Water and wastewater CFD and validation: are we losing the balance?

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ABSTRACT

A literature screening on computational fluid dynamics (CFD) modelling in water treatment applications showed a vast range of validation ranging from no validation at all, over residence time distribution (RTD) and tracer testing, to velocity field, species concentration and, finally, turbulence properties measurements. The validation level also differs depending on process scale (laboratory, pilot, full) and type of system (rheology, single phase vs. multiphase). Given the fact that CFD is in more widespread use, a discussion on the extent and need of validation needs to be initiated. This paper serves as a discussion starter on the topic.

Key words | computational fluid dynamics (CFD), validation

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INTRODUCTION

Computational fluid dynamics (CFD) has become a mature modelling framework in the water sector and is still gaining ground. Where it used to be a tool for troubleshooting, its application spans further to be used for model-based reactor design and virtual piloting for scale-up. In view of such decisions, the validation step as mentioned in the Good Modelling Practice guidelines for CFD modelling for water applications (Wicklein *et al.* 2016) becomes important with respect to trust in the model and, hence, the decisions based on it. However, there is not really a detailed description on how this validation needs to be performed and to what extent.

In the literature, the validation of CFD models spans a wide variety with respect to the level of detail (Table 1). Through screening 28 papers (no full review was envisioned), measurement variables used included velocity profiles (48%), gas holdup (13%) concentrations of solutes including oxygen (13%) and shear stress (6%). Only a few papers use multiple variables to validate and full-scale validation examples in literature are nearly non-existent. Direct, quantitative comparison to measurement data is scarce, and often (dis)agreement between model prediction and measurement data is assessed by visually comparing trends (e.g. using colour maps). Also, within a certain validation measurement 'category' (e.g. 'velocity'), a multitude of different sensors and methods are used (e.g. velocity can be measured using a wide array of acoustic and other methods). No clear quantitative level is recommended for a CFD model to be perceived as adequate.

CFD models are based on first principles and come in different levels of complexity depending on the required ingredients. For more simple cases (e.g. single phase/laminar) there are not really a suite of parameters that can be calibrated. However, in more complex cases (e.g. multiphase, occurrence of turbulence) models already come with certain calibration of models to provide closure. These are based on detailed studies at laboratory-scale and sufficient data collection at full-scale would be cumbersome. That is why in a CFD model development project there is not such a thing as calibration. Indeed, when validation is insufficient, the modeller needs to look back to the different steps in the development in order to adapt the model structure, the mesh, the solver settings, etc. In many cases, wrong assumptions lead to models with insufficient predictive power (i.e. prediction capability under different conditions). This can be sitting in details that are often thought to be of no influence. The objective of this paper is to initiate a discussion on the need and extent of validation required for CFD models. In what follows, we do so by providing some examples to illustrate the different

doi: 10.2166/wst.2020.181

Table 1 | A summary of CFD validation approaches and measurement methodologies used in 28 papers reviewed

	Type of measurement	Measurement method	Type of fluid	Type of technology	Volume of system	Scale	How data were collected	How validity was assessed	Reference
1	velocity	electromagnetic	wastewater	activated sludge bioreactor	n/a	full scale	4 points	generally mentioned in text (no graphical comparison)	Elshaw *et al.* (2016)
2	velocity	acoustic	wastewater	activated sludge bioreactor (aeration)	10 L	lab scale	5 points	vector maps compared	Karpinska & Bridgeman (2017)
		laser					n/a		
	dissolved oxygen	portable dual channel multimeter					n/a	n/a	
		digital luminescent DO probes					n/a		
3	RTD (mixing time)	radiotracer (BuOH)	water	bubble column reactor	10 L	lab scale	n/a	CFD and experimental results compared on diagrams (in every point)	Pant *et al.* (2004)
		NaCl tracer (additional experiments)					n/a		
4	velocity	laser Doppler velocimetry	wastewater	activated sludge bioreactor	n/a	lab scale	2 planes – 3 heights each	CFD and experimental results compared on diagrams (in every point)	Le Moullec *et al.* (2008)
	liquid phase residence time distribution	tracer (NaCl)					1 point		
5	velocity/turbulence	laser Doppler velocimetry	wastewater	stirred tank	0.5 m i.d. vessel	lab scale	13 points	CFD and experimental results compared on diagrams (in every point)	Sahu *et al.* (1999)
6	velocity/turbulent kinetic energy dissipation rate	laser Doppler anemometry	wastewater	stirred tank	approx. 1 L	lab scale	8 points	CFD and experimental results compared on diagrams (in every point)	Yeoh *et al.* (2004)
7	instantaneous velocity	acoustic Doppler velocimetry	wastewater	storm-water tank	547 L	lab scale	n/a	colour maps compared	Dufresne *et al.* (2017)
	mean velocity	particle image velocimetry				lab scale	n/a		
8	velocity	laser Doppler anemometry	water	flocculator	1.725 L	lab scale	23 points at different depth	CFD and experimental results compared on diagrams (in every point)	Bridgeman *et al.* (2010)
	power dissipation	power input measurements				lab scale	n/a	n/a	
9	velocity	acoustic Doppler velocimetry	water	n/a	n/a	full scale	5 points	CFD and experimental results compared on diagrams (in every point)	Andersson *et al.* (2013)

