CHEMICAL ENGINEERING TRANSACTIONS

VOL. 32, 2013

A publication of AIDIC
The Italian Association of Chemical Engineering
Online at: www.aidic.it/cet

Chief Editors: Sauro Pierucci, Jiří J. Klemeš

ISBN 978-88-95608-23-5; **ISSN** 1974-9791

DOI: 10.3303/CET1332239

Particle Tracing Based Validation for CFD Models of Stirred Reactors

Attila Egedy*, Tamás Varga, Tibor Chován

University of Pannonia, Department of Process Engineering, Egyetem Str. 10, H-8200 Veszprém, Hungary
egedya@fmt.uni-pannon.hu

Modeling the flow field in a stirred tank is always a challenging task because multiple processes (e.g. heat and component transport processes, reaction) must be considered to build an adequate model. Nowadays Computational Fluid Dynamics (CFD) models can be used to examine the different physical phenomena in a stirred tank. However the validation of these models is not an easy task. In this work particle tracing methods were used to analyze the flow patterns in a laboratory glass reactor. The particle movements were recorded from two different angles to follow the trajectories of the particles in three dimensions. Beside the physical experiments, the geometry and the momentum balance model were implemented in CFD software. Based on the experimental results the CFD models were validated. A statistical analysis was applied in the model validation. MATLAB/Simulink was applied for video processing and COMSOL Multiphysics for CFD model implementation and simulation studies. In our experience the proposed method can significantly simplify the validation of CFD models.

1. Introduction

Stirred reactors are widely used in the process industries for example in biotechnologies pharmaceutical, polymerization and crystallization technologies. The stirring system of a mixed tank is always an important factor of design, because the involved processes (such as reactions, heat or component transport) usually require proper contact and homogeneity of the existing phases. For the suitable homogeneity the design and size of the moving parts are also important problems. In certain situations the attachment of static parts to a stirred tank (such as baffles) may have an important effect too. Modeling of the developing flow pattern is difficult, especially in complex geometries (multiple impellers, baffles etc.). Based on the detailed hydrodynamic modeling of the system the critical parameters and operation limits can be determined. Using adequate models the practical knowledge can be expanded, and can lead to a better understanding of the behavior of reactors, and the macro mixing phenomenon. Computational Fluid Dynamic (CFD) models can support modeling (Maggioris et al., 1998), development (Wei, 2010) safe operation or other engineering tasks (Rudniak et al., 2004). CFD models use partial differential equations, and a unique mesh for every single problem. The momentum, heat and component balances can be computed together, due the growing computation performance. The most important advantage of the CFD approach is the possibility to model entire geometries in three dimensions, and analyzes whole technologies, even multiphase systems (Tamburini et al., 2011). Moreover three dimensional simulation allows engineers to examine the operation of the plant, and prevent dangerous situation by discovering inhomogeneities in a reactor (such as thermal hot spots, thus preventing runaway situations) (Milevska and Molga, 2010). However CFD simulation has a quite large computation need (based on the applied fluid flow model), and the proper validation of the developed model is important.
There are two major approaches of CFD model validation, the laser based methods, and mixing time measurements. The laser based methods (Laser Doppler anemometry, Particle image velocimetry) are more expensive, but provide more reliable data. The mixing time measurements, usually based on colorization, conductometry or thermometry methods, are cheaper, but less sophisticated (Paul 2004.).
Beside the classical validation techniques, there are new emerging methods to CFD model validation, such as particle tracing methods. The particle tracing methods use a transparent vessel, and colored

Please cite this article as: Egedy A., Varga T., Chovan T., 2013, Particle tracing based validation for cfd models of stirred reactors, Chemical Engineering Transactions, 32, 1429-1434 DOI: 10.3303/CET1332239

tracer particles to obtain the velocities in a device. The basic idea of this approach is the same as that of the particle image velocimetry methods. However video processing methods can be used instead of laser and that will lead to much cheaper measurements.

In CFD simulations particle tracing models will be different. In COMSOL Multiphysics there is a possibility to calculate particle trajectories based on the velocity field formulation in a vessel using momentum balance model implementation. On the other hand the equations behind the movement can be defined by the user applying mathematical particle tracing methods.

