

Description of the funded research project 1st Call for H.F.R.I. Research Projects to Support Faculty Members & Researchers and Procure High-Value Research Equipment **Title of the research project:** Innovative Catalyst Design via 3D Printing

Principal Investigator: Dr Eleni Heracleous

Reader-friendly title: Innovative Catalyst Design via 3D Printing

Scientific Area: Engineering Sciences & Technology

Institution and Country: International Hellenic University, Greece

Host Institution: International Hellenic University

Collaborating Institution(s): Chemical Process and Energy Resources Institute (CPERI/CERTH)

Project webpage (if applicable):







Budget: 190.000 euros

Duration: 3 years

Research Project Synopsis

Three-dimensional (3D) printing is a fabrication method that creates structures from digital models. Despite the profound impact that 3D printing has had in many fields, its application for the production of materials with chemical functionalities that can catalyze chemical conversions is still in infancy. The main goal of the 3DInnovaCat project is to prepare highly active and stable bifunctional metal/acid structured catalysts with optimized geometries for improved mass and heat transfer characteristics, exploiting the unprecedented possibilities offered by 3D printing, for the one-step conversion of CO₂ to DME.

This ambitious target will be achieved by closely linking advanced catalyst preparation with 3D printing with detailed characterization of the mechanical and physicochemical properties of the materials and testing under industrially-relevant conditions.

In order to meet the needs of the project, we have assembled a strong research team which involves collaboration among scientists expert in the fields of 3D printing and catalytic process development and collaboration among different organizations (IHU and CPERI/CERTH) with available state-of-the-art infrastructure to complete all the technical tasks of the project.

The scientific knowledge and technological know-how that will be accumulated can potentially have a major impact in the field of catalysis and the application of 3D printing for the manufacture of catalyst batches with custom geometries and sizes. The proposed project will contribute in the long-term to economic growth and improved competitiveness, as catalytic processes form the fundamentals of modern chemical and petrochemical industries. Finally, the implementation of the proposed research will offer the involved scientists the chance to collaborate and acquire expertise in areas of high interest. The multi-disciplinary character of the involved scientists will allow the development of unique synergies and transfer of knowledge between the collaborators and will in turn promote the development of specialized scientific personnel and R&D excellence.



Project originality

Despite the advancements achieved in additive manufacturing, there are still several challenges related to the application of 3D printing for catalyst preparation. Most issues are associated with the suitability of the feedstock materials for 3D printing and their compatibility with the conditions typically employed in chemical processes (high temperature and pressure). In addition, when post-treatment is required, a major challenge is to preserve both the macroporous and the micro/meso structure of the 3D printed materials. Solvent removal, required for some extrusion-based printing processes, has been reported to cause shrinkage and pore structure damage. Calcination also caused negative effects on the pore structure, especially for powder based printing. Therefore, improvements are needed to overcome the effects of the post-treatment processes. In addition, the differences in the mechanical properties and chemical stability between various 3D printed materials and materials prepared through conventional methods have not been fully studied.

To the best of our knowledge, the preparation of CuZnAl catalysts alone or supported on acidic supports such as zeolites or alumina through 3D printing has not been systematically investigated. The application of such 3D structures for the conversion of CO_2 to DME in a single step, a reaction with particular issues associated with mass and heat transfer peculiarities, has also not been explored in the past.



Expected results & Research Project Impact

The scientific knowledge and technological know-how that will be accumulated in the course of the proposed research can potentially have a major impact in the field of catalysis and the application of 3D printing for the manufacture of catalyst batches with custom geometries and sizes. The systematic study of the use of different printing materials, 3D printing technologies and synthesis strategies (direct printing and post-printing modification) for the preparation of metal/metal oxide catalysts on acidic supports will provide new insights on the requirements for the fabrication of stable, hydrothermally resilient 3D catalysts, durable under typical chemical reaction conditions, with appropriate active site distribution and good geometry for optimal heat and mass transfer in the reactor.

The proposed project will contribute in the long-term to economic growth and improved competitiveness. Catalyst market was valued at \$28,567 million, and is expected to reach \$40,000 million by 2022, supported by a CAGR of 4.8%. The development of methods for reliable, highly reproducible custom manufacturing of complex, well-defined catalyst structures in an economical and energy efficient way can potentially transform the field with major economic benefits.

On the application side, the development of efficient and economically viable value chains for CO_2 conversion to high added value products can boost the competitiveness of the Greek and European industry. Overall, the application of the proposed technology will have positive impact to the environment, the economy and the employment. The global dimethyl ether market size in terms of volume was estimated to be ~ 4 billion tons in 2014, registering an annual growth rate of 15.67% in between 2015 and 2020. Cost-competitive efficient DME production that would allow its use as transportation fuel would significantly further boost these numbers. DME is currently produced via a two-step process starting from natural gas as feedstock. The replacement of only 10% of the current global DME production by DME produced from CO_2 via the process proposed in the 3DInnovaCat proposal would lead to a displacement of more than 280.000 tons of CO_2 per year.



The importance of this funding

The funding of the research project by H.F.R.I. is giving to the involved scientists the chance to collaborate and acquire expertise in areas of very high interest. The multi-disciplinary character of the involved scientists (catalysts experts with mechanical engineering experts) will allow the development of unique synergies and transfer of knowledge between the collaborators and will in turn promote the development of specialized scientific personnel and R&D excellence.

At the same time, the Principal Investigator and the other scientists involved in the project will improve the competitiveness and extroversion of their respective research entities and will prepare for future collaborations and funding through the EU Framework Programme Horizon 2020.

The research progress and knowledge that will be generated might also become part of the educational programs offered by IHU to train scientists and engineers in making optimal use of the new possibilities enabled by digital fabrication also in the field of chemical processing and catalysis.





COMMUNICATION

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