2D numerical investigation of liquid dispersion in rotating packed bed and its comparison with experimental measurements using high-speed camera

Jakub Elcner[1*], *Ondrej* Hajek[1], and *Miroslav* Jicha[1]

[1]Brno University of Technology, Faculty of Mechanical Engineering, Energy Institute, Technicka 2896/2, Brno 616 69, Czech Republic

Abstract. Study deals with liquid dispersion of water in unstructured wire mesh of rotating packed bed, experimentally investigated using high speed camera. Dispersed water in outer region of rotating packed bed were captured by high-speed camera and droplet size were investigated using image processing. Numerical simulations were performed on two – dimensional plane with similar geometry characteristics (diameter and distance between each wire). Volume of fluid method was used to describe a multiphase behaviour of phenomena and turbulence was modelled using k-epsilon model. Results of both were compared on basis of frequency distribution of individual size fraction of dispersed water in outer region of rotating packed bed and its velocities. Discussion was focused on possibility of 2D numerical investigation and possibility of its comparison with experimental measurement.

1 Introduction

Carbon dioxide contributes to global warming with approximately 60% and Carbon Capture and Storage technology (CCS) or Carbon Capture, Utilization and Storage (CCUS) becomes a key strategy for its reduction if we leave aside sustainable sources. It is today merely accepted that the CCS or CCUS technology for coal power plants is too expensive and it’s cost of investment and operation is too high to be widely implemented unless the price of emission permits increases to about 60 to 80 EUR/tCO2. Therefore, the CCS (CCUS) technology is aimed at several intense industrial branches like cement, refineries, steel works and many small and medium industries. In the complete system of CCS technology, the most expensive is the CO2 capture that represents about 70% of the total cost for required 90% CO2 reduction. It´s quite logic that research and development focus on intensification of the capture process. According to many studies the most advanced and mature technology when comparing with other methods is chemical absorption, which is on the Technology Readiness Level 9 (TRL9), i.e. close to commercialization although it has its weaknesses on the absorption side itself (the need for intensification), and also on the solvent regeneration side. Ammonia NaOH or different amines (most often Monoethanolamine MEA) are the most used solvents. Both have some positives and negatives, but MEA became a reference liquid. Static columns or any spray systems like scrubbers are limited by gravitation and the process cannot be further intensified. Therefore, the aim is to intensify the absorption process. This can be reached by using a rotary absorber called Rotating Packed Bed (RPB). Depending on its diameter and speed, and considering dynamic forces, the rotary absorber can develop up to twenty times the gravitational acceleration and subsequently ensure up to one order of magnitude higher transfer of CO2 to the solvent, with dimensions ten times smaller than static columns or scrubbers.

Main task in the development of Rotating Packed Bed is to clarify the phenomena that occur during their operation e.g. influence of geometry, rotational speed, inlet behaviour, liquid dispersion, primary solvent distribution, and type of packing (wire mesh, metal foam or others) on liquid distribution, and liquid disintegration and film formation, i.e. phase interface inside rotating packing. The most suitable way to assess the influence of various parameters and to propose an optimal solution for RPB is to use computational fluid dynamics (CFD) to simulate the process inside the packing and validate it by experiments on identical geometry. Our previous research [1], based on experiments performed by Yang et al. [2] focused on RPB has dealt with effect of multiple liquid inlets and its affect on mass transfer inside the packing represented by liquid holdup. Thanks to own experimental model of RPB with wired packing, we are now able to perform experiments and have direct comparison/validation of our numerical research.

* Corresponding author: elcner@fme.vutbr.cz

2 Methods

2.1 Rotating packed bed

The main object of the RPB is a wired mesh consisting of 34 m long grid, twisted in 48 layers. The inner diameter of the mesh is 150 mm, and the outer diameter is 300 mm. The grid is 30 mm wide. The wire mesh is attached to the housing by six spikes of 8 mm in diameter. The diameter of single wire of the grid is 0.8 mm and the distance between the axis of the individual wires forming the grid is 3.95 mm. The housing is then a plastic enclosure with external dimensions of 400 x 405 x 100 mm, which houses a wire mesh attached to the rotor shaft, thus separating the space into three parts. Inner region - Wired mesh - Outer region. The inner region contains the fluid inlet in the form of a pipe of 0.54 mm diameter, oriented at an angle of 45° from horizontal plane of RPB. The outer region contains the fluid outlet with a height of 35 mm. All dimensions of the RPB are shown in Figure 1.

