

# Analysis of the Flow Behavior of Single and Multiphase Liquid in Packed Columns

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## Abstract

In recent decades packed columns have become very popular for distillation processes since they acquire higher loadings and a better separation efficiency than ordinary tray columns. Fluid dynamics cover an important place in the design of packed towers. Identifying the main quantities remains subject of various research works. There exists a wide range of different approaches to determine the mass transfer coefficient  $k_L$  and the specific interfacial area  $a$ . Mostly these researches use integral measurements. Since the flow behavior inside the column may change within a few centimeters packing height local investigations are more reasonable. The research work presented here follows this approach to gain information on these quantities by coupling experiments and computational fluid dynamics (CFD). The presentation focuses on some fundamental investigations on the determination of the surface area.

## Introduction

Distillation is one of the most used separation processes and therefore consumes the largest amount of energy. During the '80s the substitution of trays with packings brought a major benefit in that matter. The calculation of the separation efficiency and the design of packed towers are mainly based on empirical and semi-empirical equations [1-3]. These equations have been formulated using aqueous systems and measurements over the total packing height. Thus the local distribution and flow behavior are neglected. Since it has been shown that the flow behavior has a great impact on the separation [4] it is reasonable to formulate a model which takes the local distribution into account.

The application of computational fluid dynamics (CFD) concentrates on the simulation of the vapor phase without any liquid [5] or a given liquid profile [6] or a two-dimensional film flow [7]. The flow behavior of rivulets and droplets makes three-dimensional calculations necessary [8]. For the case of two liquid phases the flow behavior takes on very complex forms [9] with one phase flowing down as a film and the other as rivulets or droplets. It could be shown for these systems that the separation efficiency might decrease, increase or may stay the same in relation to only one liquid phase operation [10]. This makes detailed models necessary.

To develop such a model it is reasonable to first investigate relatively simple cases in order to validate the model and to identify major influences. Therefore we begin with the investigation of liquid flow down inclines. When the numerics have been validated it is possible to calculate more complex geometries of packing internals.

## Experiments

The flow behavior is very complex and changes in all three directions. Therefore it is necessary to measure all important values simultaneously. Since the film thickness is only about 0.5 mm, non-intrusive methods are preferred. The following set-up (fig. 1) meets these requirements. It makes use of a particle tracking velocimetry (PTV) method [11] to measure the velocities on the liquid surface. We use light ceramic particles, waves, and droplets as tracers. It has been observed that the velocities do not vary between the different tracer types for water flow. The flow behavior is observed with a CCD camera. These pictures are also used to obtain information on the wetted surface area. To obtain different inlet conditions the liquid can either be fed onto the plate out of a

tank with an overflowing weir or through a feeding tube with several holes. The first option enables a continuous film at the inlet while the latter is used for rivulet condition and is inevitable for the delivery of two liquid phases.

