Validation of CFD model for mixture flow in FGD reactor

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Abstract: This article describes the flow of gas mixture inside the flue gas desulfurization (FGD) reactor This reactor is self-constructed for using as experimental verification tool in research of modeling the desulfurization process. Inside the reactor space there is situated a spray nozzle for injecting water droplets into the gas. During the experimental study the velocity field in the reactor spray zone were measured. For CFD modelling the modification of standard OpenFOAM solver is used. CFD simulations were performed to model flow of multicomponent gas. Simulation results (velocity fields) are confronted with experimental data. Based on the comparison the good accordance with the real state was found. The conclusion is that the developed OpenFOAM solver could be used for future research, but further validation is recomended.

Key-Words: desulfurization, CFD, OpenFOAM, mixture, gas

1 Introduction

In the Czech Republic the most electricity is produced by coal power plants. Amount of pollutants, which are harmful for the environment (e.g. NO_x, SO_2…), has to be reduced under the legal limits. For reducing sulfur dioxide the devices called wet scrubbers are used. Process inside the scrubber is called flue gas desulfurization (FGD). Principle of wet FGD is based on absorption of sulfur dioxide into a droplets of limestone slurry. Inside the scrubber there is multicomponent multiphase flow. It could be simplified to flow of ideal gas mixture with limestone slurry droplets [1].

The aim of our work is to develop the numerical model of FGD process implemented into OpenFOAM computation software. This model should solve different physical problems like gas flow, injection of discrete phase (droplets of limestone slurry) and chemical reactions.

In previous work [2] we found that we need to build a scaled model of FGD reactor to verify the numerical results. The testing measurement and comparison of its results with results from initial CFD simulations were presented in work [3]. Based on this comparison, the recommendations for improving quality of measurement results were defined.

The CFD model was modified to reach more precise results with better compliance with experimentally measured data. Aim of this work is to show the comparison between velocity fields, measured inside the experimental reactor in comparison with velocity fields gained from modified numerical solver.

Because of needs for simulate the injection of droplets, new piping and nozzles for spraying water were mounted inside the experimental reactor.

Based on t hese modification, new geometry of CFD model was created. The CFD solver (described in [3]) has been modified to allow modelling of multiphase flow using the Euler-Lagrange approach, that have been successfully used by Marocco and Inzoli [4] for simulations of processes in wet flue gas desulphurization technology. Before multiphase flow modelling, the solver for flow inside the reactor has to be validated.

Development of the fully worked solver should be divided into several steps:

1. Modelling of simple flow of air.
2. Modelling of mixture flow.
3. Modelling of multiphase flow.
4. Modelling of chemical reactions.

This article deals with step 2 aiming on t he mixture flow modelling.

2 Experimental reactor

The scaled model for simulating the operation of flue gas desulphurization reactor was built. Based on the actual needs for our investigation, some modifications of its design were performed.

2.1 Experimental setup

The main area of the experimental reactor is the spray zone located in cylindrical part. In this zone, three different level were defined for measuring velocity field (see figure 1). In each level 33 measuring points across the section were defined. Scheme of point´s position same for all levels is shown in figure 2. These points were sorted in 4 groups for each level. These groups are labeled as L1, L2, L3, L4. Each group represents a velocity profile in one direction on defined planes Z.
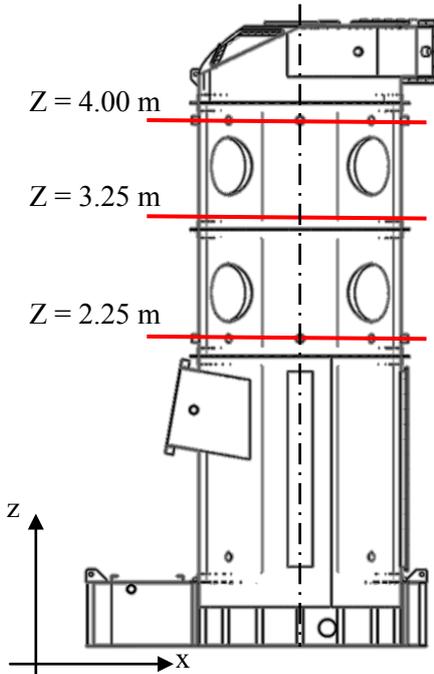