Particle tracing methods can be used for example for:

- collider, tokamak and cyclotron design using magnetic particle tracing (Gyimesi et al., 1999)
- surveillance target tracking (Han et al., 2011)
- swallow water tracking with fluorescent particles (Tauro et al., 2012)
- micromixer particle tracing (modeled in COMSOL Multiphysics) (Karniadakis et al., 2005)
- visualization of mixing with particles (Torré et al., 2008).

Processing video recordings is an easy and low cost way to quantify particle tracing measurements or mixing time measurements. Color intensity values can be calculated from frame to frame, and mixing time can be computed. (Cabaret et al., 2007; Visuri et al., 2007).

With video or image analysis methods such as Laser Sheet Image Analysis (Tamburini et al., 2009) even multiphase systems can be analyzed in a transparent reactor, and the evolving vortexes can be quantified (Busciglio et al., 2011.).

A similar approach can be followed in processing particle tracing measurements. The tracer particles must be identified from frame to frame, and from the position changes; the velocities in the device can be calculated.

The primary goal of this study is to create a video processing method capable of identifying particle trajectories from camera recordings, and then validate a CFD model of the device based on the measurements. MATLAB/Simulink was used for the video processing steps, and COMSOL Multiphysics for the CFD model implementation.

2. Experimental and video processing methods

2.1 Experimental procedures

For the particle tracing experiments a laboratory measurement system containing a 1 liter laboratory glass reactor was developed. It was equipped with different plastic impellers (3D printed based on CAD drawings), and a computer controlled IKA mixer motor. Two Sony cameras (CX 115E) were used to record videos from different impellers from two different position in 90°angle to each other in order to obtain three dimensional particle trajectories. Figure 1 (a) shows the experimental apparatus.

The parameters of the cameras (brightness, focus distance, distance from the vessel etc.) were the same in both cases to ensure the repeatability and make the video processing step easier. Figure 1 (b) shows the strategy that was applied to obtain three dimensional particle trajectories from two dimensional videos.

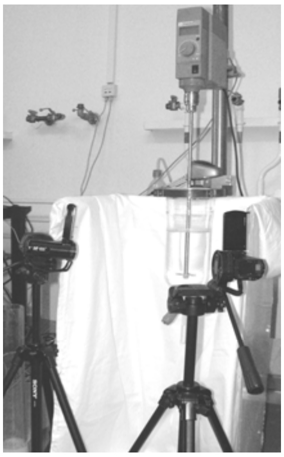
2.2 Video processing methods

One black plastic particle was used to obtain particle trajectories. In our study a static background without any particles was recorded first. Based on the detected background we are able to detect the moving edges beside the tracer particle (e. g. impeller and shaft). When the particle was added to the system, it can be traced by detecting the moving edges and removing the moving parts from the background, hence the tracer particle can be followed from frame to frame. In the video processing method the following steps were applied:

- The recording was loaded to MATLAB.
- The recording was divided into individual frames, based on the resolution of the camera (25 fps).
- A background was defined based on the frames of the video without tracing particle.
- Detection of the moving edges (impeller, shaft), by removing the static parts of the vessel, based on color intensity, and a predefined threshold.
- Detection of the moving particle by removing the movements of the impeller and shaft.
- The position of the particle was traced from frame to frame.
- The obtained data was corrected based on the recording from the other angle.
- Synchronizing the two angles.
- 3D particle trajectory calculation.

After the correction was completed the three dimensional particle trajectories were calculated.
A statistical method was developed to validate our results. The recorded particle positions were quantified using a quasi-residence time method. The whole geometry was divided into smaller subsections, and the number of appearances of the particle was computed. The 3D particle trajectories were converted to a 2D diagram by calculating radius coordinates from x-y coordinates. The number of appearances in every subsection was counted in time, and based on the percentage of appearances compared to the all appearances a graph were drawn. This graph is representing the residence time of the particle in the vessel and we are able to compare the CFD simulations to the experimental results.

