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Numerical evaluation of stresses acting on particles in high-pressure microsystems using a Reynolds stress model

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HIGHLIGHTS

- We investigate the multiphase flow fields of different micro-channels by CFD.
- A new model to calculate acting stresses on particles was used.
- Based on the Reynolds stress tensor and a stationary particle tracking a quantification of acting stresses was possible.
- Effect of steam and cavitation was reproduced.
- Peak stress seems to be the leading breakage mechanism in turbulent microchannels.

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ABSTRACT

In the present study a model was developed which enables to calculate the stress acting on particles induced by the fluid flow in microchannels. Computational fluid dynamics (CFD) was used to simulate the flow field in five different microchannel geometries. With the help of a *Reynolds-stress model* and a stationary particle tracking a quantification of stresses in different geometries at varying pressure differences is possible. Furthermore, the effect of cavitation which occurs if the fluid expands to ambient pressure was investigated. The mass flow rates determined by the simulations are in good agreement with the ones determined experimentally. Except for the z-channel the computed stresses are in good agreement with previously conducted dispersion experiments. Additionally, the computed fluid stress was compared with the calculated *Kolmogorov* length scale to validate the results.

1. Introduction

In the last couple of years the impact and influence of numerical methods for process design and optimisation largely increased. Simulations are used to get a better understanding of different processes, for the prediction of the results or as a additional tool to investigate acting mechanisms. Due to the increased computational power new, more detailed simulations can be conducted which improved the understanding of unit processes. Especially, if experimental methods are not applicable or if they are expensive (in time and costs) simulations become more and more the method of choice. In this work simulations were used as they are (often) faster, reliable and enable information which cannot be fetched out of experimental investigations. They were used to compute different types of microchannel geometries and to identify the dominant stress mechanism for the breakage of agglomerates or aggregates (in the following named particles).

The usage of microchannels in chemical and pharmaceutical engineering offers a couple of advantages, like high energy input per volume, high efficiency, narrow residence time distributions and reproducible results. As nanoparticles have become more and more important for industrial applications the microchannels are used to produce particles with a defined size and a defined, narrow size distribution. As the geometry of these devices is very flexible investigations to optimise the geometry are required. The number of possible designs is extremely high and, hence, simulations are required to get a understanding of the leading breakup mechanism. If the mechanism for the breakage of the particles in a microchannel is known the geometry can be adapted in a way which supports this mechanism.

Wengeler and Nirschl (2007) and Wengeler (2007) investigated the dispersion behaviour in nozzles with a circular cross-sectional area. They used a stress model with four different kinds of stresses

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(compressive, shear, tensile and turbulent stress) for a two-dimensional simulation to evaluate the acting stress. This model was enhanced to three dimensions and extended with a stationary particle tracking to enable a quantification of different microchannel geometries (see Beinert et al., 2012). Furthermore, in these previous published results a k–ϵ model was used to calculate the flow fields and compute the stresses acting on the particles.

As the dispersion of solid particles in microchannels is a relatively new process and not yet common in industrial application there is not much research done on it. Many research projects were done in the field of (laminar) mixing and chemical reactions in micro-devices and particle laden gas flows. The laminar mixing of different species and a possible reaction is based on the diffusion process and the interface which is very large in such micro-devices. Particle laden fluid flows, especially turbulent flows, are very common for diesel injection, solid–fluid transportation or fluidized beds.

1.1. Mixing and chemical reactions in micro- and macro-devices

Among others, micro-devices are used for continuous mixing and/or for continuous chemical reactions. Due to the fact that laminar flows are volitional only low fluid velocities, low forces and low pressures occur. Therefore, established experimental and numerical methods for laminar flow can be used to characterise and improve the geometry of the micro-devices. Pennella et al. (2012) investigated a new designed micromixer by the help of particle image velocimetry (PIV) and computational fluid dynamics (CFD). They showed that the current methods can be used to largely improve the geometry in terms of mixing quality, costs and energy input. On the other hand the micro-scale of reactive flows was investigated. For example Porta et al. (2012) looked at the global reaction rate and the space–time distributions in dependency of dimensionless quantities like *Peclet* or *Damkoehler number*.