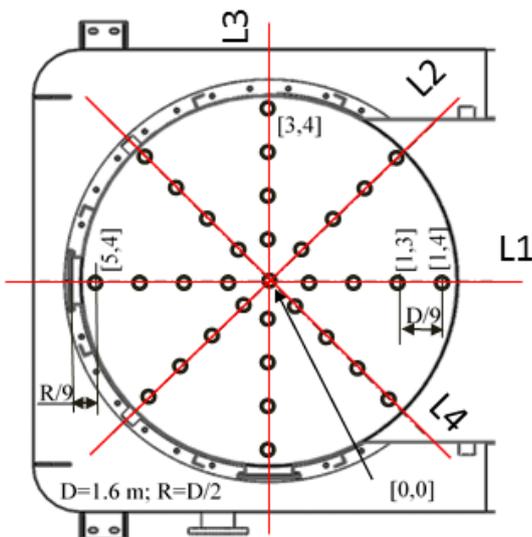**Fig. 1** – Reactor – Position of section planes

Fig. 2 – Measuring points – scheme and labeling

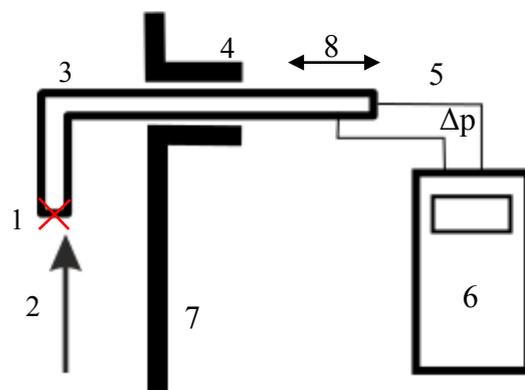For measuring velocity the system with Prandtl probe was used. The whole apparatus consists of the Prandtl probe with 1m length, connecting silicone hoses and Testo 480 climate measurement meter and data logger. This device connected to the Prandtl probe measure differential pressure and convert that directly to the value of velocity. The velocity values are given from measured pressure difference:

$$v = \sqrt{\frac{2 \cdot \Delta p}{\rho}},$$

where   v (m/s) is measured velocity,
Δp (Pa) is pressure difference between total and static pressure,
ρ (kg/m^3) is gas density before Prandtl probe.

TESTO logger uses inner algorithm for evaluating directly the velocity from measured values, where the values are all evaluated as absolute number, which means that the direction of velocity vector could not be evaluated from measured data. Values are also stored to the inner memory of the device.

The function scheme of the apparatus described in the previous paragraph is shown in figure 3. Measuring end of Prandtl probe was oriented in –Z direction, so only the z-component of velocity was measured.

1 – measuring point   5 – silicone hoses
2 – velocity vector   6 – TESTO 480
3 – Prandtl probe   7 – wall of reactor
4 – nipple   8 – traversing direction

Fig. 3 –Scheme of experimental apparatus

At each measuring point, the velocity values were measured and averaged in time by inner data logger algorithm. After that the velocity profiles in different direction through the measuring plane were created.

2.2 CFD simulation of mixture flow

For CFD simulation of flow inside the FGD reactor the self-modified OpenFOAM solver have been used. The main goal of our investigation is to numerically simulate the whole desulfurization process. Actually, the investigation is aimed to development of the suitable solver for flow of gas mixture. The solver is based on t he coalChemistryFoam solver included in OpenFOAM, which uses modified Navier-Stokes equations for describing the mathematical model of flow.

2.2.1 Geometry and mesh

Computation geometry and mesh is based on the simplified CAD model of experimental reactor. The fluid volume inside the reactor were discretized by snappyhexMesh utility. Created computational mesh is based on hexahedral elements. Size of the elements were set as 66 mm with respect to previous study of the influence of mesh element on C FD results (presented in work [3]). Computational mesh used for this study is shown in figure 6.

2.2.2 Boundary conditions

Boundary conditions were set in agreement with the experiment. Inlet velocity field has been set as non-uniform velocity field with real values in specified points, which were obtained from measurement. This field was mapped to mesh points. Interpolated velocity field at the inlet is shown in figure 4. Other boundary conditions are shown in fig. 5 and table 1.
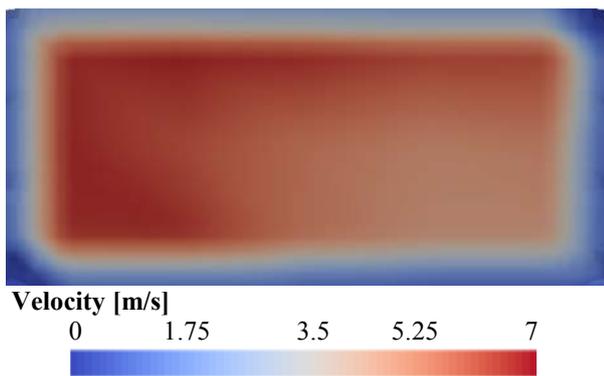

