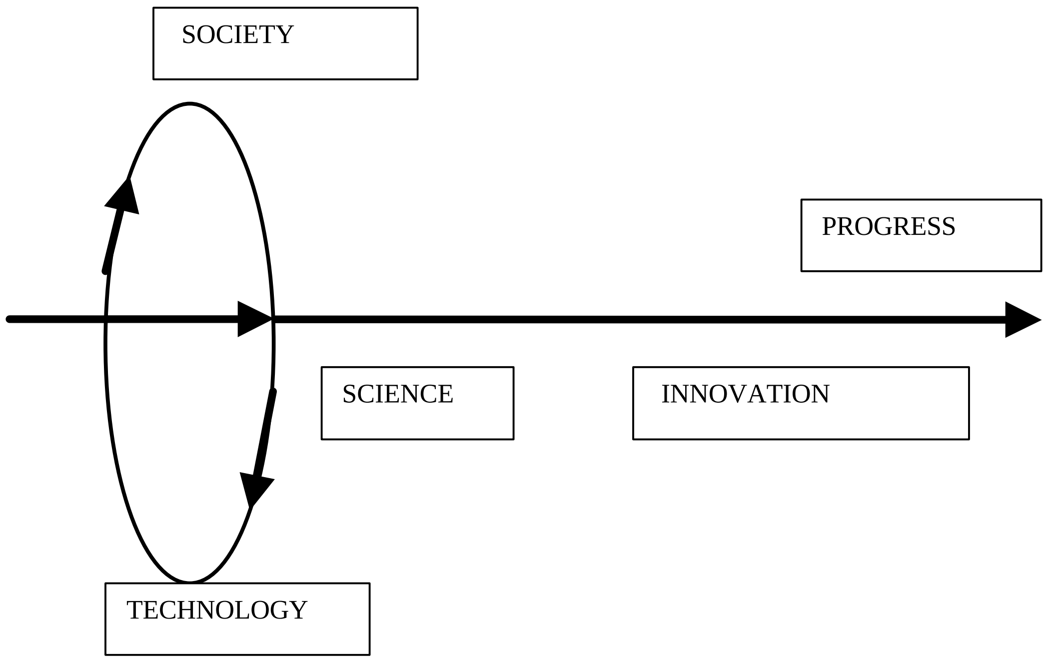
"Progress," the result of this linear process, was (and is still) measured by various indicators and highly celebrated by governments, economists; politicians, electors, etc. At the same time, modern philosophers are all saying that "progress is dead" because it results in apocalypse (Czernobyl, pollution, climatic changes, etc) instead of the expected happiness.

The linear model is based on binary interactions. For example between science and technology: the R&D activity, the scientific and technical literature, associative bodies like IUPAC, the universities' departments of engineering, ... Societal matters are almost completely absent. It's the same with the interaction technology **-** society: science is almost absent in business schools' curricula, technical magazines, etc.

The negative impacts of a certain number of technological breakthroughs (nuclear bombs, PCB, CFC,etc) and the fears of terrific dangers (real or not: radioactivity, induced cancers, GMO,...) show that the binary approach is not adequate to give a positive image of the technical progress. The triad must be considered with a ternary model, as a circular loop with continuous interaction between the three elements, two by two:



The Ternary Approach
With the ternary approach, innovation appears as a factor of intensity depending on the three interfaces on a circular loop and progress appears as a flux created by this intensity:



The central part of this loop where the three elements are interacting represents the field of activity of the various types of engineers. Their role is to transform scientific data into technical innovations useful for society. All three elements participate in their professional and social activity. Therefore, the course of a good engineering school must be a balanced mixture of :

* solid scientific background;
* technological competence
* some societal and cultural aptitudes (languages, law, ecology, management; economy, arts, etc.).

The innovation loop has interesting features. Progress is a consequence of an intensity of means exchanged between the three components (science, technology, and society). For example: a decrease in the financial support of the research activity induced a reduction in the overall progress. Through a cooperative program, the innovative loop of a developed country will induce an innovative intensity in a less developed country with the necessary condition to have a real interaction between the three components (without a scientific structure there is no chance for significant progress). And so on.

The ternary approach cannot be completely rational because it includes a societal element. We may call "neo-cartesian rationalism" the type of approach that we see applied in new concepts such as sustainable development, green chemistry, ... The courses in good engineering schools (in France, at least) are more and more conceived on this basis.

To be truly successful, a CHEMRAWN Conference must adopt such a ternary approach: the meeting itself must explore the science - technology interface with the necessity of expressing conclusions and recommendations applicable to society. The Future Action Committee has to be attentive to this aspect before and during the meeting and to be sure of the speeding of those conclusions and recommendations in the society after the meeting. A CHEMRAWN Conference is not an usual meeting of chemists for chemists, at least when its F.A.C. is efficient.

Conclusion
The chemical innovative process must progressively and urgently adopt the ternary approach at the start of any research program. Societal constraints have to be considered already at the laboratory stage. This is a mandatory

condition to restore the public image of chemistry in society.

