CHEMICAL ENGINEERING TRANSACTIONS
VOL. 69, 2018
A publication of AIDIC
The Italian Association of Chemical Engineering
Online at www.aidic.it/cet
Guest Editors: Elisabetta Brunazzi, Eva Sorensen

ISBN 978-88-95608-66-2; **ISSN** 2283-9216

Development of a Mesoscale Modeling Approach for the Gas Phase Fluid Dynamics in Structured Packings

Johannes Sacher*, Jens Uwe-Repke

Technische Universität Berlin, Straße des 17. Juni, 10623 Berlin, Germany
johannes.sacher@tu-beriln.de

The gas fluid dynamics in structured packings of distillation and absorption columns is investigated especially with respect to the mixing behavior of component concentrations. The first part comprises a fundamental experiment of a single crisscrossing junction which represents a repetitive periodic element of the packing geometry. Particularly, the mixing efficiency of a tracer component is measured. Additionally, CFD simulations are conducted and analyzed with regard to their capacity to represent the distribution of the tracer component. In the second part the implementation of a new mesoscale model for structured packings (StructuPack) is described which is motivated by the need to resolve local velocities, pressures and concentrations with low computational cost as compared to microscale CFD simulations. Finally, an exemplary scenario in a packing section is calculated both by CFD and the mesoscale model to demonstrate the model's potential to resolve local pressures, velocities and tracer concentrations using comparatively few computational resources.

1. Introduction

Structured packings occupy an outstanding position in distillative and absorptive separation processes. The separation efficiency of packings can be influenced considerably by the maldistribution of the fluid phases (Edwards et al. 1999). Whereas for the liquid phase maldistribution effects have already been investigated extensively, the gas phase has not been examined as much in this respect, but also exhibits substantial maldistribution (Stemich and Spiegel 2011). For instance, liquid collectors and distributors often create drastic gas maldistributions, which substantially increase pressure drop (Ali et al. 2003) and so far, the effect on separation efficiency in this regard has not been examined sufficiently. Further, in so-called shallow bed columns (with a height smaller than a diameter, used, e.g. in vacuum crude oil distillation) gas maldistribution can have a considerable impact on performance (Porter et al. 1993). As another example, scenarios during the operation of divided wall columns have been reported where the two vapor streams exiting the middle section did not mix sufficiently in the top section and thus jeopardized the product specification (Steffens 2007). The above examples show that more precise predictions of the three-dimensional fluid dynamic behavior of the gas phase are highly desirable and deeper physical understanding is required. Of particular relevance are the local gas velocities and concentrations, which develop over the height and cross section of the packed bed in presence of non-uniform boundary conditions. CFD simulations can give good insights in this respect and have been carried out in numerous previous works. The investigations focused mainly on dry pressure drop of structured packings, which could be successfully represented (e.g. Raynal et al. 2004). However, an analysis is still missing as to whether the different employed turbulence models also have the capability to correctly describe the distribution of concentrations. Furthermore, the computational effort of CFD simulations for complete industrial packing columns still remains enormous.
The presented work is divided into two parts: The first part describes experimental and numerical (CFD) fundamental research studies, which are particularly focused on the quantitative material distribution in a crisscrossing junction of two triangular channels, a representative elementary geometry of structured packings. Secondly, a new own mesoscale modeling approach (StructuPack) for the simulation of structured packings is expressed. The approach is supposed to enable the simulation of whole industrial columns with comparatively low computational cost and at the same time resolve the essentials of the three-dimensional distributive behavior in the packing, i.e. the local velocities, pressures and concentrations.

