USE OF OPENFOAM® FOR INVESTIGATION OF MIXING TIME IN AGITATED VESSELS WITH IMMERSED HELICAL COILS

STEFAN, A.[1], VOLKMER J.[2], SCHULTZ, H. J.[3]
[1]*University of Applied Sciences Niederrhein, alexander.stefan@hs-niederrhein.de*
[2]*University of Applied Sciences Niederrhein, jan.volkmer@stud.hn.de*
[3]*University of Applied Sciences Niederrhein, heyko_juergen.schultz@hs-niederrhein.de*

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In process engineering and especially in chemical industry, agitated vessels are commonly used for a multitude of applications. They have therefore been investigated in numerous papers and monographs [1]-[7]. Typical basic operations are heating, homogenizing, suspending, blending and chemical reactions. For an appropriate design and effective operation of agitated vessels, it is necessary to understand the hydrodynamics and the transfer phenomena under the given circumstances. In previous works, good models for different aspects of stirred processes have been given for vessels with and without baffles. It is however not possible to give a universal model for different design scales of vessels foremost not for different equipments and internals. It is therefore necessary to look at each case individually. Experimental investigation quickly reaches its limits concerning applicability and costs. At this point numerical simulation appears to be of large value. The results of numerical calculations have to be validated and verified though. The objective of the present work is to provide an experimental based CFD-model for the determination of the mixing time in an agitated vessel with immersed helical coils.

Description of Experiment

Up to now, little research has been published for this special configuration due to the very elaborate metrological approach. For noninvasive optical methods, complex geometries pose a challenging obstacle concerning measurement accuracy. This can be circumvented by fabrication of the geometry out of a translucent material and adaptation of the refractive index of the fluent. Figure 1 shows the meassurement setup for laser-induced-fluorescense (LIF). A 10 L beaker glas was used as vessel, the coil was made out of perspex and ammonium thiocyanate solution was used as refractive index matched liquid. The mixing time was determined by using rhodamine B as tracer substance.

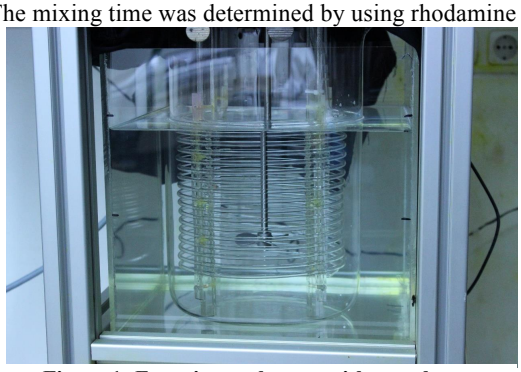

Figure 1: Experimental setup with translucent internals.

Mixing time is one of the central feature sizes in a stirred process. It has fundamental influence on both, material and thermal transport phenomena. Its value is the basis for process design and the key to the determination of the operating parameters and the estimation of energy requirement. However, the experimental determination is highly individual for each problem and even experimental setup. Though, it is very important to ensure acurate projection of the experiment to the numerical calculation.

CFD-method

This work deals with the implementation of a simulation method using the CFD-software OpenFOAM® and gives an evaluation of the simulation results with regard to pre-processing and modelling effort, the calculation time, certain numerical criteria and validity by comparison with measurement data.
For the inverstigation of the mixing time it is necessary to bring the agitated system to a quasi-steady state, where the main flow field is already developed. The OpenFOAM-solver pimpleDyMFoam (cf. [8]) was used for this issue. To ensure that the state is quasi-steady, the volume averaged values for the field values (velocity U, pressure p, turbulent kinetic energy k and energy dissipation rate epsilon) were observed. For the cases in this work, the quasi-steady state could be reliably reached after 15 s real time simulation. The results were then used as start condition for the real issue.

As no adequate precompiled solver could be found in the current OpenFOAM version, there had to be built a new solver with the demand to be capable to simulate transiently two miscable liquids with a dynamic mesh and turbulent flow. The twoLiquidMixingFoam from the actual version could be identified as a reasonable basis for the observed issue. It was compiled as user-own solver after adding the dynamicMesh library to it like instructed in [9]. The resulting solver was obviously named twoLiquidMixingDyMFoam. The tracer substance was mapped for a definite volume at the spot where it was injected in the experiment. After initial stability issues, the simulation could be brought to convergency by adjusting the numerical schemes. Exactly like in the experimental approach, several probe points in the vessel domain were selected for determination of the mixing time. The volume fraction alpha is being observed until it reaches a convergent value. Since statistical fluctuations cannot be avoided, the convergent value is uncertain and has to be calculated as a mean value over a period of time. Due to this issue, a convergence criterion has to be found. Following the recommendation in [4], a deviation of 5 % of the mean value was taken as mixing time criterion, i.e. the mixing time is specified as the time interval between injection of the tracer up to the time where it enters the ± 5 % margin-box for the last time (Figure 2).

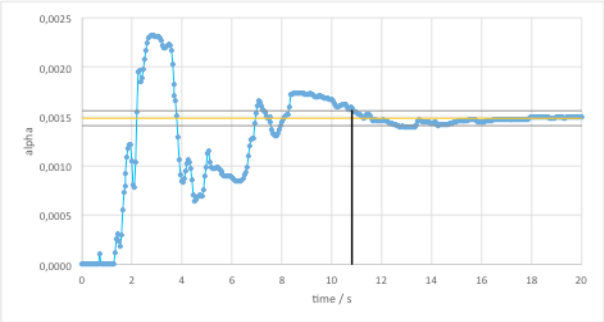

Figure 2: Mixing time via the tracer concentration at a certain probe location.

Within the scope of verification, the simulation was performed for successivly refined meshes in order to determine the convergence order. This analysis allows to make a tradeoff between results acuracy and time efficiency. Since the analytical solution is not known, the results of the finest mesh were considered to be correct and compared to the results of the remaining meshes. The volume-of-fluid method was furthermore checked for conservation of alpha, as parts of the mesh are strongly nonorthogonal and arbitrary mesh interfaces are involved. For the final validation, the simulations were compared to the experimental results. First results are very promising but need further attention yet. The method ought to be transferred to industrial scale where mixing time often is the only possible validation method for a CFD-model due to the fact that the measurement possibilities are very limited in an industrial reactor, sample points however exist in the most reactors.

The implemented CFD method for investigation of the mixing time is suitable for the utilization for an agitated vessel with complex internals like immersed helical coils. For this purpose, an existing OF-solver was provided with the dynamicMesh library. Simulation results were analyzed and compared to experimental meassurements. Further potential for research and industrial applicability could be identified.

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