Velocity [m/s]

| 0 | 1.75 | 3.5 | 5.25 | 7 |

Fig. 4 – Inlet velocity field

Table 1 – Boundary conditions

	Inlet	Wall	Outlet
U	mapped	0	inletOutlet
p	zeroGrad	10^5	zeroGrad
T	290	zeroGrad	Zerograd
TKE	0.079	0.135	0.041
Omega	0.047	inletOutlet	omegaWallFc

Table 2 –Mixture components mass fractions

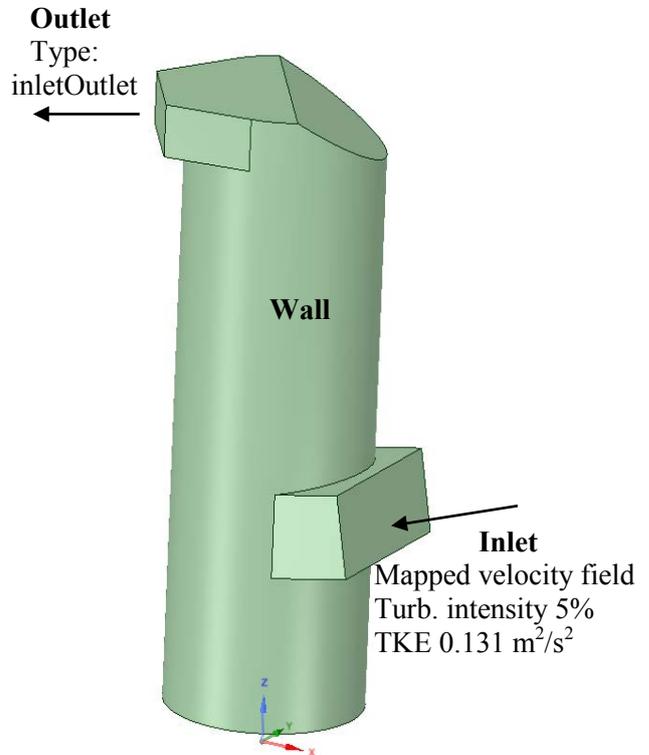| Mass fraction [1]	N_2	O_2	SO_2
Inlet	0.75	0.22	0.03

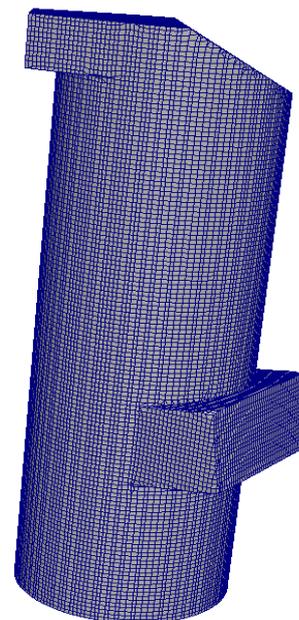

Fig. 5 – Fluid volume with boundaries

Fig. 6 – Computational mesh

2.2.3 Calculation setup

Calculation is conceived as t ransient flow of mixture of gases that are contained in the flue gas. For simplification of the CFD solver, only several gases were considered (see table 2). The *reactingMixture* model were used for calculations of mixture thermophysical properties with respect to perfect gas law. Viscosity of mixture species were modeled by Sutherland´s model, which uses the Sutherland coefficients from OpenFOAM thermal database. Enthalpy model *janafThermo* was used for enthalpy calculations. Turbulence k-ω SST model was used. Residuals of momentum and turbulent quantities were set to 10^{-3}, residuals of energy to 10^{-6}. Only 1st order schemes were used for all solved equations because of limitations for janafThermo model, which allows only 1st orders discretization schemes.

3 Results assessment

Obtained results from experiments and CFD simulations are the velocity fields in previously described areas.

3.1 Experimental data

From measurement with Prandtl probe the velocity fields in three levels of the scrubber totally in 99 measuring points were obtained. Results of measuring velocity for different section planes and 4 cut lines in each plane are shown in figures 7 - 10. Experimental data series are labeled by text ,,*EXP*" at the end of the label.