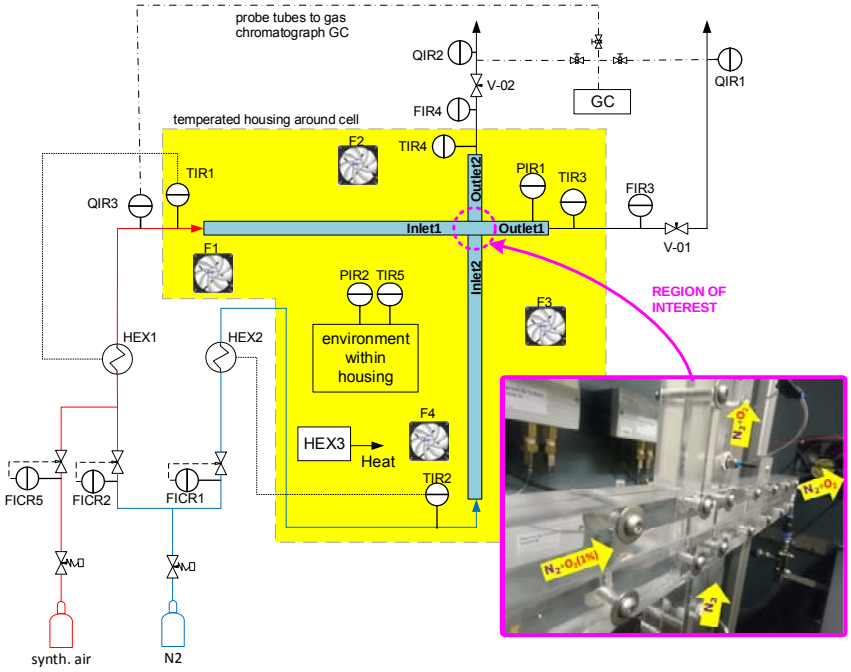


Figure 1: Flow sheet of experimental set up and photograph of region of interest.

2. Fundamental investigation of mass transport in a single crisscross junction

2.1 Experimental set up

The goal of the experiments is to measure quantitatively the distribution of a tracer concentration in a small representative geometry for structured packings and thus deliver data for the validation of CFD models. Hence, a crisscross junction of two triangular channels was manufactured from acrylic glass as shown in the photograph in Figure 1. In order to ensure defined developed inlet velocity profiles, the inlet lengths were chosen to 115 cm. The dimensions of the channels are analogous to the geometry of the Montz-Pak B1-250 packing with a channel base length of 22 mm (Figure 2c). Both inlets were supplied with pure nitrogen whereas in the first inlet (inlet1, Figure 1) a tracer concentration of 1 mol% oxygen can be added. System pressure was controlled by the outlet valves (Figure 1) and held constant at 1200 mbar (+/- 2 mbar). The system was further tempered to uniformly 25 °C (+/- 0.2 °C) by means of a temperature controlled ventilated housing and by control of the inlet stream temperatures (Figure 1). The mass flows were controlled and measured with mass flow controllers of type Bronkhorst EL-FLOW select. The tracer concentrations at the outlets were measured with a gas chromatograph (type Agilent 490 Micro-GC, molsieve5A-column). In this study the symmetric scenario was investigated, i.e. both inlet velocities and both outlet velocities were equal. Thereby, eight experimental points at different inlet velocities were measured. The velocities ranged from low values of 0.5 m/s (equivalent packing F-factor of 0.412 $Pa^{0.5}$, channel Reynolds number of 347.7) up to 5 m/s (F-factor of 4.12 $Pa^{0.5}$, channel Reynolds number of 3476.5). The equivalent packing F-factor is defined as $F = v_{sup} \cdot \sqrt{\rho} = v_{chann} \cdot 1/\sqrt{2} \cdot \sqrt{\rho}$, considering that in a 45°-packing the superficial velocity v_{sup} and effective channel velocity v_{chann} are related by $v_{chann} = \sqrt{2} \cdot v_{sup}$.

2.2 CFD set up

The goal of the CFD simulations was a validation against the experimental tracer outlet concentrations and thus evaluate their capacity to predict the distribution of component concentration in structured packings. The simulations were conducted in OpenFOAM with the incompressible solver simpleFoam. The computational domain is shown in Figure 2c and had the same dimensions as the physical domain. The inlet and outlet lengths of the computational domain measure 60 mm, which corresponds to about 6 hydraulic diameters of the triangular channel. The fully developed velocity profiles for the inlets were obtained from prior consecutive calculations on a single triangular channel with an identical mesh resolution and mapped onto the inlets of the crisscross junction.

