

## **DIRECT NUMERICAL SIMULATION OF REACTIVE FLOW THROUGH A FIXED BED OF CATALYST PARTICLES**

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Many catalytic refining and petrochemical processes involve two-phase reactive systems in which the continuous phase is a fluid and the porous phase consists of rigid particles randomly stacked. Improving both the design and the operating conditions of these processes represents a major scientific and industrial challenge in a context of sustainable development. Thus, it is above all important to better understand all the intricate couplings at stake in these flows: hydrodynamic, chemical and thermal contributions. The objective of our work is to build up a multi-scale modelling approach of reactive particulate flows and at first to focus on the development of a microscopic-scale including heat and mass transfers and chemical reactions for the prediction of reactive flows through a dense or dilute fixed bed of catalyst particles. A first step is the upgrading and the validation of our numerical tools via analytical solutions or empirical correlations when it is feasible. Then we illustrate the assets of our simulation method on a reactive flow through a pack of different shapes of particles. Our method is implemented in our massively parallel numerical platform PeliGRIFF ([www.peligriff.com](http://www.peligriff.com)) that already enable us to improve the accuracy of predictions in scales which interest engineers in process engineering. In fine, this processus will enable to take a step towards the enhanced design of semi-industrial processes.