3.2 CFD analysis

From CFD analysis were obtained velocity fields in different section planes across the Z axis. Because only the z-direction velocities was obtained from the experiments, the results from CFD are shown in the same way, only velocities in z-direction. All values are shown in absolute values. It means no distinguish of velocity vector direction.

Post-processing of CFD results allows to obtain data from various section planes through the reactor. For evaluation results, totally nine planes were defined in the range for Z between 2.25 meters to 4.25 meters with a constant step 0.25 meters.

3. 3 Data comparison

Comparison of CFD results with experimental data was performed by the key shown in table 3 t o compare data of neighboring cutting planes. Corresponding charts are shown in figures 7-9.

Influence of Z coordinate on the velocity profile is shown in figure 10.

Table 3 – Comparison of CFD simulations and experimental cases

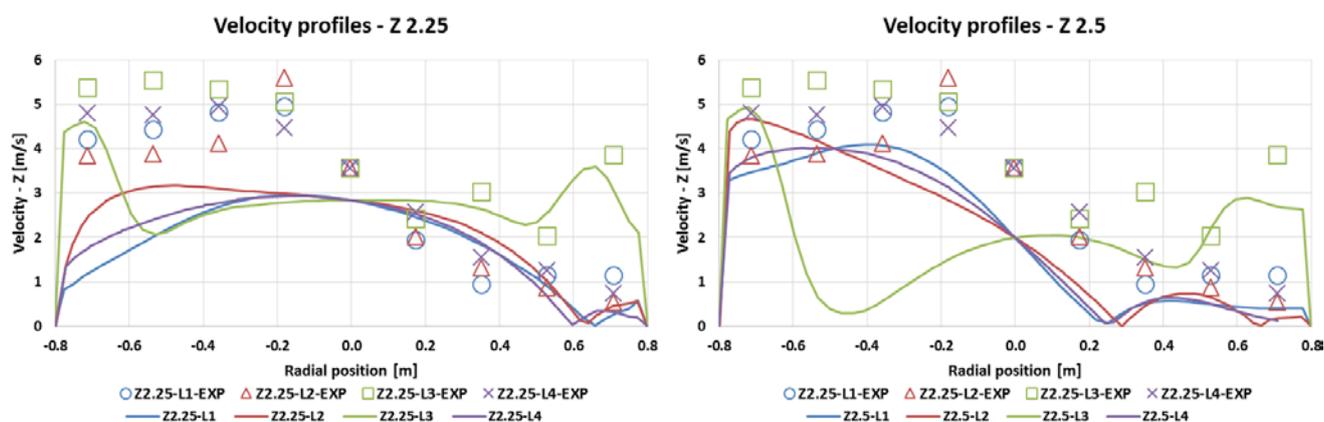| CFD	Z2.25-EXP	Z3.25-EXp	Z4.00-EXP
Z2.25	X		
Z2.50	X		
Z2.75		X	
Z3.00		X	
Z3.25		X	
Z3.50		X	
Z3.75			X
Z4.00			X
Z4.25			X