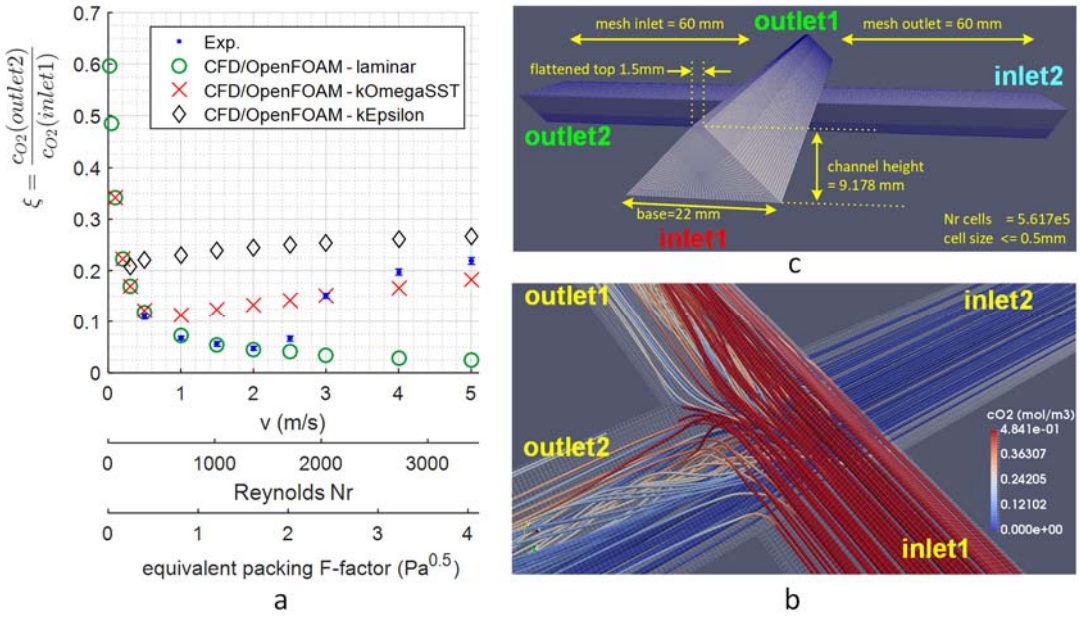
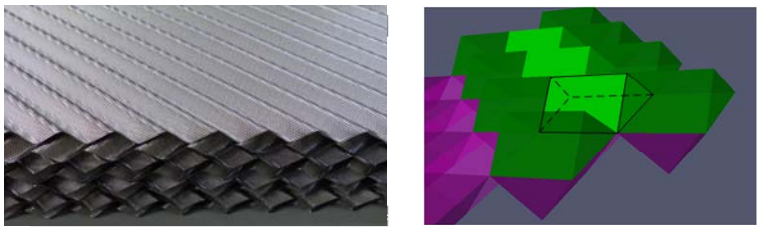


Figure 2: Tracer distribution in a single crisscross junction with equal velocities at inlets: a) Comparison of experimental and CFD results; b) streamlines and tracer transport for w=2 m/s (F=1.65 Pa$^{0.5}$) of the CFD/OpenFOAM simulation with kOmegaSST-turbulence model; c) geometry and computational mesh.

The mesh consists purely of hexahedrons (Figure 2c) and it was found that for cell sizes smaller 0.5 mm grid independence could be established. In this study two different reynolds-averaged (RANS) turbulence models were employed: Firstly the k-omega-SST-model which got very popular over the past decade and secondly the standard k-epsilon model, which is traditionally one of the most employed turbulence models. Further, laminar calculations were performed, i.e. without turbulence modeling.