Session D. Summary of Presentations and Discussion Held on 12 August

J.A. Kopytowski, CHEMRAWN Committee Member and Secretary 2004-2005

Introduction

Innovation is much more than invention. Innovation has its specific dimensions and instrumentation. Innovation has real impact in the following dimensions:

- economic—it has real impact on the national income and turnover of companies
- social—it changes the behavior of the society and consumption pattern
- financial—it creates the targets for investment
- scientific—it opens new areas of know-how, advancing the understanding of the rules of nature

Innovation also results in advanced techniques and instrumentation. Often major innovations require changes on a variety of levels:

- social—organizing people around the goals of development
- human resources—developing new ways to manage and organize human capital
- instruments—designing and engineering new instruments or envisioning new applications using existing instruments
- information technology—improving computer technology in order to collect and process large amounts of data
- economic—creating new methods to continually assess the economic impact of the innovation

There are no systematic studies analyzing and evaluating the progress achieved through innovations, including the impact of new processes on new products, or of new products on new applications. Progress is rather evaluated according to the following parameters:

- increase in the living standard at lower social cost
- development of new ways of thinking
- new frontiers of knowledge

Until around 1975, the innovation process was ruled according to a simple linear rationalism by which scientific research impacts on technology development, and the later impacts on societal application. However, and as presented by R. Hamelin (see figure), science, technology, and society are all part of a more complex interaction, by which innovation appears as a factor of intensity depending on the three interfaces on a circular loop and progress appear as a the flux created by this intensity.

Some companies are measuring the impact of the innovative process by analyzing the number (turnover) of new products introduced on the market during the last five years and the proportion between traditional and new products from that period of time. However, these statements are made using the non-transparent methodology that makes it difficult to objectively judge the impact of the innovative process (e.g., GDP growth). Some examples were given by Dr. Norling.

Keeping with the tradition of examining a world need, the goal of CHEMRAWN XVI was to examine the innovation process in the chemical industry; specifically to look at techniques for more efficient development of new products and processes, and approaches to overcoming the significant barriers encountered in these efforts. The proof that this initiative was timely and well oriented is the recent establishment in the United States of the National Innovation Initiative, which was created by the Council on Competitiveness. The previously underestimated management of the technology has become crucial for further development.

Organization of CHEMRAWN XVI

CHEMRAWN XVI was organized as a one-day Consultation Forum in Ottawa in the framework of the IUPAC General Assembly. The Forum has been organized in three panels. The 16 speakers has presented their papers ; four invited speakers: UOP, BP Chemicals, CEFIC, SRI) and twelve were members of the CHEMRAWN Committee representing industry and academia. Overall participation in Forum was 27 . The summary has been presented at the joint COCI and CHEMRAWN Committees meeting on 12 August.

Summary of the Presentations and Discussion

Present Character of the Innovative Process

As A. Smith showed with his example of the United Kingdom, the restructuring of the chemical industry in the last decade was due in large measure to globalization trends. This fact has large-scale implications for research and development (R&D) and innovation in the chemical industry. Following are some of the issues surrounding globalization that speakers discussed:

- As G. Intille reported, R&D is no longer a local activity—it has worldwide components. He also pointed out that competition in the chemical industry might arise from any corner of the world.
- P.M. Norling noted that a 5% yield from R&D is fairly typical for most chemical companies (some report better than 20%). To finance such a low yield is beyond the means of small and medium-sized companies, according to Norling. Therefore, R&D has become concentrated in the multinational companies, many of which have spent more on R&D than on direct investments during the last several years.
- As reported by M. Evans, the implementation of innovations on an industrial scale requires more and more investment due to the global capacities of the industrial units. (e.g., BP Chemicals first plant of fluidized bed process for vinyl acetate monomer has a capacity of 250 000 t/year).
- As discussed by M.C. Chon, M. Imanari, M. Evans, and R.H. Jensen, a trend in the innovation process is to apply the most sophisticated computer modeling and analytical devices to speed up industrial design and implementation. This has been mainly true in areas such as reactions scaling, catalyst selection, and testing of reactor models.
- Innovations are usually related to the chemical reaction, which may be regarded as a central processing unit in the frame of the technological unit. The technological unit is also composed of process units that feed the reaction conditions, as well as process the products of the reaction into commercial form. The selection and engineering assessment of these adjacent units in the majority of cases is established mainly by the computerized systems and is not necessarily part of the innovative process.
- G. Intille pointed out that companies often rush to evaluate the cost-effectiveness of innovation, but as J.A. Kopytowski discussed, it is often necessary to apply heuristic rules to assess the size and pattern of specific units involved in the implementation of an innovative process. Regular assessments are needed for decision-making purpose, resulting in a “kill” or “continue” decision. Use of heuristic rules results in many fewer errors according to Kopytowski. Companies have developed specific rules of assessment from the point of view of algorithms (according to P.M. Norling) and supervision organization (i.e. Degussa Project Houses, presented by M. Droescher).
- It was clear from the presentations that biochemistry is dominating chemistry research. A survey of worldwide abstracts has shown that 42% are oriented toward biochemistry and 20% to applied research. In 2000, 25% of U.S. patents were related to biochemistry. However, it should not be forgotten that each bioprocess also requires unit processes defined by chemical engineering.
- Through “octopusing,” chemical processes are being applied in other industries and are being used to develop new products outside the “classic” chemical industry. The examples given by F. Kuznietsov showed the amazing applications of advanced chemistry and physico-chemistry in the fields of energy production and distribution. It is expected that this trend will lead to the establishment of new scientific disciplines.
- There are growing numbers of qualified chemists worldwide who are outside of the traditional research centers of the industrialized countries and who can't find jobs at universities because they are already staffed beyond capacity. However, as P. Moyna discussed, the technological changes that are occurring throughout the industry are requiring new development strategies, which should provide new options for research chemists in these areas.