(*continued*)

Table 1 | continued

	Type of measurement	Measurement method	Type of fluid	Type of technology	Volume of system	Scale	How data were collected	How validity was assessed	Reference
10	velocity	acoustic velocimetry	water	n/a	ok 6 m^3	lab scale	12	CFD and experimental results compared on diagrams (in every point) and table	Baghalian *et al.* (2012)
11	velocity	acoustic Doppler velocimetry	water	n/a	13.4 m^3	lab scale	10	CFD and experimental results compared on diagrams (in every point)	Baranya *et al.* (2012)
12	velocity	propeller flowmeter	water	n/a	approx. 10 m^3	lab scale	1	CFD and experimental results compared on diagrams and in the table (in every point)	Erduran *et al.* (2012)
13	velocity	ultrasonic Doppler velocimeter	river water	n/a	n/a (10 m long)	full scale	40	results not compared	Greco *et al.* (2004)
14	velocity	horizontal acoustic Doppler current profiler (H-ADCP)	river water	n/a	n/a	full scale	1 point	experimental and numerical methods compared on diagrams	Nihei & Kimizu (2008)
15	velocity	horizontal acoustic Doppler current profiler (H-ADCP)	river water	n/a	n/a	full scale	1	H-ADCP validated with ADCP in summary and on diagram	Sassi *et al.* (2011)
16	velocity	acoustic Doppler profiler (aDp)	river water	n/a	n/a	full scale	1 point	no validation	Szupiany *et al.* (2007)
17	velocity gas hold-up oxygen transfer	mono-directional flow-meter optical probe measurement probe	wastewater	activated sludge bioreactor	200 dm3 – 142 m^3	lab scale and full scale	20 points 15 8	CFD and experimental results compared on diagrams (in every point)	Fayolle *et al.* (2007)
18	concentration of benzoic acid	UV spectrophotometer	water	annular reactor	$2 \times 0,2$ L	lab scale	1	CFD and experimental results compared on diagrams (in every point)	Duran *et al.* (2009)
19	flow rate thickness of water film (shear)	weighing method n/a	water	water film n food contact surface (not water treatment)	5m2 – testing surface	lab scale	n/a 10	no validation CFD and experimental results compared on diagrams (in every point)	Suthanarak & Nunak (2018)
20	velocity gas fraction (hold up) mass transfer	particle image velocimetry n/a n/a	water	ozonation column	350 m^3	full scale	? (some measurements were taken in lab scale)	experimental data not shown; no grpahic comparison of calculated and measured results	Cockx *et al.* (1999)

