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Publication date:
2012

Document Version
Publisher's PDF, also known as Version of record

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Citation (APA):
Krühne, U., Bodla, V. K., Møllenbach, J., Laursen, S., Theilgaard, N., Christensen, L. H., & Gernaey, K. (2012). *Computational Fluid Dynamics at work - Design and Optimization of Microfluidic Applications*. Poster session presented at 11th International Symposium on Process Systems Engineering, Singapore.

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Computational Fluid Dynamics at work Design and Optimization of Microfluidic Applications

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Motivation

Computer aided process engineering has many potential applications. One of the most eloquent ways of applying computational tools is to predict the performance of systems and to use the predictions for optimization of future designs. Computational fluid dynamics (CFD) has throughout the last decades undergone a breathtaking development and is used increasingly in industrial applications. The prediction quality has indeed reached such a level of maturity that many scientific and industrial users increasingly apply the method for a broad range of applications. A well suited field of use for CFD supported design or analysis is in the area of fluid dynamic conditions with low Reynolds numbers. Typical applications can be found where the flow channel geometries are in the range of micrometers, giving the field the name microfluidics. From a mathematical point of view the equation system is reduced to the Navier Stokes equation and hence no turbulent terms have to be implemented. Therefore the prediction quality of the CFD models is expected to supply excellent qualitative and quantitative results for such systems. This poster presents three different case studies applying CFD in designing microfluidic systems.

Results

1. Scaffold 3D geometry design and optimization

A biological model [1] has been implemented into a commercial CFD platform (ANSYS® CFX) considering the beneficial impact of shear stress. Hence the cost function is optimized considering the maximal area and the optimal shear strain rate (SSR). A similar approach is described in [2]

- Starting geometry with shear strain rate (SSR) plot;
- intermediate result;
- Final 3D geometry in optimized form. The new form is optimized with respect to the homo-geneous shear strain rate field as well as for the maximum surface area.

Conclusions

CFD has been demonstrated as a powerful tool for development of new theoretical qualitative insight or quantitative understanding of difficult measurable key components in microfluidic applications. Due to the lack of turbulent flow conditions in miniaturized systems the CFD results have a high predictive quality and results can be obtained with relatively small effort

Acknowledgments

The work was partly financed by the Danish Research Council for Technology and Production and the 'AUTOBONE' Strep RTD project supported by the EC under the 6th Framework Programme under contract number 505711-1.

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- [3] P. Tufvesson et. al., 2011, Process considerations for the asymmetric synthesis of chiral amines using transaminases, *Biotechnology and Bioengineering*, 108 (7), 1479-1493.

2. CFD as software sensor

3. The design of a microfluidic biocatalytic reactor

Simulation of the interdigitated fluidic array (fast diffusion coefficients for both media);

Experimental setup with dyed liquid streams. Obviously the diffusion of the dye is relatively slow compared to the simulated substances.