2.3 Results and discussion

The experimental and CFD-results are shown in Figure 2a, where the mixing efficiency ξ, defined as the ratio of tracer concentrations at outlet2 and inlet1, is plotted over the inlet velocity. The corresponding Reynolds number and equivalent packing F-factor are also shown on the abscissa axis. The mixing efficiency can also be described as the proportion of oxygen changing to the second channel. The experimental results in Figure 2a firstly show a decline of ξ within the laminar regime for velocities smaller than 2 m/s. In this laminar range convective mechanisms are responsible for the decrease of mixing characteristics. For small velocities a great portion of the flow is redirected to the adjacent channel due to pressure driven effects and the wall geometry. This effect can even redirect more than half of the flow leading to ξ-values over 0.6 for very small velocities, as could be observed in the CFD-simulations. As velocities increase inertial effects get stronger and keep a bigger portion of each stream in its channel, which explains the decrease of mixing for increasing velocities. However, as can be nicely seen from Figure 2a, at a velocity of 3 m/s (Re=2085.9) a sudden increase in mixing could be observed which is due to the onset of the turbulent regime. Within the turbulent regime the mixing efficiency further increases with velocity as turbulent transport intensifies.
The laminar CFD calculations could describe the experimental results within the laminar regime quite well with a deviation of less than 6%. The k-epsilon model performed poorly, which is no surprise since it is a high-reynolds-model which cannot resolve well the viscous sublayer and is not suitable for this regime, where y+-values (required dimension of first cell for wall function) are violated. On the other hand the k-omega-SST model can describe the tendencies of the mixing behavior over both the laminar and turbulent regimes. However, it is not capable to reproduce the transition from laminar to turbulent and also the gradient of the increasing mixing efficiency is not matched quantitatively. Admittedly, the k-omega-SST model was just applied with the standard parameters which could be adjusted for the packing geometry in future studies.
From the comparison it can be concluded, that CFD can correctly model the essential mechanisms for the mixing of components in structured packings, but care has to be taken with regard to the mesh resolution and employed turbulence model, e.g. no high-Reynolds models should be used. Nevertheless, a more precise quantitative prediction is desirable and has to be sought by means of parameter adjustment and a more complete screening of the big variety of low-Reynolds turbulence models.



a b

Figure 3: a) Sheets of structured packing (Montz-Pak B1-250) with characteristic geometry of crisscrossing channels; b) basic cell geometry of the mesoscale model matching exactly half of a crisscrossing junction.

3. Mesoscale model for structured packings (StructuPack)

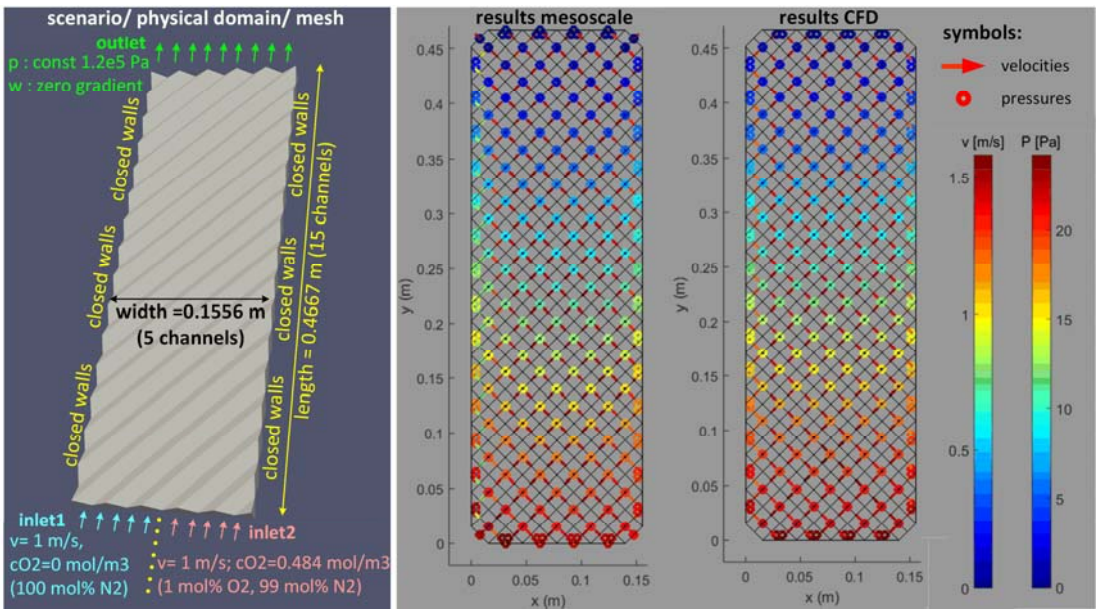
The results of the previous section are used to justify CFD as a meaningful comparative tool in order to develop and validate the coarser mesoscale model.

