Computational Fluid Dynamics (CFD) for catalytic micro-structured reactors design: an overview and successful case studies

Inés Reyero[1], Ainara Moral[1], Pedro M. Diéguez[2], Fernando Bimbela[1], Luis M. Gandía[1,*]

1 Grupo de Reactores Químicos y Procesos para la Valorización de Recursos Renovables, Institute for Advanced Materials (InaMat), Universidad Pública de Navarra, E-31006 Pamplona, Spain. 2 Escuela Técnica Superior de Ingenieros Industriales y de Telecomunicación, Universidad Pública de Navarra, E-31006 Pamplona, Spain

**Corresponding author: lgandia@unavarra.es*

Highlights

- Computational Fluid Dynamics (CFD) is a very valuable tool in chemical reactor design.
- Process intensification can be notably boosted by the use of catalytic-wall microreactors.
- An overview of various case studies and experiences carried out using CFD are presented.

1. Introduction

The recent advances ongoing and continued progress in computing hardware and software are significantly changing the approaches adopted to chemical processes equipment analysis and design. Particularly, Computational Fluid Dynamics (CFD) is becoming an increasingly used tool in many fields within Chemical Engineering and in many other disciplines, such as Biomechanics and Biomedical Engineering, Conventional Energy Production and Renewables, Aeronautics, Automotive, Environmental and Civil Engineering, Architecture, Meteorology, Oceanography, etc. A plethora of scientific articles making use of this tool can be found in the literature, with more than 13,000 works published in the field of Chemical Engineering, experiencing a significant boost in the last 20 years and having reached a plateau of more than 1,000 publications per year in the last 5-year period. It is worth mentioning that the first CFD codes developed date back to the 1960s. Besides, thanks to the joint efforts of different researchers and companies working under multidisciplinary environments, the development of CFD software tools was successfully achieved in the 1980s and has relentlessly evolved until present day. This has resulted in unprecedented levels of detail, accuracy and intricacy in the output results provided in the simulation studies carried out using different commercial and open-code CFD software programs.

Chemical reactors have been notably benefitted by the abovementioned progress, the design of which may be notably improved by the use of CFD. This is because this tool is capable of describing the hydrodynamics of very complex situations; for instance, as occurs in most of the multiphase reactors. Furthermore, CFD modeling allows a complete description of the phenomena governing reactor performance, thus becoming a powerful tool to guide design and scale-up [1].

Structured catalysts and reactors are being successfully employed in a number of processes, mostly related with environmental and energy generation applications. In the case of the micro-structured systems, such as microreactors and catalytic-wall microchannel reactors, the very small characteristic dimensions (typically below 1 mm) prevailing in these devices allow a significant enhancement of the mass and heat transport rates. This results in an incomparable intensification of the process with an excellent temperature control, and improved product quality and process safety. Structured catalysts normally consist of a ceramic or metallic substrate that can adopt several configurations, such as parallel channels monoliths, open cell foams, stacked wire meshes, and microchannel reactors. The substrate provides structural entity and determines the flow pattern inside the reactor. The catalyst, typically composed of a porous support, the active component, and eventually modifiers to tune some properties or provide new ones, is incorporated in the form of a thin layer that coats the substrate walls or even forming micro-packed-beds inside the substrate cavities.

Within this context, the aim of the present work is to present an overview of the status, recent studies and successful case studies achieved in the field of micro-structured chemical reactor design using CFD. Different studies and experiences developed by this research group through the years will be discussed. To cite just a few: hydrogen and syngas production by steam reforming of several fuels (methane, ethanol, methanol) [2–5], preferential oxidation of CO [6,7], production of synthetic fuels by means of the Fischer-Tropsch synthesis [8,9] and photocatalytic production of hydrogen from water-ethanol mixtures [10].

In these studies, CFD models were developed at various description levels depending on the objectives to be accomplished. Parametric studies on the effect of the characteristic dimension, microchannel geometry, catalyst loading, space velocity, feed-stream composition and reaction temperature were performed with models including between 1 and 4 microchannels. These investigations have revealed the great capacity of microchannel reactors for process intensification since they allow working at extremely high space velocities achieving satisfactory conversions and selectivities to the desired products. In general, the effect of reducing the characteristic dimension within the 1 mm–300 μm range is very positive on the microreactor productivity. On the other hand, as the characteristic size increases the negative effects of transport limitations appear very soon as they have been found to start to be present, though slightly, at sizes above only 2 mm.

The microchannel level was scaled-up to a level consisting in two plates with up to 10 parallel channels each. These models have allowed to investigate the thermal integration in the same micro-device of endothermic (fuels reforming reactions) and exothermic (fuels combustion) processes. It has been found that microreactors are very effective for thermal integration. By adjusting the space velocity in each plate it is possible to operate nearly isothermal at very high reaction temperatures which was essential for attaining good productivities and selectivity which was very important for methanol steam reforming and CO-PROX.

Finally, CFD models for complete microreactors and micro-monoliths with up to 100 x 100 microchannels were developed to study the influence of the flow distribution headers, magnitude of the heat losses and effective thermal conductivity of the substrate on microreactor performance. The results serve to illustrate the great potential of CFD for microreactor design [11,12].

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Catalytic-wall microreactor; Computational Fluid Dynamics (CFD), Chemical reactor design, Process intensification.

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