In the work of Makowski et al. (2012) large eddy simulations (LES) were used to calculate the mixing process of particles in a rectangular channel reactor. The results were compared with different simulations and experimental data. They showed that for high *Reynolds numbers* and low concentration the k–ϵ model offers similar results. With decreasing *Reynolds number* and higher concentration large scale inhomogeneities and non-linear effects have to be taken into account and, therefore, the usage of a LES is required.

Similar investigations were performed in Gradl et al. (2006) and Gradl and Peukert (2009). They investigated a t-mixer with the help of experimental and numerical methods. They used coupled direct numerical simulations (DNS) and population balance equations (PBE) to model the influence on the resulting particle size distribution. With the help of a derived micro-mixing model they were able to predict the particle size distribution in the precipitation process. For unstable conditions they extended their coupling with the DLVO theory which improves the possibilities to stabilise the production of particles.

1.2. Particle laden flows

In contrast to the work shown above a lot of investigations have taken place in the field of particle laden turbulent flows in non-micro-devices. In Messa et al. (2013, 2014) different process parameters for turbulent flows were computed and compared with experimental data. They compared their computed results based on a turbulence model including physical mechanisms with experimentally measured pressure drops, solid volume fractions or spatial particle distributions and particle velocities. Furthermore, DNS can be used to calculate micro- and macro-time scales (compare the work of Wang and Manhart, 2012).

(Gui et al., 2010) simulated the particle–vortex interaction in turbulent, swirling jets with the help of DNS and studied the influence of the particles on a plane jet in Gui et al. (2013). They showed that the DNS is a good method to simulate those interactions if the *Reynolds number* is not to high due to the rapidly increased computational costs. Furthermore, they pointed out that for high volume fractions of the dispersed phase the two-way interactions between the fluid and the particles have to be taken into account.

1.3. Stress mechanism in dispersion processes

A general overview of the acting stresses on particles in a fluid is given in Raasch (1961) and a general overview of dispersion experiments in different dispersing devices is given by Schilde et al. (2010, 2011).

Investigations of dispersion and aggregation behaviour of particles in non-uniform shear flows were performed and described by Masuda et al. (2013b) (backward facing step) and Masuda et al. (2013a) (parallel plates). These investigations were performed for low *Reynolds numbers* and two-dimensional flow simulations. They introduced a model which enables the prediction of size distribution of particle clusters (based on coagulation and breakup) and compared the gained results with experimental data.

Rotor–stator devices are often used for the production of dispersions or emulsions as they produce high shear stresses. Jasińska et al. (2013, 2014) simulated the three-dimensional flow in a rotor stator with the k–ϵ model to predict the power input and turbulence within the flow and/or linked it with the population balance equations to predict the droplet size distribution over time.

CFD coupled with the discrete element method (DEM) can be used to evaluate the stress acting on agglomerates in an pharmaceutical dry powder inhaler. Tong et al. (2013) used this approach to identify agglomerate-device impacts as the dominant stress mechanism beside multiple impacts between agglomerates. A similar approach to describe the dispersion progress in a stirred media mill is shown in Beinert et al. (2014). Coupled CFD-DEM simulations were performed to evaluate the contacts between grinding media to estimate – with the help of PBE – the particle size distribution over time.

2. Methods and models

In the first section the microchannels, experimental set-up and material properties are described. Further information on the experimental part of this project are given in Gothsch et al. (2011, 2014). The second part describes the software and used boundary conditions while the third part describes the turbulent model. The fourth part denotes how the acting stress is calculated, while the last section takes the effect of turbulence on particles into account.

2.1. Experimental set-up

A fluid was pumped through the microchannels (containing particles) with a pressure difference up to $\Delta p = 500\,\text{bar}$ and expanded to ambient pressure or into a pressure vessel at various pressures. These microchannels were manufactured by the Institute for Microtechnology of TU Braunschweig (compare Lesche et al., 2011). The pressure in the vessel is called “backpressure” while the difference between the inlet and the outlet is called “pressure” or “pressure difference”. The backpressure experiments were performed to investigate the influence of cavitation. Two