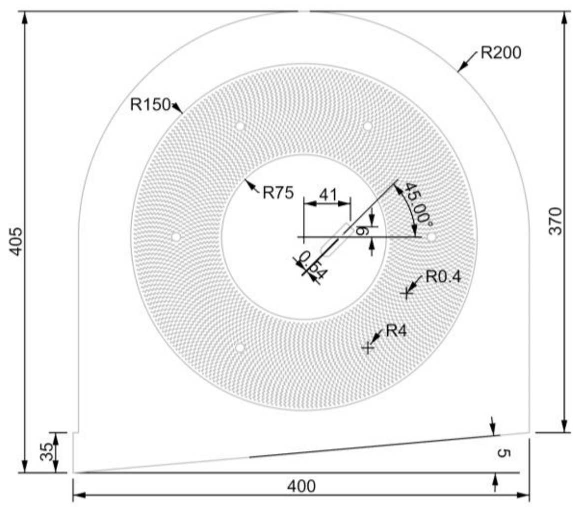

Fig. 1. Dimensions of rotating packed bed

2.2 Experimental setup

The experiments were performed on a test rig, which scheme can be found in Figure 2. The wired mesh was made of 1.4301 stainless steel. Its porosity was 0.82 and specific surface area was 874 m^2/m^3. The packing was connected to a motor of rotary speed of 10Hz. This value corresponds to the real speed of the wired mesh of 409.5 rpm. The flow rate of the water injected by the inlet was 3.8 kg/h and it flowed through a nozzle located in half of thickness of wired mesh. At a distance of 115 mm (horizontal) and 90 mm (vertical) from the axis of rotation of the wired mesh, the lower left corner of the measured area was located, and an image was captured using a Photron FASTCAM SA-Z type 2100K-M-16GB high-speed camera. The area of 23.4 x 23.4 mm (1024 x 1024 px) was recorded at a frame rate of 20,000 fps and a shutter speed of 1.25 μs, for the time of 0.05 s. This produced 1000 contiguous frames.

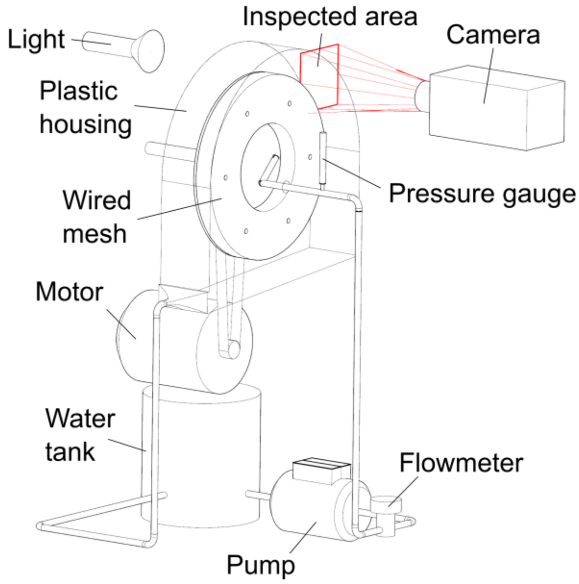

Fig. 2. Test rig

2.3 Numerical setup

2.3.1 Geometry and mesh

In order to reduce the hardware requirements, a two-dimensional representation of the RPB region was created containing an inner region with an inlet boundary condition of dimension corresponding to diameter of the nozzle. The wired mesh region is represented by circular obstacles of 0.8 mm in diameter, at a distance of 3.95 mm, helically arranged in 48 rows of geometry with inner and outer diameters ranging from 150 to 300 mm, respectively. The area of the inner region was constrained (see Figure 3 green line) in order to reduce the final number of control volumes and thus reduce the computational requirements.

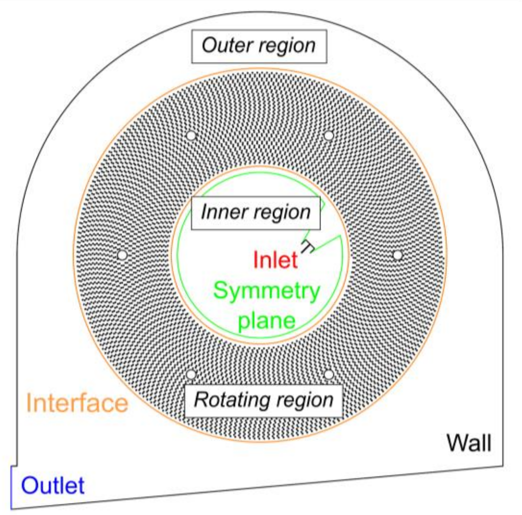

Fig. 3. Boundary conditions

A computational mesh of 5.5 million cells (0.2 inner region; 1.4 mil wired mesh; 3.9 mil outer region) was then created on this geometry. Since the Volume of Fluid method (VOF) has specific requirements for describing the interfaces between the phases and the aim of the research was to capture the smallest possible droplets formed due to dispersion, it was necessary to choose the smallest possible element size of the computational mesh. The base size was chosen to be 0.25 mm with the inner and outer region being further refined to 0.125 mm. Due to the large number of circular objects, the surface curvature value was reduced from the standard 36 points per circle to 18 pts/cycle to maintain the circular shape of the wires and reducing the number of cells in computational mesh. The resulting computational mesh is shown in Figure 4.