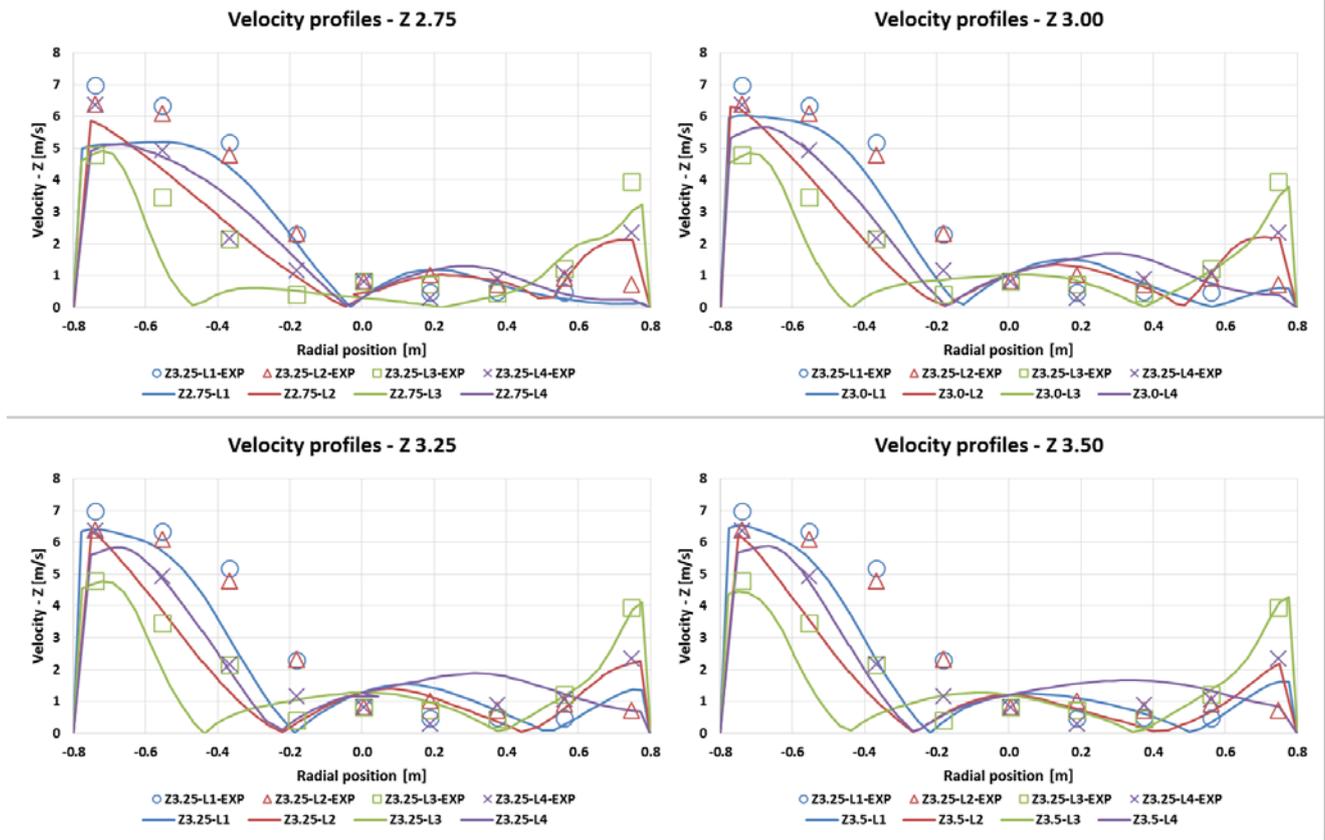**Fig. 7** – Velocity profiles compared with experimental results - Z = 2.25 m

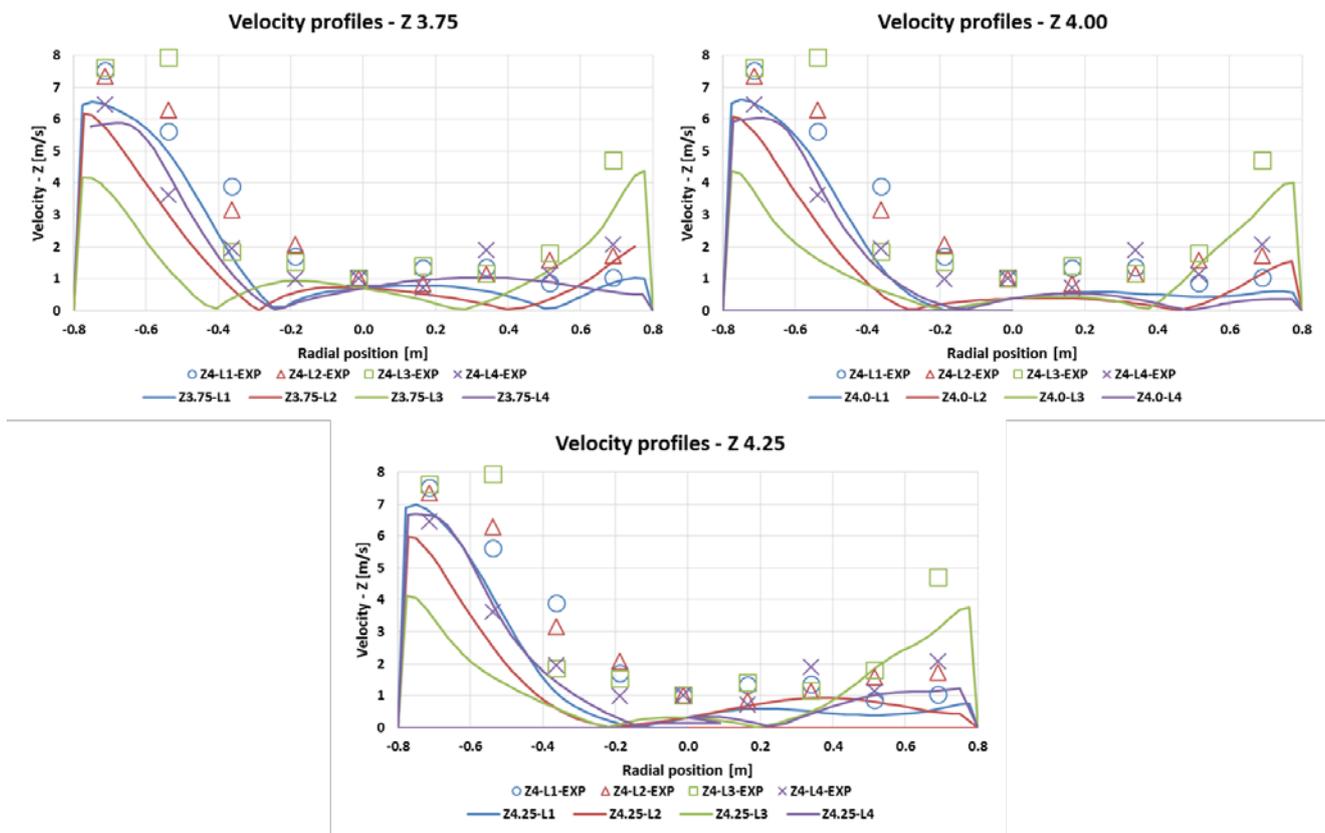**Fig. 8** – Velocity profiles compared with experimental results- Z = 3.25 m