21	velocity	particle image velocimetry	wastewater	airlift reactor (activated sludge)	700 L	lab scale	1 points	CFD and experimental results compared on diagrams and in the table (in every point)	Cockx *et al.* (2001)
	gas hold up	n/a							
	mass transfer	n/a							
	axial dispersion	n/a							
22	velocity	particle image velocimetry	wastewater	activated sludge bioreactor	587,5 L	lab scale	11 points	CFD and experimental results compared on diagrams (in every point)	Do-Quang *et al.* (1998)
	average gas retention (gas hold up)	n/a					9 points		
23	velocity shear rates	laser Doppler velocimetry (shear calculated based on LDV results)	glycerine & Carbopol polymer	mixing tank	70 L	lab scale	n/a	CFD and experimental results compared on diagrams (in every point)	Kelly & Gigas (2003)
24	local gas holdup	double-sensor conductivity probe	air and water	internal loop reactors	385 L	lab scale	5 points	CFD and experimental results compared on diagrams (in every point)	Lu *et al.* (2009)
25	velocity	pH probes (H2SO4 tracers)	air and water	internal loop air lift reactor	50 L	lab scale	4 points	CFD and experimental results compared on diagrams (in every point)	Šimčík *et al.* (2011)
	gas holdup	U-tube manometers					4 points		
26	velocity	laser Doppler anemometry	air and water	bubble column	12 L	lab scale	8 points	CFD and experimental compared on graph (not clear)	Buwa & Ranade (2004)
	average bubble size	high-speed digital imaging system					n/a	n/a	
	wall pressure fluctuations	pressure transducers					n/a	n/a	
	voidage fluctuation measurements	electrical conduction					n/a	n/a	
	time-averaged gasholdup	high-speed imaging					n/a	n/a	
27	nitrate concentration ammonium concentration and soluble COD	ion chromatography standard HACH protocols	wastewater	activated sludge bioreactor	130 L	lab scale	13 points	CFD and experimental results compared on diagrams (in every point)	Le Moullec *et al.* (2010)
	oxygen concentration	standard oxygen probe							
	velocity/turbulent kinetic energy	laser Doppler velocimetry						colour maps compared	
28	shear rates	electrodiffusion measurement method	wastewater	stirred-tank reactor	n/a	lab scale	n/a	n/a	Vlaev *et al.* (2007)

level of validation detail required/available/possible to assess the accuracy of CFD models.

CASE STUDIES HIGHLIGHTING THE DIFFERENT LEVELS OF VALIDATION FOR CFD MODELS

Case of high detailed velocity measurements (mechanical stirrer) at laboratory scale

This case illustrates the setup to gather high detailed velocity measurements for a scaled-down mechanical stirrer at laboratory scale (Fernandes del Pozo *et al.* 2020; Figure 1). The high quality dataset allows derivation of time-dependent highly detailed velocity measurements as well as derived quantities for a complete CFD validation study (local turbulent kinetic energy, local shear rate, local viscosity, etc.; Figure 2).

Mechanical stirrers mixing viscous fluids such as the ones encountered in anaerobic digesters (AD) are often considered black-boxes due to the difficulty of obtaining any data from inside the reactor. In this line, the use of rheologically mimicking fluids (surrogates) such as Carbopol provide a promising technique to study the mixing mechanism of sludges in high level of detail and can provide sufficient

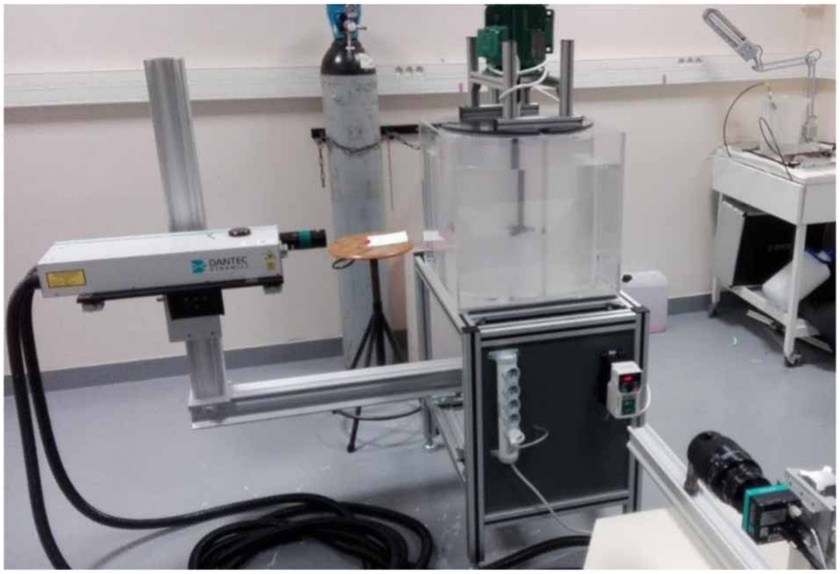

Figure 1 | Particle image velocimetry (PIV) setup for an axially stirred tank with a medium-viscosity fluid mimicking the rheology of a digested sludge (Carbopol).