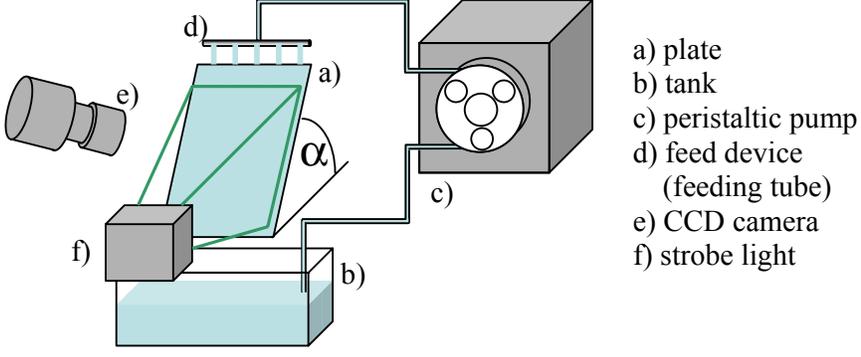


Fig. 1: Experimental Setup for one liquid phase with the feeding tube option

**Numerics**

The numerical calculations are carried out with the commercial tool CFX 5. This CFD program makes use of finite volumes for discretization and a Eulerian-Eulerian algorithm for the multiple phases. The surface tension is accounted for by the continuous surface force model of Brackbill et al [12]. Contact angles are included as static contact angles and used to fix the surface normal to a given direction within the cell at the wall. For the case of relatively strong drag at the interfaces it is reasonable to reduce the model to only one field of equations and a scalar value for the phase fraction forming a model similar to the well-known volume-of-fluid (VOF) [13] model. This vastly reduces the calculation effort. Nevertheless this model simplification might lead to problems where the phases act very differently e.g. at countercurrent flow.

The modeled geometry is shown in Fig. 2. The velocity profile at the inlet is analog to the Nusselt profile. The gas phase is considered to be static and only accelerated by the liquid at the interface. At the outlet a relative pressure of zero is fixed. The other boundaries are taken as walls with only the top as a free-slip boundary. Contact angles are given at the plate and the sides. On the right hand side a detail of the mesh is shown. The cell height in neighborhood to the plate is very small. A refinement study of the mesh showed that a ratio of 1:10 for cell height to Nusselt film thickness should be used.

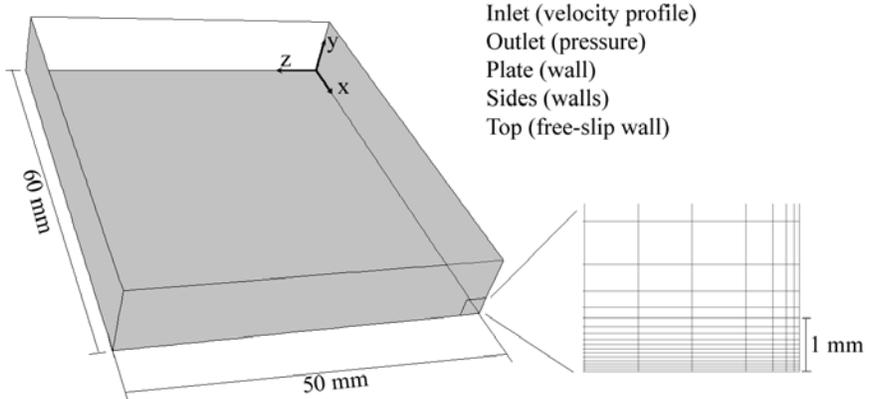


Fig. 2: Numerical geometry and conditions, detail of mesh

## Results

Since the flow behavior is clearly different for one and two liquid phases (Fig. 3), the two cases will be discussed separately. The simpler case of one liquid phase and vapor (also called two-phase flow) focuses on the detection of the velocity, film thickness and the wetted area. One specific value which can be easily validated is the critical liquid load at which the liquid is not able to form a closed film anymore but instead forms rivulets or droplets.