Fig. 9 – Velocity profiles compared with experimental results – Z = 4.00 m
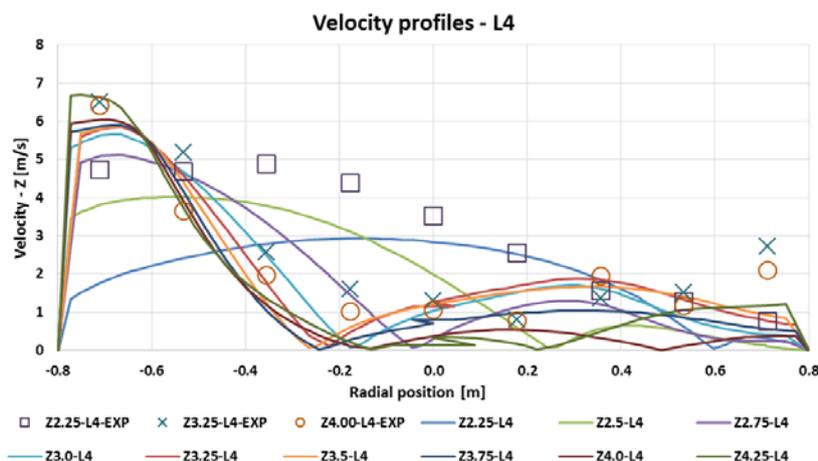
Fig. 10 – Velocity profiles compared with experimental results - Z = 4.00 m

4   Conclusion

In this work the investigation of velocity fields inside the scaled model of FGD reactor by experimental and numerical methods have been performed. Initial conditions and parameters of CFD model, especially velocities at inlet area, were set to correspond well with experimental setup.

Experimental part was performed with using the possibilities and components of experimental reactor (e.g. nipples as entrances for inserting Prandtl probe) and available equipment. Experimental device consists of Prandtl probe and TESTO 480 data logger. Measuring points have been divided into three groups (each with 33 points) which represents three different height level inside the spray zone of the reactor. Experiments were performed by one flow regime (40% of the fan power).

As we can see from the results published in figures 7-9, the velocity field is very variable across the section of reactor. The typical feature inside the profiles is that velocity increases very significantly with the distance from the center. Maximum speeds are located in regions that are opposite to the inlet. It is probably caused by the inertia of flow from the inlet rectangular channel. Velocity in planes with Z coordinate close to the inlet area (shown in figures 7,10) have a worse match with experimental data. It could be caused by the effects of other velocity components (X and Z), that are connected to turbulence phenomena and wake in these areas.

The turbulence effects are not included in experimental data, because the velocity values are time-averaged.

Generally it c ould be said that the velocity profiles obtained from CFD simulations are in a good accordance with experimental data. In the regions, where the main flow stream is located, the difference between experimental and numerical data do not exceed over 15 %.

Finally it can be recommended to the future work to validate the CFD solver using experimental data for different flow regime (power of fan) and then continue with development of the solver by adding the solution for multiphase flow with water droplets.

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