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CFD analysis of hydrodynamic and thermal behaviour of Advanced-Flow™ Reactors

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Corning® Advanced-Flow™ glass reactors are continuous flow reactors with hydraulic diameter in the range of millimetres. These devices make possible the switch of chemical reactions from batch mode to continuous processing through more efficient, more economical and safer processes. In addition, these reactors provide a platform for developing innovative chemistries that have never been considered industrially practical, either for hazard or yield reasons.
Corning proprietary apparatuses are compact, adaptable and scalable, optimizing overall production cost and quality of high-value specialty, fine, and pharmaceutical chemicals. Corning Advanced-Flow™ glass reactors are composed of multiple inter-connected glass devices having different designs, offering the advantages of process intensification and glass-specific qualities like transparency and very good chemical resistance.
This paper presents the comparison between experimental and CFD modelling results of a family of Corning glass devices aiming at achieving and maintaining very efficient mixing along the dwell time path. Numerical results are compared to experimental data: velocity profiles measured by micro-PIV means, pressure drop and heat transfer coefficient.
The satisfactory agreement between experimental results and CFD modelling proved the utility of numerical simulations in the development of new designs. Therefore, CFD tools help on one hand to predict the performance of new devices and on the other hand to optimize their design in order to improve their behaviour. Thus, CFD simulation facilitates the design and reduces time and cost for the investigation.

1. Introduction

Process miniaturization and microreaction technology provide opportunities for improving process capability and control in chemical/biochemical synthesis and can allow safer and more efficient chemical/biochemical kinetic investigations. Compared to normal scale reactors, microreactors have the following advantages: decrease of linear dimensions, increase of surface to volume ratio, fast and efficient process development, decreased potential of environmental impact, and increased safety. The large surface-to-volume ratios of the micro channels improve heat transfer for

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exothermic reactions, thus preventing either thermal degradation or explosive evolution (Mae, 2007, Watts and Wiles, 2007, Hessel et al., 2008). The operating conditions, controlled better and more accurately than for classical reactors, are more aggressive, attaining regimes previously out of reach, which imply higher yields, making the separation process cost effective. Side reactions could be avoided or reduced by operating the microreactor in a tight window of parameters where the process selectivity and product purity have the highest values.

Microreactor technology provides relatively simple and quick means towards commercialization of a process. The economic production of large numbers of microreactors enables the shift from the present production paradigm of batch process and "scaling up" to a new paradigm of continuous process and "numbering up", i.e., running numerous microreactors in parallel for mass production (Lavric and Woehl, 2009). This would lead to short lead times from laboratory development to industrial production as well as the ability to produce chemicals on demand on-site.

Corning has developed proprietary continuous micro-reactor processing technologies that are compact, adaptable and scalable, optimizing overall quality of high-value specialty, fine, and pharmaceutical chemicals. The devices, which are as small as beneficially needed, are glass-made, offering the advantages of process intensification and glass-specific qualities like transparency and very good chemical resistance. Corning fluidic modules are devices composed of a reaction chamber stacked between two heat exchanger layers, thus integrating mixing and/or dwell time with heat transfer.

Computational fluid dynamics (CFD) is a powerful simulation tool, based on numerical solutions of equations for the conservation of mass, momentum, energy, offering an alternative technique to traditional experimental methods for accelerating equipment design and optimization while gaining additional fundamental understanding of transport processes. Once validated, CFD can be utilized for design purposes.

Before CFD can be used confidently, the results must be validated against experimental values. The primary benefit of CFD models lies within their capacity for testing and optimizing numerous scenarios quickly compared to designing and building an experimental/laboratory model.

CFD has been widely used to investigate the characteristics of flow and heat transfer inside microfluidic devices (Tomomura et al., 2002, Haeberle et al., 2005, Feng and Yang, 2009).

The velocity field, pressure drop and temperature profiles in a device were computed assuming steady-state, laminar flow in the reaction channel and turbulent flow on heat exchange side. Navier–Stokes and energy transport (governing) equations have been solved for water, imposing as boundary conditions the inlet velocity (flow rate) and exit pressure for a device having the reactive channel of 1.1 mm height. Numerical results are compared to experimental data: velocity profiles measured by micro particle image velocimetry (μ-PIV) means, pressure drop and heat transfer coefficient.