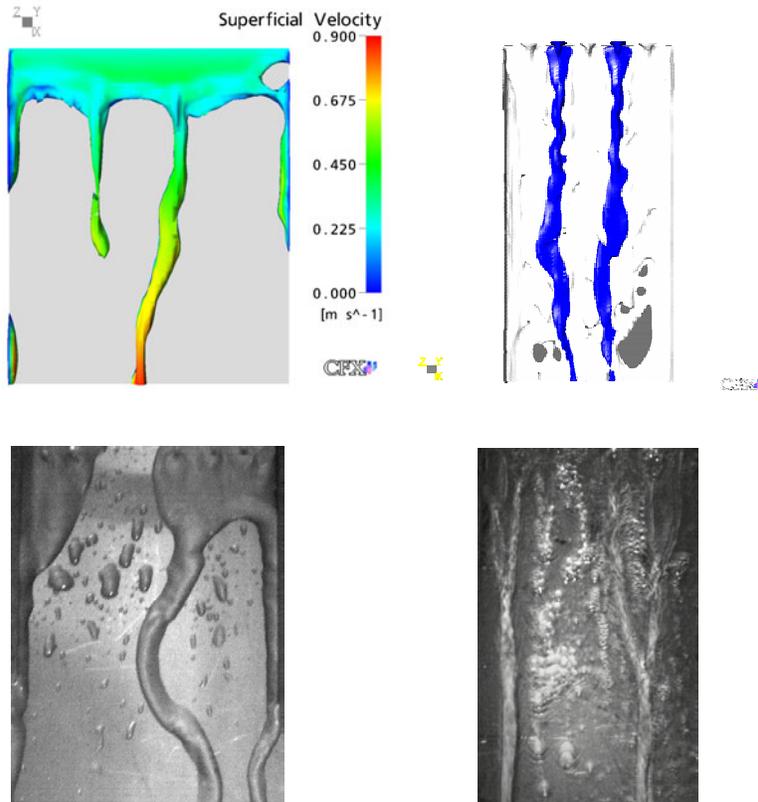


Fig. 3: Comparison of calculated and experimentally observed liquid flows with one and two liquid phases

Exemplarily in Fig. 4 the wetted area is plotted over the Reynolds number for the case of water on a  $60^\circ$  inclined steel plate. It can be seen that the simulated specific wetted area agrees well with the experimental data. Nevertheless the liquid covers less area for a specific liquid load than in the experiments. This can be explained as follows. For one the plate used in the experiments is not treated before the measurements. Furthermore the plate used has a very rough surface. Both characteristics have an effect on the contact angle. The simulated values shown here do not take these into account. The static contact angle measured varies between  $60^\circ$  and  $80^\circ$ . The simulation uses a constant contact angle of  $70^\circ$ . The calculated values with smooth ideal surfaces more or less form a lower bound to the measured data. Experiments in progress with accurately treated plates confirm that observation. The simulated critical liquid load for film break-up is in good agreement with the experiments.

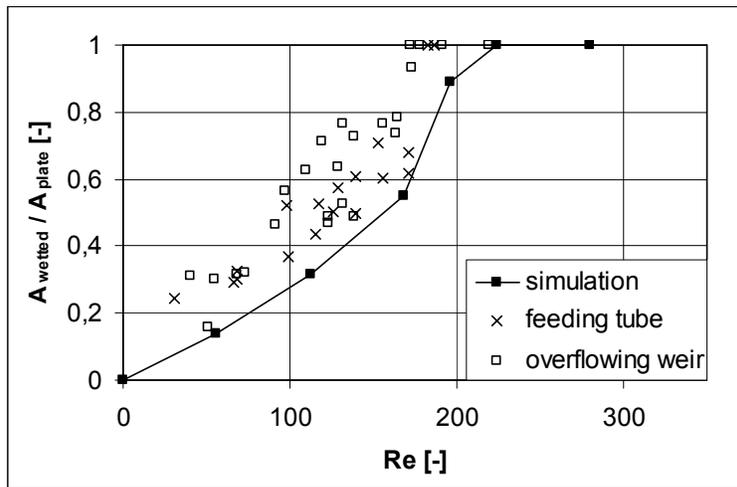


Fig. 4: Specific shadow area  $a$  over liquid load  $Re$  for water on a  $60^\circ$  inclined steel plate

Taking a look at the surface velocities it can be seen that the results match each other very good provided the inlet conditions are the same. Shown in Fig. 5 is the surface velocity of a rivulet flow condition at the liquid load of  $Re = 110$ . The simulation with a film inlet boundary condition and the experiments with an overflowing weir agree well. The application of the feeding tube results in higher surface velocities. This is reasonable if we take the higher inlet velocity through the holes into account. Here we observe regions of different film thickness. This leads to higher surface velocities in the thicker regions.

