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CFD Characterization of a Well-Structured Porous Medium milli-Scale Flow Reactor

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Highlights

- Geometrical parameters of well-structured porous media are systematically studied.
- RTD and mixing in various porous media are characterized using CFD.
- Introducing a rotational variation in the fiber stacking improves mixing.

1. Introduction

One of the major drawbacks of micro reactors limiting their applicability in the industrial context is their low throughput. Scale-out, i.e. increasing the channel size, could be a remedy for this shortcoming [1], and in this study we investigate fibrous periodic porous media as an open cellular structure embedded in a milli-scale reactor as a scale-out approach. The aim of this approach is to combine the enhanced mass and heat transfer of the micro-scale with the throughput of milli-scale reactors. In general, the geometrical parameters of this type of porous structure, such as fiber shape, inter-fiber distance, orientation with respect to the mean flow direction, and the fiber size can be altered more readily in contrast to typical metal foams (with tetrakaidecahedron unit cell shape) [2,3]. However, the relationship between these porous media characteristics and mixing performance is not yet fully established. Therefore, computational fluid dynamics (CFD) is utilized in this study to investigate the impact of the porous media geometry on mixing, RTD, and pressure drop.

2. Methods

In this study, the porous structures consist of cylindrical fibers with an outer diameter of 250 µm, which are arranged as stacks in consecutive layers in a tube with an inner diameter of 3.4 mm. In all structures, subsequent fiber layers are shifted relatively to each other by a third of the inter-fiber distance (see Figure 1a). In addition, we also introduce rotations between fiber layers with respect to the mean flow direction and plane normal to mean flow direction as shown in Fig. 1 b) and c). Starting from a basic structure (θ=0°, φ=0°, Figure 1 d), we focus on the tilt against a plane normal to the mean flow direction (φ), which is increased from 9° (Figure 1 e) to 22.5° (Figure 1 f) and 45° (Figure 1 g), while keeping θ constant at ±22.5° and additionally keeping φ constant at 45° while changing θ to ±9° and ±45° (Figure 1 h, i).

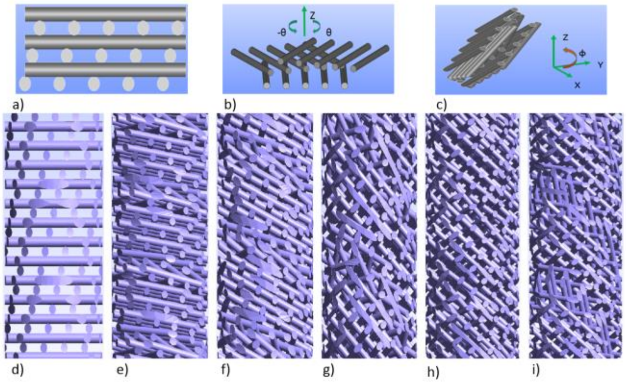

Fig. 1: a) Stacking arrangement of subsequent fiber layers; b) rotation in a plane perpendicular to the mean flow direction (θ); c) tilting against a plane parallel to the mean flow direction (φ); d) Basic porous media with θ=0, φ=0 ; e) θ=±22.5°, φ=9° ; f) θ=±22.5°, φ=22.5° ; g) θ=±22.5°, φ=45°; h) θ=±9°, φ=45°; i) θ=±45°, φ=45°.

The stereolithography (stl) files of the porous structures are generated in SALOME, and the utility SnappyHexMesh is used for mesh generation. The open-source software package OpenFOAM® is utilized to investigate the effect of the porous media geometry on hydrodynamics and mixing. Simulations are performed for three flow rates of 1, 3 and 6ml/min, corresponding to pore-scale Reynolds numbers of 2, 6 and 11.9. First, a steady-state flow field is calculated using the simpleFoam solver. In a second step, the transport of a passive scalar is simulated using the scalarTransportFoam solver. For this, a defined tracer pulse upstream of the porous structures (tracer concentration in predetermined computational cells) is implemented.

3. Results and discussion

Figure 2 depicts contours of the tracer concentration inside the porous structures. For the structure without rotation $(\phi,\Theta=0)$ limited radial mixing is observed, as a peak concentration in the center of the plume is still visible. All other structures with introduced rotation lead to a more evenly tracer concentration distribution. In addition, it is observed that increasing the inclination of the porous structures against the mean flow direction (i.e. increasing ϕ) from 9° to 45° will increase radial transport of the tracer. Furthermore, changing the fiber orientation with respect to the main flow direction (i.e. increasing θ) also promotes an increased radial concentration distribution. This observation can be explained by the increased deflection of fluid elements by the fibers and the tube wall.

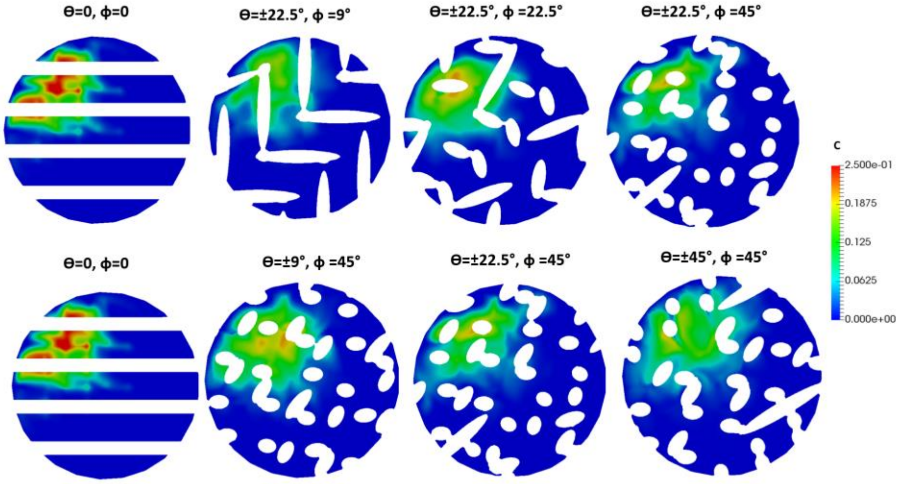

Fig. 2: Concentration profile of the tracer inside the porous mediums on 25% of the length.

4. Conclusions

The mixing performance of porous media with different fiber configurations has been investigated. The study shows that a considerable improvement of tracer distribution can be achieved by utilizing well-structured porous media in comparison to an empty tube case. The RTD study reveals that using the fibrous porous media results in a behavior closer to plug flow reactors. Furthermore, the scalar transport simulation results show that introducing tilting in the stack of fibers will enhance the chaotic mixing by deflecting more fluid elements and consequently dispersing the tracer more radially. In addition, it is observed that increasing the inclination of the stack against the mean flow direction increases the pressure drop. This study reveals the potential of well-structured milli-scale reactors as a scale up method and the link between geometrical parameters and mixing improvements.

References

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Keywords
Porous media; CFD; Mixing