a



b

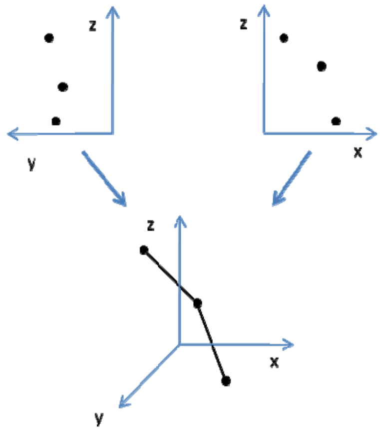


Figure 1 (a) The experimental apparatus (glass reactor, two cameras with different angles and the IKA mixer motor) (b) Strategy to obtain three dimensional particle trajectories

3. CFD model

This part of the study focuses on the physical phenomena and the structure of the CFD model. In this investigation the revolution speed was 500 1/min. In our study different impellers were implemented (blade and turbine). The geometry was the same in the experimental and the simulation cases.
The first implemented physical phenomenon was the momentum balance. It is based on the Navier-Stokes equation extended with k-ε turbulence terms (Wilcox et. al, 1998). The particle tracing part of the model contains terms calculating the particle trajectories based on the developed flow field (drag and gravity forces).
After the models were solved the particle trajectories can be extracted from the program and can be compared to the experimental results.

4. Results

Due to the similar conditions of the two cameras we do not need a time stamp to synchronize the videos; instead the changes in z coordinate provide an excellent way, to synchronize the dynamics of the video recordings. Figure 2 shows the z-coordinates of the videos from two angles before and after the synchronization.

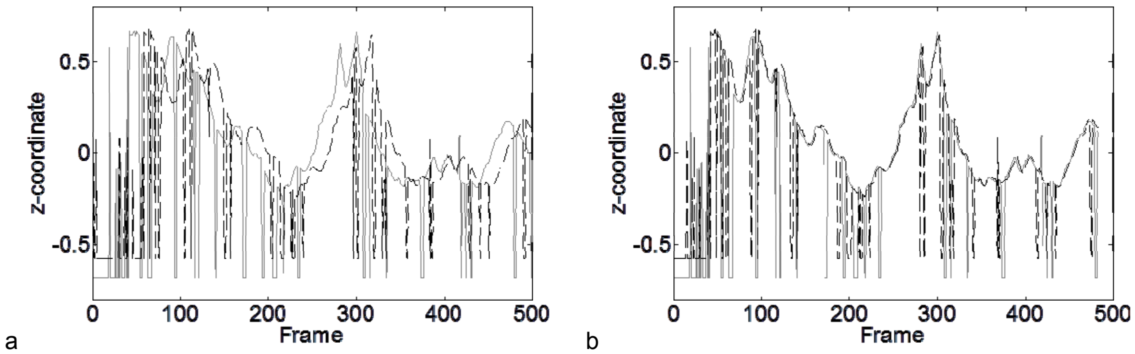


Figure 2 The z-coordinate of the videos before (a) and after synchronization (b).

After the synchronization step we are able to calculate 3D trajectories. The computed trajectories can be enhanced using a spline interpolation, and scaling. In the simulation case after model implementation we have to solve the momentum balance model, and particle tracing model and the results can be extracted as 3D coordinates. Figure 3 shows a three dimensional particle trajectory from measurement (a) and the 3D representation of a few particle trajectories from CFD simulations (b) in the case of blade impeller.

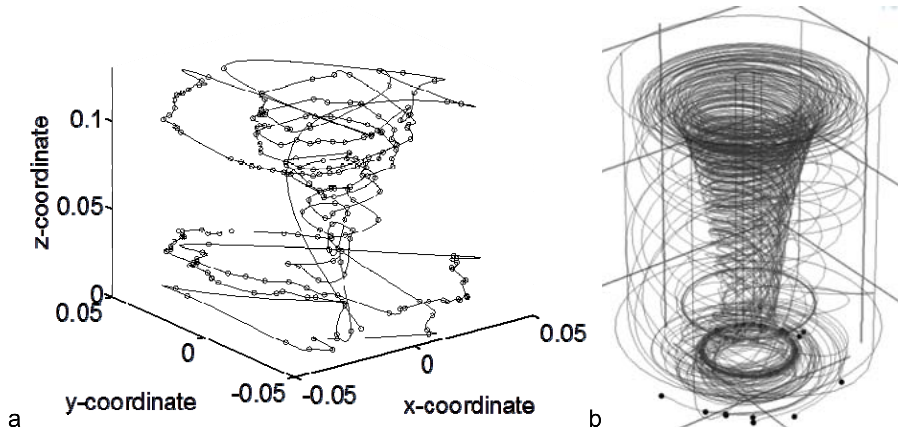


Figure 3 3D particle trajectories from measurement (a) and from simulation (b) in the case of blade impeller