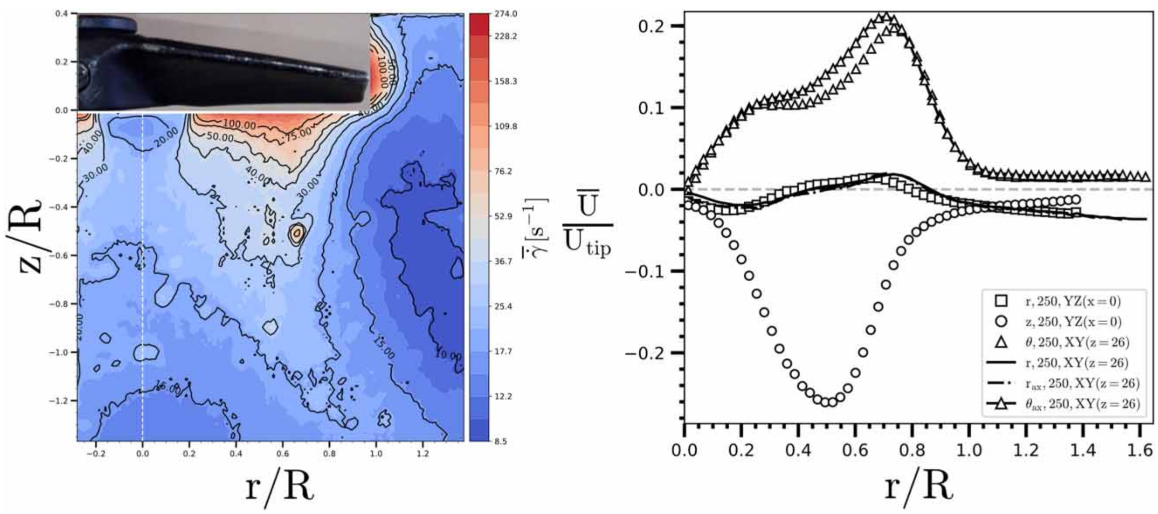

Figure 2 | Contour plot of shear rate below the impeller (left) and normalised axial, radial and tangential velocity profiles (right) at 26 mm below the impeller. R = 0.075 m.

metrics for tedious validation of CFD stirrer models. It is noted that a high level of detail is required for anaerobic digesters due to the complexity in modelling non-Newtonian flows (Dapelo & Bridgeman 2018).

Case of WWTP Eindhoven (Waterboard De Dommel, The Netherlands)

This case simulates the outer ring of a concentric bioreactor which is partly aerated. Different levels of validation were pursued here. First, a plain hydrodynamic model was validated using velocity measurements obtained by an acoustic Doppler current profiler (ADCP). The limitation is that such a measurement is only possible in a non-aerated zone. A first approach used the density of water and resulted in a large offset with the data (Figure 3, left). Accounting for sludge density led to a vast improvement (Figure 3, middle). Further improvement was achieved by including the swirl boundary condition of propellers present (Figure 3, right). At first, this was not accounted for as it complicated the modelling effort quite a bit (instead of defining a boundary condition, the motion of multiple impellers needs to be accounted for, requiring a moving reference frame and finer mesh) and it was assumed that this was likely not going to influence the macroscopic flow behaviour. This assumption proved to be too harsh leading to a deterioration in predictive power.

A next level of validation was by means of dissolved oxygen (DO) measurements at 99 locations conducted by a construction crane (Figure 4). This qualitatively shows that model predictions of the integrated CFD-biokinetic model (Rehman et al. 2017) were in line with measured patterns.

