**Development of a computational approach for the CFD simulation in OpenFOAM of fixed and fluidized catalytic bed reactors for hydrogen production**

**Summary of the research project**

Environmental and geopolitical concerns drive the development and exploitation of new and improved energy production systems. To this end, the use of biogas and synthetic natural gas to produce CO2-free or CO2-negative captive H2 from catalytic processes offers a promising solution. In fact, sustainable biogas as a feedstock may contribute to capture CH4 emissions from agriculture thus leading to a C negative H2. Similarly, the adoption of synthetic natural gas may contribute to reduce CO2 emissions. Alongside the cutting-edge experimental research based on the production and characterization of novel catalyst formulations and their applications in fixed and fluidized bed reactors, a modelling effort is needed to help bridging the knowledge from lab to industrial scales. Some of the most important challenges encountered in the scale up of fixed and fluidized catalytic bed reactors are related to the complex fluid dynamics effects inside the equipment, that in turn affect the energy, momentum, and mass transfer phenomena.

To this end, Computational Fluid Dynamics is a powerful tool to study the interplay of these different transport phenomena, analyze and troubleshoot different aspects of the process and suggest action to help the design and the scale-up of the whole catalytic process. A robust and accurate modelling of such processes must set foot from the realistic representation of the reactor geometry, its operative conditions and reaction kinetics. Whenever possible, ad-hoc experimental data must be used to validate the computational approach in known operative conditions or correlations from the open literature must be employed for validation purposes.

The goal of this project is the development of a computational approach for the CFD simulation of fixed and fluidized catalytic bed reactors for the production of H2 from biogas and synthetic natural gas. The open source CFD software OpenFOAM will be used, and the objectives of this study will be met through:

1. The design and discretization of the computational domain to closely match the catalytic reactors adopted in the parallel experimental campaign;
2. The study of the fluid dynamics in the system without chemical reactions, to develop and test single phase solvers;
3. The development, testing and validation of solvers to couple the chemical reaction kinetics and the thermal effects;
4. The analysis of the predictions of the developed and validated computational approach.

The study will focus on the development, implementation, and validation of OpenFOAM solvers, exploiting the available C++ libraries and coding the system specific solvers needed for the application. The developed libraries will then be used to perform simulations in support of the parallel experimental campaign.

**Activity Plan**

The study will begin from the analysis of results from literature, and it will lead to the development and implementation of numerical models for the simulation of fixed and fluidized catalytic bed reactors with the CFD software OpenFOAM. The activity will continue with the 3D CAD design of the studied geometries and their spatial discretization by means of the generation of a computational grid (mesh), the analysis of the sensitivity of the results to changes in discretization (grid convergence study), the formulation of a computational model describing the phenomena of interest coupled with the catalytic reaction kinetics, within the computational domain, and the subsequent numerical solution of the model equations. The modelling will be validated with experimental results, with particular attention to the integral quantities and local profiles of the variables of interest.