The satisfactory agreement between experimental results and CFD modelling proved the utility of numerical simulations in the development of new designs.

2. Device

Typically, CFD analysis involves the decomposition of the structure into a mesh of cells or elements, performing the fluid-flow calculations at the nodes of each cell. The results

can be presented in graphic form, allowing immediate visualisation and interpretation of flow and thermal profiles.
The devices analyzed in the present study are composed of chains of identical cells having variable cross sections and internal elements which force the liquid to split and recombine (Figure 1). Thus, the velocity fields are modified continuously, the result being an efficient and continuous mixing along the dwell time path (Chevalier et al., 2008, Lavric and Woehl, 2009). The device incorporates an injector, enabling feeding and mixing two fluids, but can also be used as dwell only; the recommended operating flow rate is in the range of 30 to 120 g/min for water-like fluids.

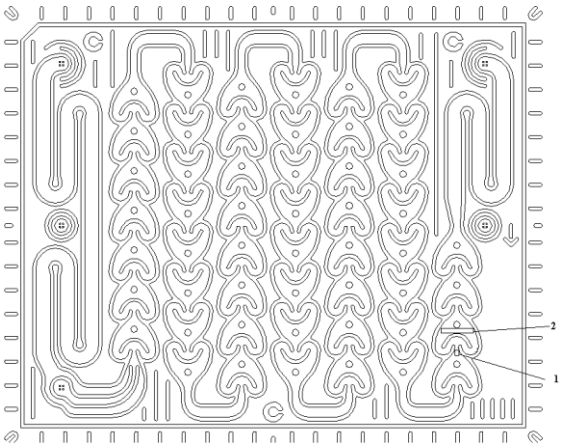

Figure 1: Mixing and/or dwell time fluidic module for multi-phase applications

Numerical mesh for calculations was developed using pre-processor Gambit. It was found that a hexahedron element type is most efficient during pressure drop and mixing quality calculation in terms of mesh size and convergence. Since reaction and heat-exchange layers have different 2D designs, each layer was meshed separately by extruding of their 2D mesh. The whole fluidic module mesh was obtained by coupling the layers into one model using mesh interface mechanism. For the considered device, the whole mesh size consists of 25 million cells and it takes about 30 hours to achieve convergence.

3. Results and discussions

3.1 Velocity field

Flow field has been observed and quantified by μ-PIV measurements (Musteti, 2008), with an exposure time of 10^6 μs. This technique, developed specifically for the determination of instantaneous fluid velocity fields within microchannels, is a non-intrusive optical technique that enables local analysis of the flow at a high spatial resolution, down to ~ 1 μm (Aubin, 2010). The flow was illuminated by a dual laser-head Nd:YAG laser and image pairs were acquired by a dual-frame CCD camera (DaVis 7.2, LaVision GmbH). Since the liquid phase was seeded with fluorescent microspheres PMMA – Rhodamine B –(d_{Sphere} = 1 to 20 μm), the liquid velocity profile

in the channel centre plane could be determined. Optical distortions as reflection or refraction had been corrected during the calibration procedure. As examples, averaged velocity profiles obtained for 40 g/min in sections 1 and 2 (in Figure 1) are presented in Figures 2; the dimensionless coordinate is done with respect to the channel width. For the working conditions, typical velocity ranges from 0.25 m/s to 0.5 m/s. Figure 2 left shows some spurious vectors outside the fluid channel, due to the glass non-uniformities detected by the laser light and interpreted in DaVis as vector fields. A mask could not be defined because this would have lead to the loss of some important vector areas, but such false information is disregarded easily since it is outside fluid channel.
As expected, very low velocities are shown in the space situated between the internal elements by both μPIV measurements and numerical calculations (Figure 2 right).
Fair agreement has been obtained between numerical results and experimentally measured data (Figure 2).