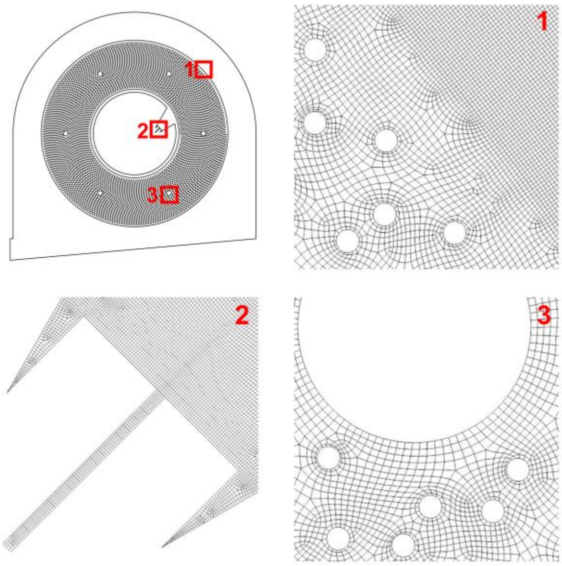

Fig. 4. Details of computational mesh

2.3.2 Physics

The numerical calculations were performed by the Siemens software, Star-CCM+ in version 2019.2 build 14.04.011. The physical setup is based on the assumption that the domain contains two immiscible newtonian fluids, water and air, both incompressible and mutually immiscible. The surface tension between the phases is 0.0728 N/m. The VOF method was used for the calculation, which solves the interactions between air (density = 1.18415 m3/kg; dynamic viscosity = 1.85508E-5 Pa/s) and water (density = 998.2 m3/kg; dynamic viscosity = 1.003E-3 Pa/s). The contact angle on the wires was set to 150° to simulate hydrophilic material, while the contact angle on the walls of RPB was prescribed to 30° (hydrophobic material) based on information from [3]. The calculation was performed on a two-dimensional domain. Turbulence was modelled using unsteady Reynolds Averaging of Navier-Stokes equations (RANS) approach with Realizable K-Epsilon Two-Layer model with all-y^+ wall treatment which calculates velocity profile of near-wall region for low values of wall-y^+ (>1) and model it for higher values. An implicit unsteady solver was set up with time step of 5×10^{-6} s with 2nd order of temporal discretization for time period of 0.55 second of phenomena. To decide whether the airflow field inside the RPB was stabilized, the liquid holdup values were monitored in all regions of the domain. The wired mesh motion was solved with a rigid body motion model with a rotation setting of 409.5 rpm in the direction corresponding to the experiment. Through the inlet (see Figure 3) in the inner region, 100% of the water fraction was injected into the domain at a velocity of 4.62 m/s corresponding to the flow rate during the experiment. The calculations were performed on 64 cores of Intel Xeon E5-2690 processors which are contained in the computing cluster located at Brno University of Technology. The run time to calculate 0.55 seconds of phenomena was 200 hours.

3 Results

With respect to intercomparison, the same area and time period was recorded in the numerical simulation as during the experiment. A comparison of the results obtained during the experiment and the numerical simulation is presented in Figure 5.

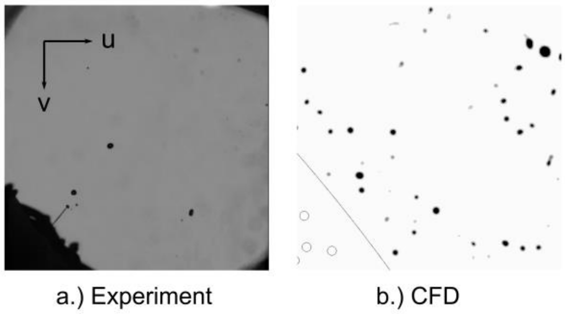

Fig. 5. Comparison of data obtained from experiment and CFD

The size and velocity of the passing water particles were then analyzed in MATLAB® (PIVlab addon) from the obtained images. In the experimental images a 37 particles were recorded and in the CFD images a 347 particles were recorded. The diameters of recorded particles were analyzed and compared in a histogram according to size classes in 0.1 mm increments (Figure 6).