Case of large drinking water storage basin (PWN, The Netherlands)

This case concerns the CFD modelling of a large surface water storage basin for drinking water treatment (6Mm³ volume; operated by the Dutch drinking water utility PWN). Figure 5 shows the transport of a virtual tracer introduced at the inlet (a), a satellite image (b) and a drone image (c). The basin contains one coarse bubble aerator (white spot in Figure 5(b)). Also different levels of validation were pursued here. Detailed velocity measurements across the basin depth were performed using ADCP (the ten measurement points are indicated in Figure 5(b)). Further, the visible transport of the 'white plume' of precipitated calcium carbonate was compared to the virtual tracer transport.

Initially, the basin was modelled using one-phase CFD, not accounting for the coarse bubble aeration. Large deviations between predicted and measured velocities were observed. The model was extended to a simple two-phase aeration model with improved outcomes. However, after further refinement of the aeration model, good predictive power was observed (Figure 6). It is worth mentioning that the model also incorporated the impact of wind speed and direction by introducing momentum source on the top of the basin.

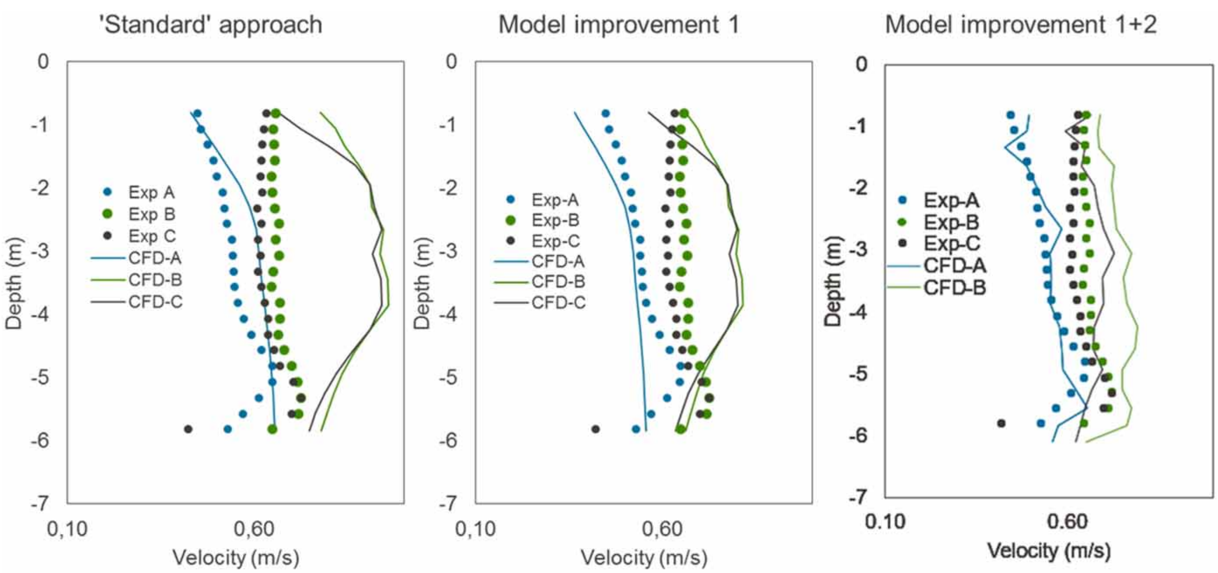

Figure 3 | Improved validation of velocity along the depth of the bioreactor by accounting for more ingredients in the CFD model: density of water (left), density of sludge (middle) and account for swirling motion of propeller (right).