3.1 Description of the mesoscale modeling approach

The idea of the newly developed mesoscale simulation code (named StructuPack) comes from the observation within CFD simulations, that gas flow is predominantly oriented along the crisscrossing triangular channels formed by the packing sheets (Figure 6a and 3a). The channels are discretized in cells that match exactly the half of a crisscross junction as depicted in Figure 3b. The cells at the packing borders differ somewhat from the geometry of the inner cells, but are treated in the same manner by the code's framework which allows for arbitrary cell geometry. Pressures are stored at cell centers whereas velocities are stored at the cell faces. The pressure-velocity field is solved by a coupled solution of momentum and continuity equations. At this stage the code allows for steady state solutions, but transient calculations will be implemented in the future.

The steady state continuity equations have the form $0 = \sum_f \left(\rho_f \cdot \vec{A}_f \circ \vec{v}_f\right)$ with density ρ, velocities of each face $\vec{v}_f$ and oriented face area $\vec{A}_f$. <∘> denotes the scalar product.

The momentum balances have the form $0 = F_{conv} + F_P + F_{fric} + F_{wall} + F_{cross}$. Here F_{conv}, F_P and F_{wall} represent the convective momentum transport (i.e. local local acceleration), pressure force and the orthogonal wall force respectively. F_{fric} is the wall friction and described by $F_{fric} = \overline{\tau_w} \cdot A_{wall,parallel}$, with the mean wall shear stress $\overline{\tau_w}$ and wall area (portion parallel to flow) $A_{wall,parallel}$. The mean wall shear stress is obtained from an analytical solution for triangular channels (Mortensen et. al 2005).



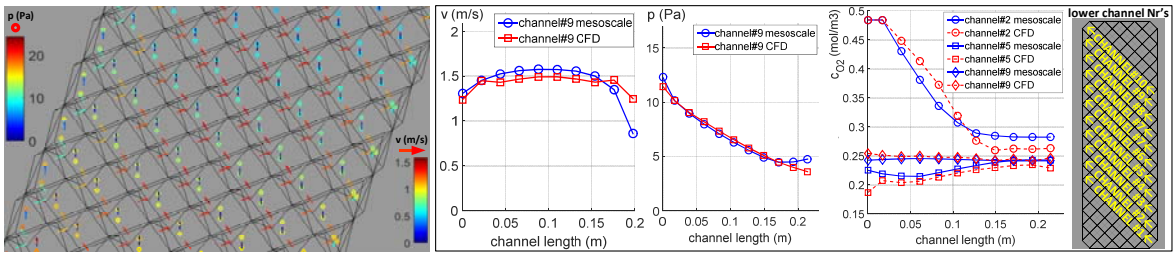
a b

Figure 4: a) Depiction of the geometry and boundary conditions of the scenario; b) Simulation results for local pressures and velocities of the mesoscale simulation (4.8 seconds CPU-time) and CFD (4963 seconds CPU-time).

F_{cross} is an interesting additional force which is produced at the shear layer at the open (cross) side between two adjacent channel cells (i.e. the middle of the crisscross junction). The mechanisms of this phenomenon are quite complex and will be more accurately modeled and investigated in the future. For now a rather simple model is used: $F_{cross} = \zeta_{cross} \cdot \frac{\rho}{2} v_{chann}{}^2 \cdot A_{chann}$, with a constant friction coefficient ζ_{cross}, density ρ and the velocity v_{chann} and cross sectional area A_{chann} in the channel's mainstream direction. This simple model is justifiable when velocities are uniformly enough distributed within a packing, as is normally the case.