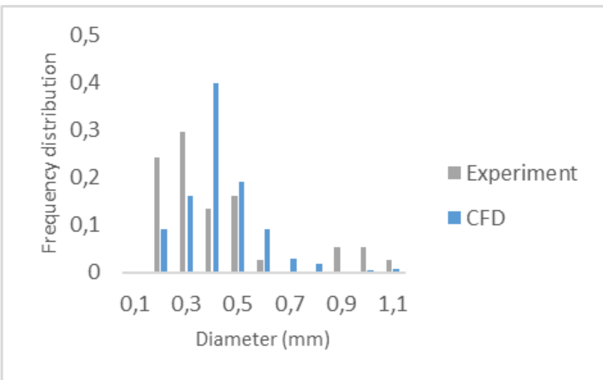

Fig. 6. Comparison of water droplet distribution in RPB

The observed particles were also evaluated for their velocity. The tracking was based on the analysis of the acquired images. The magnitudes and velocities in the direction of the individual components (see Fig. 4) were averaged and results are shown in Table 1. The analysis was based on the change in the position of each droplet within successive set of imaged obtained by high-speed camera and by numerical simulation.

Table 1. Velocity inside investigated region of RPB.

	Experiment	**CFD**
Velocity (mag)	*5.17 m/s*	*6,61 m/s*
Velocity (u)	*4,19 m/s*	*4,87 m/s*
Velocity (v)	*2,84 m/s*	*4,4 m/s*

The main difference between the compared cases is the number of samples analysed. Although the condition of the same time period and the same frame rate was observed, different amounts of fluid dispersed in examined space were realistically analysed. While in the case of the experiment, a thin slice through the domain of wire mesh, dependent on the depth of field of the camera, was observed and liquid droplets, located outside this depth, were not recorded, and thus could not be evaluated. In the case of CFD, which was solved on a 2D domain, an identical amount of fluid is concentrated in one plane and the amount of liquid droplets that can be analysed is consequently larger. This fact significantly affected the statistical sample size of the experimental data. Due to the density of the computational mesh, the VOF method is able to resolve droplets larger than the size of the control volume of the mesh, which in our case is 0.125 mm, while the high-speed camera should theoretically resolve droplets of one pixel size (0.023 mm).

4 Discussion

Although the numerical simulations were performed on a domain constrained in one dimension, thus neglecting the breakup due to the wires running in the RPB plane, the compared data show good agreement between experiments and numerical simulations. Disregarding the different number of liquid droplets captured during experiment and simulation, agreement in the capturing of the droplet size fraction is evident. The range of droplet sizes measured in both cases was between 0.2 - 1.1 mm. Both methods also capture the main size spectrum of particles moving in the investigated region in the range of 0.2 - 0.5 mm. These results suggest the suitability of using the VOF method to capture liquid dispersion on 2d geometry. Comparison of velocities in the measured region shows more than 20% difference in the case of magnitude and velocity in the v component direction. Since there is a significant turbulence inside the RPB due to the motion of the wire mesh, it is likely that the velocity component in the direction parallel to the axis of rotation of the RPB is non-zero and the liquid droplets captured by the high-speed camera do not move along the scanning plane and thus their velocity evaluated by the camera is distorted. The problem of the 2d numerical simulation lies mainly in the mass fraction of fluid present in the domain. Since there is no volumetric spread of the fluid injected by the inlet and a given velocity, the geometry will be overwhelmed and consequently the fluid will collide at the edge of the geometry, which does not correspond to reality.

Due to the smallest droplet size (0.1 mm in diameter) which needs to be solved using the VOF method, and the large range of length scales of the geometry (wire diameter vs. casing diameter), a full solution in 3D would require a minimum mesh size of about 80 million cells [4]. The number of elements in the mesh could be reduced by using an adaptive mesh refinement method or by prescribing a cyclic boundary condition and solving a slice of geometry [5], but the simulation demands due to the number of elements and the need to choose a short time step with respect to CFL < 1 [5] would still be too large. This comparison shows that the 2D approach, despite raising questions about the neglect of one dimension, is meaningful and may offer interesting results.

This work was financially supported by the project "Computer Simulations for Effective Low-Emission Energy" funded as project No. CZ.02.1.01/0.0/0.0/16_026/0008392 by Operational Programme Research, Development and Education, Priority axis 1: Strengthening capacity for high-quality research. And project Czech Grant Agency 21-45227L. The financial support is gratefully acknowledged.

References

1. J. Elcner, M. Jicha, MATEC Web Conf, *AEaNMiFMaE-2020*, **328**, 4 (2020)
2. Y.C. Yang, Y. Xiang, G.W. Chu, H.K. Zou, Y.Luo, M. Arowo, J.F. Chen, Chem. Eng. Sci. 138 (2015)
3. P. Xie, X. Lu, X. Yang, D. Ingham, L. Ma, M. Pourkashanian, Chem. Eng. Sci 172 (2017)
4. Y. Liu, Y. Luo, G. Chu et al., Chem. Eng. Sci 170 (2017)
5. W. Zhang, P. Xie, Y. Li et al., Chem. Eng. Journal 427 (2021)