Then a particle residence method was used to calculate average particle residence in the smaller parts (1/100) of the vessel. The 3D trajectories were mapped to a 2D representation by replacing the x-y coordinates with the radius coordinate. Figure 4 shows the results in the case of measurement and simulation based on different impellers.

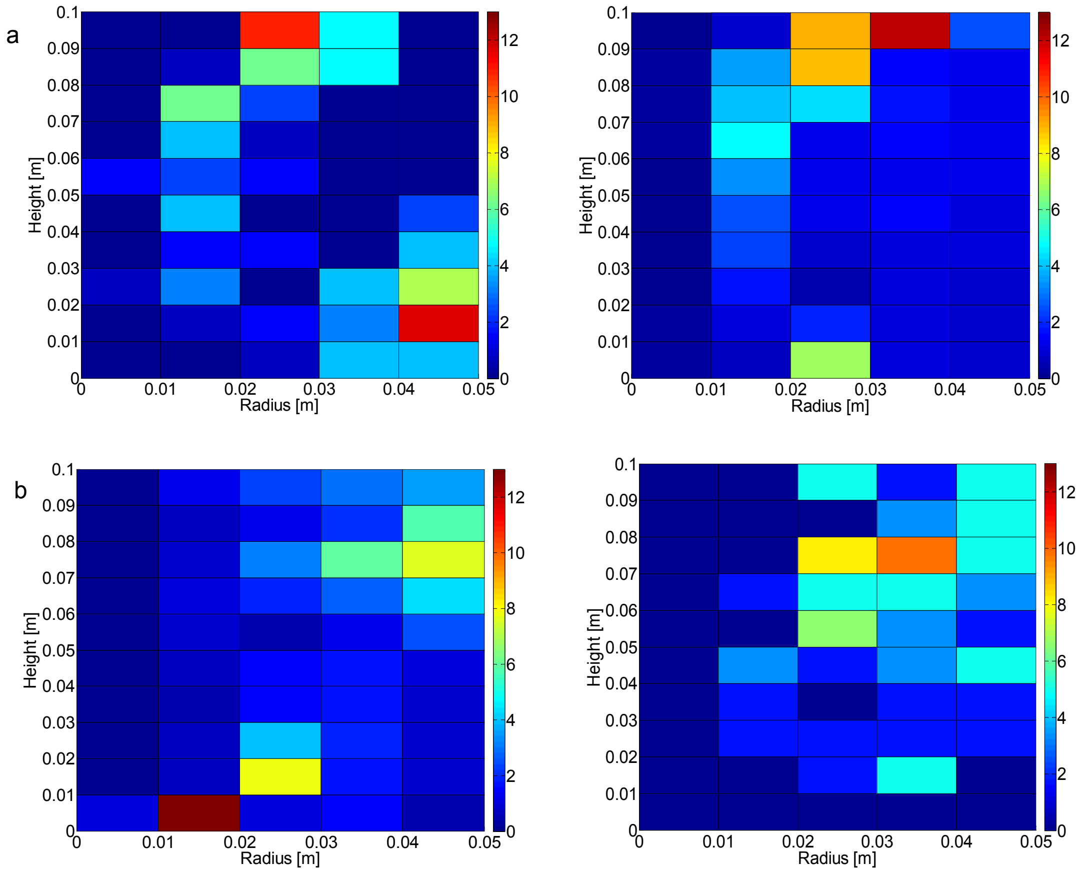


Figure 4 Statistical analysis of the particle trajectories from measurement (left) and from simulation (right), in case of (a) blade, (b) turbine impeller)

After the statistical analysis we compared the measured and the calculated graphs to each other. There is a dead zone near the impeller shaft and both diagrams shows a vortex near the impeller. In case of the blade and the turbine impeller the measurement and simulation results show similar characteristics, however to find the causes of the differences more experiments might be needed.