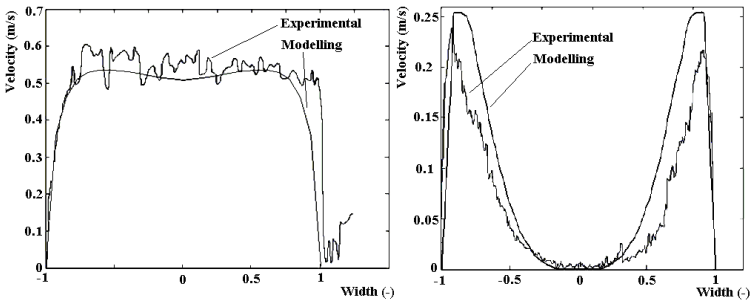

Figure 2. Velocity profiles as function of non-dimensional channel width

3.2 Pressure drop

For the examined system, comparison of numerical and experimental results for pressure drop is a vital element of validation, since pressure drop could be a limiting factor for increasing the throughput of fluidic modules. Design of all process equipment involves a critical trade-off between pressure drop and other performances like mixing and/or heat transfer. CFD simulations predicted the pressure drop with high accuracy over the entire operating range (Figure 3).

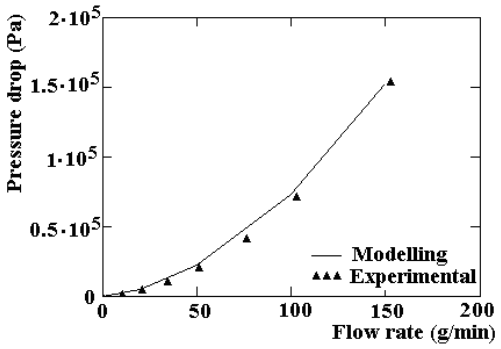

Figure 3. Dependency of pressure drop on flow rate

3.3 Heat transfer

Solving the energy transport equation together with the conservation of mass and momentum allowed obtaining temperature profiles along reaction and heat exchange paths. Thermal boundary conditions used were inlet temperatures of fluids and adiabatic external walls. Once temperature profiles are known, overall heat transfer coefficient can be easily calculated using heat transfer equation.

CFD simulation results showed close proximity to the experimental result, although it simulated a higher heat transfer coefficient at 100 g/min (Figure 4). Taking into account that the experimental error measurement is ± 10 %, one can conclude that numerical results are consistent with experimental data.

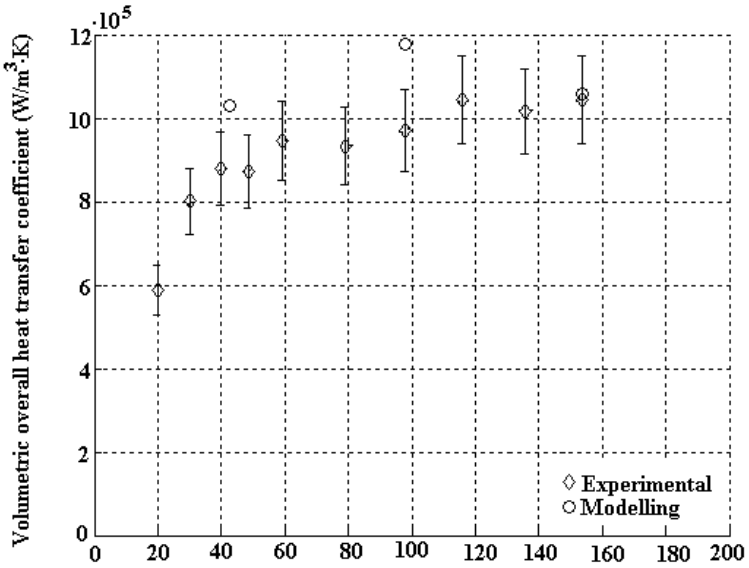

Figure 4. Predicted and measured volumetric heat transfer coefficients

Conclusions

Flow and heat transfer behaviour of devices belonging to one family of designs of Corning glass microstructures was studied. Experimental velocity profiles, pressure drop and heat transfer coefficient were compared with numerical results obtained using CFD software Fluent® for solving Navier–Stokes and energy transport equations for steady-state flow for water-like fluids.

Simulated velocity profiles agree reasonably well with μ-PIV measurements.

Pressure drop was accurately predicted by numerical simulations, with a precision within experimental measurement error (less than 10 %).

The numerical calculations for heat transfer coefficient are also consistent with experimental data.

The very good agreement between experimental results and CFD modelling proved the utility of numerical simulations in the development of new designs. Due to this, one can

conclude that CFD modelling can be used to develop and optimise new designs, reducing time and cost for the investigation.

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