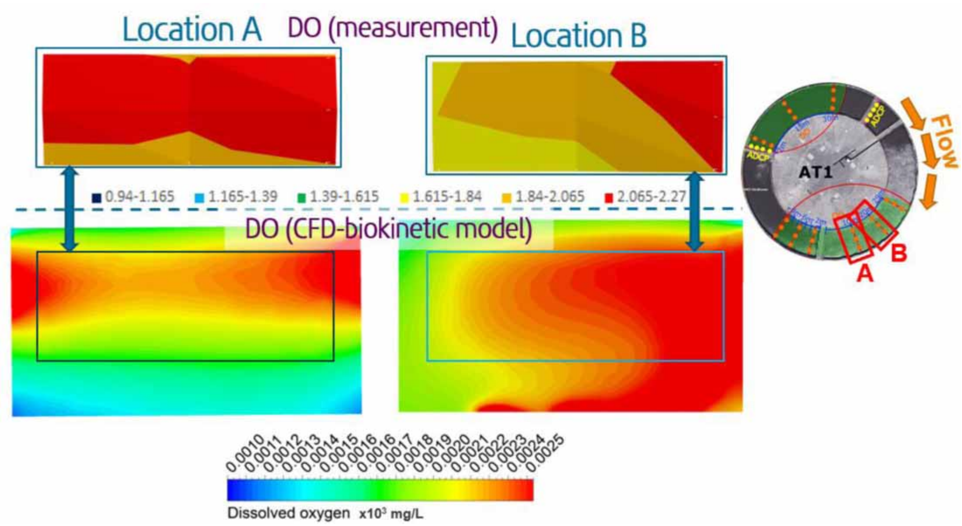

Figure 4 | Validation of predicted DO with interpolated DO measurements (grid of 9 points) at two locations ('A and B') in the outer ring.

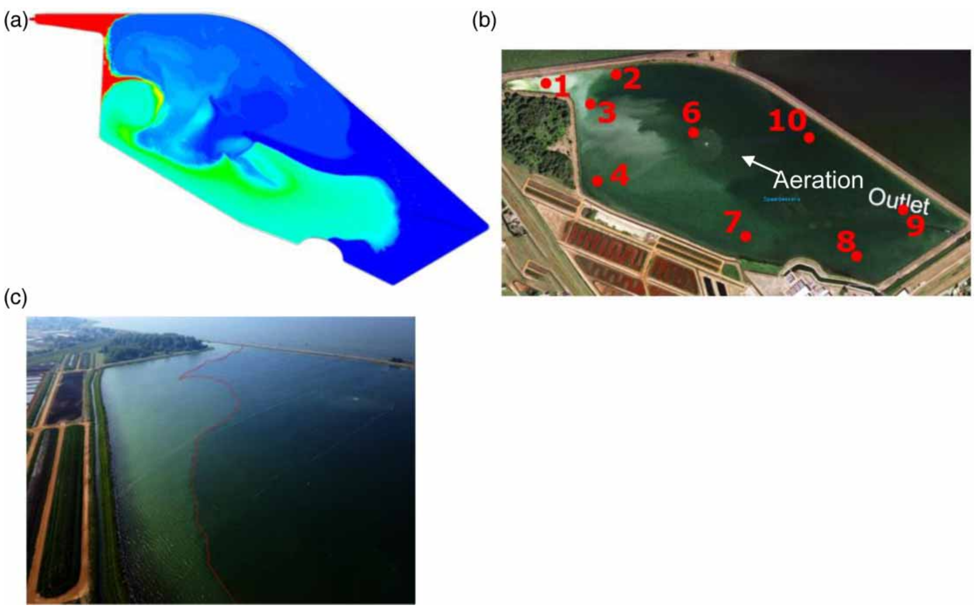

Figure 5 | The storage basin modelled: CFD simulation (a), satellite image (b) and drone image (c).

The general transport behaviour of the white precipitate was also reproduced by the model. The shape of the white front was indicated by the red line in Figure 5(c). Transport patterns in Figure 5(b) and 5(c) corresponded very well with the predicted front of the virtual tracer in 5a.

Very important to note is that in this case, the impact of aeration was significant, even though the basin had a huge volume. Validation measurements led to significant improvements of the CFD model, with high trust in the model as a result.

DISCUSSION

As a first lesson, all cases clearly illustrated that often details in the CFD modelling process (i.e. finer mesh, including (more detailed description of) phenomena, using better submodels for rheology) are the reason for insufficient predictive power. Adding certain mechanisms or more geometry detail can increase predictive power quite drastically. Another lesson learned (although this was not new) is that data collection is not straightforward, especially at full-scale.

