A summary of remarks

Sessions:

1- ***New experimental and simulation tools f*****or material design, synthesis and formulation**
Use of molecular modeling and virtual experiments to understand fundamental phenomena, produce new experimental data beyond the possibilities of current experimental technologies, High Throughput Synthesis (HTS) of molecules (solvents, materials, etc.) for a given industrial application or for obtaining missing properties, catalytic reaction kinetics.
Use of in silico molecular experiments for the design of products and processes.
The laboratory of the future will combine complementary real and virtual experiments for the more efficient and safer design of processes and products using the multiscale approach (nanoparticle synthesis, crystallization, aerosols, sol-gel processes, etc.).

2- **Innovative tools and methods for the evaluation and characterization of materials**
Use of microfluidic and unconventional millifluidic tools to sustain chemical and process development and obtain basic kinetic data for chemical processes. Innovative tools to characterize materials on different scales (atom, nano, micro, etc.) and development of the instrumentation for these systems.
Use of powerful thermal tools enabling catalyst characterization during reactions or the use of in situ spatially resolved methods to determine spatial characteristics within a catalyst under reaction conditions.
Large-scale research facilities to characterize the nano and microstructures of materials (e.g. drug discoveries).

3- **High-throughput Experimentation (HTE) to speed up the discovery, characterization and evaluation of materials**
Use of robotic systems for HTE experiments in catalyst synthesis and parallelized slug flow reactors for material characterization. Development of various equipment platforms for use by different projects and companies taking into account safety and confidentiality aspects. Issues related to the human resources (engineers, technicians, etc.) required to handle a large quantity of experiments. Need for planning of experiments and requirement to handle large quantities of data.

4- **Numerical and experimental tools for process scale-up**

CFD and simulation tools for understanding and designing heterogeneous catalysts. Need for process simulation, intensification and scale-up for the "factory of the future". Useful tools - especially in the case of numerical ones - to avoid unnecessary experimentation.. Illustrations with H2 purification with PSA or a dynamic transient approach to study and optimize 3-phase reactors, as well as the use of CFD for characterizing flows in reactors, etc.

5- **New analytical tools for process monitoring**

A variety of equipment, such as Raman, IR, GC, HPLC, NMR, MS, LIBC, UV-VIS, etc., as well as microfluidic devices, such as analytical tools, miniaturized silicon MEMS columns for oil field applications, have been developed. Process analytical tools with in situ analysis at the "heart of the process" were described and presented. Enhancing process optimization using new analytical tools and a product and process characterization approach (resulting in improved process control). New projects and platforms have been constructed for the development and testing of new technologies, microanalysis, in situ characterization, etc. used by a variety of projects and companies.

6- **Round Table: "Laboratory of the Future". Vision, Integration with the Factory of Future, New methods of collaboration"**

Participants:
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- **To create the concept of the laboratory of the future, find inspiration in real life (observation, art, market, etc.). Life should drive creation. Find research subjects from the market.**

- **The laboratory of the future : 2 different viewpoints**
  - **The incremental lab (research, quality, manufacturing, etc.) to provide answers and knowledge (i.e. Science is the object): modeling, size/time modification, in situ/ in operando, ab initio modeling, in silico experiments, etc.**
  - **The breakthrough lab (creativity, innovation) to provide inspiration (i.e. Science is the tool): Big Data (let the computer think), Design Thinking (Mixer experiment), Art and Science, Crowdfunding experiment**

- **Be able to work in a multidisciplinary environment: the borders between biology, chemistry, physics, material science and mathematics should disappear.**

- **Experiments conducted on a small scale, using minute amounts of products, reducing the environmental impact of laboratories and exposure of researchers (miniaturization).**

- **Network and communication tools are needed to share knowledge, ensuring confidentiality. Data from different labs are available in real-time to distribute to research teams.**

- **Use of various high-tech devices (smartphones, tablets, smartglasses, etc.) to replace or complement computers.**

- **Be able to deal with the large amounts of data produced and be able to process and analyze it.**

- **Use the right tool to get the right level of information**. Being open minded and continuously improving methodologies at lower cost and with faster development times by :
    - Identifying the bottleneck in the R&D innovation process and solving it by combining a variety of skills, simulation improvement, enhancement of available tools, implementation of new technologies, downsizing and parallelization, breakthrough methodologies, etc.
    - Paying attention to local process control and in situ analysis for a better understanding of what is actually measured.
    - No universal, perfect, definitive tool ever, because knowledge, technology and targets are constantly evolving.
    - Use the right tool to get the right level of information.

- **Increase automation and robotics to speed up processes.**

- **Use the potential offered by computational chemistry, in silico experiments and modeling as standard tools for the chemist, reducing the need for expensive experimentation.**

- **Optimize human resources: Small team in the laboratory with a large network (virtual team). One manager, coordinating:**
    - Technical and research team experts from various partners around the world.
    - Academic and private companies and PhD students, engineers, master's students, etc.

- **Partnership with a network of SMEs and research centers.**

- **Pooling of tools: technological platforms with pilots and experimental facilities used by different companies.**
- **The laboratory of the future may be a unit composed of several expert laboratories, with different geographic locations, mobilized on the basis of the specific research requirements (chemical reaction, separation methods, purification, modeling, etc.)**