Modelling Methods for Improving the Scale-up of Industrial Multiphase Reactors

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Multiphase reactors are increasingly adopted in the chemical industry in a variety of innovative processes, ranging from the conversion of CO_2 and H_2 into chemicals or fuels to a wide spectrum of chemical productions from renewable raw materials. In case of mass transfer limited reactions, reactor scale-up is particularly challenging and traditional methods are often not adequate to achieve optimized performances.

In this work we aim at contributing to the development of predictive methods combining fundamental knowledge on the phase interactions obtained by fully resolved Direct Numerical Simulations (DNS) and the full-scale description of the turbulent multiphase fluid dynamics in the reactors by Reynolds Averaged based models. The work is complemented by the results of an experimental activity run in parallel, which is specifically designed for guiding towards a robust simulation workflow.

The results of the experimental campaign consisting of overall gas hold-up, power consumption, bubble size distribution in gas-liquid and gas-solid-liquid systems are exploited to assess the multiphase model capability and to provide a physically sound basis for the identification of suitable closure models. Starting from the integral results and the meso-scale distributions, turbulence parameters of critical local portions of the tank are identified and reproduced in the two-phase DNS. The insight gained from experiments and DNS are adopted to improve the reactor modelling.

The resulting modelling framework is exploited to specifically investigate the scale up of a laboratory stirred tank for carbon mineralization in the realm of a project supported from ICSC – Centro Nazionale di Ricerca in "High Performance Computing, Big Data and Quantum Computing" and exploiting HPC resources of ENI and the European supercomputer Leonardo, hosted and managed by Cineca.

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