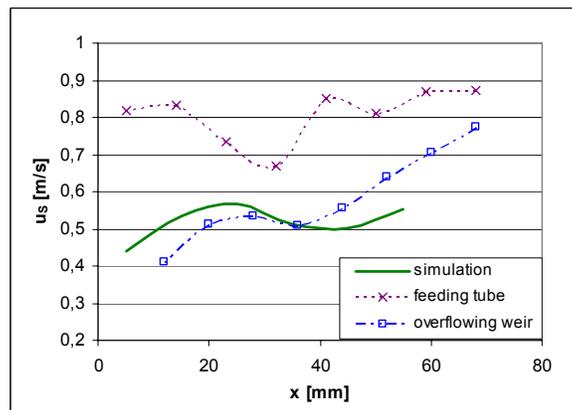


Fig. 5: Comparison of measured and calculated surface velocity profiles in flow direction at  $Re = 110$  with a specific wetted area of 60%

In Fig. 6 a comparison of three simulations with different liquid loads is shown. If we consider film flow, which occurs at higher liquid loads, the surface velocity approaches a constant value. Reducing the load results into film break-up. Where the film breaks we observe a deceleration followed by a slight acceleration in the rivulet again. When we get droplet flow this effect becomes even stronger. In this case we get velocities which are in the same range as the ones at film flow conditions which occur at much higher loadings. This leads to strongly reduced residence times.

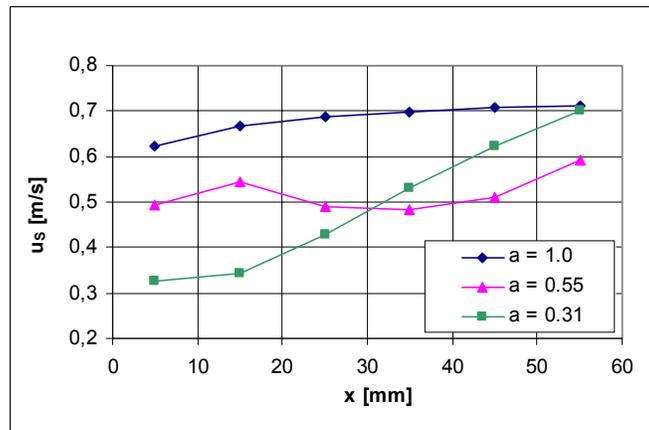


Fig. 6: Velocity profiles at different liquid loads, identified by the specific shadow area  $a$

As mentioned above the flow behavior of two liquid phases is much more complex. The right-hand side of Fig. 3 shows the flow of water and toluene down a  $45^\circ$  inclined steel plate. This leads to new questions for experiments as well as numerics. What can be observed here is a film flow of the organic phase and rivulet or droplet flow of the aqueous phase. This behavior is also modeled by the CFD simulations but the simulations behave far less stable than with only one liquid phase. The grid has to be refined and the calculation time increases strongly. The phases interact with each other. The slower organic film is accelerated by the faster water rivulets and droplets. This can be shown in the simulations as well as in the experiments. In the experiments it could be shown that the influence of the organic liquid load on the water surface velocity is stronger than influence of the water load and vice versa.

## Conclusion

It is shown that for two phase flow the CFD models for multiphase flow are able to predict the flow behavior correctly. Morphological and quantitative comparison with the experiments shows a good agreement. The boundary conditions have a great impact on the results. Their major effects are identified and taken into account. In the case of three phase flow the simulated flow behavior seems to agree with the experiments very well. The velocities also show good agreement. Further investigations are in progress to validate these observations.

Therefore it is reasonable to use CFD simulations to investigate the flow behavior inside column packings. With modern computers it is still not possible to simulate more than small regions in detail. Thus the important regions inside the packing section have to be identified and investigated separately. The results found here are used to develop a model for packed columns which takes into account the flow behavior.

## Acknowledgements

The authors would like to thank the DFG (German Research Foundation) for their financial support and the Center of Fluid Systems Technology for organizational support of the Graduiertenkolleg (Research Training Group) 827. We also appreciate the support of the post graduate school PIPES.

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