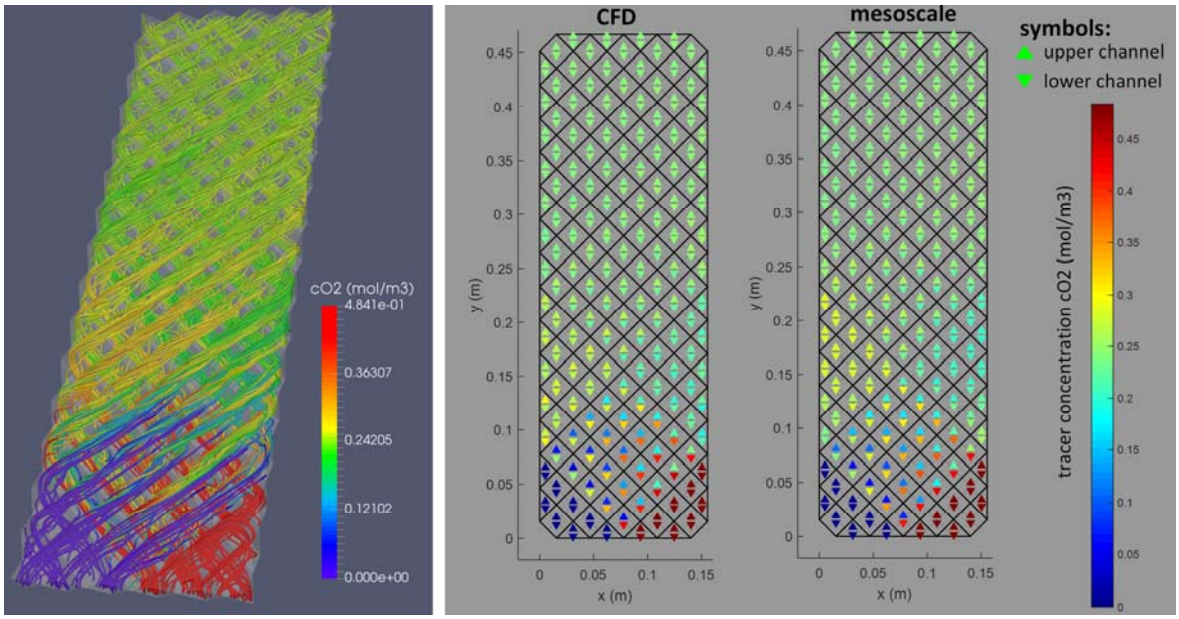
3.2 Comparison of the mesoscale model with CFD on a single packing layer

An exemplary scenario for gas flow in a packing layer is simulated by both the mesoscale model and by CFD in order to evaluate the mesoscale model's capacity to represent local velocities, pressures and concentrations. The specifications of the scenario are depicted in Figure 4a. Like in section 2, the packing geometry corresponds to Montz-Pak B1-250 with a channel base width of 22 mm. The right and left borders are completely closed with walls, so that the flow of each ending channel enters completely into one adjacent beginning channel. The inlet is supplied with nitrogen at a velocity of 1 m/s (corresponding to an F-factor of 1.16 $Pa^{0.5}$) whereas only at the second half of the inlet a tracer concentration of 1 mol% (0.4841 mol/m3) is added. The outlet boundary is specified with a constant pressure of 1200 mbar.



a b

Figure 5: a) Mesoscale simulation with position and values of local velocities and pressures in a packing section; b) quantitative comparison of CFD and mesoscale values along different packing channels.



a b

Figure 6: a) Streamlines of CFD calculation with representation of tracer concentration; b) local tracer concentrations in the packing for both mesoscale and CFD simulation.

The CFD was performed in a laminar manner, i.e. without a turbulence model in compliance with results of section 2 in Figure 2a at F-factors below 2 $Pa^{0.5}$. The streamlines and tracer transport can be seen in Figure 6a. Figure 5a gives an impression of the mesoscale cell geometry and its position of the stored pressures and velocities in a packing section. Figure 4b allows a direct comparison between the mesoscale and CFD results (calculated as mean values of pressure and velocity at the mesoscale cell volumes and faces). It can be seen that the profiles correspond very well, though it has to be noted, that the pressure loss over the packing length