Identified Deficiencies in the Innovative Process

CHEMRAWN XVI explored the external and internal deficiencies of the innovative process in the chemical industry. The external deficiencies discussed were as follows:

- The introduction of biotechnology into many processes has resulted in a new impact on the environment that requires large capital expenditures to sustain conditions of operation and commercialization or require changes to laws or rules.

- The new processes used in the chemical industry are of higher capacity and automated, which means that less labor is required and fewer workers are needed.
- The R&D process is concentrated in the large multinational chemical companies. While small- and medium-sized chemical companies provide about 90% of the employment, they are mostly excluded from the innovation process.
- In many countries, young people are avoiding scientific careers, especially in the chemical sciences, because there is a lack of jobs for scientists. The establishment of "technology parks" has been explored as a means of facilitating interaction between academia and industry and generating interest in scientific careers.
- Government attitudes and funding are mostly inadequate. In the United States and the European Union, government funding of R&D exceeds the gross domestic product (GDP) of many countries. Therefore, one could expect that these funds would be distributed wisely and in conformity with the merits of the projects. However, many problems have been identified with the way R&D funds are distributed:
  —Funds are going mainly to the "high sciences" and politicized projects, and are not oriented to solving problems that concern private industry.
  —Under pressure from different political and pseudo-political groups, some governments are establishing rules and regulations that are suppressing the innovation process. This is easily observed in EU countries where the cost of implementation and bureaucratic delays are much higher and longer then in the United States.
  —The governments of many countries do not have clear strategies in regard to the macroeconomic parameters of R&D. This is especially valid in developing countries or countries in transition where a meager 0.1%-0.4% of their already low GDP is allocated to R&D. The self-organization of the industrial community may largely improve the actions of governments. In particular, the role of large professional organizations should not be overestimated if their influence is used properly and in a timely manner.

The following internal deficiencies were discussed and concluded at the joint meeting of the IUPAC Committee on Chemistry and Industry (COCI) and CHEMRAWN, the day after the forum:

- The scientific community—academe in particular—is only oriented toward the first part of the innovative process: invention. Often, when an industry approaches universities with the intention of implementing new processes, it finds that more research is needed (usually a long and costly process) to prove the invention's profitability.
- The scientific community is seeking research funding in "politicized" areas (e.g., the "climate warming" problem), while many important social and economic problems remain unresolved.
- The scientific community has established a pattern of "self support" when projects are competitively selected. This means that funding is not necessarily based on the merits of the proposal.
- The potential of R&D is decreasing around the world due to the effects of multinational companies; small groups of researchers are losing out to large companies in their search for funding. Large companies prefer to kill the competition in research instead of cooperating, although they very often use the creativity of small R&D companies. In addition, these large companies seldom subcontract with small research companies in the developing world.
- Process engineering, which is crucial to innovation implementation, is under-funded and funds are decreasing. In many countries this is due to budgetary difficulties, but in others it is because of underestimation by liberal politicians of the potential impact of innovation. However, it must be acknowledged that the unit cost of R&D is constantly growing mainly due to the need for expensive research instrumentation. Despite these cost barriers, examples at the forum showed that combination and new usage of existing equipment resulted in fruitful research advancement.

FORUM RECOMMENDATIONS

I. The CHEMRAWN Committee and other related IUPAC bodies should actively participate in the planned INNOVATION CONFERENCE in Beijing at the next IUPAC General Assembly meeting.

II. For the purpose of disseminating the crucial innovative process features, particularly for developing countries, the following "white papers" should be prepared:

   a) Evaluation methodology of the assessment of the innovative process

b) System of establishing technology parks: the roles of universities, industry, and governments in the organization, financing, and implementation of the innovative processes.

III. COCI may consider preparing a position paper on the introduction of the processes for generic products in developing countries, weighing on the one hand the expected losses to global companies and on the other hand the development of the scientific and engineering capability of the developing countries.

IV. Considering the complexity of modern scientific instrumentation used in the innovative process, it is recommended that universities train chemistry students (not just teach) on the software and hardware needed for innovation. The IUPAC Education Committee should consider preparing a framework.