

# Characterization of radial flow dynamics in gyroid structures: A case study of the SCR reaction

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## Motivation

In recent years, Triply Periodic Minimal Surface (TPMS) structures have attracted interest in heat transfer applications and reaction engineering due to their high surface to volume ratio. Among the various TPMS topologies, gyroid structures have been shown to be promising candidates for catalytic applications, owing to their continuous, open, and fully interconnected pore network leading to improved mass transport in radial direction. [1,2]

Radial mass transport is a critical, yet often overlooked parameter in catalytic reactor design, especially in systems exhibiting pronounced radial reactant gradients. A relevant example is the selective catalytic reduction (SCR) of nitrogen oxides ( $\text{NO}_x$ ) in exhaust gas aftertreatment. Despite their widespread use, conventional monolith catalysts suffer from radial maldistribution of  $\text{NH}_3$  (Uniformity-Index of 0,59 to 0,87 [3]) caused by insufficient residence time and mixing of ammonia precursor solutions injected upstream the SCR monolith. In addition, unfavorable injection angles promote wall impingement and diminish droplet evaporation. This maldistribution leads to locally reduced catalyst utilization and decreased  $\text{NO}_x$  conversion limiting the overall efficiency of current SCR systems. [3,4]

Because of their interconnected pore network, gyroid structures could mitigate concentration gradients and improve catalyst utilization. However, the relationship between gyroid geometric parameters and radial mass transport remains insufficiently examined. This study presents a parametric analysis aiming to identify promising gyroid architectures capable of homogenizing radial reactant distribution.

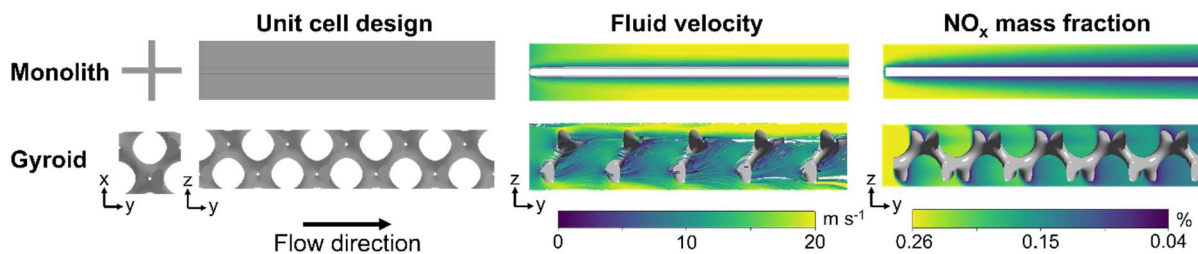
## Methodology

In this work, the ratio of radial to axial mass transport in gyroid structures is systematically quantified as a function of unit cell size and porosity using computational fluid dynamics (CFD) simulations performed in ANSYS Fluent. For this purpose, structures with unit cell sizes in the range of 1 to 10 mm and a porosity between 55%

to 85% are generated. The computational domain consists of an inlet channel, a structural section and an outlet channel. A fluid inlet and outlet are defined in the streamwise direction, while periodic boundary conditions are applied on the lateral boundaries. A particle tracking model is used to systematically evaluate the effects of unit cell size, porosity and flow velocity are systematically evaluated. Consequently, the simulation results on radial mass transport are utilized to design gyroid structures for improved SCR efficiency.

## Results

Figure 1 presents a comparison between the monolith and gyroid structures with respect to fluid velocity and  $\text{NO}_x$  mass fraction. The three-dimensional streamlines of the fluid velocity reveal that, in the monolith, the flow proceeds predominantly in the axial direction. In contrast, the gyroid structures exhibit helical flow patterns and enhanced radial mass transport between adjacent unit cells. With regard to the  $\text{NO}_x$  mass fraction, the results indicate that the conversion efficiency increases by improving reactant transport to the catalytic surface. The obtained insights into radial mass transport highlight the potential of gyroid structures for process intensification, particularly in reaction systems exhibiting pronounced radial concentration gradients.



**Figure 1:** Comparison of the fluid velocity and  $\text{NO}_x$  mass fraction within a monolith and gyroid structure.

## References

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- [2] Ellebracht, Nathan et al., *Energy & Environmental Science*, 2023, 16, 1752-1762
- [3] Vedagiri, Praveena et al., *Environmental Science and Pollution Research*, 2021, 28, 11988-11999
- [4] Jang, Jaehwan et al., *energies*, 2021, 14, 5788