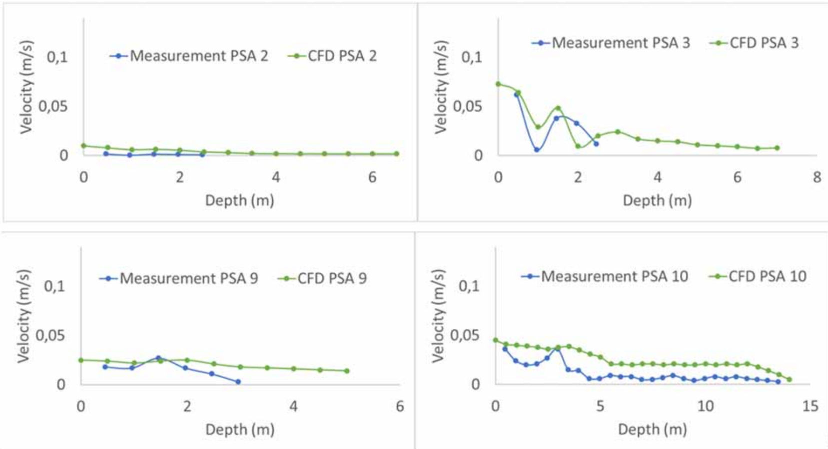

Figure 6 | Comparison of measured and predicted velocity profiles obtained using the final two-phase CFD model (points 2, 3, 9 and 10 in Figure 5(b)).

It is time and resource demanding and one can ask the question whether this effort is required for every new case.

In contrast, further generalising, one could argue that it would be more useful to gather experiences where validation has been performed and rather list recommendations for the model development (geometry details, mesh, turbulence model choice, rheological model) for future users, keeping them from performing detailed validation experiments infinitely. It would therefore be valuable to start collecting successful CFD validation cases in a database including all the data and metadata as well as all settings of the CFD model and specifically highlighting the important details leading to a high predictive power. Obviously, the level of validation currently required will depend on the system complexity and the objective. There is likely not going to be anyone still validating the parabolic profile of a laminar flow in a tube. However, it becomes more cumbersome for more complex systems, such as multiphase systems. Here, it is likely more efforts are still required to build this knowledge base. In the region of intermediate complexity, we need some guidance to nail down knowledge (just like the laminar pipe flow) to avoid continued large investments in measurement campaigns.

In the whole discussion above, one should also not lose the link with the modelling objective. Depending on the goal, validation needs might be different. Take the example of a sand filter. If one is interested in the design of the inlet and outlet structures and how they affect flow, a one-phase liquid model suffices and a tracer test could be used for validation. However, if one is interested in the detailed capturing of solids in the voids of the sand bed, a more sophisticated two-phase model would be needed, along with a filter bed autopsy to evaluate the non-homogeneity of the depositions. Noteworthy is that, apart from its value for model improvement, validation drastically increases the practitioner's trust in the model. High trust leads to increased weight of decisions people take based on model outcomes, markedly increasing its value.

Finally, it is of utmost importance that the modeller knows the limitations of the model and software being used. This is especially true for commercial software as not all equations and settings are clearly accessible. Open-source codes could be helpful here as it provides full flexibility with regards to adapting solvers. However, they present a steep learning curve for swift application given the fact that the graphical user interface is less user-friendly.

CONCLUSIONS

In view of the increasing usage of CFD, the demand for predictive power through validation pops up continuously. We argue that this demand should be put in perspective and not force people to eternally validate systems for which knowledge has been built up. We propose a knowledge base of validation cases to be developed that scrutinizes the need for explicit validation of future CFD models. The need for validation will in this way dynamically shift towards more complex modelling cases. For simple cases, this is already widely accepted. We need to bring this to practice for intermediate complexity problems. Complex cases still require further validation efforts to be performed and might also require more flexible open source software tools for accurate validation.

ACKNOWLEDGEMENT

We acknowledge Waterboard De Dommel and PWN for providing access to their systems to study the detailed hydrodynamics.

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First received 7 January 2020; accepted in revised form 2 April 2020. Available online 16 April 2020