was matched by adjusting the additional friction coefficient at the crisscrossings to $\zeta_{cross} = 0.37$. Without this friction effect the pressure loss in the mesoscale calculation would be of factor 5 lower, which indicates the shear layer's dominant effect on pressure drop in packings. A more quantitative comparison is given in Figure 5b, where velocity and pressure profiles are taken along one channel (9nth fully crossing channel from the bottom). It can be seen that the profiles match very well between CFD and StructuPack in concavity (or convexity). However, at the channel endings differing values can be observed. This could be due to stronger energy dissipation effects at the channel endings, where the gas flow is heavily redirected. These effects have not yet been modeled in StructuPack and have to be analyzed more profoundly.
When comparing the behavior of tracer transport, Figures 6b and 5b show that the concentration distribution can be very well represented by the mesoscale model. However, it has to be noted here that the comparison matched this well when a mixing efficiency at the crisscrosses of $\xi = 0.14$ was assumed. This value is much higher than the one found in the fundamental investigations in section 2 (see $v = \sqrt{2} \cdot 1$ m/s in Figure 2). This observation indicates that mass transfer depends heavily on the inlet velocity profiles, which are periodic in a packing and different from the fully developed profiles in section 2. The mesoscale simulation of this scenario needed 4.8 seconds on a 2.6 GHz desktop computer, whereas the CFD-calculation took 4963 seconds at the same computer with one core.

4. Conclusion

The conducted fundamental experiments of tracer distribution in a single representative crisscrossing junction in combination with CFD and mesoscale model development show first of all that a combination of all these three approaches can lead to a deeper understanding of the physical mechanisms of the gas phase in structured packings that eventually determine relevant engineering questions: how quickly do gases mix in a packing? What role has the F-factor on mixing in a packing?
Thereby, CFD turns out to be a useful tool to give insight in the physical mechanisms which enable the development of appropriate mesoscale models. However, CFD only delivers meaningful results when exerted with care regarding mesh resolution and submodels.
The CPU-time required for the developed mesoscale model is about 3 orders of magnitude lower than in the conducted CFD simulations, which could be demonstrated for a single packing layer. This factor could even rise by more orders of magnitude when CFD-simulations with highly resolved boundary layers and transient eddies turn out necessary. When translating the computational cost to scenarios of whole industrial columns with meters in diameter this could make mesoscale calculations the only feasible option that still resolves local information within structured packing columns. Meanwhile, the mesoscale approach showed to have the capacity to represent the packing's internal mechanisms in a physical first principle manner, allowing for the simulation of very diverse scenarios in the future. This is mainly due to the fact that the model's core consists of proper momentum balances that determine the velocity profiles in a coupled pressure-driven manner. However, a broader investigation through experiment and CFD has to be done to give a better description of the individual contributions in the mesoscale balance equations and finally the use of parallel computing will be inevitable also for the mesoscale computations in order to achieve acceptable CPU times for industrial columns.

References

Ali A. M., Jansens P.J., Olujić Ž., 2003, Experimental Characterization and Computational Fluid Dynamics Simulation of Gas Distribution Performance of Liquid (Re)Distributors and Collectors in Packed Columns, Chemical Engineering Research and Design, 81, 108-115

Edwards D. P., Krishnamurthy K. R., Potthoff R. W., 1999, Development of an Improved Method to Quantify Maldistribution and Its Effect on Structured Packing Column Performance, Chemical Engineering Research and Design, 77, 656-662

Mortensen N. A., Okkels F., Bruus H., 2005, Reexamination of Hagen-Poiseuille Flow: Shape Dependence of the Hydraulic Resistance in Microchannels, Physical Review E, 71, 057301

Porter K. E., Ali Q. H.; Hassan A. O., Aryan A. F., 1993, Gas distribution in shallow packed beds, Industrial & Engineering Chemistry Research, 32, 2408-2417

Raynal L., Ballaguet J.-P., Barrere-Tricca C., 2004, Determination of mass transfer characteristics of co-current two-phase flow within structured packing, Chemical Engineering Science, 59, 5395 - 5402

Stemich C., Spiegel L., 2011, Characterization and quantification of the quality of gas flow distributions, Chemical Engineering Research and Design, 89, 1392 - 1396

Steffens F., 2017, Untersuchungen zur Gasverteilung und Gasdurchmischung in Trennwandkolonnen, Jahrestreffen der ProcessNet-Fachgruppe Fluidverfahrenstechnik 2017, Cologne, Germany