5. Conclusions

A video processing particle tracing based method was developed to validate CFD model of stirred systems. The method was based on an off-line method using edge detection to follow the movement of a plastic particle. The movement of the particle was recorded and 3D particle trajectories were reconstructed from the data. Both the measured and the simulated data sets were evaluated using a statistical method. A quasi-residence time was calculated and with the statistical method, the simulated cases were validated. The proposed method makes the CFD model validation much easier.

Acknowledgements

This work was supported by the European Union and financed by the European Social Fund in the frame the TAMOP-4.2.2/B-10/1-2010-0025 and TÁMOP-4.2.2/A-11/1/KONV-2012-0071 projects.

References

Busciglio A., Grisafi F., Scargiali F., Davi M.L., Brucato A., 2011, Vortex Shape in Unbaffled Stirred Vessels: Experimental Study via Digital Image Analysis, Chemical Engineering Transactions, 24, 1387-1392

Cabaret F., Bonnot S.,Fradette L., Tanguy P.A., 2007., Mixing time analysis Using colorimetric methods and image processing, Industrial Engineering Chemistry and Research, 46, 5032-5042

Gyimesi M., Zhulin V., Ostergaard D., 1999, Particle trajectory tracing in ANSYS, Nuclear Instruments and Methods in Physics Research A, 427, 408-411

Han, H., Ding Y-S., Hao K-R., Liang X., 2011, An evolutionary particle filter with the immune genetic algorithm for intelligent video target tracking, Computers and Mathematics with Applications, 62, 2685–2695

Karniadakis G., Beskok A., Aluru N., 2005, Microflows and Nanoflows, Springer, New York, USA

Maggioris D., Goulas A., Alexopoulos A.H., Chatzi E.G., Kiparissides C., 1998, Use of CFD in prediction of particle size distribution in suspension polymer reactors, Computers and Chemical Engineering, 22, 315-322

Milevska A., Molga E., 2010, Safety aspects in modelling and operating of batch and semibatch stirred tank chemical reactors, Chemical Engineering Research and Design, 88, 304-319

Paul E.L., 2004, Handbook of Industrial Mixing Science and Practice, John Wiley & Sons, New Jersey, USA

Rudniak L., Machniewski P. M., Milewska A., Molga E., 2004, CFD modelling of stirred tank chemical reactors: homogeneous and heterogeneous reaction systems, Chemical Engineering Science, 59, 5233 – 5239

Tamburini A., Gentile L., Cipollina A., Micale G., Brucato A., 2009, Experimental investigation of dilute solid-liquid suspension in an unbaffled stirred vessels by a novel pulse based image analysis technique, Chemical Engineering Transactions, 17, 531-536

Tamburini A., Cipollina A., Micale G., 2011, CFD Simulation of Solid Liquid Suspensions in Baffled Stirred Vessels Below Complete Suspension Speed, Chemical Engineering Transactions, 24, 1435-1440

Tauro F., Pagano C., Porfiri M., Grimaldi S., 2012, Tracing of shallow water flows through buoyant fluorescent particles, Flow Measurement and Instrumentation, 26,93-101

Torré J-P., Fletcher D.F., Lasuye T., Xuereb C., 2008, An experimental and CFD study of liquid jet injection into a partially baffled mixing vessel: A contribution to process safety by improving the quenching of runaway reactions, Chemical Engineering Science, 63, 924-942

Visuri O., Laakkonen M., Aittamaa J., 2007, A digital imaging technique for the analysis of local inhomogenities from agitated vessels, Chemical Engineering Technology, 30, 1692-1699

Wei, H, 2010, Computer-aided design and scale up of crystallization processes: Integrating approaches and case studies, Chemical Engineering Research and Design, 88, 1377-1380

Wilcox D.C., 1998, Turbulence Modeling for CFD, 2nd ed., DCW Industries, La Canada, CA